# DEVELOPING AND EVALUATING RESEARCH-BASED LEARNING TOOLS FOR QUANTUM MECHANICS

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Here I present my work on developing and evaluating research-based learning tools for quantum mechanics. In particular, I will discuss the development and evaluation of two Quantum Interactive Learning Tutorials (QuILTs) focusing on Degenerate Perturbation Theory (DPT) and a System of Identical Particles. The QuILTs are guided by several learning theories from cognitive science and strive to help students develop a more robust understanding of the concepts covered. The investigation was carried out in advanced quantum mechanics courses by administering free-response and multiple-choice questions and conducting individual interviews with students. It was found that students share many common difficulties related to relevant physics concepts. They had difficulty with mathematical sense-making and applying linear algebra and combinatorics concepts correctly in this novel context of quantum mechanics. I describe how the research on student difficulties was used as a guide to develop and evaluate the QuILTs, which strives to help students develop a functional understanding of concepts necessary for DPT and a system of identical particles. I also discuss the development and validation of the DPT QuILT focusing on these issues and its in-class evaluation in the undergraduate and graduate courses that focused on these issues.

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# PREFACE

I am very thankful for all the support bestowed upon me by my family. I would like to thank my wife, Kayla, for all of her sacrifices and continued support during this very rewarding but also very challenging endeavor. I would like to thank my daughters, Abigail and Gwendolyn, for the inspiration to see this goal all the way through to the end. I would like to thank my parents for instilling in me the value of hardwork, the importance of education, and the desire to help others achieve their goals.

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## 1.0 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. There have been a number of research studies aimed at investigating student reasoning in QM [15, 16, 17, 18, 19, 20, 21, 22, 23, 24] and improving student understanding of QM [25, 26, 27, 28, 29, 30, 31, 32, 33]. However, there have been relatively few investigations into student difficulties with fundamental concepts involving degenerate perturbation theory (DPT) or a system of identical particles. Through researching students' understanding and reasoning about DPT or a system of identical particles, I have found many common student difficulties that may hinder their development of a consistent and coherent knowledge structure pertaining to this topic. These common student difficulties were then used as a guide to help develop a research-based learning tool, i.e., a Quantum Interactive Learning Tutorial (QuILT) [34, 35, 36, 37, 38, 39]. I describe the methodology for investigating these student difficulties along with the development and evaluation of the corresponding research-based QuILT that strives to help students develop a functional understanding of the fundamental concepts involved in constructing the many-particle stationary state wavefunction for a system of identical particles.

The QuILT incorporates guided inquiry-based learning sequences which consist of a set of questions, each building upon the previous question(s) that require the students to take a stand and actively engage in the learning process. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether they are correct and explain why they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being

that students would identify an inconsistency in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include excerpts that strive to present the students with a contradiction between the answer to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining difference between the correct reasoning and their own reasoning before moving on the next section.

## 1.1 FRAMEWORKS FOR LEARNING THAT INSPIRED MY RESEARCH

### 1.1.1 Cognitive Apprenticeship Model

The Cognitive Apprenticeship Model describes how the traditional apprenticeship model, which has been a primary instructional method for centuries, can be applied in the context of formal education [40]. Collins, Brown, and Newman state that the learning environment is most effective when it includes the following elements: modeling, coaching, and fading of the scaffolding support. In modeling, the instructor demonstrates approaches to critical thinking, problem-solving, and metacognition from an expert perspective. The coaching step is where the instructor provides scaffolding support to the students. This is a very important step that is often missing in traditional, lecture-based instruction. The final step involves slowly removing the scaffolding support until the students are able to complete the desired task on their own.

### 1.1.2 Zone of Proximal Development

Vygotsky's Zone of Proximal Development (ZPD) states that the level of instruction should be aimed just beyond the students' current knowledge state [41]. The ZPD focuses on the aspects of learning necessary for scaffolding support required to move individuals from an initial knowledge state to the desired final knowledge state. As the students learn and move towards the desire final state, the level of instruction continually changes to be just beyond the students' current level. It is the instructors' responsibility to choose the appropriate level of instruction and to create an environment in which the students receive the scaffolding support necessary to move to the desired final knowledge state. This scaffolding support can come from the instructor or from peers. It is often said that one goal of focusing on the ZPD is to ensure that what an individuals are able to do today with help, they are able to do tomorrow on their own.

### 1.1.3 Assimilation, Accomodation and Optimal Mismatch

Piaget stated that when one is faced with a new situation or an inconsistency in their knowledge structure, they may be motivated to adapt [42]. According to Piaget, it is during this adaptation that the learning process is taking place. This adaptation can be achieved by either assimilation or accomodation or both. In assimilation, an individual is able to use their existing knowledge structures (or schema) to make sense of the new situation and correct the inconsistencies. Accomodation occurs when one's current knowledge structures are not sufficient and need to be changed in order to fully understand the concepts. Piaget's "optimal mismatch" is one technique used to provide guidance and promote the adaptation in the learning process. The key idea behind Piaget's "optimal mismatch" framework is to allow students to discover their mistakes on their own and allow them to correct the inconsistencies in their own knowledge structures. One method to achieve this is to scaffold student learning using a guided inquiry-based approach which focuses on the necessary skills and concepts students should learn and strives to help the students develop a functional understanding of the underlying concepts.

### 1.1.4 Preparation for Future Learning

Additionally, the QuILT strives to incorporate Bransford and Schwartz's Preparation for Future Learning (PFL) framework with a special focus on instruction that incorporates elements of both innovation and efficiency [43]. In the PFL framework, innovation and efficiency can be viewed as two orthogonal components of instructional design that must be balanced for effective learning outcomes. One interpretation of this framework in this context is that innovation refers to presenting students with novel tasks that are just beyond students' current understanding that allows them to grow and strive for more robust knowledge. Efficiency can be viewed as a characteristic of instruction that allows the students to practice what they are learning and become skilled at a particular type of task. The framework suggests that instruction should attend to both these aspects. The concern is that if instruction only focuses on one of these aspects there is danger that the students will become frustrated when instruction is too innovative beyond their current knowledge state (the instruction is too innovative without allowing for efficiency) or when the instruction focuses too much on rote learning and procedural redundancy (the instruction is too efficient without the creative aspects associated with innovation).

## 1.2 MEMORY AND COGNITIVE LOAD

At a coarse-grained level, the human information processing system can be classified as consisting of two types of memory: long-term memory and short-term (or "working") memory [44]. Long-term memory encompasses all that an individual has learned and that can be recalled at a given instance. There appears to be no limit to the amount of information that can be stored in the long-term memory. Working memory, on the other hand, is where information is processed while solving a problem or performing a task before it can be stored in the long-term memory. Working memory is also responsible for synthesizing new information with prior knowledge to form new knowledge structures in a given domain. In general, an individual's working memory is restricted to $7 \pm 2$ "slots" or "chunks" available to ded-

icate to a given task [45]. If more slots are required in working memory than is available to perform a task or solve a problem, one may experience cognitive overload and may no longer have cognitive resources available to process the information appropriately or engage in metacognition to ensure one's reasoning is consistent and correct. As one gains expertise in a given domain, one is able to make connections between different concepts and combine individual concepts into larger chunks each of which occupy a single slot in the working memory.

## 1.3 SEMANTIC NETWORK

A semantic network has been used as a method to visualize an individual's knowledge structures. A semantic network consists of nodes representing individual concepts and links between these nodes that represents a connection between different concepts [46]. As one gains expertise in a given domain, one reorganizes their knowledge structures and it becomes more hierarchical. One is able to make connectiion between concepts important in that domain and the more important concepts are moved to the top of the hierarchical network.

## 1.4 BOUNDED RATIONALITY

Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of the individual who is solving the problem, Simon's framework of "bounded rationality" and "satisficing" posits that an individual will make decisions while solving problems based upon their current level of expertise, which may not be optimal [47]. When faced with a decision in problem-solving tasks, individuals can be categorized as either satisficers or maximizers. Satisficers are interested in what is referred to as satisficing and often only look for a solution that is satisfactory to them in which they see no inconsistencies rather than searching for additional pathways in the problem space which may be more optimal. Satisficers often

only make decisions that are sub-optimal and do not discuss the need to consider alternative pathways in the problem space which may yield more optimal solutions. In other cases, they may realize that there are additional pathways in the problem space that may be more optimal but choose not explore these pathways for the more optimal solution. Maximizers are those who are motivated to look for the optimal solution pathways among all of the infinitely many possible pathways in the problem space. However, if the individual's level of expertise is not sufficient and they are not provided with appropriate scaffolding support, they may experience cognitive overload and may not be able to obtain the optimal solutions [48]. Many of the student difficulties discussed here may be attributed in part to students' bounded rationality and satisficing in that they may be satisfied with a sub-optimal solution that does not cause cognitive overload and may not search for optimal solution pathways in the problem space that may yield the correction solution. Resorting to satisficing may sometimes amount to sense-making which is commensurate with students' current level of expertise and inappropriate integration of mathematical and physical concepts to solve problems may occur due to students' evolving expertise. Since the paradigm of QM is novel, these issues of satisficing become critical in the work presented in this thesis.

## 1.5 MATHEMATICAL SENSEMAKING IN PHYSICS

Prior research suggests that students often have difficulty applying mathematical concepts in the context of a concrete physical problem. In particular, students have difficulty connecting and applying mathematics correctly in physics contexts (e.g., see Refs. [49, 50, 51, 52, 53]). Mathematical sense-making in the context of solving physics problems can often be more difficult than when solving equivalent mathematics problems without the physics context [49, 50, 51, 52, 53]. Since working memory is constrained to a limited number of chunks and students' knowledge chunks pertaining to a concept are small when they are learning and developing expertise in physics, use of mathematics in physics can increase the cognitive load during problem solving especially if students are not proficient in mathematics [48] and they may struggle to integrate physics and mathematics concepts. Thus, mathematical

sense-making while focusing on solving a physics problem is often challenging and students sometimes make mathematical mistakes that they otherwise would not make if the physics context was absent [49, 50, 51, 52, 53].

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# 2.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DEGENERATE PERTURBATION THEORY: BASIC FOR DEGENERATE PERTURBATION THEORY

## 2.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics. Prior investigations suggest that many students struggle to develop intuition with quantum mechanical phenomena due to the abstract nature of the subject matter and pedagogical approaches such as tutorials and visualization tools can improve student learning [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. Our group has also conducted a number of studies aimed at investigating student reasoning in QM [14, 15, 16, 17, 18, 19, 20, 21] and improving student understanding of QM [22, 23, 24, 25]. For example, some of the studies from our group have focused on helping students learn about Dirac notation, quantum measurements, expectation values and their time dependence [26, 27, 28, 29, 30]. Guided by research studies conducted to identify student difficulties with QM and findings of cognitive research, we have been developing a set of research-based learning tools including the Quantum Interactive Learning Tutorials (QuILTs) [31, 32, 33, 34, 35, 36].

There has been relatively little research conducted into student understanding of advanced topics in quantum mechanics, e.g., degenerate perturbation theory (DPT) [37, 38]. Here, we discuss an investigation of student difficulties with DPT and the development and evaluation of a research-based Quantum Interactive Learning Tutorial (QuILT) that makes use of student difficulties as resources to help them develop a solid grasp of DPT. We first summarize the basics of DPT that students should learn. Then, we describe the methodology

for investigating student difficulties and the common student difficulties found. We describe how the difficulties were used as a guide to develop the QuILT and its in-class evaluation in undergraduate and graduate QM courses.

## 2.2 BASICS FOR DPT

Perturbation theory is a powerful approximation method for finding the energies and the energy eigenstates for a system for which the Time-Independent Schrödinger Equation (TISE) is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$. The TISE for the unperturbed Hamiltonian, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, is assumed to be exactly solvable where $\psi_n^0$ is the $n^{th}$ unperturbed energy eigenstate and $E_n^0$ the unperturbed energy. Perturbation theory builds on the solutions of the TISE for the unperturbed case. Using perturbation theory, the energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \cdots$ where $E_n^i$ for $i = 1, 2, 3..$ is the $i^{th}$ order corrections to the $n^{th}$ energy of the system. The energy eigenstates can be approximated as $\psi_n = \psi_n^0 + \psi_n^1 + \psi_n^2 + \cdots$ where $\psi_n^i$ is the $i^{th}$ order correction to the n$^{th}$ energy eigenstate. We focus on the first order perturbative corrections to the energies and energy eigenstates, which are usually the dominant corrections. In nondegenerate perturbation theory, the first order corrections to the energies are

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle, \tag{2.1}$$

and the first order corrections to the energy eigenstates are

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle. \tag{2.2}$$

In Eqs. 6.1 and 6.2, $\{|\psi_n^0\rangle\}$ is a complete set of eigenstates of $\hat{H}^0$.

When the eigenvalue spectrum of $\hat{H}^0$ has degeneracy (i.e., two or more eigenstates of $\hat{H}^0$ have the same energy and two or more diagonal elements of $\hat{H}^0$ are equal), Eqs. 6.1 and 6.2 from nondegenerate perturbation theory are still valid provided one uses a *good* basis. For a

given $\hat{H}^0$ and $\hat{H}'$, we define a *good* basis as consisting of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. Therefore, the terms $\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle$ in Eq. 6.2 for the wavefunction are zero when $m \neq n$ so that the expression for the corrections to the wavefunction in Eq. 6.2 does not have terms that diverge when $E_m^0 = E_n^0$. Only if a *good* basis is chosen, Eq. 6.1 is valid for finding the first order corrections to the energies (which are the diagonal elements of the $\hat{H}'$ matrix as given by Eq. 6.1). Since $\hat{H}^0$ is the dominant term and $\hat{H}'$ provides only small corrections to the energies, we must ensure that the basis states used to determine the perturbative corrections to the energies in Eq. 6.1 are eigenstates of $\hat{H}^0$.

If $\hat{H}^0$ and $\hat{H}'$ commute, it is possible to diagonalize $\hat{H}^0$ and $\hat{H}'$ simultaneously to find a complete set of simultaneous eigenstates and the exact results are obtained. However, if a complete set of simultaneous eigenstates of $\hat{H}^0$ and $\hat{H}'$ cannot easily be identified, because $\hat{H}^0$ and $\hat{H}'$ have degeneracy, then it is useful to recognize that diagonalizing $\hat{H}'$ only in each degenerate subspace of $\hat{H}^0$ produces a *good* basis and both $\hat{H}^0$ and $\hat{H}'$ become diagonal in that basis. In this case, the first order corrections in DPT (the diagonal elements of $\hat{H}'$) are exact results. If $\hat{H}^0$ and $\hat{H}'$ do not commute, perturbation theory must be used and a *good* basis is found by diagonalizing $\hat{H}'$ *only* in each degenerate subspace of $\hat{H}^0$.

## 2.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

As can be seen from the brief review in the previous section, there are many concepts that students must consider when applying DPT correctly. It is not surprising that students struggle to develop a consistent and coherent knowledge structure and a functional understanding of DPT. Student difficulties with finding the corrections to the energies and energy eigenstates using DPT were first investigated using five years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts to 64 upper-level undergraduates in a second-semester junior/senior level QM course and 42 first-year physics graduate students in the second-semester of the graduate core QM course. Additional insight was gained concerning these difficulties via responses of

13 students (graduate and undergraduate students) during a total of 45 hours of individual interviews. A "think aloud" protocol was used during the interviews in which students were asked to think aloud as they answered the questions posed without being disturbed [39]. Once the students had answered each question to the best of their ability, we asked them to clarify their reasoning and probed deeper into certain difficulties. The interviews were generally conducted in one sitting, but there were two interviews that took place over the course of two days.

In all the questions discussed here, students worked through examples involving DPT that are restricted to a three-dimensional Hilbert space (with a two-fold degeneracy in $\hat{H}^0$). The purpose for restricting the problem solving to three dimensions was to ensure that students focus on the fundamental concepts instead of working through cumbersome calculations that may detract from the focus on why it is important to determine if the initial basis is a *good* basis to find perturbative corrections. In all the questions discussed, the Hamiltonian operator was given in matrix form and we will refer to the basis used to generate these initial matrix representations of the Hamiltonian operator as the initially chosen basis.

To probe student understanding of a *good* basis for finding perturbative corrections to the energies and energy eigenstates, we posed questions regarding the following four systems (given by the Hamiltonians **H1**-**H4**) in which the Hilbert space is three dimensional and $\epsilon$ is a small parameter ($\epsilon \ll 1$). For each system, the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.3}$$

**H1.**

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \tag{2.4}$$

**H2.**

$$\hat{H}^0 = V_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & 0 & -4\epsilon \\ 0 & 2\epsilon & \epsilon \\ -4\epsilon & \epsilon & 2\epsilon \end{pmatrix} \tag{2.5}$$

**H3.**

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 2\epsilon & 0 \\ 2\epsilon & 0 & 3\epsilon \\ 0 & 3\epsilon & -2\epsilon \end{pmatrix} \tag{2.6}$$

**H4.**

$$\hat{H}^0 = V_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & 0 & -4\epsilon \\ 0 & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix} \tag{2.7}$$

The basis given in Eq. A.11 is a not *good* basis for the Hamiltonians **H1** and **H2** as each $\hat{H}'$ matrix is not diagonal in the degenerate subspace of the corresponding $\hat{H}^0$. The basis given in Eq. A.11 is a *good* basis for the Hamiltonians **H3** and **H4** since each $\hat{H}'$ matrix is diagonal in the degenerate subspace of the corresponding $\hat{H}^0$.

## 2.4 STUDENT DIFFICULTIES

Throughout our analysis of student responses to the multiple choice and open-ended questions, we found that many students struggled to determine a *good* basis and the corrections to the energies and energy eigenstates. It was often the case that students had difficulty even starting some of the open-ended problems after traditional lecture-based instruction in relevant concepts. We conducted individual think-aloud interviews to gain a better understanding of student difficulties. Below, we discuss some of the common student difficulties with DPT found via interviews in the context of a three-dimensional Hilbert space with a two-fold degeneracy in $\hat{H}^0$. It was not possible to discern the underlying cognitive mechanism and reasoning for student responses via the students' written responses to multiple-choice or open-ended questions. It was during the interviews that we probed further into the students' reasoning and were able to uncover reasoning for some of the common student difficulties

with DPT. When possible, in the discussion below, we will give the percentage of the interviewed students who displayed a given difficulty. We note that certain student responses generated further probing and so those probing questions may not have been asked to all of the interviewed students. Therefore, we will only report the percentage of difficulties for interviewed students for questions that were common to all the interviewed students. In the results section, we present in-class student performance data that suggest that students gained a better understanding of the concepts related to DPT after working through the QuILT.

Interviews suggest that many of the following difficulties may partly be a result of the students' overloaded working memory [40, 41, 42, 43] and the fact that they did not have a strong background in linear algebra or they struggled to apply linear algebra concepts correctly in the context of DPT. In DPT, students must integrate a number of different concepts to solve a single problem and some students struggled to incorporate these concepts coherently to solve problems involving degeneracy. For example, one cannot simply focus on the unperturbed Hamiltonian $\hat{H}^0$ or the perturbation $\hat{H}'$, but one must conisder both $\hat{H}^0$ and $\hat{H}'$ when determining a *good* basis and the first order corrections to the energies and energy eigenstates. The unperturbed Hamiltonian dictates whether one should use DPT and the perturbating Hamitlonian $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ determines whether the initial basis is a *good* basis. It is often difficult for students who are still developing expertise in the context of DPT to apply all these concepts correctly. Additionally, DPT problems require the application of linear algebra concepts in the context of QM. It is not enough to simply diagonalize a matrix, which is a familiar task for many students from their mathematics courses. In DPT, one must be able to identify whether a basis is a *good* basis, whether a matrix must be diagonalized, what needs to be diagonalized ($\hat{H}'$ in each degenerate subspace of $\hat{H}^0$), and also understand that the degeneracy in the energy spectrum of $\hat{H}^0$ is what allows us to diagonalized $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ while keeping $\hat{H}^0$ diagonal everywhere. The difficulties found are consistent with many prior studies focusing on student difficulties in connecting the mathematics and physics concepts and how constraints on working memory can negatively impact student performance in areas in which their expertise is still evolving [40, 41, 42, 43].

### 2.4.1 Difficulty realizing that a *good* basis is required for corrections to the energies

Most of the interviewed students (85% of the interviewed students) realized that the first order corrections to the energy eigenstates $|\psi_n^1\rangle$ are not valid unless we choose a *good* basis. When examining Eq. 6.2, they identified that there will be terms in which the denominator is zero due to the degeneracy in the energy spectrum. However, many of these same students (38%) thought that Eq. 6.1 is still valid to find the first order corrections to the energies since no divergent terms appear in Eq. 6.1. They claimed that any basis which consists of eigenstates of $\hat{H}^0$ is a *good* basis for finding the first order corrections to the energies, but that this same basis may not be a *good* basis for finding the first order corrections to the energy eigenstates. These students did not realize that if a basis is not a *good* basis for finding the corrections to the energy eigenstates, then that same basis cannot be a *good* basis for finding the corrections to the energies. When calculating the first order corrections to the energies, students with this difficulty used the diagonal matrix elements of $\hat{H}'$ as the first order corrections to the energies whether the initially chosen basis was a *good* basis or not (whether $\hat{H}'$ in that basis was a diagonal matrix in the degenerate subspace of $\hat{H}^0$ or not). For example, when given the system with Hamiltonian **H1** in Eq. 2.4, students with this difficulty incorrectly claimed that the initially chosen basis was a *good* basis for finding the first order corrections to the energies. They incorrectly stated that the first order corrections to the energies are all zero. However, when diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ in Eq. 4, one finds that the first order corrections to the energies are $\epsilon V_0$, $-\epsilon V_0$, and 0, respectively.

### 2.4.2 Difficulty identifying $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$

Many students had difficulty identifying the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ when the Hamiltonian $\hat{H}$ for the system was provided in a matrix form. In particular, students had difficulty with the fact that, in order to determine $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, they should start by identifying whether there is any degeneracy in the energy spectrum of $\hat{H}^0$. In fact, we found that some students (31% of the interviewed students) incorrectly

focused on the diagonal elements of the perturbation $\hat{H}'$ to determine whether there was "degeneracy" in $\hat{H}'$ and whether they should use DPT. For example, students were given the Hamiltonian in **H2** in Eq. 2.5 and were asked in a multiple choice format to identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Some interviewed students incorrectly identified $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ as $\begin{pmatrix} 2\epsilon & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$ because $2\epsilon$ appears twice as a diagonal matrix element of $\hat{H}'$. However, the same diagonal matrix elements of $\hat{H}'$ has nothing to do with whether one should use DPT.

Additionally, many students (38% of the interviewed students) were unable to identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ given the Hamiltonian $\hat{H}$ in the matrix form if the degenerate basis states were not in adjacent rows/columns. For example, in the system given by the Hamiltonian **H3** in Eq. A.19, students were asked to identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. In this system, the degenerate states are $|\psi_1^0\rangle$ and $|\psi_3^0\rangle$. Thus, $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ is $\begin{pmatrix} -\epsilon & 0 \\ 0 & -2\epsilon \end{pmatrix}$, which is diagonal. The initially chosen basis is a *good* basis. Several students (38% of the interviewed students) who correctly identified the matrix elements of $\hat{H}^0$ corresponding to the degenerate unperturbed energies were unable to correctly identify $\hat{H}'$ in that degenerate subspace of $\hat{H}^0$ because the degenerate states are not in adjacent rows/columns. Some of the interviewed students (31% of the interviewed students) with this difficulty would then look for "degeneracy" in the diagonal elements of $\hat{H}'$ and determine if the initially chosen basis was a *good* basis based upon whether $\hat{H}'$ had same diagonal elements (in other words, they looked for the "degenerate" subspace of $\hat{H}'$ as opposed to the degenerate subspace of $\hat{H}^0$).

### 2.4.3 Difficulty determining whether the initially chosen basis is a *good* basis

A *good* basis is one that keeps the unperturbed Hamiltonian $\hat{H}^0$ diagonal while diagonalizing the perturbation $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. However, many students had difficulty determining whether the basis in which the Hamiltonian was given in matrix form was a *good* basis. For example, students were given the system with the Hamiltonian **H2** in Eq. 2.5 and were asked if the initially chosen basis is a *good* basis. In this case, $\hat{H}'$ in the degenerate

subspace of $\hat{H}^0$ is $\begin{pmatrix} 2\epsilon & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$, which is not diagonal. Therefore, the initially chosen basis is not a *good* basis. However, some students (15% of the inteviewed students) incorrectly stated that the initially chosen basis is a *good* basis because it consists of a complete set of eigenstates of $\hat{H}^0$ ($\hat{H}^0$ is diagonal in the initial basis) without considering whether $\hat{H}^0$ had any degeneracy and the implications of the degeneracy in $\hat{H}^0$ for finding a *good* basis. These students did not consider the $\hat{H}'$ matrix before determining whether the initial basis was a *good* basis for finding the perturbative corrections.

Other students only examined the basis in a general manner and did not focus on either $\hat{H}^0$ or $\hat{H}'$. For example, one student incorrectly stated that the basis is a *good* basis if "it forms a complete Hilbert space." Another student incorrectly claimed that the only condition to have a *good* basis is that "the basis vectors are orthogonal," regardless of the fact that the unperturbed Hamiltonian $\hat{H}^0$ had degeneracy in the situation provided.

Another common difficulty students had with identifying a *good* basis was considering only $\hat{H}^0$ or $\hat{H}'$ when determining whether a basis was a *good* basis. For example, students were asked to consider the system with the Hamiltonian **H4** in Eq. 2.7 and asked if the basis in which the Hamiltonian is written in the matrix form is a *good* basis. Since $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ is $\begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}$, which is diagonal, the initially chosen basis is a *good* basis. However, many students (46% of the interviewed students) had a tendency to focus on either $\hat{H}^0$ or $\hat{H}'$, but not both, as is necessary to correctly answer the question. For example, during the interview, one student said, "$\hat{H}'$ must be diagonal (everywhere) in the *good* basis". Equivalently, another student incorrectly claimed that the basis was not a *good* basis "since $\hat{H}'$ has off-diagonal terms in this basis." These types of incorrect responses suggest that students have difficulty with the fact that a *good* basis is one in which $\hat{H}'$ need only be diagonal in the degenerate subspace of $\hat{H}^0$. Students with these types of responses often focused on diagonalizing the entire $\hat{H}'$ matrix (rather than diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$). They did not realize that if $\hat{H}^0$ and $\hat{H}'$ do not commute, $\hat{H}^0$ will become non-diagonal in a basis that diagonalizes the entire $\hat{H}'$ matrix, which is inappropriate since we are finding small corrections in perturbation theory.

Moreover, some students (31% of the interviewed students) had difficulty with the fact that even when the initially chosen basis is not a *good* basis, it may include some states that are *good* states that can be used to find the first order corrections to the energies using Eq. 6.1. For example, when asked to consider the system with the Hamiltonian **H2** in Eq. 2.5, many students claimed that none of the three basis states in Eq. A.11 are *good* basis states. However, the state $|\psi_1^0\rangle$ corresponding to the non-degenerate subspace of $\hat{H}^0$ is a *good* state and $|\psi_2^0\rangle$ and $|\psi_3^0\rangle$ are not *good* basis states for the Hamiltonian **H2** in Eq. 2.5. Roughly one-third of the students were unable to correctly identify whether each state in the initially chosen basis is a *good* basis state or not. For example, during the interview, one student said, "We cannot trust nondegenerate basis states for finding corrections to the energy. We must adjust all the basis states since we can't guarantee any will be the same." This student and others with this type of response assumed that if the unperturbed Hamiltonian has degeneracy, none of the initially chosen basis states are *good* states. However, any state belonging to the nondegenerate subspace of $\hat{H}^0$ is a *good* state.

Other students struggled with the fact that if $\hat{H}'$ is already diagonal in a degenerate subspace of $\hat{H}^0$, the initially chosen basis is a *good* basis and Eq. 6.1 can be used to determine the perturbative corrections without additional work to diagonalize $\hat{H}'$ in the subspace. For example, students were given the system with **H4** in Eq. 2.7 and were asked to find the first order corrections to the energies. Some students (15% of the interviewed students) with this difficulty attempted to diagonalize the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$. Since the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ is $\begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}$, these students attempted to diagonalize a matrix that was already diagonal. They appeared to have memorized a procedure for finding the first order corrections and often made mistakes when diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Interviews corroborated the fact that students with this type of response did not have a functional understanding of DPT partly because of difficulties with linear algebra and also not thinking globally about the problem.

### 2.4.4 Difficulty understanding why diagonalizing the entire $\hat{H}'$ matrix is problematic

Many students (45% of the students after traditional lecture-based instruction) did not realize that when the initially chosen basis is not a *good* basis and the unperturbed Hamiltonian $\hat{H}^0$ and the perturbing Hamiltonian $\hat{H}'$ do not commute, they must diagonalize the $\hat{H}'$ matrix *only* in the degenerate subspace of $\hat{H}^0$. For example, students were given the system with Hamiltonian **H4** in Eq. 2.7 on a written test and asked to determine the first order corrections to the energies. In the Hamiltonian **H4**, $\hat{H}^0$ and $\hat{H}'$ do not commute. In this situation, 45% of the students diagonalized the entire $\hat{H}'$ matrix instead of diagonalizing the $\hat{H}'$ matrix only in the degenerate subspace of $\hat{H}^0$. When presented with a similar system and asked to determine the first order corrections to the energies, one interviewed student who attempted to diagonalize the entire $\hat{H}'$ matrix justified his reasoning by incorrectly stating, "We must find the simultaneous eigenstates of $\hat{H}^0$ and $\hat{H}'$." This student, and others with similar difficulties, did not realize that when $\hat{H}^0$ and $\hat{H}'$ do not commute, we cannot simultaneously diagonalize $\hat{H}^0$ and $\hat{H}'$ since they do not share a complete set of eigenstates. Students struggled with the fact that if $\hat{H}^0$ and $\hat{H}'$ do not commute, diagonalizing $\hat{H}'$ produces a basis in which $\hat{H}^0$ is not diagonal. Since $\hat{H}^0$ is the dominant term and $\hat{H}'$ provides only small corrections, we must ensure that the basis states used to determine the perturbative corrections in Eqs. 6.1 and 6.2 remain eigenstates of $\hat{H}^0$.

### 2.4.5 Difficulty understanding why it is always possible to diagonalize $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$

Some students (23% of the interviewed students) did not realize that $\hat{H}'$ can be diagonalized in the degenerate subspace of $\hat{H}^0$ while keeping $\hat{H}^0$ diagonal even when $\hat{H}^0$ and $\hat{H}'$ do not commute. For example, when considering the Hamiltonian **H4** in Eq. 2.7 in which $\hat{H}^0$ and $\hat{H}'$ do not commute, one student in the interview stated, "We cannot diagonalize a part of $\hat{H}'$, we must diagonalize the whole thing." In general, students had great difficulty with the fact that the degeneracy in the eigenvalue spectrum of $\hat{H}^0$ provides flexibility in the choice of basis in the degenerate subspace of $\hat{H}^0$ so that $\hat{H}'$ can be diagonalized in that subspace (even if $\hat{H}^0$

and $\hat{H}'$ do not commute) while keeping $\hat{H}^0$ diagonal. For example, if we consider the case in which $\hat{H}^0$ has a two-fold degeneracy, then $\hat{H}^0\psi_a^0 = E^0\psi_a^0$, $\hat{H}^0\psi_b^0 = E^0\psi_b^0$, and $\langle\psi_a^0|\psi_b^0\rangle = 0$ where $\psi_a^0$ and $\psi_b^0$ are normalized degenerate eigenstates of $\hat{H}^0$. Any linear superposition of these two states, e.g. $\psi^0 = \alpha\psi_a^0 + \beta\psi_b^0$ with $|\alpha|^2 + |\beta|^2 = 1$, must remain an eigenstate of $\hat{H}^0$ with the same energy $E^0$. Many students (31% of the interviewed students) did not realize that since any linear superposition of the initial basis states that correspond to the degenerate subspace of $\hat{H}^0$ remains an eigenstate of $\hat{H}^0$, one can choose a special linear superposition of the initial basis states which diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

## 2.5 METHODOLOGY FOR THE DEVELOPMENT OF THE QUANTUM INTERACTIVE LEARNING TUTORIAL (QUILT)

### 2.5.1 Development and Validation of the QuILT

The difficulties described show that many students struggle in determining a *good* basis for finding corrections to the energies in the context of degenerate perturbation theory (DPT). Therefore, we developed a QuILT that takes into account these difficulties. The development of the DPT QuILT started by investigating of student difficulties via open-ended and multiple-choice questions administered after traditional instruction to advanced undergraduate and graduate students and conducting a cognitive task analysis of the requisite knowledge from an expert perspective [44]. The QuILT strives to help students build on their prior knowledge and addresses common difficulties found via research, some of which were discussed in the previous section.

The QuILT is inspired by Piaget's "optimal mismatch" framework [45] as well as the preparation for future learning framework of Bransford and Schwartz [46]. In Piaget's "optimal mismatch" framework, students are intentionally placed in a situation in which their current knowledge structure of relevant concepts is inadequate and they are then given the opportunity and support to reorganize their existing knowledge structures or develop new

structures to reconcile this conflict. Bransford and Schwartz's preparation for future learning framework emphasizes that learning occurs when elements of innovation and efficiency are both present. Although there are many interpretations of the framework, in one interpretation, innovation and efficiency describe two orthogonal components of instructional design. Innovation describes aspects that are new to students, such as new concepts or new problem-solving skills. Efficiency is a measure of the structure and organization of the instructional design and learning tools, as well as how proficient the student is with the instructional design and learning tools. Instructional design that incorporates only one of these elements leads to students becoming disengaged. If instruction is too innovative, students cannot connect what they are learning with their prior knowledge and may become frustrated. When the instruction is too efficient, students may become disengaged with the repetitious material that is too easy and that does not provide intellectual stimulation.

In the QuILT, innovation is incorporated by presenting students with novel tasks. Whether by examples, hypothetical conversations, or quantitative reasoning, the QuILT strives to help students develop a deeper understanding by actively working through the guided inquiry-based sequences. Student difficulties are incorporated in these questions to create a cognitive conflict after which the students are provided scaffolding support designed to resolve these issues and develop a robust knowledge structure. Efficiency is addressed in the QuILT in several ways. First, the QuILT follows a guided inquiry-based learning sequence laid out in the cognitive task analysis. It is organized to build on the students' prior knowledge and each guided inquiry-based sequence in the QuILT builds upon the previous guided inquiry-based sequences. This organization strives to help students build their own knowledge structures in a coherent manner. Second, students are provided scaffolding support to help address common difficulties, thus resolving the cognitive conflicts. Third, the QuILT progressively reduces the scaffolding support so that students develop self-reliance and are able to solve the problems without any assistance. Finally, as the students work through the different tasks, they develop proficiency in applying the concepts in diverse contexts.

The development of the QuILT went through a cyclic, iterative process. The preliminary version was developed based upon the task analysis and knowledge of common student

difficulties. Next, the QuILT underwent many iterations among the three physics education researchers and then was iterated several times with three physics faculty members to ensure that they agreed with the content and wording. It was also administered to graduate and advanced undergraduate students in individual think-aloud interviews to ensure that the guided approach was effective, the questions were unambiguously interpreted, and to better understand the rationale for student responses. The next step involved evaluating student responses during the interviews and their corresponding posttest responses to determine the impact of the QuILT on student learning and whether difficulties remained. Finally, modifications and improvements were made based upon the student and faculty feedback before it was administered to students in various courses.

### 2.5.2 Structure of the QuILT

The QuILT uses a guided inquiry-based approach to learning and actively engages students in the learning process. It includes a pretest to be administered in class after traditional instruction in DPT. Next, students engage with the tutorial in small groups in class (or alone when using it as a self-paced learning tool in homework), and then a posttest is administered in class. As students work through the tutorial, they are asked to predict what should happen in a given situation. Then, the tutorial strives to provide scaffolding and feedback as needed to bridge the gap between their initial knowledge and the level of understanding that is desired. Students are also provided checkpoints to reflect upon what they have learned and to make explicit the connections between what they are learning and their prior knowledge. They are given opportunities to reconcile differences between their predictions and the guidance provided in the checkpoints before proceeding further.

The DPT QuILT uses a blend of qualitative and quantitative reasoning to improve students' understanding. For example, the QuILT requires qualitative understanding while students respond to the hypothetical conversations and quantitative reasoning to determine the first order corrections to the energies and energy eigenstates. In addition, students are asked to verify predictions about the validity of the statements in hypothetical conversations via quantitative reasoning by working through problems. The QuILT strives to help

students with linear algebra difficulties relevant for DPT by incorporating a combination of quantitative and qualitative questions in the guided inquiry-based sequences. Students are asked to reflect upon their answers and reasoning and then provided checkpoints to reconcile their initial reasoning with the correct reasoning.

### 2.5.3 Addressing Student Difficulties

In the QuILT, students actively engage with examples involving DPT that are restricted to a three-dimensional Hilbert space (with two-fold degeneracy in $\hat{H}^0$). In this manner, students focus on the concept of a *good* basis in DPT without working through complex calculations. In particular, for a given $\hat{H}^0$ and $\hat{H}'$, when there is degeneracy in the eigenvalue spectrum of $\hat{H}^0$, students learn about why some bases are not *good* even though they may consist of a complete set of eigenstates of $\hat{H}^0$. The QuILT strives to help students develop a functional understanding of whether the basis is a *good* basis and how to change the basis to one which is *good* (if the initial basis is not *good* for a given $\hat{H}^0$ and $\hat{H}'$) so that Eqs. 6.1 and 6.2 can be used to find the first order corrections. Below, we discuss how the QuILT addresses student difficulties and strives to help students learn about a *good* basis for finding perturbative corrections.

**Helping students realize that a *good* basis is required even for finding first order corrections to the energies:** By engaging with the QuILT, students learn to reason about why a basis that is not a *good* basis for Eq. 6.2 cannot be a *good* basis for Eq. 6.1. There are several questions in which students must identify that $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$ and therefore is not a *good* basis. For example, students consider the following system and are asked to determine whether the basis is a *good* basis:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} -3\epsilon & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix}.$$

The terms $\langle\psi_1^0|\hat{H}'|\psi_2^0\rangle$ and $\langle\psi_2^0|\hat{H}'|\psi_1^0\rangle$ are not zero so that Eq. 6.2 contains divergent terms since $E_1 = E_2$. Thus, it is not a *good* basis for finding perturbative corrections to the energies and energy eigenstates. The following is an excerpt from a hypothetical student

conversation in which the students must consider each hypothetical student's statement and explain why they agree or disagree with each statement. The conversation strives to help students reflect upon the fact that the same basis cannot be a *good* basis for Eq. 6.1 while at the same time NOT be a *good* basis for Eq. 6.2.

Student 2: We cannot use equation (6.2) when the unperturbed energies are degenerate with $E_1^0 = E_2^0 = V_0$ and in the degenerate subspace of $\hat{H}^0$, the perturbing Hamiltonian $\hat{H}'$ is $V_0 \begin{pmatrix} -3\epsilon & 2\epsilon \\ 2\epsilon & 0 \end{pmatrix}$. The first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ "blow up" because the denominators go to zero! But we can use Eq. 6.1 for corrections to the energies since nothing "blows up" in that equation.

Student 3: If $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$, we can neither use equation (6.1) nor (6.2) in the initially chosen basis $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$. The initially chosen basis is not a *GOOD* basis. We need to find a *GOOD* basis in order to use equations (6.1) and (6.2).

After the students work through the question and consider the validity of each statement in the hypothetical conversation, they are provided further scaffolding. They are then asked to summarize when Eqs. 6.1 and 6.2 are valid if there is degeneracy in the energy spectrum of $\hat{H}^0$ and are provided opportunities to reconcile any differences between their initial understanding and the correct understanding via the checkpoints. The QuILT strives to help students learn that care must be taken to determine a *good* basis to ensure Eqs. 6.1 and 6.2 are valid.

**Helping students identify that if $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$, it is a *good* basis:** In the QuILT, students work through different examples in which the same unperturbed Hamiltonian $\hat{H}^0$ is provided with different perturbations $\hat{H}'$ and are asked to identify whether the initially chosen basis is a *good* basis for a given $\hat{H}'$. In the initial examples in the QuILT, they are given opportunities to reflect upon situations in which $\hat{H}'$ is already diagonal in the degenerate subspace of $\hat{H}^0$ in the basis provided and

therefore the initial basis is a *good* basis. For example, students work through the following guided inquiry sequence aimed at helping those who have difficulty identifying $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ given the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ and who have difficulty determining if the basis is a *good* basis.

**Q1(A).** Consider the following example, in which the Hilbert space is three dimensional and $\epsilon$ is a small parameter ($\epsilon \ll 1$) and answer the following questions:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \text{ and } \hat{H}' = V_0 \begin{pmatrix} \epsilon & 2\epsilon & 0 \\ 2\epsilon & \epsilon & 0 \\ 0 & 0 & 3\epsilon \end{pmatrix}$$

in which the normalized basis states are $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

All of the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ are eigenstates of

(i) $\hat{H}^0$ only

(ii) $\hat{H}'$ only

(ii) Both $\hat{H}^0$ and $\hat{H}'$

(iv) Neither $\hat{H}^0$ nor $\hat{H}'$

Explain your reasoning.

In question Q1(A), students must identify that since $\hat{H}^0$ is diagonal in the initially chosen basis, the basis consists of a complete set of eigenstates of $\hat{H}^0$. Thus, the initially chosen basis satisfies one of the conditions for a *good* basis.

The next question Q1(B) asks students to identify whether there is degeneracy in the energy spectrum of $\hat{H}^0$ so that DPT must be used. Students must identify $2V_0$ as the two-fold degenerate unperturbed energy in order to correctly identify the degenerate subspace of

$\hat{H}^0$.

The subsequent question in the guided inquiry-based sequence asks students to identify $\hat{H}^0$ and $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ after identifying the degeneracy in $\hat{H}^0$ in question Q1(B) as follows:

**Q1(C).** Choose one of the following options to fill in the blank. In the degenerate subspace of $\hat{H}^0$, the matrix representation of $\hat{H}'$ is _____ and the matrix representation of $\hat{H}^0$ is _____, respectively.

(i) $V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$, $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$

(ii) $V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$, $V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

(iii) $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$, $V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$

(iv) $V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$, $V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$

Option (ii) is the correct answer to Q1(C). Students must correctly identify the degenerate subspace of $\hat{H}^0$ and identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ for question Q1(C). Option (i) is given as a distractor because students often incorrectly focused on the matrix elements of $\hat{H}'$ when determining the degenerate subspace of $\hat{H}^0$. In option (i), the matrix representation of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ is incorrectly given as the matrix representation of $\hat{H}'$ in the "degenerate" subspace of $\hat{H}'$.

The final part to this inquiry-based sequence asks the following:

**Q1(D).** Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a *GOOD* basis? Explain.

In Q1(D), the initially chosen basis is a *good* basis since it consists of a complete set of eigenstates of $\hat{H}^0$ (probed in Q1(A)), and $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ (probed in Q1(C)). However, students who had difficulty identifying whether the initially

chosen basis is a *good* basis for finding the perturbative corrections often selected option (i) in Q1(C) and they determined that the initially chosen basis is NOT a *good* basis as $\hat{H}'$ in option (i) is not diagonal in the given subspace. Scaffolding is provided after this question in the form of student conversations and checkpoints to help students reconcile the differences between their initial responses and correct ideas.

After students work through several examples to determine whether the initially chosen basis is a *good* basis when the degenerate states are in adjacent rows/columns of $\hat{H}^0$, students are also given an example to help them identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ when the degenerate states are not in adjacent rows/columns.

**Helping students identify that if $\hat{H}'$ is *not* diagonal in the degenerate subspace of $\hat{H}^0$, it is *not* a *good* basis for finding the perturbative corrections:** In other examples in the QuILT, students learn that if $\hat{H}'$ is *not* diagonal in the degenerate subspace of $\hat{H}^0$, it is *not* a *good* basis for finding the perturbative corrections. For example, the following is an excerpt from a guided inquiry-based sequence in the QuILT

**Q2(A).** Consider the following example, in which $\epsilon$ is a small parameter ($\epsilon \ll 1$), and answer the following questions:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -3\epsilon & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix}. \tag{2.8}$$

The normalized basis states are

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Choose one of the following options to fill in the blank. In the degenerate subspace of $\hat{H}^0$, the matrix representation of $\hat{H}'$ is _____ and the matrix representation of $\hat{H}^0$ is _____, respectively.

(i) $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}$, $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$

(II) $V_0 \begin{pmatrix} -3\epsilon & 2\epsilon \\ 2\epsilon & 0 \end{pmatrix}$, $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

(III) $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $V_0 \begin{pmatrix} -3\epsilon & 2\epsilon \\ 2\epsilon & 0 \end{pmatrix}$

(IV) $V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$, $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}$

**Q2(B).** Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a *GOOD* basis? Explain.

This example and other guided inquiry-based sequences strive to help students with difficulties identifying whether the initially chosen basis is a *good* basis for finding the perturbative corrections. In particular, to help students identify that the initially chosen basis is not a *good* basis, students are asked the same questions as in Q1, but in these examples they identify that the $\hat{H}'$ matrix is not diagonal in the degenerate subspace of $\hat{H}^0$. Therefore, the initially chosen basis is not a *good* basis. The tutorial includes several examples in which the initially chosen basis is a *good* basis and several examples in which it is not a *good* basis. After students engage with each example, they are asked to reflect upon and summarize in their own words why the initial basis is a *good* basis or not in each situation.

**Helping students understand why diagonalizing the entire $\hat{H}'$ matrix is problematic when $\hat{H}^0$ and $\hat{H}'$ do not commute:** In the QuILT, students focus on why it is inappropriate to diagonalize the entire $\hat{H}'$ matrix if $\hat{H}^0$ and $\hat{H}'$ do not commute. For example, the following is an excerpt taken from a hypothetical student conversation which is designed to present the students with a cognitive conflict:

Student 1: We should not diagonalize the entire $\hat{H}'$ matrix, but rather only the part of $\hat{H}'$ that corresponds to the degenerate subspace of $\hat{H}^0$.
Student 2: I disagree. If we diagonalize part of the $\hat{H}'$ matrix then we cannot guarantee that it will give us a *GOOD* basis. We must diagonalize the entire $\hat{H}'$ matrix.
Student 3: Actually, it is equally valid to diagonalize either the entire $\hat{H}'$ matrix or only the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$. We usually

choose to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ simply because it requires less work to diagonalize a matrix with a lower dimension.

After students contemplate which hypothetical student is correct (which is Student 1 and possibly agree with the wrong student due to the common difficulty mentioned earlier), they check their responses to Q3 via quantitative reasoning as follows.

**Q3**. Let's see what happens when we diagonalize the entire $\hat{H}'$ matrix. Consider the example

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 5 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{bmatrix}, \qquad (\epsilon \ll 1). \tag{2.9}$$

Due to the degeneracy in the energy spectrum of $\hat{H}'$, the eigenstates of $\hat{H}'$ are not unique. One possible set of eigenstates of $\hat{H}'$ is

$$|\phi_1^0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, |\phi_2^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, |\phi_3^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \tag{2.10}$$

written in terms of the basis states used to write equation (A.21). If we use the eigenstates of $\hat{H}'$ as the basis states, the $\hat{H}^0$ matrix becomes

$$\hat{H}^0 = \begin{bmatrix} \frac{7}{3} & -\frac{4}{\sqrt{6}} & -\frac{4}{\sqrt{6}} \\ -\frac{4}{\sqrt{6}} & 3 & \frac{5}{2} \\ -\frac{4}{\sqrt{6}} & \frac{5}{2} & 3 \end{bmatrix}. \tag{2.11}$$

Can this basis be used for finding the corrections to the energies and energy eigenstates in perturbation theory for the Hamiltonian in equation (A.21)? Explain.

This guided inquiry-based sequence strives to help students learn that when $\hat{H}^0$ and $\hat{H}'$ do not commute, we cannot simultaneously diagonalize $\hat{H}^0$ and $\hat{H}'$. Therefore, diagonalizing $\hat{H}'$ results in a basis in which $\hat{H}^0$ is NOT diagonal. The objective is to have students examine the effect that diagonalizing $\hat{H}'$ has on $\hat{H}^0$. Therefore, rather than having the students work through all the steps to diagonalize the entire $\hat{H}'$ matrix and then express the $\hat{H}^0$ matrix in the basis of the eigenstates of $\hat{H}'$ (as opposed to eigenstates of $\hat{H}^0$), they are provided the $\hat{H}^0$ matrix when the basis is chosen to be the eigenstates of $\hat{H}'$. They can now focus on making sense of the fact that $\hat{H}^0$ is not diagonal if the basis is chosen to be a complete set of eigenstates of $\hat{H}'$ (and therefore, $\hat{H}'$ is diagonal in the basis). They are then guided to reason about the fact that when $\hat{H}^0$ and $\hat{H}'$ do not commute, it is impossible to simultaneously diagonalize them. They are also guided to make sense of the fact that, in a *good* basis, $\hat{H}^0$ must be diagonal since the basis states must be eigenstates of $\hat{H}^0$ (the dominant term in the Hamiltonian) since we are finding small corrections to the energy in DPT.

**Helping students understand why it is always possible to diagonalize $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ (even when $\hat{H}^0$ and $\hat{H}'$ do not commute):** In the QuILT, students reason about why it is possible to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ while still keeping $\hat{H}^0$ diagonal. For example, the following excerpt from an inquiry-based sequence in the QuILT strives to help students understand why it is always possible to diagonalize $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ (i.e., even when $\hat{H}^0$ and $\hat{H}'$ do not commute):

**Q4(A).** Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ in which

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \text{ and } \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \ (\epsilon \ll 1) \tag{2.12}$$

and the normalized eigenstates of $\hat{H}^0$ given by $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, are

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.13}$$

Fill in the blanks using equations (A.14) and (A.15).

(i) $\hat{H}^0|\psi_1^0\rangle =$ _____

(ii) $\hat{H}^0|\psi_2^0\rangle =$ _____

(iii) $\hat{H}^0(a\ |\psi_1^0\rangle +\ b\ |\psi_2^0\rangle) =$ _____

**Q4(B).** Is $a\ |\psi_1^0\rangle +\ b\ |\psi_2^0\rangle$ a normalized eigenstate of $\hat{H}^0$, where $a$ and $b$ are any arbitrary complex numbers that satisfy $|a|^2 + |b|^2 = 1$? Explain.

**Q4(C).** Can $\hat{H}^0$ still be diagonal if $a\ |\psi_1^0\rangle + b\ |\psi_2^0\rangle$ and $c\ |\psi_1^0\rangle + d\ |\psi_2^0\rangle$ are used as new basis states instead of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ and $a, b, c$ and $d$ are chosen such that $a\ |\psi_1^0\rangle + b\ |\psi_2^0\rangle$ and $c\ |\psi_1^0\rangle + d\ |\psi_2^0\rangle$ are orthonormal and $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$? Explain.

Students are then asked to find values of $a, b, c$, and $d$ that diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

In parts (a) and (b) of question Q4, students verify that the linear combination of eigenstates of $\hat{H}^0$ from the same degenerate subspace of $\hat{H}^0$ is an eigenstate of $\hat{H}^0$. Q4(C) strives to help students learn that we can find a particular linear combination that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ while keeping $\hat{H}^0$ diagonal to find a *good* basis for DPT. Students are given the opportunity to check their answer in Q4 via quantitative reasoning.

## 2.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate QM classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts in DPT but before working through the tutorial. The pretests were never returned to the students. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest. The posttest was similar to the pretest with minor changes to the degenerate subspaces. The pretest, tutorial, and posttest each counted as components of the students' course grades. The pretest was scored

for completeness for both groups. The posttest was scored for correctness for the undergraduates in all three years. However, the posttest was scored differently for the graduate students in the two different years. In Year 1, the graduate students' posttest was scored for completeness while in Year 2 it was scored for correctness. For the undergraduate students, the QuILT (including pretest, tutorial, and posttest) contributed to roughly 2.5% of their course grade in Year 1 and Year 2. In Year 3, for the undergraduate students, it contributed to roughly 7% of their course grade. For the graduate students, roughly 1% of the course grade was associated with the QuILT. Regardless of how the pretest and posttest counted towards the students' course grade, each was scored for correctness to investigate the effectiveness of the QuILT for research purposes. These scores are the scores that are reported here.

The entire pretest and posttest each consist of 10 questions related to DPT. We will present the results from the three questions that focused on finding a *good* basis and first order corrections to the energy for a system restricted to a three-dimensional Hilbert space. To probe student understanding of DPT in the context of three dimensional Hilbert space, the following questions QI-QIII were administered on the QuILT pretest and/or the QuILT posttest. All the questions were asked on both the pretest and posttest in Years 1 and 3. In Year 2, question QI(B) was posed only on the pretest and question QI(A) was posed only on the posttest.

**QI**. Consider the unperturbed Hamiltonian $\hat{H}^0 = V_0 \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 7 \end{bmatrix}$.

(a) Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis forms a *good* basis (so that one can use the same expressions that one uses in non-DPT for perturbative corrections). Use $\epsilon$ as a small parameter.

(b) Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis does NOT form a *good* basis (so that we cannot use the basis for perturbative corrections using Eq. 6.1).

Use $\epsilon$ as a small parameter.

**QII**. Given $\hat{H} = \hat{H}^0 + \epsilon\hat{H}' = V_0 \begin{bmatrix} 5 & 0 & -4\epsilon \\ 0 & 1-4\epsilon & 0 \\ -4\epsilon & 0 & 1+6\epsilon \end{bmatrix}$ with $\epsilon \ll 1$, determine the first order corrections to the energies. **You must show your work.**

**QIII**. Given $\hat{H} = \hat{H}^0 + \epsilon\hat{H}' = V_0 \begin{bmatrix} 2 & \epsilon & \epsilon \\ \epsilon & 2 & \epsilon \\ \epsilon & \epsilon & 3 \end{bmatrix}$, with $\epsilon \ll 1$, determine the first order corrections to the energies. You must show your work.

In order to answer QI correctly, students must first identify the degenerate subspace of $\hat{H}^0$. Since $\hat{H}^0$ is diagonal in the given basis, a *good* basis is one in which $\hat{H}'$ is also diagonal in the degenerate subspace of $\hat{H}^0$. Therefore, in part QI(A), students must provide an $\hat{H}'$ matrix that is diagonal in the degenerate subspace of $\hat{H}^0$ and in part QI(B), students must provide an $\hat{H}'$ matrix that is not diagonal in the degenerate subspace of $\hat{H}^0$.

For QII, students must first identify $\hat{H}'$ and $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$. Once they identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, they must determine whether the initially chosen basis is a *good* basis. In particular, they must realize that in QII, $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ and therefore the initial basis is a *good* basis. The diagonal matrix elements of $\hat{H}'$ are the first order corrections to the energies.

In QIII, students must first identify $\hat{H}'$ and $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$. Once they identify $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, they must determine whether the initially chosen basis is a *good* basis. In QIII, $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$. Thus, the initial basis is not a *good* basis and students first must determine a *good* basis in order to find the perturbative corrections. Since $\hat{H}^0$ and $\hat{H}'$ do not commute, students must diagonalize $\hat{H}'$ only in the degenerate subspace of $\hat{H}^0$. In a *good* basis, the diagonal matrix elements of $\hat{H}'$ are the first order corrections to the energies.

The open-ended questions were graded using rubrics which were developed by the researchers together. A subset of questions was graded separately by them. After comparing

the grading, they discussed any disagreements and resolved them with a final inter-rater reliability of better than 95%. Table 1 shows the performance of undergraduate and graduate students on the pretest and posttest. Table 1 also includes the average gain, $G$, and normalized gain [47], $g$. The normalized gain is defined as the (posttest percent - pretest percent)/(100 - pretest percent). The undergraduate students had the same instructor (Instructor 1) in Year 1 and Year 2. The instructor (Instructor 3) for the graduate level course was the same in Year 1 and Year 2 (it was a different instructor than the undergraduate course). Performance on questions QII and QIII on pretest were comparable in Years 1 and 2 and were combined into a single percentage in Table 1. Similarly, the posttest scores for the undergraduate and graduate students on QII and QIII in Years 1 and Years 2 were comparable and were combined. Both the undergraduate and graduate instructors in Years 1 and 2 used a traditional lecture-based approach. Instructor 2 for the undergraduate students in Year 3 used active-engagement teaching involving in-class clicker questions with peer discussion. The performance of the undergraduates on the pretest in Year 3 is significantly better than that of the performance of the undergraduate students on the pretest in Years 1 and 2. However, after engaging with the QuILT, there is no statistically significant difference in the performance of the undergraduate students on the posttest based upon instructor and all classes performed well regardless of the instructor. These results are encouraging and suggest that the QuILT is effective at reducing the gap between courses taught with traditional lecture-based instruction and those that incorporate active engagement activities while also achieving a high normalized gain for the students regardless of their performance on the pretest. The posttest scores are significantly better than the pretest scores on all of these questions for both undergraduate and graduate students with the exception of Q1(B) in Year 3 (in which the active learning instructor's students performed well on both the pretest and the posttest).

To investigate retention of learning, the undergraduates in Year 1 were given questions QI(A) and QI(B) again as part of their final exam. The final exam was six weeks after students engaged with the tutorial. The average score on QI(A) was 97.8% and on QI(B) was 91.0%. In QI(A), all 11 students provided an $\hat{H}'$ matrix that was diagonal in the degenerate subspace of $\hat{H}^0$. In QI(B), 10 out of 11 students provided an $\hat{H}'$ matrix that was

Table 1: Average pretest and posttest scores, gains ($G$) and normalized gains ($g$) for undergraduate students (number of students $N = 11$ in Year 1 , $N = 12$ in Year 2, $N = 12$ in Year 3) and graduate students (number of students $N = 19$ in Year 1 and $N = 19$ in Year 2). Also, the average score of the undergraduates is given for two problems that were given on the final exam six weeks later.

| | Undergraduate Students | | | | | | | Graduate Students | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Question | Instructor | N | Pre (%) | Post (%) | G (%) | g | Final (%) | Instructor | N | Pre (%) | Post (%) | G (%) | g |
| QI(A) | 1 | 11 | 23.1 | 100 | +76.9 | 1.00 | 97.8 | 3 | 19 | 67.5 | 88.2 | +20.7 | 0.64 |
| | 1 | 12 | - | 97.9 | - | - | - | 3 | 19 | - | 93.4 | - | - |
| | 2 | 12 | 69.8 | 91.7 | +21.9 | 0.73 | - | - | - | - | - | - | - |
| QI(B) | 1 | 11 | 15.4 | 100 | +84.6 | 1.00 | 91.0 | 3 | 19 | 51.3 | 73.7 | +22.4 | 0.46 |
| | 1 | 12 | 43.8 | - | - | - | - | 3 | 19 | 36.8 | - | - | - |
| | 2 | 12 | 89.6 | 92.8 | +3.2 | 0.31 | - | - | - | - | - | - | - |
| QII | 1 | 23 | 19.8 | 92.7 | +72.9 | 0.91 | - | 3 | 19 | 25.0 | 90.8 | +65.8 | 0.88 |
| | 2 | 12 | 33.3 | 94.4 | +61.1 | 0.92 | - | - | - | - | - | - | - |
| QIII | 1 | 23 | 1.2 | 91.3 | +90.0 | 0.91 | - | 3 | 19 | 12.9 | 83.0 | +70.1 | 0.80 |
| | 2 | 12 | 33.3 | 95.0 | +61.7 | 0.93 | - | - | - | - | - | - | - |

not diagonal in the degenerate subspace of $\hat{H}^0$.

Table 1 shows that the performance of the undergraduate students on all the questions in the posttest was exceptional. However, as can be seen from the pretest scores in Table 1, traditional lecture-based instruction was not particularly effective at developing a functional understanding of these topics. We also note that this second semester upper-level undergraduate QM course is an elective honors physics course that majority of the students take in preparation for graduate school to pursue a Ph.D. They are highly motivated to learn the material if appropriate guidance and support is provided (which the QuILT, that uses research on student difficulties as a guide, strived to do). This may help to explain why the undergraduate students did so well on the posttest after engaging with research-validated guided inquiry-based learning tutorial. The majority of these honors students are high achieving undergraduate students and a large fraction go on to graduate school at top universities. In addition, we note that while many students were able to answer Questions QI-QIII correctly, it is encouraging that most students provided correct reasoning along with

their work on the posttest questions. Students' written reasoning indicated that they had developed a good understanding of how to determine a *good* basis and the first order corrections to the energy rather than simply memorizing an algorithm. Figure 1 shows a written response from an undergraduate student on the posttest in Year 1 to question QIII. The student began by expressing the Hamiltonian as the sum of the unperturbed Hamiltonian $\hat{H}^0$ and the perturbating Hamiltonian $\hat{H}'$. He then boxed the degenerate subspace of $\hat{H}^0$ and $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Next, he noted that $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$ and proceeded to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Then he correctly identified the first order corrections to the energies as 0 and $\pm\epsilon V_0$. Many students provided similar solutions that clearly justified their reasoning and demonstrated a correct problem-solving approach to questions QI-QIII.

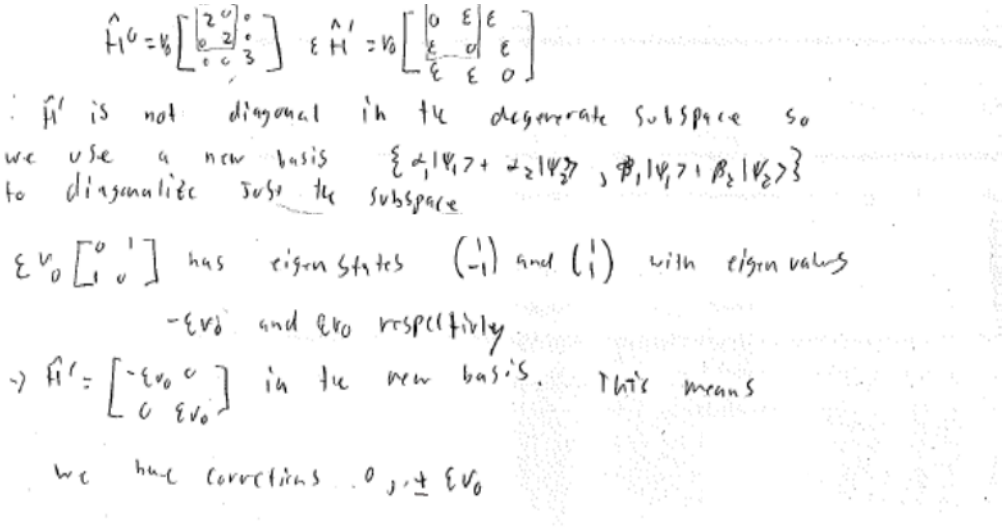


Figure 1: Written student response from an undergraduate student on the posttest to question QIII

We also note that this investigation was part of a larger study of student understanding of DPT. The QuILT focusing on DPT in a 3-dimensional Hilbert space was one of a series of QuILTs developed to help improve student understanding of DPT. The QuILT discussed here was developed to help students gain a functional understanding of fundamental concepts in DPT in the context of a 3-dimensional Hilbert space which are necessary for understanding

more complex applications of DPT. For example, we have developed a QuILT that builds on the QuILT discussed here and strives to help students find a *good* basis and the first order corrections to the energy spectrum of the hydrogen atom placed in an external magnetic field. In this situation, students must determine a *good* basis and find the first order corrections to the energies for principal quantum number $n = 2$ in an eight-dimensional subspace. We note that in these more complex situations involving the hydrogen atom, the students do not perform as well on the posttest as they do on the posttest described in this paper that focused on DPT in a 3-dimensional Hilbert space. However, they still show a dramatic improvement over their pretest scores after traditional lecture-based instruction only. We plan to discuss these investigations in future work.

As can be seen in Table 7, the graduate students generally performed better than the undergraduates on the pretest. However, the undergraduates outperformed the graduate students on the posttest on most questions (see Table 7). One possible explanation for the undergraduates outperforming the graduate students on the posttest could be the grade incentive associated with the QuILT. As discussed earlier, the QuILT accounted for a larger percent of the undergraduates overall course grade and the components of the QuILT were accounted for differently for the course grade for the two groups of students. In particular, the posttest for the undergraduate students was graded for correctness in all three years while the posttest for the graduate students was graded for completeness in Year 1 and for correctness in Year 2. Additionally, the undergraduate students knew that the material from the QuILT could appear on their examinations while the graduate students were told but the graduate instructor that this material was a review of the undergraduate quantum mechanics and that no material from the QuILT would appear on their examinations, instead, more complex problems on the DPT would appear on the exams. The fact that the graduate students were given very small grade incentive to learn the material in the QuILT may have decreased their motivation to engage as deeply with the QuILT as the undergraduates and may explain why the graduate students did not perform as well as the undergraduate students on the posttest. We also note that prior studies in the context of introductory physics suggest that more time on task does not improve student understanding and students need to engage with research-based approaches in a meaningful way for them to develop a good grasp of

concepts [48].

## 2.7 SUMMARY

We developed and evaluated a research-based QuILT which focuses on helping students reason about and find perturbative corrections to the energies using DPT. We found that the advanced physics students who are still developing expertise in QM had difficulty after traditional lecture-based instruction in reasoning about the DPT concepts while solving problems. This difficulty is in part due to the fact that students' working memory can get overloaded by the demands of the DPT problems (partly due to the fact that the paradigm of quantum mechanics is novel and partly due to the difficulty with mathematical sense making in a physics context involving degeneracy). One major cause of the difficulties is the fact that DPT relies heavily on applying linear algebra in the context of QM and many students struggled to apply these mathematical concepts correctly in the context of DPT. In particular, a majority of students were not able to integrate all the different concepts coherently to solve a given problem after traditional lecture-based instruction. We used the common difficulties of advanced students with DPT found via research as resources in order to develop and validate the QuILT. The research-validated QuILT strives to provide appropriate scaffolding and feedback using a guided inquiry-based approach to help students develop a functional understanding of DPT. The preliminary evaluation shows that the QuILT is effective in improving undergraduate and graduate students' understanding of a *good* basis in the context of DPT. Future investigations will focus on evaluating the effectiveness of the QuILT at other universities where the student in this type of undergraduate QM course are not so selective.

## 2.8 ACKNOWLEDGEMENTS

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# 3.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DEGENERATE PERTURBATION THEORY: DETERMINING A BASIS IN WHICH AN OPERATOR IS DIAGONAL

## 3.1 INTRODUCTION

Quantum Mechanics (QM) is a challenging subject for upper-level undergraduate and graduate students in physics (e.g., see Refs. [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]). There have been a number of research studies aimed at investigating student reasoning in QM [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23] and improving student understanding of QM [24, 25, 26, 27, 28, 29, 30, 31, 32]. Guided by research studies conducted to identify student difficulties with QM and findings of cognitive research, we have been developing a set of research-based learning tools including the Quantum Interactive Learning Tutorials (QuILTs) which strive to help students develop a solid grasp of QM [33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44].

Students' ability to apply linear algebra concepts in various QM contexts and interpret the physical results appropriately depends on whether they have developed a robust knowledge structure and a functional understanding of relevant upper-level QM concepts. Moreover, in the context of degenerate perturbation theory (DPT), the degeneracy makes it even more important that students have a deep understanding of linear algebra concepts and procedures in order to apply them appropriately to solve quantum physics problems involving DPT.

Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of

the individual who is solving the problem, Simon's framework of "bounded rationality and satisficing" posits that an individual will make decisions while solving problems based upon their current level of expertise, which may not be optimal [45]. While solving a problem, satisficers are often interested in what is referred to as "satisficing" and only look for a solution consistent with their current level of expertise that is satisfactory to them in which they see no inconsistencies rather than searching for additional pathways in the problem space which may yield a more optimal solution [45]. In some of these cases, satisficers are content with their efforts in solving the problem and see no reason to consider whether there are alternative pathways in the problem space. In other cases, they may realize that their satisficing may not yield an optimal solution and there may be more productive pathways in the problem space but choose not to explore those additional pathways for a more optimal solution due to the increased mental effort required in this process [45]. Other students may be motivated to find an optimal solution to the problem by searching for many possible pathways in the problem space. However, if their level of expertise is not sufficient to solve the problem on their own and they have not been provided with appropriate guidance and scaffolding support, they may experience cognitive overload and may not be able to determine an optimal solution to the problem posed [45, 46].

Many of the student difficulties discussed here in the context of DPT may be attributed in part to students' bounded rationality and satisficing while sense-making in that they may be satisfied with a sub-optimal solution that does not cause cognitive overload and may not search for optimal solution pathways in the problem space that may yield the correct solution [45, 46]. Those students who resort to satisficing are, in general, satisfied to engage in sense-making which is commensurate with their current level of expertise and their integration of mathematical and physical concepts to solve the problem may not be appropriate for the problem solving task since they are still developing expertise in these areas [45]. Since the paradigm of QM is novel, these issues related to satisficing and difficulty in sense-making become critical when students solve problems in this non-intuitive abstract context unless they are provided appropriate guidance and scaffolding support to engage in productive sense-making.

Here, we discuss an investigation of student difficulties with the representations in which

an operator is diagonal in the context of DPT involving the Zeeman effect in a hydrogen atom and how that research was used as a guide in the development, validation, and in-class evaluation of a research-based QuILT that makes use of student difficulties as a guide and strives to help students develop a good grasp of relevant concepts.

## 3.2 BACKGROUND

### 3.2.1 Background for DPT

Perturbation theory (PT) is a powerful approximation method for finding the energies and the energy eigenstates of a system for which the Time-Independent Schrödinger Equation (TISE) is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$. The TISE for the unperturbed Hamiltonian is $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$. $\psi_n^0$, the $n^{th}$ unperturbed energy eigenstate, and $E_n^0$, the $n^{th}$ unperturbed energy, are exactly solvable. PT builds on the solutions of the TISE for the unperturbed case. Using PT, the energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \cdots$ where $E_n^i$ for $i = 1, 2, 3..$ are the $i^{th}$ order corrections to the $n^{th}$ energy of the system. The energy eigenstate can be approximated as $\psi_n = \psi_n^0 + \psi_n^1 + \psi_n^2 + \cdots$ where $\psi_n^i$ are the $i^{th}$ order corrections to the $n^{th}$ energy eigenstate. We focus on the first order perturbative corrections to the energies since they are usually the dominant corrections. In nondegenerate perturbation theory (NDPT), the first order correction to the $n^{th}$ energy is $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ and the first order correction to the $n^{th}$ energy eigenstate is $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle$. When the eigenvalue spectrum of $\hat{H}^0$ has degeneracy (two or more eigenstates of $\hat{H}^0$ have the same energy, i.e., two or more diagonal elements of $\hat{H}^0$ are equal in the basis consisting of eigenstates of $\hat{H}^0$), the equations for the first order corrections to the energies and energy eignestates from NDPT are still valid provided one uses a *good* basis. For a given $\hat{H}^0$ and $\hat{H}'$, we define a *good* basis as consisting of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. In a *good* basis, $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$ so that the divergent

terms do not appear in the first order corrections to the energy eigenstates and expressions for the corrections to the energies and energy eigenstates in NDPT are valid.

### 3.2.2 Background for DPT involving the Zeeman effect in the hydrogen atom

One application of DPT that students learn about in upper-level undergraduate and graduate QM courses involves a hydrogen atom placed in an external magnetic field (known as the Zeeman effect). Using standard notations, the Hamiltonian of a hydrogen atom placed in an external magnetic field is $\hat{H} = \hat{H}^0 + \hat{H}'$ in which the unperturbed Hamiltonian, $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$, accounts only for the interaction of the electron with the nucleus via Coulomb attraction and the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $\hat{H}'_Z$ is the Zeeman term and $\hat{H}'_{fs}$ is the fine structure term. The Zeeman term accounts for the potential energy of the magnetic moments due to the orbital and spin angular momenta in the external magnetic field. The Zeeman term is given by $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ in which $\vec{B}_{ext} = B_{ext}\hat{z}$ is a uniform, time-independent external magnetic field along the $\hat{z}$-direction, $\mu_B$ is the Bohr magneton and $\hat{L}_z$ and $\hat{S}_z$ are the operators corresponding to the z component of the orbital and spin angular momenta, respectively. The fine structure term includes a relativistic correction and the spin-orbit coupling for the kinetic energy and is expressed as $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Here, $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term and $\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S}$ is the spin-orbit interaction term (all notations are standard).

For each subspace corresponding to the principal quantum number $n$, the energy spectrum of $\hat{H}^0$ is $2n^2$-fold degenerate. Therefore, a *good* basis for finding the perturbative corrections consisting of eigenstates of $\hat{H}^0$ must also diagonalize the perturbation $\hat{H}'$ in the $2n^2$ dimensional subspace corresponding to each $n$. We note that the unperturbed Hamiltonian $\hat{H}^0$ is spherically symmetric since $[\hat{H}^0, \hat{\vec{L}}] = 0$. Therefore, for a fixed $n$, $\hat{H}^0$ for the hydrogen atom is diagonal when any complete set of orthogonal states is chosen for the angular part of the basis (consisting of the product states of orbital and spin angular momenta). Thus, so long as the radial part of the basis is always chosen to be a stationary state wavefunction $R_{nl}(r)$ for the hydrogen atom (for a given principal quantum number $n$ and azimuthal quantum number $l$), which we will assume throughout, the choice of a *good*

basis amounts to choosing the angular part of the basis (or angular basis) appropriately, i.e., ensuring that the perturbation is diagonal in each degenerate subspace of $\hat{H}^0$. Therefore, we focus on the angular basis to find a *good* basis and the corrections to the energies for the perturbation $\hat{H}'$ corresponding to the intermediate field Zeeman effect in the hydrogen atom. Below, we individually consider the operators $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ representing perturbations on the unperturbed Hamiltonian $\hat{H}^0$ since we probed student understanding of a basis in which a perturbation Hamiltonian is diagonal in each degenerate subspace of $\hat{H}^0$ for each of these cases.

We note that, similar to $\hat{H}^0$, the relativistic correction term $\hat{H}'_r$ is also spherically symmetric but the corresponding energies depend on $n$ and $l$. Thus, $\hat{H}^0$ is diagonal and $\hat{H}'_r$ is diagonal in the degenerate subspace of $\hat{H}^0$ if any complete set of orthogonal states consisting of the product states of orbital and spin angular momenta with a fixed $n$ and $l$ is chosen for the angular basis. Therefore, in DPT, for a given $n$, any complete set of orthogonal states with the same $l$ forms a *good* angular basis for finding the corrections to the energies of a hydrogen atom due to the relativistic correction term $\hat{H}'_r$.

In order to determine a *good* angular basis for the spin-orbit interaction term $\hat{H}'_{SO}$, we must determine the angular basis which makes the operator $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$. A basis in the "coupled representation" consists of a complete set of states $|n,\ l,\ s,\ j,\ m_j\rangle$ (which are eigenstates of $\hat{J}^2$ and $\hat{J}_z$) in which the total angular momentum is the sum of the orbital and spin angular momenta such that $\vec{J} = \vec{L} + \vec{S}$ and for each quantum number $j$, the quantum numbers corresponding to the $z$ component are given by $m_j = -j, -(j-1), \ldots, j-1, j$ (all notations are standard). A basis in the "uncoupled representation" consists of a complete set of states $|n,\ l,\ s,\ m_l,\ m_s\rangle$ which are eigenstates of $\hat{L}_z$ and $\hat{S}_z$ (all notations are standard). Students were given the following equations that are useful when reasoning about the representation in which the matrix $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ (all of the notations are standard):

$\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{r^3}\vec{L}\cdot\vec{S}$,

$\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$,

$\hat{J}^2|n,\ l,\ s,\ j,\ m_j\rangle = \hbar^2 j(j+1)|n,\ l,\ s,\ j,\ m_j\rangle$,

$\hat{L}^2|n,\ l,\ s,\ j,\ m_j\rangle = \hbar^2 l(l+1)|n,\ l,\ s,\ j,\ m_j\rangle$,

$\hat{S}^2|n,\ l,\ s,\ j,\ m_j\rangle = \hbar^2 s(s+1)|n,\ l,\ s,\ j,\ m_j\rangle,$

$\hat{L}^2|n,\ l,\ s, m_l,\ m_s\rangle = \hbar^2 l(l+1)|n,\ l,\ s, m_l,\ m_s\rangle$

$\hat{L}_z|n,\ l,\ s, m_l,\ m_s\rangle = \hbar m_l|n,\ l,\ s, m_l,\ m_s\rangle$

$\hat{S}^2|n,\ l,\ s, m_l,\ m_s\rangle = \hbar^2 s(s+1)|n,\ l,\ s, m_l,\ m_s\rangle$

$\hat{S}_z|n,\ l,\ s, m_l,\ m_s\rangle = \hbar m_s|n,\ l,\ s, m_l,\ m_s\rangle$

$\hat{S}_\pm|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1))}|n,\ l,\ s,\ m_l,\ m_s \pm 1\rangle,$

$\hat{L}_\pm|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar\sqrt{l(l+1) - m_l(m_l \pm 1))}|n,\ l,\ s,\ m_l \pm 1,\ m_s\rangle.$

Focusing on the expression for $\hat{H}'_{SO}$ in which $\vec{L}\cdot\vec{S}$ is proportional to $\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$, one can infer that the product states in the "coupled" representation $|n,\ l,\ s,\ j,\ m_j\rangle$, which are eigenstates of the operators $\hat{J}^2$, $\hat{L}^2$, and $\hat{S}^2$, diagonalize $\hat{H}'_{SO}$ in each degenerate subspace of $\hat{H}^0$. Thus, the coupled representation is a *good* angular basis for finding the corrections to the energies using DPT. However, it is NOT the case that $\hat{H}'_{SO}$ is diagonal in the degenerate subspace of $\hat{H}^0$ if any linear combination of states in the coupled representation is chosen as the angular basis. From the expression in which $\hat{H}'_{SO}$ is proportional to $\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$, one can infer that the product states in the "uncoupled" representation $|n,\ l,\ s,\ m_l,\ m_s\rangle$ (notations are standard) are eigenstates of $\hat{L}_Z$ and $\hat{S}_Z$ (and also $\hat{L}^2$ and $\hat{S}^2$), but are not eigenstates of the operators $\hat{S}_\pm$ and $\hat{L}_\pm$. Thus, $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ if a basis consisting of states in the uncoupled representation is chosen as the angular basis. Since $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ if a basis consisting of states in the uncoupled representation is chosen as the angular basis, $\hat{H}'_{SO}$ cannot be diagonal in each degenerate subspace of $\hat{H}^0$ if a basis consisting of any linear combination of states in the uncoupled representation is chosen as the angular basis.

Lastly, we consider the perturbation $\hat{H}'_Z$. The following equations are useful when reasoning about the representation in which the perturbation $\hat{H}'_Z$ is diagonal (all notations are standard): $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z), \hat{L}_z|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar m_l|n,\ l,\ s,\ m_l,\ m_s\rangle$, and $\hat{S}_z|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar m_s|n,\ l,\ s,\ m_l,\ m_s\rangle$. Thus, the product states in the uncoupled representation, $|n,\ l,\ s,\ m_l,\ m_s\rangle$, are eigenstates of both the operators $\hat{L}_z$ and $\hat{S}_z$ and are, threrefore, eigenstates of $\hat{H}'_Z$. Thus, an angular basis consisting of states in the uncoupled representation will make the $\hat{H}'_Z$ operator diagonal and such a basis will be a *good* basis for finding the corrections to the energies using DPT with $\hat{H}^0$ and $\hat{H}'_Z$ (in that case, if $\hat{H}'_Z$

was the only perturbation, the perturbative corrections to first order PT give exact results, correct to all orders).

## 3.3 METHODOLOGY

Student difficulties with the representation in which a perturbation Hamiltonian is diagonal in each degenerate subspace of $\hat{H}^0$ in the context of DPT were first investigated using five years of data involving responses to open-ended and multiple-choice questions administered after traditional, lecture-based instruction in relevant concepts from 64 upper-level undergraduates in a second-semester junior/senior level QM course and 42 first-year physics graduate students in the second-semester of the graduate core QM course. Additional insight was gained concerning these difficulties via responses of 13 students during a total of 45 hours of individual interviews using a "think aloud" protocol in which they answered the questions posed without being disturbed [47]. At the end of the interview, they were asked to clarify any additional issues they had not made clear themselves.

In all questions asked in the investigation, students were given that the radial part of the basis for PT is always chosen to be stationary state wavefunctions $R_{nl}(r)$ for the hydrogen atom (for a given principal quantum number $n$ and azimuthal quantum number $l$). Thus, students must only focus on the angular basis in order to find a *good* basis for DPT for a given $\hat{H}^0$ and $\hat{H}'$ for a hydrogen atom placed in an external magnetic field. Additionally, in all questions, students were asked to consider the $n = 2$ subspace for which the unperturbed energy $E_2^0 = -\frac{13.6\text{eV}}{4}$ is 8-fold degenerate. Students were provided with all of the relevant equations discussed in the background section and had learned about the coupled and uncoupled representations via traditional, lecture-based instruction.

After analyzing responses of 32 undergraduates on questions about DPT administered in two previous years, we posed the following questions to 45 undergraduate and 42 graduate students in the following four years as part of an in-class quiz after traditional lecture-based instruction. We discuss student facility with both conceptual and procedural knowledge relevant in this case. In particular, students were asked probing questions that focused on

concepts as well as evaluation of matrix elements of relevant operators in different representations in various situations.

To probe whether students were able to determine the matrix elements of an operator that may be relevant for determining if an angular basis (e.g., coupled representation, uncoupled representation, etc.) is *good* for the perturbations $\hat{H}'_Z$ and $\hat{H}'_{SO}$, the following are two examples of questions that were posed:

**Q1(a).** Evaluate the following matrix element useful for $\hat{H}'_Z$ for $n = 2$, in which the states are written in the coupled representation $|n,\ l,\ s,\ j,\ m_j\rangle$. **In order to receive credit, you must show your work or explain your reasoning.**

$$\left\langle 2,\ 1, \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2} \left| (\hat{L}_z + 2\hat{S}_z) \right| 2,\ 1, \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2} \right\rangle$$

**Q1(b-d).** Evaluate the following matrix elements useful for $\hat{H}'_{SO}$ for $n = 2$, in which the states are written in the uncoupled representation $|n,\ l,\ s,\ m_l,\ m_s\rangle$. **In order to receive credit, you must show your work or explain your reasoning.**

(b) $\langle 2,\ 1,\ \frac{1}{2},\ 1, \frac{1}{2} | \, (\vec{L} \cdot \vec{S}) \, | 2, 1,\ \frac{1}{2}, -1, \frac{1}{2} \rangle$

(c) $\langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2} | \, (\vec{L} \cdot \vec{S}) \, | 2, 1,\ \frac{1}{2}, 1, \frac{1}{2} \rangle$

(d) $\langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2} | (\vec{S} \cdot \vec{L}) | 2\ 1\ \frac{1}{2}\ 1\ -\frac{1}{2} \rangle$

Students were provided a table which contained relevant states in the coupled representation written in terms of a linear combination of states in the uncoupled representation. One method for answering Q1(a) is to write the state $|n,\ l,\ s,\ j,\ m_j\rangle = |2,\ 1,\ \frac{1}{2}, \frac{3}{2},\ \frac{3}{2}\rangle$ in the uncoupled representation as $|n,\ l,\ s,\ m_l,\ m_s\rangle = |2, 1,\ \frac{1}{2}\ 1,\ \frac{1}{2}\rangle$. Since the states in the uncoupled representation $|n,\ l, s,\ \ m_l\ m_s\rangle$ are eigenstates of $\hat{L}_z$ and $\hat{S}_z$ with eigenvalues $m_l\hbar$ and $m_s\hbar$, respectively, the answer to Q1(a) is $[1 + 2(1/2)]\hbar = 2\hbar$.

Students were provided the equations $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ as well as the relevant eigenvalue equations and the equations for the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$ acting on states in the uncoupled representation that are helpful in answering Q1(b). Since $\hat{H}'_{SO}$ is proportional to $\vec{L} \cdot \vec{S}$, the student must choose which equation is appropriate to calculate the matrix elements for a basis consisting of states in the uncoupled representation. For a basis consisting of states in the uncoupled

representation, the equation $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ is more useful as states in the uncoupled representation are eigenstates of $\hat{L}_z$ and $\hat{S}_z$ and equations for the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$ acting on states in the uncoupled representation were provided to the students. For Q1(b), after acting with the operator $\vec{L}\cdot\vec{S}$ on the ket state $|2,1,\ \frac{1}{2},-1,\frac{1}{2}\rangle$ in the uncoupled rerpesentation, the resulting states are orthogonal to the bra state $\langle 2,\ 1,\ \frac{1}{2},\ 1,\frac{1}{2}|$. Therefore, the answer to Q1(b) is zero. For Q1(c), $\left\langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2}\right|(\vec{L}\cdot\vec{S})\left|2,1,\ \frac{1}{2},1,\frac{1}{2}\right\rangle = \left\langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2}\right|\hat{L}_z\hat{S}_z\left|2,1,\ \frac{1}{2},1,\frac{1}{2}\right\rangle = \frac{\hbar^2}{2}$. For Q1(d), $\langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}\ 1\ -\frac{1}{2}\rangle = \langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|\hat{L}_-\hat{S}_+|2\ 1\ \frac{1}{2}\ 1\ -\frac{1}{2}\rangle = \frac{\sqrt{2}\hbar^2}{2}$.

In Q2, students were asked to identify the representations that make each of the operators $\hat{H} = \hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ (that make up the different parts of the Hamiltonian for the Zeeman effect) diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ to probe the common difficulties.

***Q2***. *Circle* **ALL** *of the angular bases which make the Hamiltonian operator $\hat{H}$ diagonal in the $n = 2$ subspace of $\hat{H}^0$ and explain your reasoning. Assume that for all cases, the principal quantum number $n = 2$.*

*i. Coupled representation,*

*ii. Uncoupled representation,*

*iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*v. Neither coupled nor uncoupled representation.*

In Q2, the operator $\hat{H}$ is a proxy for $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ listed individually in four separate questions. Since $\hat{H}^0$ for a hydrogen atom is spherically symmetric with eigenvalues $E_n = -\frac{13.6\text{eV}}{n^2}$ and is diagonal when any complete set of orthogonal states with a fixed $n$ is chosen for the angular basis, options i, ii, iii, and iv are all correct for the operator $\hat{H}^0$ in Q2. The operator $\hat{H}'_r$ is also spherically symmetric with eigenvalues depending on $n$ and $l$ and is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ if the options i, ii, iii, or iv in Q2 are chosen

as the angular basis. The operator $\hat{H}'_{SO}$ is diagonal in the $n = 2$ subspace if the angular basis consists of states in the coupled representation (option i only) in Q2. The operator $\hat{H}'_Z$ is diagonal if the angular basis consists of states in the uncoupled representation (option ii only) in Q2.

### 3.4 STUDENT DIFFICULTIES

We find that when students were asked to determine the angular part of the basis states for a *good* basis in order to find the perturbative corrections for the Zeeman effect, many struggled with the representation in which a particular Hamiltonian matrix is diagonal. Students also struggled to evaluate the matrix elements relevant for various Hamiltonians in different representations. Some students admitted to memorizing the representation to choose for the angular basis in a given situation (for a given $\hat{H}^0$ and $\hat{H}'$) rather than using systematic reasoning. For example, one interviewed student noted: "I was always confused with coupled and uncoupled representation. I just memorized when to use which." Memorization of which representation to use in different situations often masked the fact that students did not have a functional understanding of the relevant linear algebra concepts in order to apply them in this QM context.

In question Q2, students were asked to determine which bases in various options make each individual Hamiltonian $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ diagonal in the $n = 2$ subspace of $\hat{H}^0$. Table 2 shows the percentages of students who correctly answered Q2. Furthermore, 40% of the graduate students and 34% of the undergraduates did not choose a basis consisting of states in the uncoupled representation in order to diagonalize the Zeeman term $\hat{H}'_Z$. Also, 33% of the graduate students and 34% of the undergraduates did not choose the coupled representation as a basis to diagonalize the spin-orbit interaction term $\hat{H}'_{SO}$ in the $n = 2$ subspace of $\hat{H}^0$. Below, we discuss specific difficulties with choosing a basis that makes an operator diagonal in the $n = 2$ subspace of $\hat{H}^0$.

Table 2: Percentages of undergraduate and graduate students who selected all of the possible correct representations in which a given operator is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ in Q2.

| Operator | Correct Answer | Undergraduate | | Graduate | |
|---|---|---|---|---|---|
| | | N | (%) | N | (%) |
| $\hat{H}^0$ | i, ii, iii, iv | 32 | 34 | 42 | 33 |
| $\hat{H}'_r$ | i, ii, iii, iv | 32 | 22 | 42 | 21 |
| $\hat{H}'_{SO}$ | i | 32 | 34 | 42 | 36 |
| $\hat{H}'_{fs}$ | i | 12 | 33 | - | - |
| $\hat{H}'_Z$ | ii | 32 | 38 | 32 | 33 |

### 3.4.1 Difficulty calculating matrix elements when the basis did not consist of a complete set of eigenstates of the given operator

Being able to calculate the matrix elements of the perturbation is crucial to determining the first-order corrections to the energy spectrum for the intermediate field Zeeman effect. In a *good* basis, the off-diagonal elements of the perturbation matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ must be zero in each degenerate subspace of $\hat{H}^0$. Also, in a *good* basis, the diagonal elements of the perturbation matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ are the first order corrections to the energy spectrum of the hydrogen atom for the Zeeman effect. The off-diagonal elements of the perturbation matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in a *good* basis are needed to determine the higher order corrections to the energy spectrum and energy eigenstates. Therefore, to ensure meaningful calculations of the corrections to the energies and energy eigenstates, one must be able to calculate the matrix elements of $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ correctly. For example, in order to determine a *good* basis for the intermediate field Zeeman effect for finding perturbative corrections, one can initially choose a basis consisting of states in the coupled representation or a basis consisting of states in the uncoupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$. This requires students to be able to calculate the matrix elements of $\hat{H}'_{fs}$ and $\hat{H}'_Z$, e.g., in a basis consisting of the states in the uncoupled representation or a basis

consisting of the states in the coupled representation. Many students struggled to determine both the diagonal and off-diagonal matrix elements particularly when the basis did not consist of a complete set of eigenstates of the given operator.

For example, in Q1(a), students were asked to calculate the matrix elements of $\hat{H}'_Z$ if the coupled representation $|n,\ l,\ s,\ j,\ m_j\rangle$ is chosen as the basis. One method for calculating these matrix elements of $\hat{L}_Z + 2\hat{S}_Z$ is to write the basis states in the coupled representation in terms of a linear combination of states in the uncoupled representation $|n,\ l,\ s,\ m_l,\ m_s\rangle$, for which relevant tables for such transformations were provided. Many students who incorrectly answered Q1(a) did not write the given state in terms of a linear combination of states in the uncoupled representation and instead answered Q1(a) as though the given states in the coupled representation were eigenstates of $\hat{L}_Z + 2\hat{S}_Z$. These students often incorrectly applied the given eigenvalue equations $\hat{S}_z|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar m_s|n,\ l,\ s,\ \ m_l,\ m_s\rangle$ and $\hat{L}_z|n,\ l,\ s,\ m_l,\ m_s\rangle = \hbar m_l|n,\ l,\ s,\ m_l,\ m_s\rangle$ for states in the uncoupled representation. For example, in Q1, some students incorrectly evaluated the expression as $(\hat{L}_z + 2\hat{S}_z)\left|2,\ 1,\ \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2}\right\rangle = [\frac{3}{2} + 2(\frac{3}{2})]\hbar\left|2,\ 1,\ \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2}\right\rangle = \frac{9}{2}\hbar\left|2,\ 1,\ \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2}\right\rangle$. Interviews suggest that these students often incorrectly used the expression $(\hat{L}_z + 2\hat{S}_z)\,|n,\ l,\ s,\ j,\ m_j\rangle = (j + 2m_j)\hbar\,|n,\ l,\ s,\ j,\ m_j\rangle$. However, states in the coupled representation are not eigenstates of either $\hat{L}_z$ or $\hat{S}_z$.

In Q1(b), students were asked to calculate the matrix elements of $\hat{H}'_{SO}$ if the basis was chosen in the uncoupled representation. In the operator $\hat{H}'_{SO}$, $\vec{L}\cdot\vec{S}$ can equivalently be expressed as $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$. For a basis consisting of states in the uncoupled representation, the expression $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ is best suited to calculate the matrix element. Instead, some students chose the expression $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$ even though a matrix element in the uncoupled representation is to be calculated and incorrectly calculated the matrix elements as though states in the uncoupled representation were eigenstates of $\hat{J}^2$.

For Q1(a) and Q1(b), some students only focused on the operator acting on the ket state and failed to consider the inner product of the bra and ket states. Since basis states in the coupled representation are orthonormal (and similarly in the uncoupled representation), the inner product of two states is zero unless the bra and ket states correspond to the same

state. For example, the following is one student's response taken from the pretest for Q1(b):

$$
\begin{aligned}
(\vec{L}\cdot\vec{S})|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle &= \left[\tfrac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z\right]|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle \\
&= \tfrac{1}{2}[\hbar^2\sqrt{2}\sqrt{1}]|2,1,\tfrac{1}{2},0,\tfrac{1}{2}\rangle + (-1)(\tfrac{1}{2})\hbar^2|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle \\
&= \tfrac{\hbar^2\sqrt{2}}{2}|2,1,\tfrac{1}{2},0,\tfrac{1}{2}\rangle - \tfrac{\hbar^2}{2}|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle.
\end{aligned}
$$

After taking the inner product with the bra state $\langle 2,1,\frac{1}{2},1,\frac{1}{2}|$, the student's final answer for Q1(b) was $\hbar^2[\frac{\sqrt{2}}{2}-\frac{1}{2}]$. All the steps in the above calculation are correct before taking the inner product. However, when taking the inner product with the bra state, both terms in the above expression are zero as the inner product $\langle 2,1,\frac{1}{2},1,\ \frac{1}{2}|2,1,\frac{1}{2},0,\ -\frac{1}{2}\rangle = 0$ and $\langle 2,1,\frac{1}{2},\ 1,\ \frac{1}{2}|2,1,\frac{1}{2},\ -1,\ \frac{1}{2}\rangle = 0$. Thus, the correct answer is that the matrix element is zero. This student and others who made similar mistakes did not take the inner product between the bra and ket states.

This type of difficulty is particularly problematic in that many of the interviewed students resorted to explicitly evaluating matrix elements when asked to determine whether a given operator is diagonal in the degenerate subspace of $\hat{H}^0$ in various representation. However, many of them were unable to evaluate these matrix elements correctly. In contrast, when asked to determine whether a given operator is diagonal in the degenerate subspace of $\hat{H}^0$ in various representations, an expert is more likely to use qualitative arguments in his/her reasoning and not necessarily explicitly calculate various matrix elements to convince themselves whether a matrix is diagonal or not in a given representation. For example, when considering the operator $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$, an expert would use the fact that a basis consisting of states in the coupled representation forms a complete set of eigenstates for the operators $\hat{J}^2$, $\hat{S}^2$, and $\hat{L}^2$ and that an operator is diagonal when the basis is chosen to be a complete set of eigenstates of that operator to determine that $\vec{L}\cdot\vec{S}$ is diagonal in the coupled representation. Using similar considerations, basis states in the uncoupled representation are eigenstates of $\hat{S}^2$ and $\hat{L}^2$, but not $\hat{J}^2$ and therefore, are not eigenstates for the operator $\vec{L}\cdot\vec{S}$. Thus, $\vec{S}\cdot\vec{L}$ is not diagonal if the uncoupled representation is chosen as the basis. A student who is developing expertise in this area will have difficulty in reasoning in this manner without resorting to explicit calculations of matrix elements in different representations. Since

solving a problem using qualitative reasoning is often more challenging for students than solving an equivalent problem using quantitative manipulations [48], this type of difficulty with qualitative reasoning without reliance on explicit quantitative manipulation has been observed even for introductory physics students [48].

### 3.4.2 Claiming that a basis in which an operator is diagonal is dependent on the symbols used to represent the operator

Often students incorrectly selected a basis and claimed that, for a fixed $n$, a Hamiltonian operator is diagonal in that basis based upon certain symbols for various operators that were explicitly given in the expression for the operator. For example, if an operator explicitly involving the symbol $J$ in any form was present ($\hat{J}$, $\hat{J}^2$, $\hat{J}_z$, or $\vec{J}$), many students incorrectly claimed that the states in the coupled representation must make that operator diagonal. If the symbol $J$ was not explicitly present in the expression for the operator, then they incorrectly claimed that the states in the coupled representation cannot make the operator diagonal (without realizing that it is possible to express an operator in terms of $J$ even if the operator is NOT diagonal in the coupled representation). Similarly, if terms explicitly involving $L$ ($\hat{L}$, $\hat{L}^2$, $\hat{L}_\pm$, $\hat{L}_z$, or $\vec{L}$) and/or $S$ ($\hat{S}$, $\hat{S}^2$, $\hat{S}_\pm$, $\hat{S}_z$, or $\vec{S}$) were present, many students incorrectly claimed that the states in the uncoupled representation must definitely form the basis in which that operator is diagonal. Conversely, if there were no terms in the operator explicitly written in terms of the symbols $L$ or $S$, then these students claimed that the basis consisting of the states in the uncoupled representation would not make the operator diagonal.

Based upon this type of reasoning, students often incorrectly claimed that the spin-orbit interaction term, $\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S}$, is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ when the uncoupled representation is chosen as the basis due to the presence of $\vec{L}$ and $\vec{S}$ in the expression for $\hat{H}'_{SO}$. These same students often also incorrectly claimed that the operator $\hat{H}'_{SO}$ is not diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ if the coupled representation is chosen as the basis since there is no term involving the symbol $J$ in the expression. Moreover, some students used the expression $\hat{H}'_{SO} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$

and, since this expression also involves the symbols $L$ and $S$, they incorrectly claimed that the spin-orbit coupling Hamiltonian $\hat{H}'_{SO}$ is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ when the uncoupled representation is chosen as the basis. Some students who used the expression $\hat{H}'_{SO} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ when determining the basis that makes $\hat{H}'_{SO}$ diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ stated that the states in the uncoupled representation are eigenstates of $\hat{L}_z$, $\hat{S}_z$, $\hat{L}_\pm$ and $\hat{S}_\pm$. While it is true that states in the uncoupled representation are eigenstates of the operators $\hat{L}_z$ and $\hat{S}_z$, these states are not eigenstates of the operators $\hat{L}_\pm$ and $\hat{S}_\pm$. These students did not realize that when the raising and lowering operators act on a state in the uncoupled representation, they do not return a constant times the same state and, therefore, states in the uncoupled representation cannot be eigenstates of $\hat{L}_\pm$ or $\hat{S}_\pm$. Thus, they struggled with the fact that $\hat{H}'_{SO}$ is not diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ in the uncoupled representation.

Other students incorrectly claimed that both the coupled and uncoupled representations will make $\vec{L} \cdot \vec{S}$ diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$. For example, one student claimed that "since $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$, we could use either coupled or uncoupled (to find the perturbative corrections to the energy spectrum)."

### 3.4.3 Difficulty identifying that, in general, a linear combination of eigenstates of an operator is not an eigenstate of that operator

Many students incorrectly chose both options i and iii or ii and iv on Q2. For example, the operator $\hat{H}'_Z = (\mu_B B_{ext}/\hbar)(\hat{L}_Z + 2\hat{S}_Z)$ is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ in the uncoupled representation so that option ii is the correct answer to question Q2. However, many students selected both options ii and iv. During an interview, one student who selected options ii and iv for $\hat{H}'_Z$ incorrectly stated: "If the uncoupled [states] are eigenstates [of $\hat{H}'_Z$] then so is their linear combination." In general, it is not true that linear combinations of states in the uncoupled representation will remain eigenstates of $\hat{H}'_Z$ (although certain special linear combinations of states in the uncoupled representation remain eigenstates of $\hat{H}'_Z$ due to the degeneracy). The percentages of students who selected options i and iii or options ii and iv for at least one operator were 38% for graduate students and 60% for undergraduates.

A similar difficulty has been found in prior investigations [11] when students were asked to consider two stationary states, $\psi_1$ and $\psi_2$, for the TISE $\hat{H}\psi = E\psi$, such that $\hat{H}\psi_1 = E_1\psi_1$ and $\hat{H}\psi_2 = E_2\psi_2$. Many students had a tendency to overgeneralize the TISE $\hat{H}\psi = E\psi$ and claimed that if $\psi_1$ and $\psi_2$ are stationary states, then their linear combination $\psi_1 + \psi_2$ will also be a stationary state. However, $\hat{H}(\psi_1 + \psi_2) = E_1\psi_1 + E_2\psi_2 \neq E(\psi_1 + \psi_2)$ unless there is degeneracy in the energy spectrum so that $E = E_1 = E_2$.

#### 3.4.4 Difficulty recognizing that if an operator is spherically symmetric, then the operator matrix will be diagonal for each $n$ if any complete set of orthogonal states consisting of the product states of the orbital and spin angular momenta with a fixed $n$ and $l$ is chosen as the angular basis

In order for an operator to be diagonal in each degenerate subspace of $\hat{H}^0$ for all angular bases with a fixed $n$ and $l$ (see options iii and iv on question Q2), the operator must be spherically symmetric. Students did not realize that since both $\hat{H}^0$ (corresponding energy spectrum depends on $n$) and $\hat{H}'_r$ (corresponding energy spectrum depends on $n$ and $l$) are spherically symmetric, they will be diagonal matrices in each degenerate subspace of $\hat{H}^0$ when any complete set of orthonormal states consisting of the product states of the orbital and spin angular momenta with a fixed $n$ and $l$ form the basis. They struggled with the fact that these spherically symmetric operators are represented by diagonal matrices in each degenerate subspace of $\hat{H}^0$ in both the coupled and uncoupled representations because the angular part of the matrix elements of the spherically symmetric operators for each fixed $n$ and $l$ will involve $\langle n, l, s, j, m_j | n, l, s, j', m'_j \rangle = \delta_{j,j'}\delta_{m_j,m'_j}$ if we choose the coupled representation or $\langle n, l, s, m_l, m_s | n, l, s, m'_l, m'_s \rangle = \delta_{m_l,m'_l}\delta_{m_s,m'_s}$ if we choose the uncoupled representation and the off-diagonal matrix elements will be zero due to the Kronecker deltas in either case. Table 3 summarizes the percentages of students with this difficulty on question Q2.

Table 3: Percentages of undergraduate (U) ($N = 32$) and graduate (G) students ($N = 42$) not selecting both options iii and iv for the unperturbed Hamiltonian $\hat{H}^0$ or relativistic correction $\hat{H}'_r$ in Q2.

| Operator | U (%) | G (%) |
|---|---|---|
| $\hat{H}^0$ | 59 | 62 |
| $\hat{H}'_r$ | 78 | 79 |

Table 4: Percentages of undergraduate (U) ($N = 32$) and graduate (G) students ($N = 42$) who selected option iii but did not also select options i, ii, or iv and who selected option iv but did not also select options i, ii, or iii in Q2 for at least one of the four operators.

| Option Selected | Option Not Selected | U | G |
|---|---|---|---|
| iii | i | 31 | 36 |
| | ii | 56 | 60 |
| | iv | 47 | 57 |
| iv | i | 47 | 67 |
| | ii | 19 | 36 |
| | iii | 38 | 64 |

### 3.4.5 Difficulty recognizing that a state in the uncoupled representation is a special linear combination of states in the coupled representation, and vice versa

In Q2, if an operator is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ for any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation (option iv), then one such linear combination would be states in the coupled representation and therefore, option i in question Q2 should also be correct. By the same reasoning, performing the necessary change of basis, students can rationalize that the states in the coupled representation can be expressed as linear combinations of states in the un-

coupled representation. Therefore, if option iii is correct in question Q2, then option ii is also correct since the uncoupled representation is special set of linear combinations of states in the coupled representation. Table 4 shows the percentage of students not selecting option i despite having selected option iv or not selecting option ii despite having selected option iii for at least one of the four operators in Q2. We note that students *were* given a table with states in the $n = 2$ subspace in the coupled representation and the corresponding linear combinations of the same states in the uncoupled representation using the Clebsch-Gordon table. Having this table did not help them recognize that states in the coupled representation could be expressed as linear combinations of states in the uncoupled representation (and vice versa).

### 3.4.6 Difficulty recognizing that if any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation is correct, then any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation must also be correct

In question Q2, some students did not realize that option iii is equivalent to choosing any complete set of orthogonal states for the angular basis for a fixed $n$ and $l$. They also struggled with the fact that since option iv in question Q2 is also any complete set of orthogonal states for the angular basis, options iii and iv are equivalent. Table 4 shows the percentages of students not selecting option iii despite having selected option iv or not selecting option iv despite having selected option iii.

### 3.4.7 Difficulty recognizing that the coupled representation is one special set of linear combinations of states in the coupled representation

Another common difficulty displayed by students on question Q2 was selecting option iii but not selecting option i. Students did not realize that if any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with fixed $n$ and $l$ (option iii) is correct, then the coupled representation (option i) is also correct

since the coupled representation is one particular set of linear combinations of states in the coupled representation. Similarly, students did not realize that if option iv (any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with fixed $n$ and $l$) is correct, option ii (uncoupled representation) is also correct since the uncoupled representation is one particular set of linear combinations of states in the uncoupled representation. Table 4 summarizes the percentages of students who displayed this type of difficulty in question Q2.

## 3.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 3.5.1 Development and Validation of the QuILT

The difficulties described show that many students struggle in determining a representation in which an operator is diagonal. Therefore, we developed a QuILT that takes into account these difficulties and strives to help them build a robust knowledge structure of these concepts. The development of the DPT QuILT started with an investigation of student difficulties via open-ended and multiple-choice questions administered after traditional instruction to advanced undergraduate and graduate students and conducting a cognitive task analysis from an expert perspective of the requisite knowledge [49]. The QuILT strives to help students build on their prior knowledge and addresses common difficulties found via research, some of which were discussed in the preceding section.

The QuILT is inspired by Piaget's "optimal mismatch" as well as the preparation for future learning framework of Bransford and Schwartz. In Piaget's "optimal mismatch" framework, students are intentionally placed in a situation in which their current knowledge structures are inadequate and they are then forced to reorganize existing structures or develop new structures to reconcile this conflict [50]. Bransford and Schwartz's preparation for future learning emphasizes that learning occurs when elements of innovation and efficiency are both present [51]. Innovation and efficiency describe two orthogonal components of instruction.

Innovation describes aspects that are new to students, such as new concepts or new problem solving skills. Efficiency is a measure of the structure and organization of the material, as well as how proficient the student is with the material. Instruction that incorporates only one of these elements leads to students becoming disengaged. If instruction is too innovative, students cannot connect the material with their prior knowledge and become frustrated. When the instruction is too efficient, students interact with repetitious material that does not provide intellectual stimulation and may become routine experts. They will not be able to transfer their learning to new situations.

In the QuILT, students are presented with innovative tasks. Whether it be examples, hypothetical conversations, or calculations, the QuILT strives to help students develop a robust understanding by actively working through the inquiry-based learning sequences. Student difficulties are incorporated in these examples and conversations to create a cognitive conflict in which the students are then guided through subsequent tasks designed to resolve these issues. Efficiency is addressed in the QuILT in several ways. First, the QuILT follows the sequence laid out in the cognitive task analysis. It is organized in a manner which attempts to build on the students' prior knowledge, and each section in the QuILT builds upon the previous section. Second, students are provided scaffolding designed to help address common difficulties, thus reducing the cognitive conflict. Third, the QuILT progressively reduces the scaffolding such that the students are able to solve the problems without any assistance. Finally, as the students work through the different tasks, they develop more proficiency at identifying the concepts and answering the questions.

The development of the QuILT went through a cyclic, iterative process. The preliminary version was developed based upon the cognitive task analysis and knowledge of common student difficulties. Next, the QuILT underwent many iterations among the three researchers and then was iterated several times with three physics faculty members to ensure that they agreed with the content and wording. It was also administered to graduate and advanced undergraduate students in individual think-aloud interviews to ensure that the guided approach was effective, the questions were unambiguously interpreted, and to better understand the rationale for student responses. During these semi-structured interviews, students were asked to "think aloud" while answering the questions. Students first read the questions on

their own and answered them without interruptions except that they were prompted to think aloud if they were quiet for a long time. After students had finished answering a particular question to the best of their ability, they were asked to further clarify and elaborate on issues that they had not clearly addressed earlier. The next step involved evaluating the impact of the QuILT on student learning and determining if the difficulties remained. Finally, modifications and improvements were made based upon the student and faculty feedback before it was administered to students in various courses.

### 3.5.2 Structure of the QuILT

The QuILT uses a guided inquiry-based approach to learning and actively engages students in the learning process. It includes a pretest to be administered in class after traditional instruction in DPT. Then, students engage with the tutorial in small groups in class (or alone when using it as a self-paced learning tool in homework), and then a posttest is administered in class. As students work through the tutorial, they are asked to predict what should happen in a given situation. Then, the tutorial strives to provide scaffolding and feedback as needed to bridge the gap between their initial knowledge and the level of understanding that is desired. Students are also provided checkpoints to reflect upon what they have learned and make explicit connections between what they are learning and their prior knowledge. They are given opportunities to reconcile differences between their predictions and the guidance provided in the checkpoints before proceeding further.

The DPT QuILT uses a blend of qualitative and quantitative reasoning to improve students' understanding. For example, the QuILT requires qualitative reasoning while responding to the hypothetical conversations, and quantitative reasoning to determine the matrix elements of the operators $\hat{H}'_{SO}$ and $\hat{H}'_{Z}$ in the coupled and uncoupled representations. Students explain whether they agree or disagree with statements in hypothetical conversations via both quantitative and qualitative reasoning.

### 3.5.3 Addressing Student Difficulties Via Guided Learning Sequences in the QuILT

The QuILT strives to help students develop a functional understanding of bases that make a given perturbation operator diagonal in each degenerate subspace of $\hat{H}^0$. Working through the qualitative and quantitative examples, students learn to reason about how to determine bases which make each of the operators $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$ and $\hat{H}'_Z$ diagonal in each degenerate subspace of $\hat{H}^0$ and how to find a *good* basis for DPT. In particular, students engage with guided inquiry-based sequences that begin by asking the students to explicitly calculate matrix elements of relevant operators in different representations followed by scaffolding support that strives to help students evaluate the matrix elements correctly as well as develop qualitative reasoning regarding whether an operator is diagonal in each degenerate subspace of $\hat{H}^0$ when a given representation is chosen as the basis. One goal is to have students develop facility with different represenations by first performing the necessary calculations involved in evaluating the matrix elements and then using the calculations as scaffolding in developing conceptual knowledge structures. Next, we provide some examples.

**Helping students learn to calculate matrix elements in the coupled and uncoupled representations:** In the guided inquiry-based learning sequences involving the operators $\hat{H}'_{SO}$ and $\hat{H}'_Z$, students first calculate several diagonal and off-diagonal matrix elements when the coupled or uncoupled representation is chosen as the basis. In DPT, when the basis chosen is a *good* basis, the diagonal matrix elements of the perturbation are the first-order corrections to the energies and the off-diagonal matrix elements are zero in each degenerate subspace of $\hat{H}^0$. Focusing on the off-diagonal matrix elements for some of the operators, students are asked to interpret why $\hat{H}'_{SO}$ is diagonal in the degenerate subspace of $\hat{H}^0$ in the coupled representation and $\hat{H}'_Z$ is diagonal in the degenerate subspace of $\hat{H}^0$ in the uncoupled representation but not vice versa. For example, questions similar to Q1 are part of the guided inquiry-based learning sequence in which students determine the matrix elements of $\hat{H}'_{SO}$ and $\hat{H}'_Z$ in both the coupled and uncoupled representations. Since the matrix elements in question Q1 are not zero in the situation posed, the students determine that in the degenerate subspace of $\hat{H}^0$, the $\hat{H}'_{SO}$ matrix is not diagonal in the uncoupled

representation and the $\hat{H}'_Z$ matrix is not diagonal in the coupled representation.

**Helping students learn that $\hat{H}^0$ and $\hat{H}'_r$ are spherically symmetric and are diagonal in each degenerate subspace of $\hat{H}^0$ for any complete set of orthogonal angular basis states for fixed $n$ and $l$:** To help students with difficulties determining a basis in which the operators $\hat{H}^0$ and $\hat{H}'_r$ are diagonal in each degenerate subspace of $\hat{H}^0$, students are asked to consider the spherically symmetric nature of the operators $\hat{H}^0$ and $\hat{H}'_r$ and guided to learn that both are diagonal in each degenerate subspace of $\hat{H}^0$ when any complete set of orthonormal states with the same $n$ and $l$ is chosen. Through explicit examples calculating matrix elements of the operator matrices and several hypothetical conversations, students determine that $\hat{H}^0$ and $\hat{H}'_r$ are diagonal in each degenerate subspace of $\hat{H}^0$ for all of the choices in Q2 (in the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled or uncoupled representation for the same $l$). These examples and conversations also address students' difficulty C, i.e., identifying that if an operator is spherically symmetric, then the operator matrix will be diagonal in each degenerate subspace of $\hat{H}^0$ if any complete set of orthogonal states (consisting of the product states of the orbital and spin angular momenta) with the same $n$ and $l$ is chosen as the basis. For example, students are given the 8-dimensional $\hat{H}^0$ matrix in the $n = 2$ subspace with the eight-fold degenerate unperturbed energy $E_2^0 = -\frac{13.6\text{eV}}{4}$ appearing as the diagonal matrix elements (and all off-diagonal matrix elements being zero). They are asked to determine whether states in the coupled or uncoupled representation were chosen as the basis to write $\hat{H}^0$ in this $n = 2$ subspace. To answer correctly, students must reason that the unperturbed energy only depends on the quantum number $n$ and therefore the $\hat{H}^0$ matrix will be diagonal in the degenerate subspace of $\hat{H}^0$ if any complete set of orthogonal basis states is chosen for the angular basis. Similarly, the QuILT strives to help students learn that since eigenvalues of $\hat{H}'_r$ depend only on $n$ and $l$, $\hat{H}'_r$ will be diagonal in each degenerate subspace of $\hat{H}^0$ if any complete set of orthogonal basis states is chosen for the angular basis with fixed $l$. Thus, both $\hat{H}^0$ and $\hat{H}'_r$ will be diagonal matrices in the degenerate subspace of $\hat{H}^0$ if angular basis states are chosen as in options i, ii, iii, and iv in question Q2.

**Helping students identify that any linear combination of eigenstates of an operator is not, in general, an eigenstate of that operator:** Many students had difficulty identifying that, in general, a linear combination of eigenstates of an operator is not an eigenstate (difficulty B). In a guided inquiry-based learning sequence in the QuILT, they were asked to analyze the following hypothetical conversation regarding whether the $\hat{H}'_Z$ matrix is a diagonal matrix if any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states is chosen as the basis for a fixed $n$. Students then contemplate which student they agree with and explain their reasoning.

**Student 1:** *Since states in the uncoupled representation are eigenstates of $\hat{H}'_Z$, any linear combination of states in the uncoupled representation must also be an eigenstate of $\hat{H}'_Z$. Thus, $\hat{H}'_Z$ is diagonal in the uncoupled representation and also when any arbitrary complete orthonormal basis is constructed with linear combinations of a complete set of the uncoupled states.*

**Student 2:** *I disagree with Student 1. If we consider $\hat{H}'_Z$, which is proportional to $(\hat{L}_z+2\hat{S}_z)$, then states in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$ are eigenstates of $\hat{H}'_Z$. However, in general, linear combinations of states in the uncoupled representation are NOT eigenstates of $\hat{H}'_Z$. For example, if we consider the states $|\psi_1\rangle = |2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}\rangle$ and $|\psi_2\rangle = |2,\ 0,\ \frac{1}{2},\ 0,\ -\frac{1}{2}\rangle$: $(\hat{L}_z + 2\hat{S}_z)|\psi_1\rangle = (\hat{L}_z + 2\hat{S}_z)\left|2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}\right\rangle = \left|2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}\right\rangle$ and $(\hat{L}_z + 2\hat{S}_z)|\psi_2\rangle = (\hat{L}_z + 2\hat{S}_z)\left|2,\ 1,\ \frac{1}{2},\ 0,\ -\frac{1}{2}\right\rangle = -\left|2,\ 1,\ \frac{1}{2},\ 0,\ -\frac{1}{2}\right\rangle$. But a linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ is not an eigenstate of $\hat{H}'_Z$: $(\hat{L}_z + 2\hat{S}_z)(|\psi_1\rangle + |\psi_2\rangle) = (\hat{L}_z + 2\hat{S}_z)\left(\left|2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}\right\rangle + \left|2,\ 1,\ \frac{1}{2},\ 0,\ -\frac{1}{2}\right\rangle\right) = \left|2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}\right\rangle - \left|2,\ 1,\ \frac{1}{2},\ 0,\ -\frac{1}{2}\right\rangle = |\psi_1\rangle - |\psi_2\rangle \neq Constant(|\psi_1\rangle + |\psi_2\rangle)$.*

In this case, students are given an explicit example and asked to reflect upon the fact that a linear combination of two eigenstates of $\hat{H}'_Z$ is not an eigenstate of $\hat{H}'_Z$. Student 2's calculation strives to provide guidance to students in their reflection upon the fact that a linear combination of eigenstates of an operator, in general, is not an eigenstate. Later, students work on other examples and reflect upon their findings to solidify these concepts. Checkpoints are provided at the conclusion of each section that allow the students to go back and reconcile any remaining difference between the correct reasoning and their own reasoning before moving on to the next section.

**Helping students realize that if any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation is correct then the coupled representation, the uncoupled representation, and any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation are also correct:** The following is one example of a conversation that strives to help students with difficulties D-G. Students are asked to consider the following excerpt from a hypothetical student conversation regarding whether the $\hat{H}'_{SO}$ matrix is a diagonal matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$ if any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states is chosen as the angular part of the basis. They are asked to choose which student(s) they agree with and explain their reasoning for agreeing or disagreeing with each student.

**Student 1:** *Since $\hat{H}'_{SO}$ is diagonal in the degenerate subspace of $\hat{H}^0$ in the coupled representation, $\hat{H}'_{SO}$ must also be diagonal in the degenerate subspace of $\hat{H}^0$ if any arbitrary complete orthonormal basis constructed with linear combinations of the coupled states is chosen as the basis.*

**Student 2:** *I disagree with Student 1. For example, the states in the uncoupled representation can be constructed with linear combinations of states in the coupled representation. Therefore, if $\hat{H}'_{SO}$ were to be diagonal in the degenerate subspace of $\hat{H}^0$ when any arbitrary complete orthonormal basis constructed with linear combinations of the coupled states is chosen as the basis, then $\hat{H}'_{SO}$ would also be diagonal if the uncoupled representation were chosen as the basis. However, this is not the case because $\hat{H}'_{SO}$ is not diagonal for the uncoupled representation in the $n = 2$ degenerate subspace of $\hat{H}^0$. But $\hat{H}'_{SO}$ is diagonal in the coupled representation for the $n = 2$ degenerate subspace of $\hat{H}^0$.*

**Student 3:** *I agree with Student 2. Also, if an operator matrix is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ when any arbitrary complete orthonormal basis constructed with linear combinations of the* **coupled states** *is chosen as the angular part of the basis, then that matrix must also be diagonal when any complete orthogonal angular basis is chosen. Therefore, the operator matrix must also be diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ if any arbitrary complete orthonormal basis constructed with linear combinations of the*

**uncoupled states** *is chosen as the basis.*

Student 2's claim that the states in the uncoupled representation can be constructed with linear combinations of states in the coupled representation focuses on difficulty D. Students are also provided a table of states in the $n = 2$ subspace of $\hat{H}^0$ in the coupled representation and the corresponding linear combinations of states in the uncoupled representation. Student 3's statement focuses on helping students reflect on difficulty E, in that if any arbitrary complete orthonormal basis found with linear combinations of the coupled states with fixed $n$ and $l$ (option iii) is chosen as a basis to make an operator diagonal, then any arbitrary complete orthonormal basis found with linear combinations of a complete set of the uncoupled states with fixed $n$ and $l$ (option iv) chosen as the basis also makes the operator diagonal.

Additionally, students engage with guided inquiry-based learning sequences and reflect upon the validity of hypothetical student conversations about the spherically symmetric nature of $\hat{H}^0$ and $\hat{H}'_r$ (so that any angular basis with fixed $n$ and $l$ form a *good* basis) and those that are designed to elaborate on the equivalence of options iii and iv.

After developing facility with determining whether the operators $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ are diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ in a given basis, they are prepared to identify a *good* basis for finding the perturbative corrections using DPT.

## 3.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts in DPT but before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both

Table 5: Average pretest and posttest scores for Q1 for undergraduate students.

| Question | N | Pre (%) | N | Post (%) |
|---|---|---|---|---|
| Q1(a) | 13 | 3 | 32 | 80 |
| Q1(b) | 20 | 56 | - | - |
| Q1(c) | - | | 13 | 92 |
| Q1(d) | - | | 13 | 60 |

groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest. There were 46 undergraduates and 42 graduate students enrolled in the respective QM courses over a four-year period. One undergraduate student in the first year dropped the course in the time between the pretest and the posttest and therefore 45 undergraduate students took the posttest.

For the undergraduate students, Q1(b) was asked on the pretest in the first two years of the study. Q1(a) was asked on the posttest in the first three years of the study. In the fourth year, the undergraduates were asked Q1(a) on the pretest and Q1(c) and Q1(d) on the posttest.

Q1 was graded using a rubric which was developed by the researchers together. Each question was worth two points. For example, when grading Q1(b), students were given one point for correctly choosing the appropriate form of the operator $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ for the basis states in the uncoupled representation and one point for correctly evaluating the matrix element. A subset of student responses (roughly 50%) were graded separately by the researchers with a final inter-rater reliability of nearly 100%. Table 5 shows the performance of the undergraduate students on the pretest and posttest.

The percentages of students who answered Q2 correctly on the pretest and posttest are given in Table 6. In particular, over 75% of the graduate students identified all the options in Q2 for which the given operators are diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ on the posttest. For the undergraduate students, over 85% correctly identified all the options in Q2 for which the operators $\hat{H}^0$ and $\hat{H}'_r$ are diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ on

the posttest. Roughly 75% of the undergraduate and graduate students correctly identified all the options in Q2 for which the operator $\hat{H}'_{SO}$ is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$. For both groups of students, 81% correctly identified all the options in Q2 for which the operator $\hat{H}'_Z$ is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$.

Table 7 shows the percentages of undergraduates and graduate students who displayed the given difficulty for at least one of the listed operators on the pretest and posttest. After working through the QuILT, the percentage of students displaying these difficulties was greatly reduced. While the number of students who displayed the difficulty that any linear combination of eigenstates is an eigenstate (difficulty C) decreased, Table 7 shows that students selecting linear combinations of eigenstates of an operator as an eigenstate was a particularly persistent difficulty. The implications of choosing any arbitrary set of orthonormal linear combinations of states in either the coupled or uncoupled representation proved to be a challenging connection for many students to make. As seen in Table 7, the number of students who correctly chose option iii/iv and also chose options i/ii (difficulty G), ii/iii (difficulty E), and iv/iii (difficulty F) increased after working though the QuILT. However, there is still a high percentage of students who did not realize that if any arbitrary complete set of orthonormal linear combinations of states in either the coupled or uncoupled representation with fixed $l$ (option iii or iv) makes an operator diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$, then the coupled representation (option i), uncoupled representation (option ii) or any arbitrary complete set of orthonormal linear combination of states in the uncoupled or coupled representation with fixed $l$ (option iv or iii) must also make the operator diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$. This is an area to improve upon in future refinements and implementations of the QuILT to address these difficulties more effectively.

Since there can be more than one correct option for the four multiple-choice questions posed in Q2, it was graded using a rubric which was developed by the researchers together. Each question was worth four points. For example, when grading Q2 for the operator $\hat{H}'_{SO}$, students were given four points for correctly choosing only the coupled representation (option i). If they chose the coupled representation (option i) and any arbitrary complete set of orthonormal linear combinations of states in the coupled representation with fixed $l$ (iii), they we given two out of four points. We found that some interviewed students

Table 6: The percentage of students who chose all the possible correct representations to diagonalize the listed operator $\hat{H}'$ in the $n = 2$ degenerate subspace of $\hat{H}^0$ in Q2 on the pretest and posttest for undergraduates and graduate students.

| $\hat{H}'$ Operator | Correct Answer | Undergraduate Students(%) | | | | Graduate Students(%) | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | N | Pre | N | Post | N | Pre | N | Post |
| $\hat{H}^0$ | i, ii, iii, iv | 32 | 34 | 31 | 94 | 42 | 33 | 42 | 83 |
| $\hat{H}'_r$ | i, ii, iii, iv | 32 | 22 | 31 | 87 | 42 | 21 | 42 | 83 |
| $\hat{H}'_{SO}$ | i | 32 | 34 | 31 | 74 | 42 | 36 | 42 | 76 |
| $\hat{H}'_{fs}$ | i | 12 | | 33 | 100 | - | - | - | - |
| $\hat{H}'_Z$ | ii | 32 | 38 | 31 | 81 | 42 | 33 | 42 | 81 |

correctly reasoned that the degeneracy in the energy spectrum of $\hat{H}'_{SO}$ allowed for linear combinations of states in the coupled representation with the same $n$, $l$, and $j$ (but different $m_j$) to diagonalize $\hat{H}'_{SO}$. However, it is not the case that any linear combination of states in the coupled representation with fixed $l$ diagonalizes $\hat{H}'_{SO}$ in the $n = 2$ degenerate subspace of $\hat{H}^0$. While these students did not show entirely correct reasoning, they were correctly thinking about issues caused by the degeneracy in the energy spectrum but incorrectly overgeneralized these concepts to reason that any complete set of linear combination of states in the coupled representation with fixed $l$ diagonalizes $\hat{H}'_{SO}$ in the degenerate subspace of $\hat{H}^0$. Students were given one out of four points if they chose both the coupled and uncoupled representation (options i and ii) as a basis that diagonalizes $\hat{H}'_{SO}$ in the $n = 2$ subspace. As mentioned in the student difficulties section (Section IV), some students incorrectly claimed that the operator $\hat{H}'_{SO}$ is diagonal in the $n = 2$ subspace in both the coupled and uncoupled representations because $\hat{H}'_{SO} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$. Although states in the coupled representation are eigenstates of the operators $\hat{J}^2$, $\hat{L}^2$, and $\hat{S}^2$, states in the uncoupled representation are eignestates of $\hat{L}_Z$ and $\hat{S}_Z$ but they are not eigenstates of the operators $\hat{L}_\pm$ and $\hat{S}_\pm$. Therefore, in the $n = 2$ degenerate subspace of $\hat{H}^0$, $\hat{H}'_{SO}$ is diagonal

Table 7: The percentage of students displaying difficulties C-G for at least one of the listed operators on the pretest and posttest for undergraduates (number of students $N = 32$ for the pretest and $N = 31$ for the posttest) and graduate students ($N = 42$).

| Difficulty | Operator | Undergraduate Students | | Graduate Students | |
|---|---|---|---|---|---|
| | | Pre (%) | Post (%) | Pre (%) | Post (%) |
| C | $\hat{H}'_{SO}$, $\hat{H}'_{Z}$ | 50 | 19 | 38 | 19 |
| D | $\hat{H}^{0}$, $\hat{H}'_{r}$ | 75 | 7 | 60 | 10 |
| E | $\hat{H}^{0}$, $\hat{H}'_{r}$, $\hat{H}'_{SO}$, $\hat{H}'_{Z}$ | 66 | 22 | 74 | 29 |
| F | $\hat{H}^{0}$, $\hat{H}'_{r}$, $\hat{H}'_{SO}$, $\hat{H}'_{Z}$ | 59 | 18 | 48 | 29 |
| G | $\hat{H}^{0}$, $\hat{H}'_{r}$, $\hat{H}'_{SO}$, $\hat{H}'_{Z}$ | 28 | 7 | 40 | 10 |

in the coupled representation but not diagonal in the uncoupled representation. This type of response shows some correct reasoning ($\hat{H}'_{SO}$ is diagonal in the $n = 2$ subspace in the coupled representation) and was awarded partial credit. No points were awarded for any other combination of answers for the operator $\hat{H}'_{SO}$ in Q2.

A subset of student responses was graded separately by the researchers with a final inter-rater reliability of nearly 100%. Table 8 shows the performance of undergraduate and graduate students on the pretest and posttest. Table 8 also includes the average gain, $G$, and normalized gain [52], $g$. The normalized gain is defined as the (posttest percent - pretest percent)/(100 - pretest percent). Both undergraduate and graduate students struggled with this topic as can be seen by the scores on the pretest. However, both groups showed significant improvement after working through the QuILT.

## 3.7 SUMMARY

Many of the difficulties described here are consistent with the patterns of student reasoning found in other areas of quantum mechanics [53]. In order to develop a functional understanding of DPT, one must be able to synergistically apply several appropriate concepts to solve

Table 8: Average pretest and posttest scores for Q2, gains ($G$) and normalized gains ($g$) for undergraduate students (number of students $N = 32$ for the pretest and $N = 31$ for the posttest) and graduate students ($N = 42$).

| | Undergraduate Students | | | | Graduate Students | | | |
|---|---|---|---|---|---|---|---|---|
| Operator | Pre | Post | G | g | Pre | Post | G | g |
| $\hat{H}^0$ | 55 | 98 | +43 | 0.96 | 50 | 87 | +37 | 0.74 |
| $\hat{H}'_r$ | 42 | 94 | +52 | 0.90 | 38 | 88 | +50 | 0.81 |
| $\hat{H}'_{SO}$ | 50 | 89 | +39 | 0.78 | 56 | 86 | +30 | 0.68 |
| $\hat{H}'_{fs}$ | 29 | 100 | +71 | 1.00 | - | - | - | - |
| $\hat{H}'_Z$ | 54 | 92 | +38 | 0.83 | 49 | 90 | +41 | 0.80 |

a DPT problem. Moreover, using DPT to find approximate solutions to the energy spectrum of the hydrogen atom placed in an external magnetic field requires students to apply advanced mathematical concepts in the context of a concrete physical QM problem. Prior research studies have found that students have difficulty connecting and applying mathematics concepts correctly in introductory physics contexts, (e.g., see Refs. [55, 56, 57, 54]). Many of the difficulties advanced students had with DPT stem from students' lack of deep understanding of the linear algebra concepts and procedures and the difficulties in connecting the mathematical and quantum mechanical concepts.

The student difficulties discussed here can be interpreted using Simon's bounded rationality and satisficing framework (in that students are limited in their cognitive resources when solving these types of QM problems so they may resort to satisficing [45]) and Sweller's cognitive load framework (in that if appropriate scaffoldng support commensurate with students' current level of expertise is not provided, they will experience cognitive overload [46]). In satisficing while solving the QM problems posed in this study, students often only looked for a solution that was satisfactory to them in which they saw no inconsistencies (even though there were inconsistencies based upon expert cognitive task analysis of the problems) rather than searching for additional pathways in the problem space and to determine

an optimal solution. In other words, students who satisficed while solving the problem posed (e.g., about the calculation of various matrix elements in a particular representation relevant for determining whether a basis was good or not for finding the corrections to the energies) were satisfied with their sub-optimal solution commensurate with their current level of expertise and did not search for more optimal approaches to solving problems. Resorting to satisficing for students who are still developing expertise in this novel QM context often amounted to novice-like sense-making and inappropriate integration of mathematical and physical concepts to solve problems. For example, students struggled to identify that basis states in the coupled representation comprise one special arbitrary orthonormal basis constructed with linear combinations of states in the coupled representation (or one special arbitrary orthonormal basis constructed with linear combinations of states in the uncoupled representation). This type of difficulty illustrates the difference between novice and expert sense-making and reasoning when solving a DPT problem since it is central to being able to find a good basis for corrections to the energy spectrum. It is also possible that some students in this investigation recognized that their solution may not be optimal but, without sufficient guidance and scaffolding support, cognitive overload in this novel domain in which they are still developing expertise prevented them from contemplating optimal pathways in the problem space to solve the problem correctly [45, 46].

Using the common difficulties of advanced students in QM courses with determining bases in which an operator is diagonal as a guide, we developed and evaluated a research-based QuILT which strives to provide appropriate guidance and scaffolding support and focuses on helping students reason about and find bases that diagonalize the unperturbed Hamiltonian $\hat{H}^0$ completely and diagonalize the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$, and $\hat{H}'_Z + \hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$. In order to accomplish this goal, students should be able to evaluate the matrix elements of different Hamiltonians in different representations (e.g., the coupled and uncoupled representations). This is an important skill to have when determining a *good* basis for finding the perturbative corrections using DPT for a hydrogen atom placed in an external magnetic field. For example, one can determine that the angular basis in the coupled representation diagonalizes $\hat{H}^0$ and also diagonalizes $\hat{H}'_r$ and $\hat{H}'_{SO}$ in each degenerate subspace of $\hat{H}^0$ and therefore forms a *good* basis for finding the perturbative corrections to

the energies for fine structure $\hat{H}'_{fs}$, in which the diagonal matrix elements of $\hat{H}'_r$ and $\hat{H}'_{SO}$ are the first order corrections to the energies. For the perturbation $\hat{H}'_Z + \hat{H}'_{fs}$, one can determine that the angular basis in the uncoupled representation diagonalizes $\hat{H}^0$ and also diagonalizes $\hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$. However, the uncoupled representation does not diagonalize $\hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$. Thus, the uncoupled representation is not a *good* basis for $\hat{H}'_Z + \hat{H}'_{fs}$. One can determine that the Zeeman term $\hat{H}'_Z$ is not diagonal in each degenerate subspace of $\hat{H}^0$ if the coupled representation is chosen as the angular basis. In order to find a *good* basis for the pertrubation $\hat{H}'_Z + \hat{H}'_{fs}$, one is free to choose either the coupled or uncoupled representation and then diagonalize $\hat{H}'_Z + \hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$.

The QuILT strives to provide scaffolding support and feedback using a guided inquiry-based learning approach to help students develop a functional understanding of the concepts relevant for DPT. In addition to helping students develop knowledge structures, students are also guided to develop procedural skills in evaluating the matrix elements of different Hamiltonians in different representations (e.g., the coupled and uncoupled representations). The QuILT strives to have students build upon this procedural knowledge and use these explict calculations as additional scaffolding support to solidify conceptual knowledge structures.

The evaluation shows that the QuILT is effective in improving students' understanding of the bases that make an operator diagonal in the context of DPT. In particular, a majority of graduate and undergraduate students were able to correctly identify all of the possible correct representations that diagonalize $\hat{H}^0$ and diagonalize $\hat{H}'_r$, $\hat{H}'_{SO}$ and $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ in the degenerate subspace of $\hat{H}^0$. These students were able to correctly identify all of the given representations in which the operator is a diagonal matrix in the $n = 2$ subspace and were able to build upon this knowledge to help identify a complete set of states in the given representations that form a *good* basis in the context of the DPT for a hydrogen atom placed in an external magnetic field.

## 3.8 ACKNOWLEDGEMENTS

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# 4.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DEGENERATE PERTURBATION THEORY: FINE STRUCTURE

## 4.1 INTRODUCTION

The hydrogen atom has played a significant role in the development of quantum mechanics (QM). Specifically, the discrete energy levels observed by the spectroscopists for the hydrogen atom led Bohr to propose his model with quantized energy levels. Later, the Schrödinger Equation was successful in explaining many aspects of the hydrogen atom that were experimentally observed.

The fine structure term in the Hamiltonian causes shifts in the unperturbed energy spectrum of the hydrogen atom. The fine structure of the hydrogen atom is the combined effect of the relativistic correction and the spin-orbit interaction (interaction between the spin and orbital angular momenta) since the two components produce the same order of magnitude corrections to the energies of the hydrogen atom. These corrections are smaller by a factor of the fine structure constant ($\alpha \approx 1/137$) squared compared to the unperturbed energies of the hydrogen atom.

The Time-Independent Schrödinger Equation (TISE) for the hydrogen atom with the fine structure corrections cannot be solved exactly. Nevertheless, since energies corresponding to the fine structure term are significantly smaller than the unperturbed energies, perturbation theory is an excellent method for determining the approximate solutions to the TISE for finding the corrections to the unperturbed energy spectrum of the hydrogen atom due to fine structure. Moreover, due to the degeneracy in the energy spectrum of the hydrogen atom, degenerate perturbation theory (DPT) must be used to find the perturbative corrections due

to fine structure.

It is important to help students develop a functional understanding of DPT in order to find the fine structure corrections. However, QM is a challenging subject for upper-level undergraduate and graduate students in physics (e.g., see Refs. [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]). There have been a number of research studies aimed at investigating student reasoning in QM [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23] and improving student understanding of QM [24, 25, 26, 27, 28, 29, 30, 31, 32]. Here, we discuss an investigation of student difficulties with finding the first-order perturbative corrections to the energy spectrum of the hydrogen atom due to fine structure and the development and evaluation of a research-based Quantum Interactive Learning Tutorial (QuILT) that makes use of the student difficulties as resources [33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43].

## 4.2 BACKGROUND

Below we discuss the background of DPT and what students should be able to do after working through the QuILT. One goal is to help students be able to identify a *good* basis for finding the corrections to the energies due to the fine structure of the hydrogen atom and then be able to find the first order corrections due to fine structure. For a given $\hat{H}^0$ and $\hat{H}'$, we define a *good* basis as consisting of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.

### 4.2.1 Background for DPT

Perturbation theory is a powerful approximation method for finding the energies and the energy eigenstates of a system for which the Time-Independent Schrödinger Equation (TISE) is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$. The TISE for the unperturbed Hamiltonian, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, is exactly solvable, where $\psi_n^0$ is the $n^{th}$ unperturbed energy eigenstate and $E_n^0$ the unperturbed energy. Perturbation theory builds on the solutions of the TISE for the unperturbed case. Using perturbation theory, the energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \cdots$ where $E_n^i$ for $i = 1, 2, 3..$

are the $i^{th}$ order corrections to the $n^{th}$ energy of the system. Here we focus on the first-order perturbative corrections to the energy spectrum since they are usually the dominant corrections. In perturbation theory, the first-order corrections to the energies are

$$E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle, \tag{4.1}$$

and the first-order corrections to the unperturbed energy eigenstates are

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle. \tag{4.2}$$

In Eqs. 6.1 and 6.2, $\{|\psi_n^0\rangle\}$ is a complete set of eigenstates of $\hat{H}^0$. When the eigenvalue spectrum of $\hat{H}^0$ has degeneracy (i.e., two or more eigenstates of $\hat{H}^0$ have the same energy and two or more diagonal elements of $\hat{H}^0$ are equal), Eq. 6.1 from nondegenerate perturbation theory is still valid provided one uses a *good* basis.

### 4.2.2 Background for DPT involving the hydrogen atom

Using standard notation, the Hamiltonian of a hydrogen atom with fine structure is $\hat{H} = \hat{H}^0 + \hat{H}'_{fs}$ in which the unperturbed Hamiltonian, $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$, accounts only for the interaction of the electron with the nucleus via Coulomb attraction and the fine structure perturbation is $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Here, $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term and $\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}(\vec{L}\cdot\vec{S})$ is the spin-orbit interaction term. Since the relativistic correction term and the spin-orbit term are of the same order of magnitude, they are combined as the fine structure term $\hat{H}'_{fs}$.

The solution of the TISE for the hydrogen atom with Coulomb potential energy gives the unpertubed energies $E_n^0 = -\frac{13.6\text{eV}}{n^2}$, where $n$ is the principal quantum number. As mentioned in the previous section, in DPT, a *good* basis diagonalizes $\hat{H}^0$ and also diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. Since for the hydrogen atom, for each subspace corresponding to a particular principal quantum number $n$, the energy spectrum of $\hat{H}^0$ is $2n^2$-fold degenerate, a *good* basis for finding the perturbative corrections must diagonalize $\hat{H}^0$ completely (basis states must be eigenstates of $\hat{H}^0$) and must also diagonalize $\hat{H}'_{fs}$ in the $2n^2$ dimensional subspace corresponding to each $n$.

The angular part of the basis or angular basis refers to the part of the basis that combines both the spin and orbital angular momenta. Since, in order to find a good basis, the focus is on each degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$ and whether $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$, we can restrict our discussion to one value of the principal quantum number $n$. Thus, in this entire discussion below, we will focus only on the $n = 2$ degenerate subspace of $\hat{H}^0$. Also, in the questions that students were asked about the fine structure corrections to the energy spectrum of the hydrogen atom using the DPT, they were asked to fix the value of the principal quantum number to $n = 2$.

We note that $\hat{H}^0$ for the hydrogen atom is spherically symmetric (since $[\hat{H}^0, \hat{\vec{L}}] = 0$) and the unperturbed energies only depend on $n$. Thus, for a fixed $n$, $\hat{H}^0$ is diagonal when any complete set of orthonormal states is chosen for the angular basis. Thus, so long as the radial part of the wavefunctions $R_{nl}(r)$ (for a given principal quantum number $n$ and azimuthal quantum number $l$) corresponding to the eigenstates of $\hat{H}^0$ are chosen as the basis (which we will assume throughout here), the choice of a *good* basis for DPT amounts to choosing the angular basis appropriately for a given perturbation (ensuring that the perturbation matrix is a diagonal matrix in each degenerate subspace of $\hat{H}^0$). Thus, our focus here is on choosing a good angular basis.

Below, we consider each part of the perturbation $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ separately and then together in order to reason about how to determine a *good* angular basis. The operator $\hat{H}'_r$ is spherically symmetric (since $[\hat{H}'_r, \hat{\vec{L}}] = 0$) and the eigenvalues of $\hat{H}'_r$ depend on quantum numbers $n$ and $l$. Thus, for both $\hat{H}^0$ and $\hat{H}'_r$, for $n = 2$ (which is the degenerate subspace of $\hat{H}^0$ we will focus on throughout our discussion), any complete set of orthonormal states can be chosen for the angular basis so long as we take linear superpositions of states with the same values of $l$. Therefore, with fixed $n$ and $l$, any complete set of orthonormal states forms a *good* angular basis for finding the corrections to the energy spectrum of a hydrogen atom due to the relativistic correction term $\hat{H}'_r$ only. On the other hand, since $\hat{H}'_{SO}$ is proportional to $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$, it is useful to note that the product states in the coupled representation $|n,\ l,\ j,\ m_j\rangle$ are eigenstates of the operator $\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$ (in which all operators, e.g., $\vec{J} = \vec{L} + \vec{S}$, and the quantum numbers $l$, $j$ and $m_j$ are in standard notations and s has been suppressed from the states $|n,\ l,\ j,\ m_j\rangle$ since s=1/2 for the electron is a fixed

value for a hydrogen atom). Thus, $\hat{H}'_{SO}$ is diagonal in the degenerate subspace of $\hat{H}^0$ in the coupled representation and an angular basis consisting of states in the coupled representation is a *good* angular basis for $\hat{H}^0$ and $\hat{H}'_{SO}$ for DPT. Therefore, combining the relativistic and spin-orbit interaction contributions, a *good* angular basis for $\hat{H}^0$ and $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ is the coupled representation.

The uncoupled representation is another convenient angular basis. For each $n$, the states in the uncoupled representation $|n,\ l,\ s,\ m_l,\ m_s\rangle$ are eigenstates of $\hat{S}^2$, $\hat{S}_z$, $\hat{L}^2$, and $\hat{L}_z$. $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ in the uncoupled representation and therefore, an angular basis consisting of states in the uncoupled representation is not a *good* angular basis for $\hat{H}^0$ and $\hat{H}'_{SO}$ for DPT.

## 4.3 INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with finding the corrections to the energy spectrum of the hydrogen atom due to fine structure using DPT were investigated using five years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts to 64 upper-level undergraduates in a second-semester junior/senior level QM course and 42 first-year physics graduate students in the second-semester of the graduate core QM course. Additional insight was gained concerning these difficulties via responses of 13 students during a total of 45 hours of individual interviews using the "think aloud" protocol in which they were asked to answer the questions aloud that were posed without being disturbed [44]. Only at the end, they were asked to clarify any issues.

Moreover, after the development and validation of the QuILT, it was administered to 32 upper-level undergraduates in a second-semester junior/senior level QM course and 42 first-year physics graduate students in the second-semester of the graduate core QM course. The QuILT included the pretest, the tutorial, and the posttest. Students were given the pretest after traditional lecture-based instruction on DPT. Students began working on the tutorial in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest,

tutorial, and posttest were analyzed to gain insight on their understanding of corrections to the unperturbed energies of the hydrogen atom due to fine structure in the context of DPT. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

We will use student responses to the following two questions to discuss some common difficulties students had with the fine structure corrections to the energy spectrum of the hydrogen atom in the context of DPT. In both questions, students were told that the radial part of the wavefunctions $R_{nl}(r)$ corresponding to the eigenstates of $\hat{H}^0$ are chosen as the basis (Q1 and Q2 are questions posed on both the pretest after traditional lecture-based instruction on relevant concepts and posttest after students had worked on the QuILT. )

**Q1.** *Circle* **ALL** *of the bases which make the Hamiltonian operator $\hat{H}$ diagonal in the $n = 2$ subspace of $\hat{H}^0$ and explain your reasoning. Assume that for all cases, the principal quantum number $n = 2$.*

*i. Coupled representation,*

*ii. Uncoupled representation,*

*iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*v. Neither coupled nor uncoupled representation.*

In Q1, the operator $\hat{H}$ is a proxy for the operators $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ listed individually in four separate questions.

In Q1, for a fixed $n = 2$, since the $\hat{H}^0$ matrix is diagonal when any complete set of orthogonal states is chosen for the angular basis, options i, ii, iii, and iv are all correct for the operator $\hat{H}^0$. The operator $\hat{H}'_r$ is diagonal for a fixed $n$ if the options i, ii, iii, or iv in Q1 are chosen as the angular basis. On the other hand, the operator $\hat{H}'_{SO}$ is diagonal for a fixed $n$ if the angular basis consists of states in the coupled representation (option i) in Q1. Since $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$, the operator $\hat{H}'_{fs}$ is diagonal for a fixed $n$ if the angular basis consists of

states in the coupled representation (option i).

**Q2.** *A perturbation $\hat{H}'$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For the Hamiltonian $\hat{H}$, circle* **ALL** *of the representations that can be chosen as the angular part of a "good" basis and explain your reasoning. Assume that for all cases, the principal quantum number is restricted to $n = 2$.*

*i. Coupled representation,*

*ii. Uncoupled representation,*

*iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),*

*v. Neither coupled nor uncoupled representation.* In Q2, the operator $\hat{H}'$ is a proxy for the operators $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ listed individually in three separate questions. We note that options iii and iv were given without the condition of the same $l$ for operators $\hat{H}'_{SO}$ and $\hat{H}'_{fs}$ in some years of the study and that there was no difference in student performance based upon whether the wording of the question included the same $l$ or not for $\hat{H}'_{SO}$ and $\hat{H}'_{fs}$.

In Q2, for a fixed $n$ (in each degenerate subspace of $\hat{H}^0$), since $\hat{H}^0$ and $\hat{H}'_r$ are diagonal in any angular basis consisting of a complete set of orthogonal states with fixed $l$, options i, ii, iii, and iv are all correct for a *good* basis for finding the perturbative corrections for $\hat{H}'_r$ as the perturbation on $\hat{H}^0$. In each degenerate subspace of $\hat{H}^0$, the spin orbit interaction term $\hat{H}'_{SO}$ is diagonal if an angular basis consisting of states in the coupled representation is chosen. Thus, a *good* angular basis for finding the perturbative correction for $\hat{H}'_{SO}$ as the perturbation on $\hat{H}^0$ is given by option i. For the fine structure term $\hat{H}'_{fs}$, a *good* angular basis for finding the perturbative correction is a basis consisting of states in the coupled representation since the coupled representation forms a *good* angular basis for both $\hat{H}'_{SO}$ and $\hat{H}'_r$. Therefore, option i is correct for the fine structure term $\hat{H}'_{fs}$.

Below, we discuss some common difficulties with the fine structure corrections to the energy spectrum of the hydrogen atom found via research that interfere with students choosing

Table 9: Percentages of undergraduate and graduate students who selected all of the correct representations in which a given operator is diagonal in Q1 after traditional instruction.

| Operator | Correct Answer | Undergraduate | | Graduate | |
|---|---|---|---|---|---|
| | | N | (%) | N | (%) |
| $\hat{H}^0$ | i, ii, iii, iv | 32 | 34 | 42 | 33 |
| $\hat{H}'_r$ | i, ii, iii, iv | 32 | 22 | 42 | 21 |
| $\hat{H}'_{SO}$ | i | 32 | 34 | 42 | 36 |
| $\hat{H}'_{fs}$ | i | 12 | 33 | - | - |

a *good* basis and using DPT correctly in this context before discussing how those difficulties were used as a guide in developing the DPT QuILT to help students find the fine structure corrections.

## 4.4 STUDENT DIFFICULTIES

We find that when students are asked to determine a "good" basis for finding the perturbative fine structure corrections to the energy spectrum of the hydrogen atom using DPT, difficulties result from not realizing that DPT should be used. Moreover, even if students realize that DPT should be used, they may not have a functional understanding of the bases that make a perturbation Hamiltonian operator diagonal in each degenerate subspace of $\hat{H}^0$ and how this knowledge can help determine a *good* basis for finding the fine structure corrections to the energy spectrum of the hydrogen atom in the context of DPT. In Q1, many students struggled to correctly identify all sets of the angular basis states for which an operator is diagonal in the $n = 2$ subspace. Table 9 summarizes the percentages of students who selected all of the possible correct representations in which an operator is diagonal in Q1 for $n = 2$. It is important that students identify the bases in which $\hat{H}^0$ is diagonal since a *good* basis must consist of a complete set of eigenstates of $\hat{H}^0$. However, only around one-third of undergraduate and graduate students correctly identified all the angular bases in Q1 in which $\hat{H}^0$ is diagonal. Many students struggled with the fact that the operator $\hat{p}^2$ in the

unperturbed Hamiltonain $\hat{H}^0$ is spherically symmetric (since $[\hat{p}^2, \hat{\vec{L}}] = 0$) and the term $1/r$ in the Coulomb potential energy is spherically symmetric since $[1/r, \hat{\vec{L}}] = 0$ and hence, $\hat{H}^0$ is spherically symmetric ($[\hat{H}^0, \hat{\vec{L}}] = 0$). Thus, the unperturbed Hamiltonian $\hat{H}^0$ is diagonal for a fixed $n$ if the coupled representation, uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled/uncoupled representation is chosen as the basis. Many of these students attempted to explicitly determine whether states in the coupled or uncoupled representation were eigenstates of $\hat{H}^0$. They began by letting $\hat{H}^0$ act on states in the coupled or uncoupled representations (e.g, $\hat{H}^0|n,\ l,\ m_l,\ m_s\rangle$) but were not able to evaluate these expressions correctly. For example, one interviewed student who attempted to evaluate $\hat{H}^0|n,\ l,\ m_l,\ m_s\rangle$ proceeded to write the $\hat{p}^2$ operator in $\hat{H}^0$ in terms of $\hat{p}_r$, $\hat{p}_\theta$, and $\hat{p}_\phi$ and acted on the generic state $|n,\ l,\ m_l,\ m_s\rangle$ in the uncoupled representation. This is where he stopped, saying "I don't know how to find these (the components of the momentum squared operator acting on the state $|n,\ l,\ m_l,\ m_s\rangle$)." Many of these same students also had difficulty realizing that $[\hat{H}'_r, \hat{\vec{L}}] = 0$ implies that the perturbation $\hat{H}'_r$ is spherically symmetric and hence $\hat{H}'_r$ is diagonal for a fixed $n$ if the coupled representation, uncoupled representation, or any arbitrary complete orthonormal set constructed with linear combinations of states in the coupled/uncoupled representation with a fixed $l$ is chosen as the basis. They tried to determine the angular representations in which the perturbation $\hat{H}'_r$ is diagonal in the degenerate subspaces of $\hat{H}^0$ and often attempted to determine whether states in the coupled or uncoupled representation were eigenstates of $\hat{p}^4$. However, these students struggled when they attempted to explictly evaluate $\hat{p}^4$ acting on the states in the coupled and uncoupled representation (e.g., $\hat{p}^4|n,\ l,\ m_l,\ m_s\rangle$) and could not determine whether states in the coupled and uncoupled representation are eigenstates of $\hat{p}^4$ (they had similar difficulties in Q2 with any arbitrary complete set of linear combinations of states in the coupled or uncoupled representation with the same $n$ and $l$). During the interviews, many students admitted to memorizing the representation to choose for a good angular basis in a given situation (for a given $\hat{H}^0$ and $\hat{H}'$) rather than using systematic reasoning. An explicit example is the following statement from an interviewed student, "I was always confused with coupled and uncoupled representation. I just memorized when to use which." Memorization of which basis to use often masks the fact that students did not

Table 10: The percentage of students who chose all of the possible correct representations that form a *good* basis for the listed perturbation $\hat{H}'$ and the unperturbed Hamiltonian $\hat{H}^0$ in Q2 on the pretest for undergraduates (number of students $N = 32$) and graduate students ($N = 42$).

| $\hat{H}'$ Operator | Correct Answer | Undergraduate Students(%) | Graduate Students(%) |
|---|---|---|---|
| $\hat{H}'_r$ | i, ii, iii, iv | 16 | 17 |
| $\hat{H}'_{SO}$ | i | 34 | 38 |
| $\hat{H}'_{fs}$ | i | 22 | 29 |

have a functional understanding of DPT for the fine structure corrections to the energy of the hydrogen atom. Furthermore, some of these students recognized at least one representation that makes the unperturbed Hamiltonian $\hat{H}^0$ diagonal and makes the fine structure perturbation $\hat{H}'_{fs}$ diagonal in each degenerate subspace of $\hat{H}^0$, but they did not realize that this representation was a *good* basis for $\hat{H}^0$ and $\hat{H}'_{fs}$.

On Q2, students struggled to determine a *good* angular basis for each perturbation $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ on $\hat{H}^0$. The results are summarized in Table 10. For Q2, it is important that students identify that the coupled representation is a *good* basis for both $\hat{H}'_r$ and $\hat{H}'_{SO}$ and the coupled representation is the only option given in Q2 that forms a *good* basis for the fine structure perturbation $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. The percentage of students who chose the coupled representation as a *good* basis for $\hat{H}^0$ and each of the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ is given in Table 11. The percentages in Table 11 included student who correctly selected the coupled representation and may have also selected at least one additional incorrect representation as a *good* basis for $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ or may not have selected all the bases that form a *good* basis for $\hat{H}'_r$.

Below, we discuss some difficulties found regarding the fine structure corrections to the energy spectrum of the hydrogen atom in the context of DPT that hinder students' ability to select the representations that form a *good* basis in Q2. In this section, we focus on the

Table 11: The percentage of students who chose states in the coupled representation as a *good* basis for the listed perturbation $\hat{H}'$ and the unperturbed Hamiltonian $\hat{H}^0$ in Q2 on the pretest for undergraduates (number of students $N = 32$) and graduate students ($N = 42$).

| $\hat{H}'$ Operator | Undergraduate Students(%) | Graduate Students(%) |
|---|---|---|
| $\hat{H}'_r$ | 53 | 33 |
| $\hat{H}'_{SO}$ | 44 | 64 |
| $\hat{H}'_{fs}$ | 31 | 45 |

qualitative results found primarily from student responses during the think aloud interviews. Later, in the Evaluation of the QuILT section (section VI), we will discuss more quantitative results given by the percentage of students that displayed these difficulties on the pretest after traditional lecture-based instruction on relevant concepts and the posttest after engaging with the QuILT.

### 4.4.1 Not realizing that DPT must be used to find the perturbative corrections to the energies and energy eigenstates of the hydrogen atom

The unperturbed energies for the hydrogen atom only depend on the principal quantum number $n$. As noted, for each value of $n$, there are $2n^2$ degenerate states corresponding to all the possible values of $l$, $m_l$ and $m_s$ (degeneracy due to the spin degrees of freedom). Therefore, in order to find the perturbative fine structure corrections to the energy spectrum of the hydrogen atom, one must use DPT. However, many students did not realize that they had to use DPT, and instead, used non-degenerate perturbation theory to find the first-order perturbative corrections to the energies. These students did not consider the degeneracy in the energy spectrum of the unperturbed Hamiltonian $\hat{H}^0$ before using Eqs. 6.1 and 6.2. Some of these students only considered whether the given basis forms a complete set of eigenstates of $\hat{H}^0$ and gave no consideration to the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$. They did not realize that a *good* basis is one that diagonalizes $\hat{H}^0$ and also diagonalizes $\hat{H}'$ in each

degenerate subspace of $\hat{H}^0$.

### 4.4.2 Using DPT to find corrections to the wavefunction but not using DPT to find the first-order corrections to the energies

Even in the cases in which students realized that DPT must be used to find the fine structure corrections to the unperturbed energy eigenstates of the hydrogen atom, some students did not first determine a *good* basis before calculating the first-order perturbative corrections to the energies. In written responses and interviews, these students often identified the potential issue that the degeneracy in the unperturbed energies of the hydrogen atom creates for Eq. 6.2 when a given basis is not a *good* basis. They recognized that, due to the degeneracy in the unperturbed energy spectrum of the hydrogen atom, there are terms in Eq. 6.2 in which the denominator is zero and corrections to the energy eigenstates are invalid. However, they assumed that any basis could be used to determine the first-order corrections to the energy spectrum since they did not see any potentially divergent terms in Eq. 6.1. They did not realize that a *good* basis is required to find the perturbative corrections to the energy spectrum even in first-order for the hydrogen atom involving fine structure (otherwise, their first-order corrections would be incorrect).

Some students with this type of difficulty thought that any angular basis would form a *good* basis in Q2 for finding the corrections to the energy spectrum since they did not see any potentially divergent terms in Eq. 6.1 for the energy correction. They often chose options i, ii, iii, and iv for all the perturbations in Q2 since they did not have a functional understanding of DPT.

### 4.4.3 Not focusing on BOTH $\hat{H}^0$ and $\hat{H}'$ when finding a *good* basis

To probe students' understanding of the angular bases that make a perturbation Hamiltonian diagonal in a degenerate subspace of $\hat{H}^0$, Q1 was posed (both after the traditional instruction and after students had engaged with the QUILT) for each of the operators $\hat{H}^0$, $\hat{H}'_r$, and $\hat{H}'_{SO}$ (that make up the different components of the Hamiltonian of the hydrogen atom including the fine structure perturbation $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$). Many students struggled to correctly

identify all the representations in which the operators $\hat{H}^0$, $\hat{H}'_r$, and $\hat{H}'_{SO}$ are diagonal in Q1 in the $n = 2$ subspace. Sometimes students with this type of difficulty struggled with determining a representation that forms a *good* basis for DPT in Q2.

Some students did not realize that a basis that makes $\hat{H}^0$ diagonal and $\hat{H}'$ diagonal in each degenerate subspace of $\hat{H}^0$ is a *good* basis for DPT. They often answered Q1 correctly by identifying a basis that makes each operator $\hat{H}^0$ and $\hat{H}'$ diagonal in the $n = 2$ subpsace of $\hat{H}^0$ separately, but then they incorrectly answered Q2 and did not choose a *good* basis as the one that makes $\hat{H}^0$ diagonal and $\hat{H}'$ diagonal in each degenerate subspace of $\hat{H}^0$. For example, one student correctly chose options i, ii, iii, and iv as the representations that make $\hat{H}^0$ diagonal and option i as the representation that makes $\hat{H}'_{SO}$ diagonal in $n = 2$ subpsace of $\hat{H}^0$ in Q1. This same student then incorrectly chose options i, ii, iii and iv as the representations that form a *good* basis in Q2 despite not choosing options ii, iii, and iv as the representations that make $\hat{H}'_{SO}$ diagonal in the degenerate subspace of $\hat{H}^0$.

Below we discuss two types of student difficulties that involved students only focusing on $\hat{H}^0$ or $\hat{H}'$ (but not both) when finding a *good* basis.

**Only focusing on $\hat{H}^0$ to determine a *good* basis:** One difficulty that prevented students from choosing the representation that forms a *good* angular basis (e.g., in response to Q2) was focusing only on $\hat{H}^0$ and not on $\hat{H}'$ when finding a *good* angular basis. In response to Q2, students with this type of difficulty focused on the bases that make $\hat{H}^0$ diagonal but did not take $\hat{H}'$ into consideration when finding a *good* basis. For example, on question Q1, some students incorrectly selected only the uncoupled representation (option ii) as the basis that would make the operator $\hat{H}^0$ diagonal and then incorrectly chose the uncoupled representation as a *good* basis for $\hat{H}^0$ and $\hat{H}'_{SO}$ in Q2. In their explanation on the pretest, they noted that states in the uncoupled representation were eigenstates of $\hat{H}^0$, but they did not consider the fact that $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ when states in the uncoupled representation are chosen as the basis.

Similarly, some students chose a *good* basis based only upon the representation that makes $\hat{H}^0$ diagonal without considering whether the operator $\hat{H}'_{fs}$ was diagonal in each degenerate subspace of $\hat{H}^0$ in that basis. For example, in interviews, some students claimed that the uncoupled representation was a basis that would make the operator $\hat{H}^0$ diagonal,

and they then incorrectly chose the uncoupled representation as a *good* angular basis for the fine structure corrections. In their explanations, they correctly noted that states in the uncoupled representation were eigenstates of $\hat{H}^0$, but they did not consider the fact that $\hat{H}'_{fs}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ when states in the uncoupled representation are chosen as the angular basis. For example, in the $n = 2$ subspace, the $\hat{H}'_{fs}$ matrix is given below when the basis states are chosen in the uncoupled representation as $|n,\ l,\ m_l,\ m_s\rangle$ (the notations are standard and quantum numbers $m_l$ and $m_s$ correspond to the z component of the orbital and spin angular momenta, respectively) in the order $|2,\ 0,\ 0,\ \frac{1}{2}\rangle$, $|2,\ 0,\ 0,\ -\frac{1}{2}\rangle$,$|2,\ 1,\ 1,\ \frac{1}{2}\rangle$, $|2,\ 1,\ 1,\ -\frac{1}{2}\rangle$, $|2,\ 1,\ 0,\ \frac{1}{2}\rangle$, $|2,\ 1,\ 0,\ -\frac{1}{2}\rangle$, $|2,\ 1,\ -1,\ \frac{1}{2}\rangle$, and $|2,\ 1,\ -1,\ -\frac{1}{2}\rangle$ (where $\alpha$ is the fine structure constant):

$$\hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & 7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}. \tag{4.3}$$

Since many students only focused on the representation in which $\hat{H}^0$ is diagonal to determine a *good* basis, in the interviews, students were explicitly asked about the role of the perturbation term in the Hamiltonian in the choice of a *good* basis. They were asked to calculate some of the off-diagonal matrix elements of the $\hat{H}'_{fs}$ matrix or at least reason conceptually about whether some of the off-diagonal matrix elements of $\hat{H}'_{fs}$ would be non-zero in the uncoupled representation in the $n = 2$ degenerate subpsace of $\hat{H}^0$ (see Eq. 4.3). We find that the interviewed students often struggled to calculate or reason conceptually that the fine structure perturbation $\hat{H}'_{fs}$ shown in Eq. 4.3 is not diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ in the uncoupled representation and that the uncoupled representation cannot be a *good* angular basis for finding the fine structure corrections.

**Only focusing on $\hat{H}'$ to determine a *good* basis:** Some students chose a *good* basis based upon the representations that make $\hat{H}'$ diagonal in each degenerate subspace of $\hat{H}^0$

without consideration of whether the operator $\hat{H}^0$ was diagonal in that basis. For example, some students in Q1 incorrectly selected only the uncoupled representation (option ii) as the basis that would make $\hat{H}^0$ diagonal but incorrectly selected the coupled representation (option i) as the only basis that would make $\hat{H}'_r$ diagonal in the $n = 2$ subspace. These students then incorrectly chose the coupled representation as the only *good* basis for $\hat{H}^0$ and $\hat{H}'_r$ in Q2. While it is correct that states in the coupled representation form a *good* basis, they used incorrect reasoning to formulate their answer and also did not identify that all the options i, ii, iii, and iv are correct for $\hat{H}'_r$ in Q2.

## 4.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 4.5.1 Development and Validation of the QuILT

The difficulties described show that students struggle in determining a representation in which an operator is diagonal. Therefore, we developed a QuILT that takes into account these difficulties. The development of the DPT QuILT started with an investigation of student difficulties via open-ended and multiple-choice questions administered after traditional instruction to advanced undergraduate and graduate students and conducting a cognitive task analysis from an expert perspective of the requisite knowledge [45]. The QuILT strives to help students build on their prior knowledge and addresses common difficulties found via research, some of which were discussed in the previous section.

In the QuILT, students are presented with novel tasks. Whether it be examples, hypothetical conversation, or calculations, students develop a deeper understanding by actively working through the inquiry-based QuILT. Student difficulties are incorporated in these examples and conversations to create a cognitive conflict and the students are then guided through additional tasks designed to resolve these issues. The QuILT follows a guided inquiry-based learning sequence laid out in the cognitive task analysis. It is organized to build on the students' prior knowledge and each section in the QuILT builds upon the previous section. This organization helps the students build their own knowledge structures in a coherent manner. Students are provided scaffolding to help address common difficulties, thus reducing the cognitive conflict. The QuILT progressively reduces the scaffolding to the

point students are able to solve the problems without any assistance.

The development of the QuILT went through a cyclic iterative process. The preliminary version was developed based upon the cognitive task analysis and knowledge of common student difficulties. Next, the QuILT underwent many iterations among the three researchers and then was iterated several times with three physics faculty members to ensure that they agreed with the content and wording. It was also administered to graduate and advanced undergraduate students in individual think-aloud interviews to ensure that the guided approach was effective, the questions were unambiguously interpreted, and to better understand the rationale for student responses. During these semi-structured interviews, students were asked to "think aloud" while answering the questions. Students first read the questions on their own and answered them without interruptions except that they were prompted to think aloud if they were quiet for a long time. After students had finished answering a particular question to the best of their ability, they were asked to further clarify and elaborate on issues that they had not clearly addressed earlier. The next step involved evaluating the QuILT's impact on student learning and determining if the difficulties remained. Finally, modifications and improvements were made based upon the student and faculty feedback before it was administered to students in various courses.

### 4.5.2 Overview of the QuILT

The QuILT uses an inquiry-based approach to learning and actively engages students in the learning process. It includes a pretest to be administered in class after traditional instruction in DPT. Then students engage with the tutorial in small groups in class or use it as a guide for class discussions (or alone when using it as a self-paced learning tool in homework), and then they are administered a posttest in class. As students work through the tutorial, they are asked to predict what should happen in a given situation. Then, the tutorial strives to provide scaffolding and feedback as needed to bridge the gap between their initial knowledge and the level of understanding that is desired. Students are also provided checkpoints to reflect upon what they have learned and to make explicit the connections between what they are learning and their prior knowledge. They are given an opportunity to reconcile differences between their predictions and the guidance provided in the checkpoints before proceeding further.

The DPT QuILT uses a blend of qualitative and quantitative reasoning to improve students' understanding. For example, the QuILT requires qualitative understanding while responding to the hypothetical conversations and quantitative reasoning to determine the matrix elements of the operators $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ in the coupled and uncoupled representations. Students verify statements in hypothetical conversations via quantitative reasoning.

### 4.5.3 Addressing Student Difficulties

In the QuILT, students begin by engaging with examples applying DPT in the context of a three-dimensional Hilbert space before considering the infinite-dimensional Hilbert space of the hydrogen atom. These three-dimensional examples strive to help students learn why DPT must be used when there is degeneracy in the unperturbed energy spectrum. Next, the students engage with examples involving DPT in which they consider the terms $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0$. Students focus on concepts related to determining a *good* basis for the fine structure corrections to the energy of the hydrogen atom. In particular, for the unperturbed Hamiltonian $\hat{H}^0$ and the fine structure perturbation $\hat{H}'_{fs}$, students learn about (1) why DPT must be used, (2) why care must be taken to choose a *good* basis even for the first order correction to the energy spectrum even though the expression does not "blow up", and (3) how to choose a *good* basis that keeps $\hat{H}^0$ diagonal and diagonalizes $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0$. Below, we discuss how the QuILT strives to address student difficulties and help them learn about fine structure corrections to the energy spectrum of the hydrogen atom in the context of DPT.

**Helping students realize that DPT must be used to find the perturbative corrections to the energies and energy eigenstates of the hydrogen atom:** In the QuILT, students are given the unperturbed Hamiltonian

$$\hat{H}^0 = \frac{\hat{p}^2}{2m} + V(r) = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}. \tag{4.4}$$

They work through several guided inquiry-based learning sequences, such as the following, aimed at helping them reflect upon the fact that there is degeneracy in the unperturbed energy spectrum of the hydrogen atom:

**Q4(a)**. *What is one complete set of quantum numbers that describe the eigenstates of* $\hat{H}^0$

*given by equation (B.2) (include spin degree of freedom)?*

**Q4(b)**. *What is the unperturbed energy corresponding to $\hat{H}^0$ in equation (B.2) in terms of the principal quantum number $n$?*

**Q4(c)**. *Based upon your answers to the two preceding questions, should there be a degeneracy in the unperturbed spectrum of a hydrogen atom given by equation (B.2)? Explain.*

**Q4(d)**. *What is the degeneracy of an energy level with energy $E_n$ for a given $n$ (including degeneracy due to spin degrees of freedom)?*

This sequence of questions strives to help students be able to identify that there is degeneracy in the unperturbed energy spectrum of the hydrogen atom. In particular, in answering Q4(c), students reflect upon the fact that the unperturbed energy spectrum only depends on the principal quantum number $n$ and that states with different angular quantum numbers ($l, m_l, s, m_s$ or $l, s, j,\ m_j$) with the same principal quantum number $n$ are all eigenstates of $\hat{H}^0$ with the same unperturbed energy. Therefore, the answer to Q4(d) is the degeneracy of an energy level with energy $E_n$, given by $2\sum_{l=0}^{n-1}(2l+1) = 2n^2$, since for each $n$, there are $(2l+1)$ values of $m_l$ and the factor of 2 corresponds to the spin degeneracy. Having explicitly considered the degeneracy that arises due to the symmetry of the unperturbed Hamiltonian of the hydrogen atom in Q4, the QuILT strives to help students identify that DPT must be used to find the fine structure corrections to the unperturbed energies of the hydrogen atom.

**Helping students realize that a *good* basis is required even for finding the first-order corrections to the energies:** In the QuILT, students are asked to determine a *good* basis for finding the first-order corrections to the energies involving $\hat{H}^0$ and each of the individual perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$. After each question that asks the students to determine a *good* basis for finding the first-order corrections to the energy spectrum, students are provided scaffolding in the form of quantitative questions as well as conversations requiring qualitative reasoning. Additionally, students are provided checkpoints that give them an opportunity to reconcile any differences between their reasoning and the correct reasoning. Working through these questions and conversations allows the students to realize that care must be taken to ensure that a *good* basis is chosen even for finding the first-order corrections to the energies.

**Helping students with the fact that the basis that diagonalizes a Hamiltonian in each degenerate subspace of $\hat{H}^0$ may not be unique:** The following is part of a hypothetical conversation that strives to help students reflect upon the fact that in each degenerate subspace of $\hat{H}^0$, the spherical symmetry of $\hat{H}^0$ (with unperturbed energies only dependent on $n$) allows for any angular basis consisting of a complete set of orthogonal basis states to keep the $\hat{H}^0$ matrix diagonal.

**Q5.** *Consider the following conversation regarding whether the unperturbed Hamiltonian $\hat{H}^0$ is diagonal if the coupled or the uncoupled representation is chosen as the angular basis.*

**Student 1:** *Angular basis states in both the coupled and the uncoupled representations are the angular part of the eigenstates of $\hat{H}^0$ since $\hat{H}^0$ is spherically symmetric with unperturbed energies only dependent on $n$. Furthermore, for a fixed $n$, any arbitrary complete orthogonal basis constructed using linear combinations of the coupled or uncoupled states can also be chosen as the angular part of the eigenstates of $\hat{H}^0$.*

**Student 2:** *The unperturbed Hamiltonian $\hat{H}^0$ is identical in both the coupled and uncoupled representations. In fact, $\hat{H}^0$ is identical so long as, for a fixed $n$, we choose any arbitrary complete orthonormal angular basis constructed with linear combinations of states in the coupled or uncoupled representation.*

*Explain why you agree or disagree with each student.*

In Q5, Student 1 correctly notes that $\hat{H}^0$ is a diagonal matrix in both the coupled and the uncoupled representations and Student 2 adds the fact that for a fixed $n$, the $\hat{H}^0$ matrix is diagonal and identical as long as the angular basis states are chosen to consist of any orthonormal complete set of states in either the coupled or uncoupled representations. In a later conversation, students focus on the fact that since $[\hat{H}^0, \hat{\vec{L}}] = 0$, the unperturbed Hamiltonian is spherically symmetric and that the angular basis can be chosen to consisting of any complete set of orthogonal states.

After students have considered bases that diagonalize the $\hat{H}^0$ matrix, they are asked to consider $\hat{H}'_r$ and $\hat{H}'_{SO}$ separately as perturbations before considering the fine structure term as a perturbation. In particular, students work through guided inquiry-based learning sequences that strive to help them learn that the relativistic correction $\hat{H}'_r$ is diagonal in each degenerate subspace of $\hat{H}^0$ when any complete set of orthogonal angular basis states

that do not involve linear combinations of different $n$ and $l$ is chosen, so that type of basis forms a *good* basis for finding the perturbative corrections.

In the QuILT, students actively engage with examples involving the unperturbed Hamiltonian $\hat{H}^0$ and each of the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$. For all of the examples, students are scaffolded with guided inquiry-based learning sequences and conversations that strive to help them identify angular bases that keep $\hat{H}^0$ diagonal and diagonalize each of the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0$.

**Helping students with the fact that BOTH $\hat{H}^0$ and $\hat{H}'$ must be considered when finding a *good* basis:** To help students who had difficulty with determining angular bases that keep the operator $\hat{H}^0$ diagonal while diagonalizing $\hat{H}'_r$, $\hat{H}_{SO}$ and $\hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$, students work through several guided inquiry-based sequences in the QuILT.

For the operator $\hat{H}'_{SO}$, students first calculate several diagonal and off-diagonal matrix elements when the coupled or uncoupled representation is chosen as the basis. If the basis is chosen to consist of states in the coupled representation, the off-diagonal matrix elements of $\hat{H}'_{SO}$ are zero in each degenerate subspace of $\hat{H}^0$ and therefore the coupled representation forms a *good* basis for finding the perturbative corrections due to the spin-orbit interaction $\hat{H}'_{SO}$. Therefore, the diagonal matrix elements of $\hat{H}'_{SO}$ are the first order corrections to the energies if basis states are chosen in the coupled representation.

Students also work through several guided inquiry-based sequences that strive to help them learn that the unperturbed Hamiltonian $\hat{H}^0$ is spherically symmetric with the unperturbed energy spectrum only dependent on $n$ and $\hat{H}^0$ is diagonal if any complete set of orthogonal angular basis states is chosen as the basis for a fixed $n$. An angular basis consisting of states in the coupled representation is one such complete set. The following excerpt taken from a hypothetical student conversation in the QuILT strives to help students reflect upon the fact that the $\hat{H}'_{SO}$ operator is also diagonal in each degenerate subspace of $\hat{H}^0$ if states in the coupled representation are chosen as the angular basis states.

**Q6.** *Consider the following conversation about finding a "good" angular basis for the hydrogen atom with the spin-orbit interaction term as the perturbation.*

**Student 1:** $\vec{L}\cdot\vec{S}$ *is diagonal in the coupled representation because* $J^2 = (\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S}) =$

$\hat{L}^2 + \hat{S}^2 + 2\vec{L} \cdot \vec{S}$ *which implies* $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$. *The basis states in the coupled representation are eigenstates of* $\hat{J}^2$, $\hat{S}^2$, *and* $\hat{L}^2$ *and hence eigenstates of* $\vec{L} \cdot \vec{S}$.

**Student 2:** *I agree with Student 1.* $\hat{H}'_{SO}$ *is diagonal in each degenerate subspace of* $\hat{H}^0$ *when the coupled representation is chosen as the basis, but not when the uncoupled representation is chosen as the basis. The coupled representation forms a "good" basis for the given unperturbed Hamiltonian* $\hat{H}^0$ *and perturbation* $\hat{H}'_{SO}$.

*Explain why you agree or disagree with each student.*

In question Q6, both Student 1 and Student 2 are correct. Since basis states in the coupled representation are eigenstates of $\hat{J}^2$, $\hat{S}^2$, and $\hat{L}^2$, states in the coupled representation form a good basis for $\hat{H}^0$ and $\hat{H}'_{SO}$. The two conversations in questions Q5 and Q6 provide scaffolding to help students reflect upon the fact that states in the coupled representation form a good basis for $\hat{H}^0$ and $\hat{H}'_{SO}$.

Questions Q5, Q6, and similar hypothetical conversations focusing on the perturbation $\hat{H}'_{fs}$ strive to help students develop a deep understanding of the bases that make the $\hat{H}'_r$, $\hat{H}'_{SO}$ and $\hat{H}'_{fs}$ operators diagonal in each degenerate subspace of $\hat{H}^0$ and why one must consider both $\hat{H}^0$ and $\hat{H}'_{fs}$ when determining a *good* basis. Additionally, the QuILT strives to help students learn that considering both the unperturbed Hamiltonian $\hat{H}^0$ and perturbation $\hat{H}'_{fs}$ and understanding of the good bases that make the perturbation operator $\hat{H}'$ diagonal in each degenerate subspace of $\hat{H}^0$ while keeping the unperturbed Hamiltonian $\hat{H}^0$ diagonal are critical for finding the fine structure corrections to the hydrogen atom.

## 4.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts in DPT but before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework

Table 12: The percentage of students who chose all the possible correct representations to form a *good* basis for the listed perturbation $\hat{H}'$ and the unperturbed Hamiltonian $\hat{H}^0$ in Q2 on the pretest and posttest for undergraduates (number of students $N = 32$ for the pretest and $N = 31$ for the posttest) and graduate students ($N = 42$).

| $\hat{H}'$ Operator | Correct Answer | Undergraduate Students(%) | | Graduate Students(%) | |
|---|---|---|---|---|---|
| | | Pre | Post | Pre | Post |
| $\hat{H}'_r$ | i, ii, iii, iv | 16 | 87 | 17 | 79 |
| $\hat{H}'_{SO}$ | i | 34 | 94 | 38 | 74 |
| $\hat{H}'_{fs}$ | i | 22 | 81 | 29 | 86 |

assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest. The results for the pre/posttest are summarized in Tables 12 and 13, and suggest that working on the QuILT was helpful in reducing student difficulties with these concepts. In particular, over 74% of graduate students and 81% of undergraduate students were able to correctly identify all the possible correct representations that form a *good* basis for the perturbations $\hat{H}'_r$, $\hat{H}'_{SO}$ or $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ and the unperturbed Hamiltonian $\hat{H}^0$ after engaging with the QuILT. These students were able to correctly identify all of the given representations in which an operator is a diagonal matrix in each degenerate subspace of $\hat{H}^0$ and build upon this knowledge to select all of the representations that form a *good* basis for a given $\hat{H}^0$ and $\hat{H}'$.

As can be seen in Table 12, the graduate students and undergraduate students generally performed at about the same level on Q2 on the pretest. However, the undergraduates outperformed the graduate students on the posttest in identifying all the options in Q2 that form a *good* basis. One possible explanation for the undergraduates outperforming the graduate students on the posttest could be the grade incentive associated with the QuILT. The QuILT accounted for a larger percentage of the undergraduate students' overall course

Table 13: The percentage of students who answered question Q2 consistently with question Q1 and correctly for either $\hat{H}'_r$ or $\hat{H}'_{SO}$ on the pretest and posttest for undergraduates and graduate students.

| | Undergraduate Students% | | | | Graduate Students % | | | |
|---|---|---|---|---|---|---|---|---|
| $\hat{H}'$ | N | Pre | N | Post | N | Pre | N | Post |
| $\hat{H}'_r$ | 32 | 9 | 31 | 84 | 42 | 17 | 42 | 76 |
| $\hat{H}'_{SO}$ | 28 | 15 | 31 | 71 | 42 | 31 | 42 | 74 |

grade and the components of the QuILT were accounted for differently for the course grade for the two groups of students. In particular, the posttest for the undergraduate students was graded for correctness in both years while the posttest for the graduate students was graded for completeness in Year 1 and for correctness in Year 2. Additionally, the undergraduate students knew that the material from the QuILT could appear on their examinations while the graduate students were told by the graduate instructor that this material was a review of the undergraduate quantum mechanics and that no material from the QuILT would appear on their examinations; instead, more complex problems on the DPT would appear on the exams. The fact that the graduate students were given very small grade incentive to learn the material in the QuILT may have decreased their motivation to engage as deeply with the QuILT as the undergraduates and may explain why the graduate students did not perform as well as the undergraduate students on the posttest.

## 4.7 SUMMARY

Using the common difficulties of advanced students with fine structure corrections to the energies of the hydrogen atom in the context of DPT as resources, we developed and evaluated a research-based QuILT which focuses on helping students reason about and find bases which form a *good* bases for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbations $\hat{H}'_r$ and $\hat{H}'_{SO}$ separately or the fine structure perturbation $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Having a deep

understanding of the angular bases for which each of these operators is diagonal in each degenerate subspace of $\hat{H}^0$ is a prerequisite to helping students determine a *good* basis for finding the perturbative corrections using DPT for a hydrogen atom when the fine structure is treated as perturbation. In order to have a functional understanding of DPT, one must be able to synergistically apply several appropriate concepts from physics and mathematics to solve a DPT problem. This can lead to cognitive overload and students may resort to memorizing procedures rather than understanding the concepts involved and learning the process of applying those concepts appropriately [46] unless appropriate scaffolding support and feedback is provided. Additionally, our research suggests that students often did not realize that they were providing inconsistent responses within the same problem or across several closely related problems on the same quiz or test. When students are developing expertise, students' working memory may be occupied with several different aspects of a given problem and few resources may be available for metacognition, e.g., making sure that the approach is coherent and checking whether an answer makes sense and is consistent with the previous answers [46].

Solving DPT problems requires students to apply advanced mathematical concepts in the context of a concrete physical problem. Moreover, the fact that the quantum physics paradigm is novel exacerabates student difficulties [12]. Prior research studies have found that students have difficulty connecting and applying mathematical concepts correctly in introductory physics contexts (e.g., see Refs. [48, 49, 50, 47]) and they sometimes make mathematical mistakes that they would otherwise not make if the physics concept was not present. Many of the common difficulties students had with DPT were intimately entangled with students' lack of robust understanding of the underlying linear algebra concepts and difficulties connecting these mathematical and quantum mechanical concepts. For example, in order to be able to identify bases that make an operator diagonal in each degenerate subspace of the unperturbed Hamiltonian, one must have a strong background in linear algebra and be able to apply it in the context of solving a physics problem.

The QuILT strives to provide appropriate scaffolding and feedback using a guided inquiry-based approach to help students develop a functional understanding of the concepts relevant for DPT in the context of the fine structure corrections to the hydrogen atom.

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# 5.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DEGENERATE PERTURBATION THEORY: INTERMEDIATE FIELD ZEEMAN EFFECT

## 5.1 INTRODUCTION

Quantum mechanics (QM) is challenging even for upper-level undergraduate and graduate students, and students often struggle to make connections between mathematics and QM concepts in this abstract, non-intuitive and novel context (e.g., see Refs. [1, 2, 3, 6, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 15]). There have been a number of prior research studies aimed at investigating student reasoning in QM [16, 17, 18, 19, 20, 21, 22, 23, 24, 25] and using the findings as resources for improving student understanding [26, 27, 28, 29, 30, 31, 32, 33, 34]. Guided by research studies conducted to identify student difficulties with QM and findings of cognitive research, we have been developing a set of research-based learning tools including the Quantum Interactive Learning Tutorials (QuILTs), which strive to help students develop a solid grasp of QM [35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45]. However, there has been relatively little research that focuses on student understanding of advanced topics in quantum mechanics, e.g., degenerate perturbation theory (DPT) [46]. Here we discuss an investigation of student difficulties with mathematical sense-making in a physical situation in the context of DPT involving the intermediate field Zeeman effect for the hydrogen atom. We also describe the development and validation of the research-based QuILT that uses student difficulties as resources and strives to help students learn to apply mathematical concepts in linear algebra correctly to find the corrections to the energy spectrum of the hydrogen atom for the Zeeman effect.

Prior research suggests that students often have difficulty applying mathematical con-

cepts in the context of a concrete physical problem. In particular, students have difficulty connecting and applying mathematics correctly in physics contexts (e.g., see Refs. [47, 48, 49, 50, 51]). Mathematical sense-making in the context of solving physics problems can often be more difficult than when solving equivalent mathematics problems without the physics context [47, 48, 49, 50, 51]. Since working memory is constrained to a limited number of chunks and students' knowledge chunks pertaining to a concept are small when they are learning and developing expertise in physics, use of mathematics in physics can increase the cognitive load during problem solving, especially if students are not preficient in mathematics [52], and students may struggle to integrate mathematical and physical concepts. Thus, sense-making while focusing on solving a physics problem is often challenging and students sometimes make mathematical mistakes that they otherwise would not make if the physics context was absent [47, 48, 49, 50, 51].

One QM concept that involves mathematical sense-making in a physical situation is degenerate perturbation theory (DPT) in the context of the Zeeman effect for the hydrogen atom. We investigated student difficulties with finding the first-order corrections to the energies of the hydrogen atom for the Zeeman effect using DPT and used the research as a guide to develop learning tools to improve student understanding.

The hydrogen atom has played a significant role in the development of quantum mechanics (QM). Specifically, the discrete energy levels observed by spectroscopists for the hydrogen atom led Bohr to propose his model with quantized energy levels. Schrödinger proposed the wave model of particles involving the Schrödinger equation which explains features of the hydrogen atom well. The fine structure of the hydrogen atom is the combined effect of the relativistic correction and the spin-orbit interaction since the two components produce the same order of magnitude corrections to the energies compared to the unperturbed energies of the hydrogen atom. These fine structure corrections to the energies are smaller by a factor of $\alpha \approx 1/137$ squared, where $\alpha$ is the fine structure constant. The Zeeman effect represents the shift in the energy spectrum of the hydrogen atom due to the presence of a magnetic field. The shift in the energy spectrum due to the Zeeman effect is proportional to the strength of the magnetic field. The intermediate field Zeeman effect, which we will call the general case of the Zeeman effect (since it is more general than the strong or weak field Zeeman

effect), is the focus here. It is the case in which the corrections to the energy spectrum due to the fine structure and Zeeman terms are comparable. While the Bohr model accurately explained the observed unperturbed energy levels of the hydrogen atom, it cannot explain or describe the observed energy shifts due to fine structure and Zeeman terms. Only the quantum mechanical treatment using the Schrödinger equation explains that the observed shifts are due to the fine structure and Zeeman terms. Spectroscopists can also identify the energy spectrum of the hydrogen atom under different conditions, e.g., in an external magnetic or electric field. Generally speaking, the interactions of the hydrogen atom with the external magnetic or electric field create shifts and splitting in the energy spectrum.

Here, we focus on the approximate solutions to the Time-Independent Schrödinger Equation (TISE) for the intermediate field Zeeman effect using perturbation theory. While the solution for the TISE for the hydrogen atom with Coulomb potential energy can be solved exactly, the TISE for the hydrogen atom involving the Zeeman effect must include the fine structure correction term and cannot be solved exactly. The solution for the TISE for the hydrogen atom with Coulomb potential energy gives the unperturbed energies $E_n^0 = -\frac{13.6\text{eV}}{n^2}$, where $n$ is the principal quantum number. Since the fine-structure term and, in general, the Zeeman term are significantly smaller than the unperturbed term in the Hamiltonian, perturbation theory is an excellent method for computing the corrections to the energies and comparing the theoretical results with experiments. The high degree of symmetry of the potential energy of the unperturbed Hamiltonian for the hydrogen atom leads to degeneracy in the energy spectrum of the hydrogen atom and DPT must be used to find the perturbative corrections for the Zeeman effect.

## 5.2 BACKGROUND

Below, we discuss the basics of DPT with which many students struggled and the development and validation of the QuILT, which strives to help students learn about DPT in the context of the Zeeman effect. Via the QuILT, students are provided guidance and support to determine a *good* basis for finding the perturbative corrections to the energies for the

Zeeman effect, which includes corrections due to both the fine structure and Zeeman terms, and to calculate the perturbative corrections using that basis.

### 5.2.1 Basics for DPT

Perturbation theory is a useful approximation method for finding the energies and the energy eigenstates for a system for which the TISE is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$. The TISE for the unperturbed Hamiltonian, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, (where $\psi_n^0$ is the $n^{th}$ unperturbed energy eigenstate and $E_n^0$ is the $n^{th}$ unperturbed energy), is exactly solvable. The energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$ where $E_n^i$ for $i = 1, 2, 3..$ are the $i^{th}$ order corrections to the $n^{th}$ energy of the system. In PT, the first-order correction to the $n^{th}$ energy is

$$`E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle \tag{5.1}$$

and the first-order correction to the $n^{th}$ unperturbed energy eigenstate is

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle \tag{5.2}$$

in which $\{|\psi_n^0\rangle\}$ is a complete set of eigenstates of the unperturbed Hamiltonian $\hat{H}^0$. If the eigenvalue spectrum of $\hat{H}^0$ has degeneracy, the corrections to the energies and energy eigenstates are only valid provided one uses a *good* basis. For a given $\hat{H}^0$ and $\hat{H}'$, a *good* basis consists of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.

### 5.2.2 Background for DPT involving the Zeeman effect

For a hydrogen atom in an external magnetic field, one can use the DPT to find the corrections to the energy spectrum. Using standard notations, the unperturbed Hamiltonian $\hat{H}^0$ of a hydrogen atom is $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$, which accounts only for the interaction of the electron with the nucleus via Coulomb attraction. The solution for the TISE for the hydrogen atom with Coulomb potential energy gives the unperturbed energies $E_n^0 = -\frac{13.6\text{eV}}{n^2}$, where $n$ is the principal quantum number. The perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $\hat{H}'_Z$ is the Zeeman term and $\hat{H}'_{fs}$ is the fine structure term. The Zeeman term accounts for the potential energy of the magnetic moments due to the orbital and spin angular momenta in the external magnetic field. The Zeeman term is given by $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ in which $\vec{B}_{ext} = B_{ext}\hat{z}$ is a uniform, time independent external magnetic field along the $\hat{z}$-direction, $\mu_B$ is the Bohr magneton and $\hat{L}_z$ and $\hat{S}_z$ are the operators corresponding to the $z$-component of the orbital and spin angular momenta, respectively. The fine structure term includes a relativistic correction for the kinetic energy and the spin-orbit coupling, and is expressed as $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Here, $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term and $\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S}$ is the spin-orbit interaction term (all notations are standard).

We note that the unperturbed Hamiltonian is spherically symmetric since $[\hat{H}^0, \hat{\vec{L}}] = 0$. Therefore, for a fixed $n$, $\hat{H}^0$ for the hydrogen atom is diagonal when any complete set of orthogonal states is chosen for the angular part of the basis (consisting of the product states of orbital and spin angular momenta). Thus, so long as the radial part of the basis is always chosen to be a stationary state wavefunction $R_{nl}(r)$ for the unperturbed hydrogen atom (for a given principal quantum number $n$ and azimuthal quantum number $l$), which we will assume throughout, the choice of a *good* basis amounts to choosing the angular part of the basis appropriately, i.e., ensuring that the perturbation is diagonal in each degenerate subspace of $\hat{H}^0$. Therefore, we focus on the angular part of the basis (or angular basis) to find a *good* basis and the corrections to the energies for the perturbation $\hat{H}'$ corresponding to the intermediate field Zeeman effect in the hydrogen atom. For the angular basis for each $n$, states in the "coupled" representation $|n,\ l,\ j,\ m_j\rangle$ are labeled by the quantum numbers $l,\ s,\ j$, and $m_j$ (in additional to $n$) and the total angular momentum is defined as

$\vec{J} = \vec{L} + \vec{S}$ (all notations are standard and $s$ has been suppressed from the states $|n,\ l,\ j,\ m_j\rangle$ since $s = 1/2$ for the electron is a fixed value for a hydrogen atom). States in the coupled representation are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_Z$. On the other hand, for each $n$, states in the "uncoupled" representation $|n,\ l,\ m_l,\ m_s\rangle$ are labeled by the quantum numbers $l,\ m_l$, and $m_s$ (in addition to $n$), in which all notations are standard. States in the uncoupled representation are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{L}_Z$, and $\hat{S}_Z$.

An angular basis consisting of states in the coupled representation forms a *good* basis for the fine structure term $\hat{H}'_{fs}$ since with this choice of the angular basis, $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$. On the other hand, a basis consisting of states in the uncoupled representation forms a *good* angular basis for the Zeeman perturbation $\hat{H}'_Z$ (in this case, first order PT yields the exact result since $[\hat{H}^0, \hat{H}'_Z] = 0$). Therefore, for the intermediate field Zeeman effect, in which $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ and $\hat{H}'_{fs}$ and $\hat{H}'_Z$ are treated on equal footing ( we will use the notation $\hat{H}'_{fs} \approx \hat{H}'_Z$ to denote that the energy corrections corresponding to $\hat{H}'_{fs}$ are comparable to $\hat{H}'_Z$), neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* angular basis to find perturbative corrections for the hydrogen atom placed in an external magnetic field. The following procedure describes how to determine a *good* angular basis and find the first order corrections to the energy spectrum for the Zeeman effect: (1) choose an intial basis consisting of a complete set of eigenstates of $\hat{H}^0$ (e.g., one is free to choose an angular basis consisting of states in the coupled representation or a basis consisting of states in the uncoupled representation or any other basis), (2) write the $\hat{H}^0$ and $\hat{H}'$ matrices in the chosen basis, (3) identify $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$, (4) diagonalize the $\hat{H}'$ matrix in each degenerate subspace of $\hat{H}^0$ to determine a *good* basis, and (5) identify that the first-order corrections to the energy spectrum are the diagonal matrix elements of the $\hat{H}'$ matrix as given by Eq. 6.1 in the *good* basis.

## 5.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with the corrections to the energies of the hydrogen atom for the Zeeman effect using DPT were investigated using five years of data involving responses from 64 upper-level undergraduate students and 42 first-year graduate students to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts. The undergraduates were in an upper-level undergraduate QM course, and graduate students were in a graduate-level QM course. Additional insight was gained concerning these difficulties via responses of 13 students during a total of 45 hours of individual interviews using the "think aloud" protocol in which they were asked to answer the questions aloud that were posed without being disturbed [53]. Only at the end, they were asked to clarify any issues. Students were provided with all relevant information discussed in the introduction and background section and had lecture-based instruction in relevant concepts. Similar percentages of undergraduate and graduate students displayed difficulties with DPT.

We first analyzed responses of 32 undergraduates on questions related to DPT in the context of the Zeeman effect for hydrogen atom administered in two previous years. Then, we examined the difficulties that 32 undergraduate and 42 graduate students had with identifying a good basis for the Zeeman effect in the following three years as part of an in-class quiz after traditional lecture-based instruction. In all questions, students were told that the radial part of the basis is chosen to be the stationary state wavefunction $R_{nl}(r)$. The following question is representative of a series of questions that were posed after traditional lecture-based instruction on relevant concepts and after students had engaged with the QuILT (the operator $\hat{H}'$, in Q1, is a proxy for the operators $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs}$, $\hat{H}'_Z$, and $\hat{H}'_{fs}+\hat{H}'_Z$ that were listed individually in three separate questions on the pretest after traditional, lecture-based instruction and posttest after engaging with the QuILT):

**Q1.** *A perturbation $\hat{H}'$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For the Hamiltonian $\hat{H}$, circle* **ALL** *of the representations that can be chosen as the angular part of a "good" basis and explain your reasoning. Assume that for all cases, the principal quantum number is restricted to $n = 2$.*

*i. Coupled representation,*

*ii. Uncoupled representation,*

*iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same l (i.e., states with different l values are not mixed),*

*iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same l (i.e., states with different l values are not mixed),*

*v. Neither coupled nor uncoupled representation.*

We note that options iii and iv were given without the condition of the same $l$ in one year of the study and that there was no difference in student performance based upon whether the wording of the question included the same $l$ or not for $\hat{H}'_{SO}$ and $\hat{H}'_{fs}$.

In order to find the first-order corrections to the energies, one must first choose a *good* basis. Q1 focuses on the bases that form a *good* basis for the perturbation Hamiltonian for the intermediate field Zeeman effect with $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, as well as the operators $\hat{H}'_{fs}$ and $\hat{H}'_Z$ individually. Knowledge of the bases that form a *good* angular basis for the individual perturbation operators $\hat{H}'_{fs}$ and $\hat{H}'_Z$ can be helpful when determining a *good* basis for the intermediate field Zeeman effect with the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

The unperturbed Hamiltonian $\hat{H}^0$ is spherically symmetric with unperturbed energies only dependent on $n$ and therefore options i, ii, iii, and iv in Q1 all form a complete set of angular part of the eigenstates of $\hat{H}^0$. Therefore, one must consider which set of angular basis states in Q1 also diagonalizes the given $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Since the given degenerate subspace of $\hat{H}^0$ corresponds to $n = 2$, a *good* angular basis is one in which the perturbation matrix is also diagonal in that subspace.

In each degenerate subspace of $\hat{H}^0$, the fine structure term $\hat{H}'_{fs}$ is diagonal if the basis is chosen to consist of states in the coupled representation (option i in Q1) and the Zeeman term is diagonal if the basis is chosen to consist of states in the uncoupled representation (option ii in Q1), but not vice versa. Therefore, for the intermediate field Zeeman effect, in which the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis and option v in Q1 is the correct answer. In order to determine a *good* basis for the

intermediate field Zeeman effect, one may first choose an initial basis consisting of states in either the coupled or uncoupled representation and then diagonalize the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in the $n = 2$ degenerate subspace of $\hat{H}^0$. Thus, students must first express either the $\hat{H}'_{fs}$ or $\hat{H}'_Z$ matrix in an initial basis in which it is not diagonal in the degenerate subspace of $\hat{H}^0$. Then, they must be able to diagonalize the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in the degenerate $n = 2$ subspace of $\hat{H}^0$ and be able to find the corrections to the energy spectrum.

Below, we discuss some common difficulties with corrections to the energy spectrum of the hydrogen atom for the Zeeman effect found via research that interfere with students choosing a *good* basis and using DPT correctly in this context. We then discuss how the difficulties were used as a guide in the DPT QuILT to help students find the corrections to the energy spectrum due to the intermediate field Zeeman effect.

## 5.4 STUDENT DIFFICULTIES

Students had some difficulties with DPT in general (not restricted to the context of the Zeeman effect only). For example, when students were asked to determine a *good* basis for finding the corrections to the energies of the hydrogen atom, many students did not even realize that DPT should be used. Other students knew that they had to use DPT to find the corrections to the wavefunction, but they did not use DPT to find the first-order corrections to the energies. These students often incorrectly claimed that they did not need to use DPT since no terms in $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$) "blow up".

In the context of the intermediate field Zeeman effect, some students only focused on the Zeeman term $\hat{H}'_Z$ when asked to determine a *good* basis for finding the corrections to the energies of the hydrogen atom. In particular, they did not take into account the fine structure term $\hat{H}'_{fs}$ (omitted it altogether) and focused only on the Zeeman term as the perturbation. If the fine structure term $\hat{H}'_{fs}$ is neglected, then one can determine the exact energies for $\hat{H}^0 + \hat{H}'_Z$ and there is no need for perturbation theory since $[\hat{H}^0, \hat{H}'_Z] = 0$. However, the fine structure term should be considered when determining the corrections to the unperturbed

Table 14: The percentage of students who chose the listed angular representations as those that form a *good* angular basis for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ and the percentage of students who did not select any option in Q1 after traditional lecture-based instruction for undergraduates (number of students $N = 32$) and graduate students ($N = 42$).

| Option | Undergraduate Students(%) | Graduate Students(%) |
|---|---|---|
| i | 28 | 29 |
| ii | 22 | 17 |
| iii | 16 | 12 |
| iv | 13 | 12 |
| v | 44 | 33 |
| Blank | 16 | 17 |

energy spectrum.

As noted, to probe students' understanding of a *good* basis for the corrections to the energy spectrum due to the intermediate field Zeeman effect, students were asked question Q1. In the context of the intermediate field Zeeman effect, in which the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, students struggled to realize that neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis for the perturbative corrections to the hydrogen atom placed in an external magnetic field. The results are summarized in Table 14. Table 14 shows that only 44% of undergraduate students and 33% of graduate students correctly identified that option v in Q1 is the correct answer for the Zeeman effect. Additionally, 16% of undergraduate and 17% of graduate students did not provide any answer to the multiple-choice question Q1 after traditional lecture-based instruction in relevant concepts.

Below, we discuss student difficulties that hinder their ability to select the representation that forms a *good* angular basis in Q1 and find the corrections to the energy spectrum. In this

section, we focus on the qualitative results found primarily from student responses during the think aloud interviews.

### 5.4.1 Difficulty understanding why diagonalizing the entire $\hat{H}'$ matrix is problematic

Many students did not realize that when the initially chosen basis is not a *good* basis and the unperturbed Hamiltonian $\hat{H}^0$ and the perturbing Hamiltonian $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ do not commute, they must diagonalize the $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix *only* in the degenerate subspace of $\hat{H}^0$. When presented with a similar system and asked to determine the first order corrections to the energies, one interviewed student who attempted to diagonalize the entire $\hat{H}'$ matrix justified his reasoning by incorrectly stating, "We must find the simultaneous eigenstates of $\hat{H}^0$ and $\hat{H}'$." This student, and many others, did not realize that when $\hat{H}^0$ and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ do not commute, we cannot simultaneously diagonalize $\hat{H}^0$ and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ since they do not share a complete set of eigenstates. Students struggled with the fact that if $\hat{H}^0$ and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ do not commute, diagonalizing $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ produces a basis in which $\hat{H}^0$ is not diagonal. Also, since $\hat{H}^0$ is the dominant term and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ provides only small corrections, we must ensure that the basis states used to determine the perturbative corrections in Eqs. 6.1 and 6.2 remain eigenstates of $\hat{H}^0$.

### 5.4.2 Incorrectly claiming that BOTH a basis consisting of states in the coupled representation and a basis consisting of states in the uncoupled representation are *good* bases for the intermediate field Zeeman effect

Many students had difficulty identifying a *good* basis for perturbative corrections for the intermediate field Zeeman effect. For example, in Q1, many students correctly identified that the *good* angular basis for the fine structure term $\hat{H}'_{fs}$ is a basis consisting of states in the coupled representation (option i) and also correctly identified that the *good* angular basis for the Zeeman term $\hat{H}'_Z$ is a basis consisting of states in the uncoupled representation (option ii in Q1). However, after correctly identifying the *good* angular basis for the two perturbations individually, some students did not realize that neither the coupled nor the

uncoupled representation (option v in Q1) forms a *good* angular basis for the Zeeman effect in which the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$. One interviewed student incorrectly claimed that "the coupled are a *good* basis for $\hat{H}'_{fs}$ and uncoupled are a *good* basis for $\hat{H}'_Z$, so both coupled and uncoupled form a *good* basis for $\hat{H}'_{fs} + \hat{H}'_Z$." This student and others with this type of response incorrectly thought that since a basis consisting of states in the coupled representation (option i in Q1) forms a *good* basis for the fine structure term $\hat{H}'_{fs}$ and a basis consisting of states in the uncoupled representation (option ii in Q1) forms a *good* angular basis for the Zeeman term $\hat{H}'_Z$, a *good* basis for the perturbation consisting of the sum of these two perturbations is either a basis consisting of states in the coupled or uncoupled representation.

### 5.4.3 Incorrectly claiming that a *good* basis does not exist for the Zeeman effect

In Q1, some students who correctly identified that the *good* angular basis for the fine structure term $\hat{H}'_{fs}$ is a basis consisting of states in the coupled representation and also correctly identified that a *good* angular basis for the Zeeman term $\hat{H}'_Z$ is a basis consisting of states in the uncoupled representation correctly chose that neither the coupled nor the uncoupled representation forms a *good* basis for the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ (option v in Q1) but then used incorrect reasoning to do so. Two common examples are as follows:

Some students incorrectly argued that since neither an angular basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis, a *good* basis does not exist for this case. They struggled to realize that the coupled representation or the uncoupled representation were not the only two possibilities for the angular part of the basis. One interviewed student with this type of reasoning had difficulty understanding the meaning of options iii and iv in Q1, stating: "I don't know what a linear combination of coupled or uncoupled states is. I thought there were just coupled states or uncoupled states." This student and others with this type of reasoning did not realize that a good basis could be constructed from a linear combination of states in the coupled representation (or equivalently a linear combination of states in the uncoupled representation).

Some students had difficulty realizing that any linear combination of states from the same degenerate subspace of $\hat{H}^0$ are also eigenstates of $\hat{H}^0$. For example, one student who correctly identified that neither the coupled nor the uncoupled representation forms a *good* basis for the Zeeman effect argued that "no *good* basis exists since we cannot diagonalize a part of the $\hat{H}'$ matrix ($\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$) without affecting the $\hat{H}^0$ matrix." This student and others who provided similar incorrect reasoning claimed that by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, the $\hat{H}^0$ matrix would no longer be diagonal. However, due to the degeneracy, ANY linear combination of states from the same degenerate subspace of $\hat{H}^0$ are eigenstates of $\hat{H}^0$. Therefore, diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ determines the special linear combination that forms a *good* basis.

### 5.4.4 Incorrectly claiming that the choice of the initial basis affects corrections to the energy spectrum

Of the students who correctly identified that a *good* basis for the Zeeman effect will consist of a special linear combination of states in the coupled representation (or, equivalently, a special linear combination of states in the uncoupled representation), many did not realize that the first order corrections to the energy spectrum would be the same regardless of the initial choice of the basis. Since neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis, a *good* basis cannot easily be identified at the onset. In order to determine a *good* basis and the first order corrections to the energy spectrum due to the Zeeman effect, one can initially choose a basis consisting of states in the coupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$. However, one could also initially choose a basis consisting of states in the uncoupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$ to determine a *good* basis and the first order corrections to the energy spectrum due to the Zeeman effect. Regardless of the choice of the initial basis, after diagonalizing $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$, the first order corrections to the energy spectrum due to the Zeeman effect will be the same in any *good* basis. Many students thought that the first order corrections to the energies depended on

the initial choice of basis. Therefore, if one chooses a basis consisting of states in the coupled representation then the first order corrections in this case would be different than those obtained had a basis consisting of states in the uncoupled representation been chosen as the initial basis. However, it does not make sense experimentally that the observed perturbative corrections would depend upon the choice of basis. Lack of appropriate connection between physics and mathematics in the context of DPT for the Zeeman effect sheds light on the difficulty students have in mathematical sense-making in QM. It also sheds light on the physics epistemology pertaining to whether one should get the same perturbative corrections in experiments regardless of the choice of initial basis or whether the initial choice of basis should impact what is experimentally measured values of energies.

### 5.4.5 Making computational mistakes while attempting to diagonalize the entire 8-dimensional $\hat{H}'$ matrix instead of diagonalizing the two separate $2 \times 2$ submatrices of the block diagonal matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$

When asked to determine the first order corrections to the energies for the intermediate field Zeeman effect for the $n = 2$ degenerate subspace of $\hat{H}^0$, some students correctly identified that one can initially choose either a basis consisting of states in the coupled representation or a basis consisting of states in the uncoupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$ in each degenerate subspace of $\hat{H}^0$. For example, in a basis consisting of states in the coupled representation ($|n,\ l,\ j\ m_j\rangle$), the perturbation matrix $\hat{H}' = \hat{H}'_{Z} + \hat{H}'_{fs}$ corresponding to the $n = 2$ subspace is given below (in which $\gamma = \left(\frac{\alpha}{8}\right)^2$ 13.6 eV, $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c}$, $\beta = \mu_B B_{ext}$ and the basis states are chosen in the order $|2,\ 0,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|2,\ 0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|2,\ 1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|2,\ 1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|2,\ 1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|2,\ 1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|2,\ 1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, and $|2,\ 1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$):

$$\hat{H}' = \begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}.$$

However, when finding the corrections to the energy spectrum, some students attempted to diagonalize the entire $8 \times 8$ $\hat{H}'$ matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$. While this approach is correct, it is easier to diagonalize the $8 \times 8$ $\hat{H}'$ matrix by diagonalizing $\hat{H}'$ only in the block diagonal subspaces with smaller dimensions than the initial $8 \times 8$ $\hat{H}'$ matrix, i.e., the two separate $2 \times 2$ matrices $\begin{bmatrix} \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta \end{bmatrix}$ and $\begin{bmatrix} \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$. In general, an expert-like approach to diagonalizing the $\hat{H}'$ matrix involves diagonalizing $\hat{H}'$ in the block diagonal subspaces with smaller dimensions and mathematical mistakes are less likely using this approach. However, many students did not realize that in order to determine a *good* basis, one can diagonalize these block diagonal subspaces in order to diagonalize the entire $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$. In other words, they struggled with the fact that to diagonalize $\hat{H}'$ in the $n = 2$ degenerate subspace of $\hat{H}^0$, one can diagonalize the two separate $2 \times 2$ matrices instead of diagonalizng the entire $\hat{H}'$ matrix in the $n = 2$ subpsace and obtain the linear combination of the states in the coupled representation that forms a *good* basis for finding the perturbative corrections for the Zeeman effect.

## 5.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 5.5.1 Development and Validation of the QuILT

The difficulties described show that many students struggle in determining a *good* basis for finding the corrections to the energy spectrum for the Zeeman effect. Therefore, we developed a QuILT that takes into account these difficulties and strives to help students build a robust knowledge structure of these concepts. The development of the DPT QuILT started with an investigation of student difficulties via open-ended and multiple-choice questions administered after traditional instruction to advanced undergraduate and graduate students and conducting a cognitive task analysis from an expert perspective of the requisite knowledge [54]. The QuILT strives to help students build on their prior knowledge and addresses common difficulties found via research, some of which were discussed in the previous section.

The QuILT is inspired by Piaget's "optimal mismatch" framework as well as the preparation for future learning framework of Bransford and Schwartz. In Piaget's "optimal mismatch" framework, students are intentionally placed in a situation in which their current knowledge structures are inadequate and the students are required to reorganize existing structures or develop new structures to reconcile this conflict [55]. Bransford and Schwartz's preparation for future learning framework emphasizes that learning occurs when elements of innovation and efficiency are both present [56]. Innovation and efficiency describe two orthogonal components of instruction. Innovation describes aspects that are new to students, such as new concepts or new problem-solving skills. Efficiency is a measure of the structure and organization of the material, as well as how proficient the student is with the material. Instruction that incorporates only one of these elements leads to students becoming disengaged. If instruction is too innovative, students cannot connect the material with their prior knowledge and become frustrated. When the instruction is too efficient, students interact with repetitious material that does not provide intellectual stimulation and may become routine experts. However, they will not be able to transfer their learning to new situations.

In the QuILT, students are presented with innovative tasks. Whether it be examples,

hypothetical conversations, or calculations, the QuILT strives to help students develop a deeper understanding by actively working through the inquiry-based learning sequences. Student difficulties are incorporated in these examples and conversations to create a cognitive conflict in which the students are then guided through additional tasks designed to resolve these issues. Efficiency is addressed in the QuILT in several ways. First, the QuILT follows the sequence laid out in the cognitive task analysis. It is organized in a manner which attempts to build on the students' prior knowledge, and each section in the QuILT builds upon the previous section. Second, students are provided scaffolding designed to help address common difficulties, thus reducing the cognitive conflict. Third, the QuILT progressively reduces the scaffolding to help students solve problems without any assistance. Finally, as the students work through the different tasks, they develop more proficiency at identifying the concepts and answering the questions.

The development of the QuILT went through a cyclic, iterative process. The preliminary version was developed based upon the cognitive task analysis and knowledge of common student difficulties. Next, the QuILT underwent many iterations among the three researchers and then was iterated several times with three physics faculty members to ensure that they agreed with the content and wording. It was also administered to graduate and advanced undergraduate students in individual think-aloud interviews to ensure that the guided approach was effective, the questions were unambiguously interpreted, and to better understand the rationale for student responses. During these semi-structured interviews, students were asked to "think aloud" while answering the questions. Students first read the questions on their own and answered them without interruptions except that they were prompted to think aloud if they were quiet for a long time. After students had finished answering a particular question to the best of their ability, they were asked to further clarify and elaborate on issues that they had not clearly addressed earlier. The next step involved evaluating the impact of the QuILT on student learning and determining if the difficulties remained. Finally, modifications and improvements were made based upon the student and faculty feedback before it was administered to students in various QM courses.

### 5.5.2 Structure of the QuILT

The QuILT uses a guided inquiry-based approach to learning and actively engages students in the learning process. It includes a pretest to be administered in class after traditional instruction in DPT. Then, students engage with the tutorial in small groups in class (or alone when using it as a self-paced learning tool in homework), and finally a posttest is administered in class. As students work through the tutorial, they are asked to predict what should happen in a given situation. Then, the tutorial strives to provide scaffolding and feedback as needed to bridge the gap between their initial knowledge and the level of understanding that is desired. Students are also provided checkpoints to reflect upon what they have learned and make explicit connections between what they are learning and their prior knowledge. They are given an opportunity in the checkpoints to reconcile differences between their predictions and the guidance provided before proceeding further.

The DPT QuILT uses a blend of guided inquiry-based learning sequences involving both qualitative and quantitative reasoning to improve students' understanding. For example, the QuILT requires qualitative reasoning while students reason about hypothetical student conversations and quantitative reasoning to determine the matrix elements of the perturbations $\hat{H}'_{SO}$ and $\hat{H}'_{Z}$ in the coupled and uncoupled representations.

### 5.5.3 Addressing Student Difficulties via Guided Learning Sequences in the QuILT

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples involving DPT in which they consider the perturbations $\hat{H}'_{fs}$, $\hat{H}'_{Z}$, and $\hat{H}'_{fs} + \hat{H}'_{Z}$ as the perturbation on $\hat{H}^0$. In this manner, students focus on the concepts involved in determining a *good* basis for the fine structure and Zeeman corrections to the energy spectrum of the hydrogen atom separately before considering $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$. For the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$, students learn about (1) why DPT must be used (2) why care must be taken to choose a *good* basis for the Zeeman effect and (3) how to find perturbative corrections to the energy spectrum. Below, we discuss how the QuILT strives to address student difficulties and help them learn about the perturbative

corrections to the energy spectrum of the hydrogen atom due to the Zeeman effect using DPT.

Students first work through a warm-up for the tutorial that strives to help them identify the bases that consist of a complete set of eigenstates of operator $\hat{H}^0$ and the bases in which the operators $\hat{H}'_{fs}$ and $\hat{H}'_Z$ are diagonal in each degenerate subspace of $\hat{H}^0$. In addition, students also work through examples in which they must determine the matrix elements of the operators $\hat{H}'_{SO}$ or $\hat{H}'_Z$. For example, they calculate several diagonal and off-diagonal matrix elements of $\hat{H}'_{SO}$ and $\hat{H}'_Z$ in both a basis consisting of states in the coupled representation and a basis consisting of states in the uncoupled representation. Students were asked to focus on calculating the matrix elements of the operator $\hat{H}'_{SO}$ in order to help them determine whether a basis consisting of states in the coupled or uncoupled representation forms a *good* basis for the fine structure perturbation $\hat{H}'_{fs}$. Since the fine structure term is $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$, one must consider both $\hat{H}'_r$ and $\hat{H}'_{SO}$ when determining a *good* basis. However, the relativistic term $\hat{H}'_r$ is spherically symmetric with energy depending on $n$ and $l$ and so $\hat{H}'_r$ is diagonal in each degenerate subspace of $\hat{H}^0$ for a basis consisting of states in the coupled or uncoupled representation for each fixed $n$ and $l$. Students were asked to focus on the angular part of the basis that makes $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$. The warmup strives to help students learn the prerequisites for finding a *good* basis for the hydrogen atom for the Zeeman effect in the context of DPT.

**Helping students identify a *good* basis for the fine structure term $\hat{H}'_{fs}$, the Zeeman term $\hat{H}'_Z$, and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$:** The QuILT strives to help students learn that neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis for the intermediate field Zeeman effect. As part of a guided inquiry-based sequence, students are asked to evaluate the validity of the following two statements in a hypothetical student conversation in the QuILT designed to scaffold students' learning:

**Student 1:** *Since the coupled representation is a good basis for the fine structure term and the uncoupled representation is a good basis for the Zeeman term, both the coupled and uncoupled representation form good bases and are equally appropriate to find the first order*

*corrections to the energies for* $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

**Student 2:** *I disagree with Student 1. You cannot consider different bases for different parts of* $\hat{H}'$. *If we choose the coupled representation,* $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ *is not diagonal in each degenerate subspace of* $\hat{H}^0$ *since* $\hat{H}'_Z$ *is not diagonal in the coupled representation. Similarly, if we choose the uncoupled representation,* $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, *is not diagonal in each degenerate subspace of* $\hat{H}^0$ *since* $\hat{H}'_{fs}$ *is not diagonal in the uncoupled representation. Neither of these representations form a good basis.*

*Explain why you agree or disagree with Student 1 or Student 2.*

Following this conversation, further scaffolding is provided through inquiry-based learning sequences which strive to help students reconcile that Student 2 is correct.

Students are also given scaffolding support to help them determine a *good* basis and first-order corrections to the energy spectrum of the hydrogen atom for the Zeeman effect. The guided inquiry-based sequences in the QuILT strive to help students learn that neither a basis consisting of states in the coupled or uncoupled representation form a *good* basis. After diagonalizing $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in the $n = 2$ degenerate subspace of $\hat{H}^0$, a *good* basis is obtained which consists of a linear combination of states in the coupled (or, equivalently, the uncoupled) representation. Students are provided checkpoints that allow them to reconcile any differences between their initial reasoning and the correct reasoning.

**Helping students realize that the initial choice of basis cannot affect the corrections to the energy spectrum:** The QuILT strives to help students learn that one is free to choose either an initial basis consisting of states in the coupled representation or a basis consisting of states in the uncoupled representation and then diagonalize the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$ in order to determine a *good* basis (and the first order corrections to the energies due to the Zeeman effect). The following statements from a hypothetical student conversation from a guided inquiry-based sequence in the QuILT strive to help students learn that the initial choice of basis cannot change the first order corrections to the energy spectrum due to the Zeeman effect once a *good* basis has been found.

**Student 1:** *Since the diagonal matrix elements of* $\hat{H}'$ *will depend on the choice of initial basis, a different choice of the initial basis in which we diagonalize* $\hat{H}'$ *in the degenerate*

*subspace of $\hat{H}^0$ will change the first order corrections to the energies.*

**Student 2:** *I disagree with Student 1. After diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$, a good basis is obtained and the first order correction to the energy will be the same regardless of which basis, e.g., the coupled or uncoupled representation, you had initially chosen. In a good basis, you will end up with the same diagonal matrix elements of $\hat{H}'$ which are the first order corrections to the energies.*

*Explain why you agree or disagree with each student.*

Students are provided additional scaffolding support to help them reconcile that Student 2 is correct in the preceding conversation. In a *good* basis, the diagonal matrix elements of the perturbation $\hat{H}'$ are the first order corrections to the energies regardless of the choice of the initial basis.

**Helping students reflect upon the fact that diagonalizing the two separate $2 \times 2$ submatrices of the block diagonal matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ diagonalizes $\hat{H}'$ in the $n = 2$ subspace:** In the QuILT, when basis states are chosen to be states in the coupled representation in an appropriate order, the $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix is block diagonal. Students are provided scaffolding support to help them realize that one is free to choose the initial angular basis states in any order to construct the matrices without affecting the first order corrections to the energy spectrum and that choosing basis states in a certain order may make determining the first order corrections to the energy spectrum easier to calculate. In particular, the QuILT strives to help students learn that in order to determine a *good* basis for the Zeeman effect in the $n = 2$ subspace, one can diagonalize the block diagonal matrix $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ by diagonalizing the two separate $2 \times 2$ submatrices of the block diagonal $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix rather than diagonalizing the entire $8 \times 8$ $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix if the basis states are chosen in the order given earlier. The following student conversation regarding diagonalizing the $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$ for the Zeeman effect is part of a guided inquiry-based sequence in which students must reason about and explain whether each hypothetical student's statement is correct:

**Student 1:** *In the case of $n = 2$, $\hat{H}^0$ possesses an eight-fold degeneracy, which means that in order to find a good basis for the correction to the $n = 2$ energy spectrum, we must diagonalize the entire 8 x 8 $\hat{H}'$ matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$.*

**Student 2:** *We must make an effort to diagonalize $\hat{H}'$ only in those block diagonal subspaces with smaller dimensions in order to diagonalize the entire $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ to obtain the good basis set. When I calculate the $\hat{H}'$ matrix for $n = 2$ in the coupled representation and the angular basis states are chosen in the order $|\psi_1\rangle = |2,\ 0,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |2,\ 0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |2,\ 1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_4\rangle = |2,\ 1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |2,\ 1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |2,\ 1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_7\rangle = |2,\ 1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, and $|\psi_8\rangle = |2,\ 1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, I get the block diagonal matrix $\hat{H}'$ below*

$$\hat{H}' = \begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$$

*We will only need to diagonalize the $2 \times 2$ matrices* $\begin{bmatrix} \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta \end{bmatrix}$ *and* $\begin{bmatrix} \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$ *to obtain the good basis.*

*Explain why you agree or disagree with each student.*

The QuILT strives to help students learn that Student 1's approach is valid, but Student 2 uses a more efficient approach that is less prone to errors in obtaining a *good* basis. Students are asked to summarize in words how to determine a *good* basis and the first-order corrections to the energy spectrum of the hydrogen atom for the Zeeman effect. Students are then asked to calculate a *good* basis and the first-order corrections to the energy spectrum for the $n = 2$ subspace. They are provided checkpoints that allow them to reconcile any differences between their initial reasoning and the correct reasoning provided in the checkpoints.

## 5.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts in DPT but before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

The pre/posttest results for Q1 are summarized in Table 15 and suggest that the QuILT was helpful in reducing student difficulties with these concepts. In particular, 83% of the graduate students and 97% of the undergraduate students correctly identified that a *good* basis for the intermediate field Zeeman effect is option v in Q1. All of these students chose option v in Q1 as the only correct answer. In addition, many students correctly explained their reasoning for why they chose option v in Q1. For example, the following was a written response in the posttest, "Neither (coupled representation or uncoupled representation) work. We must diagonalize $\hat{H}'$ in the degenerate subspace to find a (basis consisting of a) linear combination of states (in the coupled/uncoupled representation)." After engaging with the QuILT, the majority of the students correctly chose that neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation form a *good* basis and displayed correct reasoning for their answer on the posttest.

As can be seen in Table 18, the graduate students and undergraduate students generally performed at about the same level on Q1 on the pretest. However, the undergraduates outperformed the graduate students on the posttest in identifying the options in Q1 that form a *good* basis. One possible explanation for the undergraduates outperforming the graduate students on the posttest could be the grade incentive associated with the QuILT. The QuILT accounted for a larger percent of the undergraduates' overall course grade and

Table 15: The percentage of students who chose the listed options as representations to form a *good* basis for the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$ and the unperturbed Hamiltonian $\hat{H}^0$ and the percentage of students who did not select any option in Q1 on the pretest and posttest for graduate students ($N = 42$) and undergraduate students ($N = 32$).

| | Graduate Students | | Undergraduate Students | |
|---|---|---|---|---|
| Option | Pretest (%) | Posttest (%) | Pretest (%) | Posttest (%) |
| i | 29 | 17 | 28 | 3 |
| ii | 17 | 17 | 22 | 0 |
| iii | 12 | 10 | 16 | 3 |
| iv | 12 | 10 | 13 | 0 |
| v | 33 | 83 | 44 | 97 |
| Blank | 17 | 0 | 16 | 0 |

the components of the QuILT were accounted for differently for the course grade for the two groups of students. In particular, the posttest for the undergraduate students was graded for correctness in both years while the posttest for the graduate students was graded for completeness in Year 1 and for correctness in Year 2. Additionally, the undergraduate students knew that the material from the QuILT could appear on their examinations while the graduate students were told by the graduate instructor that this material was a review of the undergraduate quantum mechanics and that no material from the QuILT would appear on their examinations. But rather, more complex problems on the DPT would appear on the exams. The fact that the graduate students were given very small grade incentive to learn the material in the QuILT may have decreased their motivation to engage as deeply with the QuILT as the undergraduates and may explain why the graduate students did not perform as well as the undergraduate students on the posttest.

## 5.7 SUMMARY

Both upper-level undergraduate and graduate students struggled with finding perturbative corrections to the hydrogen atom energy spectrum for the intermediate field Zeeman effect using DPT. Interviewed students' responses suggested that some of them held epistemological beliefs inconsistent with the framework of QM and struggled with mathematical sense-making in the context of QM in which the paradigm is novel [15]. After traditional instruction, some students claimed that different initial choice of the basis before a good basis has been found will yield different corrections to the energy spectrum of the hydrogen atom for the Zeeman effect. These students had difficulty in connecting experimental observations with quantum theory and in correctly reasoning that since the corrections to the energy spectrum can be measured experimentally, different choices of the initial basis cannot yield different physically observable corrections to the energy spectrum. Since students are still developing expertise in QM and the DPT requires appropriate integration of mathematical and physical concepts, cognitive overload can be high while reasoning about these problems [52]. Advanced students found it challenging to do metacognition [52] in this context of QM and provided responses that were not consistent with each other.

Using the common difficulties of advanced students with the corrections to the energy spectrum of the hydrogen atom for the intermediate field Zeeman effect, we developed and evaluated a research-based QuILT which focuses on helping students reason about and find a *good* basis for the Zeeman effect. Since the DPT requires students to apply advanced mathematical concepts in the context of a concrete physical problem, students often struggled to connect and apply mathematics correctly in the physics context. For example, in order to be able to determine a *good* basis and corrections to the energies for the Zeeman effect, one must have a strong background in linear algebra and be able to apply it in the context of solving quantum physics problem involving DPT for the intermediate field Zeeman effect. Since students' working memory while solving these problems involving the Zeeman effect is constrained to a limited number of "chunks", cognitive load may become high and it may become challenging for many students to be able to do sufficient metacognition without appropriate guidance and scaffolding support.

The QuILT strives to provide appropriate scaffolding and feedback using a guided inquiry-based approach to help students develop a functional understanding of relevant concepts. The evaluation shows that the QuILT is effective in improving students' understanding of the perturbative corrections to the energy spectrum of the hydrogen atom for the Zeeman effect. In particular, both on the written posttest and during interviews, student responses afforded opportunity to probe their reasoning. We find that the QuILT helped students reason about DPT more consistently and be able to reason about why neither a basis consisting of states in the coupled nor the uncoupled representation forms a *good* basis for the Zeeman effect.

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# 6.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DEGENERATE PERTURBATION THEORY: LIMITING CASES OF THE STRONG AND WEAK FIELD ZEEMAN EFFECT

## 6.1 INTRODUCTION

A major goal of physics courses, especially those for the physics majors, is to help students learn to think like a physicist [1]. In many physics courses, in addition to helping students learn physics content, there is emphasis on helping them develop problem-solving, reasoning, and metacognitive skills [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. In physics, problem-solving, reasoning, and metacognitive skills can involve, for example, planning a solution to a problem, monitoring one's problem solving, considering limiting cases appropriately and evaluating the final answer. In particular, physicists often utilize limiting cases when appropriate to simplify the problem-solving process and to check whether the results in those limits make sense. Students often learn about limiting cases throughout the physics curriculum, from introductory physics to advanced undergraduate and graduate level courses. We have been developing several Quantum Interactive Learning Tutorials (QuILTs) that strive to help students develop problem-solving, reasoning, and metacognitive skills including learning to use limiting cases and understanding their utility and applicability [27].

Here we discuss student understanding of limiting cases in the context of degenerate perturbation theory for finding the corrections to the energy spectrum of the hydrogen atom for the Zeeman effect and the development and validation of a research-based QuILT to improve student understanding. The origin of the Zeeman term in the hydrogen atom involves the

potential energy of the magnetic moments due to the orbital and spin angular momentum in an external magnetic field. The Zeeman effect is the shift in the energy spectrum of the hydrogen atom due to the presence of an external magnetic field, and it is proportional to the strength of the external magnetic field. In addition, the fine structure term in the hydrogen atom includes corrections due to the spin-orbit coupling and a relativistic correction for the kinetic energy. We focus on two limiting cases: the strong and weak field Zeeman effects. The strong field Zeeman effect occurs when the corrections to the energies due to the Zeeman term are much greater than the corrections to the energies due to the fine structure term. The weak field Zeeman effect occurs when the corrections to the energies due to the fine structure term are much greater than the corrections to the energies due to the Zeeman term.

The Time-Independent Schrödinger Equation (TISE) for the Hamiltonian with the fine structure and Zeeman corrections cannot be solved exactly. Nevertheless, since the fine-structure term and, in general, the Zeeman term are significantly smaller than the unperturbed Hamiltonian, perturbation theory (PT) is an excellent method for determining the approximate solutions to the TISE and the corrections to the energy spectrum of the hydrogen atom. Due to the degeneracy in the hydrogen atom energy spectrum, degenerate perturbation theory (DPT) must be used to find the corrections for the strong and weak field Zeeman effect.

It is important to help students develop a functional understanding of DPT in order to find the corrections to the energies for the strong and weak field Zeeman effects. However, quantum mechanics (QM) is challenging for upper-level undergraduate and Ph. D. level students (e.g., see Refs. [28, 29, 30, 33, 31, 32, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]). Since advanced students often struggle with the DPT for the limiting cases of the strong and weak field Zeeman effect, we investigated student difficulties with finding the first-order corrections to the energies of the hydrogen atom for the strong and weak field Zeeman effects using DPT.

There have been a number of prior research studies aimed at investigating student reasoning in QM [49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59] and using the findings as resources for improving student understanding [60, 61, 62, 63, 64, 65, 66, 67]. However, there have

been relaitively few studies investigating student understanding of DPT [68]. We have been developing a set of research-based learning tools that are inspired by research studies conducted to identify student difficulties with QM and findings of cognitive research. One such research-based tool is the Quantum Interactive Learning Tutorial (QuILT) which strives to help students develop a solid grasp of QM [69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79]. In this paper we describe the development and validation of the research-based QuILT focusing on DPT that uses student difficulties as resources. The QuILT strives to help students learn to find the corrections to the energy spectrum of the hydrogen atom for the limiting cases of the strong and weak field Zeeman effect.

## 6.2 BACKGROUND

We first discuss the requisite knowledge students must have to use DPT in general and in the limiting contexts of the strong and weak field Zeeman effects in particular.

### 6.2.1 Basics for DPT

PT is a useful approximation method for finding the energies and the energy eigenstates for a system for which the TISE is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$. The TISE for the unperturbed Hamiltonian, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, (where $\psi_n^0$ is the $n^{th}$ unperturbed energy eigenstate and $E_n^0$ is the $n^{th}$ unperturbed energy), is exactly solvable. The energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$ where $E_n^i$ for $i = 1, 2, 3..$ are the $i^{th}$ order corrections to the $n^{\text{th}}$ energy of the system.

In non-degenerate PT, the first-order correction to the $n^{th}$ energy is

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle \tag{6.1}$$

and the first-order correction to the $n^{th}$ unperturbed energy eigenstate is

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle, \tag{6.2}$$

in which $\{|\psi_n^0\rangle\}$ is a complete set of eigenstates of the unperturbed Hamiltonian $\hat{H}^0$. When the eigenvalue spectrum of $\hat{H}^0$ has degeneracy (i.e., two or more eigenstates of $\hat{H}^0$ have the same energy so that two or more diagonal elements of $\hat{H}^0$ are equal), Eqs. 6.1 and 6.2 from nondegenerate perturbation theory are still valid provided one uses a *good* basis. For a given $\hat{H}^0$ and $\hat{H}'$, we define a *good* basis as consisting of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. In a *good* basis, $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$. Therefore, the terms $\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle$ in Eq. 6.2 for the wavefunction are zero when $m \neq n$ so that the expression for the corrections to the wavefunction in Eq. 6.2 does not have terms that diverge. In a *good* basis, Eq. 6.1 is also valid for finding the first order corrections to the energies (which are the diagonal elements of the $\hat{H}'$ matrix as given by Eq. 6.1).

### 6.2.2 Background for DPT involving the limiting cases of the Zeeman effect

For a hydrogen atom in an external magnetic field, one can use DPT to find the corrections to the energy spectrum. Using standard notations, the unperturbed Hamiltonian $\hat{H}^0$ of a hydrogen atom is $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$, where $m$ is the reduced mass and $r$ is the radial distance between the proton and electron which accounts only for the interaction of the electron with the nucleus via Coulomb attraction (other symbols also have their usual meaning). The solution for the TISE for the hydrogen atom with Coulomb potential energy gives the unperturbed energies $E_n^0 = -\frac{13.6\text{eV}}{n^2}$, where $n$ is the principal quantum number. The perturbation is $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$, in which $\hat{H}'_Z$ is the Zeeman term and $\hat{H}'_{fs}$ is the fine structure term. The Zeeman term accounts for the potential energy of the magnetic moments due to the orbital and spin angular momenta in the external magnetic field. The Zeeman term is given by $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ in which $\vec{B}_{ext} = B_{ext}\hat{z}$ is a uniform, time independent external magnetic field along the $\hat{z}$-direction, $\mu_B$ is the Bohr magneton and $\hat{L}_z$ and $\hat{S}_z$ are the operators corresponding to the z component of the orbital and spin angular momenta,

respectively. The fine structure term includes the spin-orbit coupling and a relativistic correction for the kinetic energy and is expressed as $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Here, $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term and $\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}(\vec{L}\cdot\vec{S})$ is the spin-orbit interaction term (all notations are standard).

We note that $\hat{H}^0$ for the hydrogen atom is diagonal when ANY complete set of orthogonal states with the same $n$ is chosen for the angular part of the basis (consisting of the product states of orbital and spin angular momenta). Thus, so long as the radial part of the basis is always chosen to be stationary state wavefunctions $R_{nl}$ for the hydrogen atom (for a given principle quantum number $n$ and azimuthal quantum number $l$), the choice of a *good* basis amounts to choosing the angular part of the basis (the part of the basis that involves the product states of the orbital and spin angular momenta) appropriately. Therefore, we focus on the angular part of the basis for the $n = 2$ degenerate subspace of $\hat{H}^0$ to find a *good* basis and the corrections to the energies for the perturbation $\hat{H}'$ corresponding to the limiting cases of the Zeeman corrections to the hydrogen atom. The total angular momentum is defined as $\vec{J} = \vec{L} + \vec{S}$. For the angular part of the basis, states in the coupled representation $|l, j,\ m_j\rangle$ are labeled by the quantum numbers $l,\ s,\ j$, and $m_j$ where $l$ is the azimuthal quantum number, $s$ is the spin quantum number, $j$ is the total angular momentum number, and $m_j$ is the $z$ component of the total angular momentum quantum number (all notations are standard and $s = 1/2$ has been suppressed from the states $|l, j,\ m_j\rangle$ since $s = 1/2$ is a fixed value for a neutral hydrogen atom). On the other hand, states in the uncoupled representation $|l,\ m_l,\ m_s\rangle$ are labeled by the quantum numbers $l,\ m_l$, and $m_s$ (the quantum numbers $m_l$ and $m_s$ correspond to the $z$ component of the orbital and spin angular momenta, respectively).

In the limiting cases of the strong and weak field Zeeman effect, the perturbation $\hat{H}'$ can be separated into two terms $\hat{H}' = \hat{H}'_{strong} + \hat{H}'_{weak}$, in which $\hat{H}'_{strong}$ is the stronger perturbation and $\hat{H}'_{weak}$ is the weaker perturbation. The corrections to the energies due to the stronger perturbation $\hat{H}'_{strong}$ are larger than the corrections due to the weaker perturbation $\hat{H}'_{weak}$. In these limiting cases, in order to find the corrections to the energies, one useful approach is to use DPT via a two-step approximation. In the first step, the stronger perturbation $\hat{H}'_{strong}$ is treated as the only perturbation. A *good* basis for step 1 is one that diagonalizes

the unperturbed Hamiltonian $\hat{H}^0$ and also diagonalizes the stronger perturbation $\hat{H}'_{strong}$ in each degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$. After a *good* basis has been identified for step 1, the first order corrections for the stronger perturbation $\hat{H}'_{strong}$ are determined. In the second step of the two-step approximation, $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ is the new unperturbed Hamiltonian and the weaker perturbation $\hat{H}'_{weak}$ is treated as the perturbation. For step 2, a good basis is one that diagonalizes the unperturbed Hamiltonian $\hat{H}^0_{strong}$ and also diagonalizes $\hat{H}'_{weak}$ in each degenerate subspace of $\hat{H}^0_{strong}$. Once a *good* basis for step 2 has been identified, the first order corrections to the energies due to the weaker perturbation can be determined. The total first-order corrections to the energies are the sum of the corrections from steps 1 and 2.

As an example of one limiting case, the following steps describe how to determine a good basis and the first order corrections to the energies for the strong field Zeeman effect. (1) Treat the stronger perturbation $\hat{H}'_Z$ as the only perturbation on the unperturbed Hamiltonian $\hat{H}^0$. Identify that a basis consisting of states in the uncoupled representation forms a *good* basis for the unperturbed Hamiltonian $\hat{H}^0$ and the stronger perturbation $\hat{H}'_Z$ (since both $\hat{H}^0$ and $\hat{H}'_Z$ are diagonal in uncoupled representation, $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the uncoupled representation). Determine the first-order corrections to the energies due to the stronger perturbation $\hat{H}'_Z$. After step 1, the first-order corrections to the energies break some of the degeneracy that is present from only considering $\hat{H}^0$. (2) Treat the weaker perturbation $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$. Identify that a basis consisting of states in the uncoupled representation forms a *good* basis for the unperturbed Hamiltonian $\hat{H}^0_Z$ and the weaker perturbation $\hat{H}'_{fs}$ (since $\hat{H}^0_Z$ is diagonal in the uncoupled representation and $\hat{H}'_{fs}$ is diagonal in the degenerate subspaces of $\hat{H}^0_Z$ in the uncoupled representation). Determine the first-order corrections to the energies due to the weaker perturbation $\hat{H}'_{fs}$. (3) The sum of the first-order corrections obtained in steps 1 and 2 is the first-order corrections to the energy spectrum of the hydrogen atom.

In step 1, when the stronger perturbation $\hat{H}'_Z$ is treated as the only perturbation on the unperturbed Hamiltonian $\hat{H}^0$, basis states in the uncoupled representation ($|l,\ m_l,\ m_s\rangle$) diagonalize both $\hat{H}^0$ and $\hat{H}'_Z$. For the $n = 2$ subspace, if $l = 1$ then $m_l = -1, 0, 1$ or if $l = 0$ then $m_l = 0$ and for $s = \frac{1}{2}$, we have $m_s = -\frac{1}{2}$ or $\frac{1}{2}$. By taking all the combinations of $l$, $m_l$,

$s$, and $m_s$ one finds that the $n = 2$ subspace is eight-dimensional with basis states in the uncoupled representation ($|l,\ m_l,\ m_s\rangle$) given by $|0,\ 0,\ \frac{1}{2}\rangle$, $|0,\ 0,\ -\frac{1}{2}\rangle$, $|1,\ 1,\ \frac{1}{2}\rangle$, $|1,\ 1,\ -\frac{1}{2}\rangle$, $|1,\ 0,\ \frac{1}{2}\rangle$, $|1,\ 0,\ -\frac{1}{2}\rangle$, $|1,\ -1,\ \frac{1}{2}\rangle$, and $|1,\ -1,\ -\frac{1}{2}\rangle$. The matrices for the operators $\hat{H}^0$ and $\hat{H}'_Z$ are given below which correspond to the $n = 2$ subspace in which the basis states are chosen in the uncoupled representation in the order $|0,\ 0,\ \frac{1}{2}\rangle$, $|1,0,\ \frac{1}{2}\rangle$, $|0,0,\ -\frac{1}{2}\rangle$, $|1,\ 0,\ -\frac{1}{2}\rangle$, $|1,\ 1,\ -\frac{1}{2}\rangle$, $|1,\ -1,\ \frac{1}{2}\rangle$, $|1,\ 1,\ \frac{1}{2}\rangle$, and $|1,\ -1,\ -\frac{1}{2}\rangle$ :

$$\hat{H}^0 = -\frac{13.6\text{eV}}{4}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{6.3}$$

$$\hat{H}'_Z = \mu_B B_{ext}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \end{bmatrix}. \tag{6.4}$$

Since $\hat{H}'_Z$ is diagonal in the uncoupled representation, it is diagonal in each degenerate subspace of $\hat{H}^0$ and basis states chosen in the uncoupled representation form a *good* basis for step 1. In fact, since the basis consisting of states in the uncoupled representation simultaneously diagonalizes $\hat{H}^0$ and $\hat{H}'_Z$, the energies including the first-order corrections to the energies obtained after step 1 are the exact result for the energies. In step 2, the new unperturbed Hamiltonian is $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ and the weaker perturbation is $\hat{H}'_{fs}$. Basis states chosen in the uncoupled representation also form a *good* basis for step 2 for the strong field

Zeeman effect because $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ has lower degeneracy than $\hat{H}^0$ and $\hat{H}'_{weak} = \hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}_Z^0$. Below are the matrices for the $n = 2$ subspace in which basis states are chosen in the same order as the earlier matrix above ($\beta = \mu_B B_{ext}$ and $\alpha$ is the fine structure constant):

$$\hat{H}_Z^0 = \begin{bmatrix} \boxed{E_2 + \mu_B B_{ext}} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\ \boxed{0} & \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{E_2 - \mu_B B_{ext}} & \boxed{0} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{0} & \boxed{E_2 - \mu_B B_{ext}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{E_2} & \boxed{0} & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{0} & \boxed{E_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 + 2\mu_B B_{ext} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - 2\mu_B B_{ext} \end{bmatrix}$$

$$\hat{H}'_{fs} = \frac{(-13.6\text{eV})\alpha^2}{192} \begin{bmatrix} \boxed{15} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\ \boxed{0} & \boxed{7} & 0 & 0 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \boxed{15} & \boxed{0} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{0} & \boxed{7} & 0 & 4\sqrt{2} & 0 & 0 \\ 0 & 4\sqrt{2} & 0 & 0 & \boxed{11} & \boxed{0} & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & \boxed{0} & \boxed{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}$$

All of the unperturbed energy eigenvalues in the $n = 2$ subpsace have energy $E_2 = \frac{-13.6\text{eV}}{4}$, as given by the diagonal matrix elements in Eq. B.2. States in the uncoupled repesentation are eigenstates of $\hat{H}'_Z$ with energy $\mu_B B_{ext}(m_l + 2m_s)$. For example, the state with $l = 1$, $m_l = -1$, and $m_s = \frac{1}{2}$ has energy $\mu_B B_{ext}(-1 + 2(\frac{1}{2})) = 0$ (see Eq. 4). Thus, in step 1, the corrections to the unperturbed energies due to the Zeeman term in the strong field Zeeman limit are the diagonal matrix elements of $\hat{H}'_Z$ in Eq. C.16 in this case, it is the exact result since $\hat{H}^0$ and $\hat{H}'_Z$ commute and both are diagonal in the uncoupled representation). Moreover, even though the weaker perturbation $\hat{H}'_{fs}$ is not diagonal if basis states are chosen in the uncoupled representation, $\hat{H}'_{fs}$ *is* diagonal in each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ as noted by the boxed matrix elements for $n = 2$ (see Eq. 6). Therefore, a basis consisting of states in the uncoupled representation is a *good* basis for both step 1 and

step 2 for the strong field Zeeman effect. In step 2, the diagonal matrix elements of $\hat{H}'_{fs}$ in the uncoupled representation, which are the fine-structure corrections in the strong field Zeeman limit, are given by $\frac{(13.6\text{ eV})\alpha^2}{n^3}\left\{\frac{3}{4n}-1\right\}$ for $l=0$ and $\frac{(13.6\text{ eV})\alpha^2}{n^3}\left\{\frac{3}{4n}-\left[\frac{l(l+1)-m_l m_s}{l(l+1/2)(l+1)}\right]\right\}$ for $l=1$[80].

On the other hand, for the weak field Zeeman effect, the dominant fine structure term is the only perturbation on $\hat{H}^0$ in step 1 and the weaker perturbation $\hat{H}'_Z$ is the perturbation on the Hamiltonian $\hat{H}^0_{fs}=\hat{H}^0+\hat{H}'_{fs}$ in step 2. In the weak field Zeeman effect, the coupled representation forms a good basis for both steps 1 and 2.

## 6.3 METHODOLOGY

Student difficulties with the corrections to the energies of the hydrogen atom for the strong and weak field Zeeman effects using DPT were investigated using five years of data involving responses from 64 upper-level undergraduate students and 42 first-year Ph. D. level students to open-ended and multiple-choice questions administered after traditional, lecture-based instruction in relevant concepts. The undergraduates were enrolled in an upper-level, undergraduate QM course. Most Ph. D. students enrolled in the Ph.D. level course had already learned this material in an undergraduate quantum mechanics course but this was the first exposure beyond the undergraduate level. The Ph.D. level course was a required core course for the enrolled Ph.D. student who were in their first year of physics Ph.D. program (the completion of six core courses including two courses in quantum mechanics is mandatory for Ph.D. students to obtain a masters' degree while pursuing Ph.D. and advance to candidacy for the Ph.D. research-note that most research universities in the US do not admit students only for a masters in physics so students enroll in Ph.D. program and take Ph.D. core courses such as the quantum mechanics course discussed here in their first year after finishing their undergraduate degree). Traditional instruction was used in both the undergraduate and Ph.D. level courses and consisted of lecture style instruction along with traditional textbook homework problems. The textbook used in the undergraduate course was authored by Townsend [81], and the textbook used in the Ph.D. course was authored

by Sakurai [82]. For the majority of the classes, students listened to lectures and took notes (except in the undergraduate course when students engaged with the QuILT). The instructor for the undergraduate course was the same in both years, and the instructor for the Ph.D. level course was the same in both years. Additional insight about the difficulties was gained from 13 individual think-aloud interviews (a total of 45 hours). Interviewed students were provided with all relevant information discussed in the introduction and background sections and had traditional, lecture-based instruction in relevant concepts. Similar percentages of undergraduate and Ph.D. level students displayed difficulties with DPT.

After analyzing responses of 32 undergraduates on similar questions administered in two previous years, we posed the following question to 20 undergraduate and 42 Ph.D. level students in the following two years as part of an in-class quiz after traditional lecture-based instruction to examine student difficulties. Question Q1 was posed to identify whether students were able to determine a *good* basis for the limiting case of the strong field Zeeman effect (in which the limiting cases of the strong field and weak field Zeeman effects were listed individually in two separate questions). Students selected all the representations that form a *good* basis for strong field Zeeman effect in the multiple-choice question and were then asked to provide explanation for the options they chose in Q1:

**Q1.** *A perturbation* $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ *acts on a hydrogen atom with the unperturbed Hamiltonian* $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. *For the perturbation* $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, *circle* **ALL** *of the representations that form a good basis for the strong field Zeeman effect and explain your reasoning. Assume that for all cases the principal quantum number* $n = 2$.

*i. Coupled representation,*

*ii. Uncoupled representation,*

*iii.* **ANY** *arbitrary orthonormal basis constructed with linear combinations of states in the coupled representation,*

*iv.* **ANY** *arbitrary orthonormal basis constructed with a linear combination of states in the uncoupled representation,*

*v. Neither coupled nor uncoupled representation.*

Students were also asked to determine a *good* basis for the limiting case of the weak field

Zeeman effect (in a question identical to Q1 except that the phrase "strong field Zeeman effect" was replaced by "weak field Zeeman effect"). The correct answer for the strong field Zeeman effect is the uncoupled representation (option ii) and the correct answer for the weak field Zeeman effect is the coupled representation (option i). Below, we discuss difficulties with corrections to the energies due to the strong and weak field Zeeman effects.

## 6.4 STUDENT DIFFICULTIES

Students had several difficulties with DPT in general (i.e., not restricted to the limiting context of the strong and weak field Zeeman effects only). For example, when students were asked to determine a *good* basis for finding the corrections to the energies of the hydrogen atom due to fine structure, many students did not even realize that DPT should be used. Other students knew that they had to use DPT to find corrections to the wavefunction, but they did not use DPT to find the first-order corrections to the energies. These students incorrectly claimed that they did not need to use DPT since no terms in $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$) "blow up". Some students only focused on the Zeeman term $\hat{H}'_Z$ when asked to determine a *good* basis for finding the corrections to the energies of the hydrogen atom in the limiting cases of the strong and weak field Zeeman effect. In particular, they ignored the fine structure term $\hat{H}'_{fs}$ altogether and focused on the Zeeman term as the only term in the perturbation. Moreover, even if students realized that DPT should be used for the limiting cases of the strong and weak field Zeeman effects, many of them admitted that they had memorized which representation was a good basis in a given situation. Memorization of which basis to use often masked the fact that students did not have a deep understanding of DPT. Table 16 shows that many students struggled to identify a good basis for finding the corrections to the energy spectrum due to the limiting cases of the strong and weak field Zeeman effects. Below, we discuss some specific student difficulties:

**A. Not focusing on both $\hat{H}^0$ and $\hat{H}'$ when determining a *good* basis:** Students with this type of difficulty typically focused on the bases that make $\hat{H}^0$ diagonal but did not give consideration to $\hat{H}'$ when finding a good basis. For example, in the first step of the

Table 16: Percentages of undergraduate (U) ($N = 32$) and Ph. D. level students (P) ($N = 42$) who answered Q1 correctly.

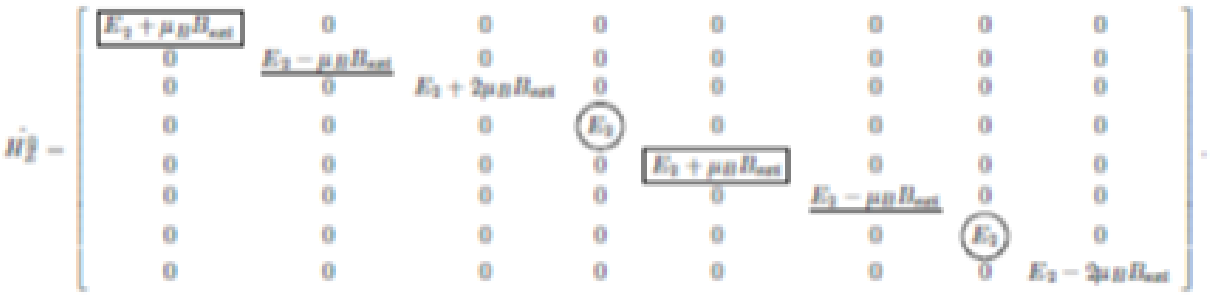
| Limiting Case | U | P |
|---|---|---|
| Strong Field | 41% | 29% |
| Weak Field | 31% | 31% |

two-step approximation for the weak field Zeeman effect, some students incorrectly claimed that the uncoupled representation forms a *good* basis because it diagonalizes the operator $\hat{H}^0$. Interviews suggest that these students often did not realize that $\hat{H}'_{fs}$ is not diagonal in the degenerate subspace of $\hat{H}^0$ if the uncoupled representation is chosen as the basis and the corrections to the energies using this representation will yield incorrect values inconsistent with experiments.

**B. Focusing on the degeneracy in the perturbation $\hat{H}'$ instead of the degeneracy in the unperturbed Hamiltonian when determining a good basis in step 1 or step 2:** When determining whether DPT should be used and whether a basis is a *good* basis, some students incorrectly focused on the degenerate subspaces of $\hat{H}'$ instead of $\hat{H}^0$. For example, when students were asked to find the energy corrections in the first step of the two-step approximation, some students incorrectly focused on the degeneracy in the stronger perturbation, $\hat{H}'_{strong}$, to determine whether DPT should be used and whether the basis provided was *good*. In particular, they focused on whether the degenerate subspaces in $\hat{H}'_{strong}$ were diagonal to determine if the basis was *good* (instead of whether $\hat{H}'_{strong}$ was diagonal in the degenerate subspaces of $\hat{H}^0$). An analogous student difficulty was also prevalent in step 2 of the two-step approximation. In particular, in order to determine whether a basis is a *good* basis for the strong or weak field Zeeman effect in step 2, students must identify the degenerate subspaces of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ and determine whether or not the weaker perturbation $\hat{H}'_{weak}$ is diagonal in each degenerate subspace of $\hat{H}^0_{strong}$. However, many students incorrectly focused on the degeneracy and degenerate subspaces of $\hat{H}'_{weak}$ instead of the degenerate subspaces of $\hat{H}^0_{strong}$ to determine whether DPT should be used

and if the basis provided was *good*.

For example, during the portion of the interview regarding the strong field Zeeman effect, in step 2, students were given the strong field Zeeman Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ from step 1 and the weaker perturbation $\hat{H}'_{fs}$ in matrix form in the uncoupled representation for $n = 2$ (since the uncoupled representation is a *good* basis for step 1 of the two-step approximation method). The students were then asked to identify the $\hat{H}'_{fs}$ matrix in each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ and explain whether or not the uncoupled representation forms a *good* basis in step 2 of the 2-step approximation method. In the $n = 2$ subspace with $s = \frac{1}{2}$, the $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ matrix provided to students to probe their understanding is the following in which the basis states are chosen in the uncoupled representation $(|l,\ m_l,\ m_s\rangle)$ in the order $|0,\ 0,\ \frac{1}{2}\rangle$, $|0,\ 0,\ -\frac{1}{2}\rangle$,$|1,\ 1,\ \frac{1}{2}\rangle$, $|1,\ 1,\ -\frac{1}{2}\rangle$, $|1,\ 0,\ \frac{1}{2}\rangle$, $|1,\ 0,\ -\frac{1}{2}\rangle$, $|1,\ -1,\ \frac{1}{2}\rangle$ , and $|1,\ -1,\ -\frac{1}{2}\rangle$:



The basis states were chosen in a different order to probe whether students were able to identify the degenerate subspace of $\hat{H}_Z^0$ when basis states with the same energies are not in the adjacent rows/columns.

The $\hat{H}_Z^0$ matrix has three separate two-fold degeneracies for the energies $E_2 + \beta, E_2 - \beta$, and $E_2$ as indicated by the boxed, underlined, and circled matrix elements of $\hat{H}_Z^0$ above. In order to determine whether a basis consisting of states in the uncoupled representation forms a *good* basis, $\hat{H}'_{fs}$ must be diagonal in each of these three degenerate subspaces of $\hat{H}_Z^0$. The $\hat{H}'_{fs}$ matrix in the $n = 2$ subspace in which the basis states are chosen in the same order as they were for the $\hat{H}_Z^0$ matrix above is as follows:

From the boxed matrix elements, $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}_Z^0$ for the degenerate energy $E_2 + \beta$ is $\frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 15 & 0 \\ 0 & 7 \end{bmatrix}$. Similarly, as given by the underlined matrix elements, $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}_Z^0$ for the degenerate energy $E_2 - \beta$ is

$$\hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} \boxed{15} & 0 & 0 & 0 & \boxed{0} & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ \boxed{0} & 0 & 0 & 4\sqrt{2} & \boxed{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}.$$

$\frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 15 & 0 \\ 0 & 7 \end{bmatrix}$ and from the circled matrix elements, $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0_Z$ for the degenerate energy $E_2$ is $\frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 11 & 0 \\ 0 & 11 \end{bmatrix}$.

However, students often did not realize that they should focus on the degeneracy of the Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ and instead they focused on the degeneracy of the weak perturbation $\hat{H}'_{fs}$ by examining the diagonal matrix elements of $\hat{H}'_{fs}$ that were equal. In particular, they incorrectly focused on whether the degenerate subspaces of $\hat{H}'_{fs}$ were diagonal in order to determine whether a given basis is a *good* basis. For example, they focused on the degenerate subspace $\frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 15 & 0 \\ 0 & 15 \end{bmatrix}$ in $\hat{H}'_{fs}$. However, the degeneracy of the weaker perturbation $\hat{H}'_{fs}$ is not relevant to determining a *good* basis. Instead, one should identify the degenerate subspaces of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ and determine if the weaker perturbation $\hat{H}'_{fs}$ is diagonal in the degenerate subspaces of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ to decide whether a given basis is a *good* basis in step 2 of the two-step process.

**C. Incorrectly claiming that $\hat{H}'_{weak}$ must be diagonal in each degenerate subspace of $\hat{H}^0$ (instead of $\hat{H}^0_{strong}$) in a good basis when using the two-step approximation:** Many students incorrectly claimed that, in a *good* basis for step 2 of the two-step approximation, $\hat{H}'_{weak}$ must be diagonal in the degenerate subspace of $\hat{H}^0$ as opposed to the degenerate subspaces of $\hat{H}^0_{strong}$. They did not realize that when using the two-step approximation in the limiting cases in step 2, the weaker perturbation $\hat{H}'_{weak}$ need only be diagonal in each degenerate subspace of the stronger Hamiltonian $\hat{H}^0_{strong}$ obtained after step 1 (as opposed to each degenerate subspace of $\hat{H}^0$). In the strong field Zeeman effect, a basis consisting of states in the uncoupled representation forms a *good* basis. The matrices to be considered in step 2 for the new unperturbed Hamiltonian $\hat{H}^0_{strong} = \hat{H}^0_Z$ and the weaker perturbation $\hat{H}'_{fs}$ are given below for the $n = 2$ subspace, in which basis states are chosen

in the uncoupled representation ($|l,\ m_l,\ m_s\rangle$) in the order $|0,\ 0,\ \frac{1}{2}\rangle$, $|1,0,\ \frac{1}{2}\rangle$, $|0,0,\ -\frac{1}{2}\rangle$, $|1,\ 0,\ -\frac{1}{2}\rangle$, $|1,\ 1,\ -\frac{1}{2}\rangle$, $|1,\ -1,\ \frac{1}{2}\rangle$, $|1,\ 1,\ \frac{1}{2}\rangle$, and $|1,\ -1,\ -\frac{1}{2}\rangle$:

$$\hat{H}'_Z = \begin{bmatrix} E_2+\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2+\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2-\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2-\mu_B B_{ext} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2+2\mu_B B_{ext} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2-2\mu_B B_{ext} \end{bmatrix}$$

$$\hat{H}'_{fs} = \frac{(-13.6\text{eV})\alpha^2}{192} \begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7 & 0 & 0 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 15 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7 & 0 & 4\sqrt{2} & 0 & 0 \\ 0 & 4\sqrt{2} & 0 & 0 & 11 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & 0 & 11 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}$$

In step 2, despite the fact that the weaker perturbation $\hat{H}'_{weak} = \hat{H}'_{fs}$ is not diagonal in the degenerate subspace of $\hat{H}^0$ (as seen by the matrix elements $4\sqrt{2}$ above for the $n = 2$ subspace) when the uncoupled representation is chosen as the basis, the weaker perturbation $\hat{H}'_{fs}$ *is* diagonal in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ after accounting for the splitting of the energy levels due to the stronger perturbation $\hat{H}'_Z$ (as seen by the boxed subspaces in the weaker perturbation $\hat{H}'_{fs}$). Many students struggled with the fact that the weaker perturbation $\hat{H}'_{fs}$ must only be diagonal in each degenerate subspace of $\hat{H}^0_Z$ in step 2. For example, one interviewed student claimed "the uncoupled is not a *good* basis (for strong field Zeeman effect) since $\hat{H}'_{fs}$ is not diagonal in the uncoupled representation. So we will have off-diagonal (matrix) elements (in $\hat{H}'_{fs}$)." Thus, many students had difficulty with the two-step approximation involving the limiting cases (strong or weak field Zeeman effect). They struggled to identify when it was valid to use the two-step approximation and in connecting these limiting cases with the intermediate field Zeeman effect in the appropriate limit.

**D. Not realizing that some of the degeneracy is broken after taking into account the stronger perturbation, allowing $\hat{H}'_{weak}$ to be diagonal in each degenerate subspace of $\hat{H}^0_{strong}$:** Many students struggled with the fact that the utility of the two-step approximation for the limiting cases of the strong and weak field Zeeman effects lies in the fact that some of the degeneracy is broken in step 1 of the two-step approximation when the stronger perturbation $\hat{H}'_{strong}$ is treated as the only perturbation on the unperturbed Hamiltonian $\hat{H}^0$. They did not realize that, in general, after taking into account the stronger perturbation in step 1, the dimension of some of the degenerate subspaces is reduced. Therefore, in step 2, when $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ is treated as the new unperturbed Hamiltonian, the degeneracy of energy spectrum $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ is less than the degeneracy of $\hat{H}^0$, making it possible for the weaker perturbation $\hat{H}'_{weak}$ to be diagonal in the degenerate subspaces of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$. For example, in the strong field Zeeman effect, a basis consisting of states in the uncoupled representation forms a good basis for $\hat{H}^0$ and $\hat{H}'_Z$ in step 1 and also in step 2 for $\hat{H}^0_{strong}$ and $\hat{H}'_{weak}$. However, students often did not realize that for $n = 2$, the degeneracy in the new unperturbed Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ is reduced to three separate two-fold degeneracies and two energies with degeneracy of one (instead of an 8-fold degeneracy in the unperturbed Hamiltonian $\hat{H}^0$). In particular, they did not realize that in step 2, in the uncoupled representation, the weaker perturbation $\hat{H}'_{fs}$ is diagonal in each of these $2 \times 2$ subspaces of the Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ so that the uncoupled representation is a good basis for finding the corrections.

In interviews, students often argued that *neither* a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation is a *good* basis even in the limiting cases since neither is a *good* basis for both the Zeeman term $\hat{H}'_Z$ and the fine structure term $\hat{H}'_{fs}$. They claimed that even in the limiting cases, one must find a basis that diagonalizes *both* the Zeeman term $\hat{H}'_Z$ and the fine structure term $\hat{H}'_{fs}$. Further probing suggests that they often did not realize that in the limiting cases, some of the degeneracy is lifted after step 1 in the two-step process so that the basis chosen in step 1 remains a good basis in step 2.

**E. Difficulty connecting the first order corrections to the energy spectrum in the intermediate field Zeeman effect with the two-step approximation in the**

**appropriate limit:** Prior to considering the limiting cases of the strong and weak field Zeeman effect during the interview, students worked through examples involving the intermediate field Zeeman effect (in which $\hat{H}'_Z \approx \hat{H}'_{fs}$). For the intermediate field Zeeman effect, the Zeeman term and the fine structure term are on equal footing and must be treated simultaneously as the perturbation on the unperturbed Hamiltonian $\hat{H}^0$. Since neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation form a *good* basis for the intermediate field Zeeman effect, students must choose an initial basis (either the coupled or uncoupled representation) and then diagonalize $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$ in order to determine a *good* basis and find the first-order corrections to the energy spectrum.

After working through examples involving the intermediate field Zeeman effect in the interview, students considered the two limiting cases of the strong and weak field Zeeman effects. For the intermediate field Zeeman effect, one obtains first order corrections to the energies in which both the Zeeman term, $\hat{H}'_Z$, and the fine structure term, $\hat{H}'_{fs}$, are treated as perturbations simultaneously on the unperturbed Hamiltonian, $\hat{H}^0$. However, in the limit that the energy corrections due to one of these two perturbations are much larger than the other, one can use the expressions for the energy corrections for the intermediate field Zeeman effect and perform a Taylor series expansion about the small parameter that accounts for the smaller correction. The results obtained by the two-step approximation method in the limiting cases (strong and weak field Zeeman effects) yield the same corrections to the energy spectrum as those obtained by the Taylor series expansion of the corrections to the energy spectrum in the intermediate field Zeeman effect when retaining terms of the same order. Many students struggled to connect these limiting cases to the intermediate field Zeeman effect. They did not realize that under the appropriate limits, the first-order corrections to the intermediate field Zeeman effect for the hydrogen atom are consistent with the first order corrections in the strong and weak field Zeeman effects when using the two-step approximation method. In fact, interviews suggest that some students viewed the limiting cases of the strong and weak field Zeeman effect as entirely separate problems and did not think of these limiting cases as related at all to their previous work on the intermediate field Zeeman effect.

Other students had difficulty correctly expressing a Taylor-series expansion of the general case (intermediate field Zeeman effect) in order to determine the first-order corrections to the energy spectrum for the limiting cases in the strong and weak field Zeeman effects. For example, one interviewed student claimed that in order to obtain the results for the weak field Zeeman effect, "for the Taylor expansion (of the intermediate field Zeeman corrections to the first order energies), we can set $B_{ext} = 0$ and all the terms for the magnetic field drop out." Another interviewed student claimed that in order to obtain the results for the strong field Zeeman effect from the general case, we should simply "let $B_{ext}$ go to infinity" in the expression for the energy corrections for the intermediate field Zeeman effect. When asked what the first-order corrections to the energies would be if we let $B_{ext}$ go to infinity, the student responded, "Well, they would go to infinity. Wait that's not right, is it? I think I need to go back and review how to do a Taylor series expansion."

It is important that students realize that the first-order corrections to the energy spectrum in the limiting cases of the strong and weak field Zeeman effects match those obtained in the intermediate field Zeeman effect when taking the appropriate limits. This realization would help students make sense of the use of the two-step approximation method for the limiting cases and recognize that the errors in the two-step approximation are comparable to those obtained by retaining terms of a certain order in a Taylor series expansion.

## 6.5 METHODOLOGY FOR THE DEVELOPMENT OF THE QUILT

### 6.5.1 Development and Validation of the QuILT

The difficulties described show that many students struggle in determining a *good* basis for finding the corrections to the energies in the limiting cases of the strong and weak field Zeeman effects. Therefore, we developed a QuILT that takes into account these difficulties and strives to help students build a robust knowledge structure of these concepts. The development of the DPT QuILT started with an investigation of student difficulties via open-ended and multiple-choice questions administered after traditional instruction to advanced

undergraduate and Ph. D. level students and conducting a cognitive task analysis from an expert perspective [83]. The cognitive task analysis was conducted by three physics education researchers together and discussed with members of the physics faculty who teach (or had taught) QM. It described not only the requisite knowledge and skills one would need in order to have a functional understanding of DPT, but also the order in which the material should be presented to help ensure that the material in each section built upon that in previous sections. The investigation of student difficulties also informed the cognitive task analysis in that we were able to fill in any "gaps" (due to expert blind spots) in the expert cognitive task analysis based upon students' perspectives. The QuILT strives to help students build on their prior knowledge and addresses common difficulties found via research, some of which were discussed in the previous section.

The QuILT is inspired by Piaget's "optimal mismatch" framework as well as the preparation for future learning framework of Bransford and Schwartz. In Piaget's "optimal mismatch" framework, students are intentionally placed in a situation in which their current knowledge structures are inadequate and the students are required to reorganize existing structures or develop new structures to reconcile this conflict [84]. Bransford and Schwartz's preparation for future learning framework emphasizes that learning occurs when elements of innovation and efficiency are both present [85]. Innovation and efficiency describe two orthogonal components of instruction. Innovation describes aspects that are new to students, such as new concepts or new problem-solving skills. Efficiency is a measure of the structure and organization of the material, as well as how proficient the student is with the material. Instruction that incorporates only one of these elements leads to students becoming disengaged. If instruction is too innovative, students cannot connect the material with their prior knowledge and become frustrated. When the instruction is too efficient, students interact with repetitious material that does not provide intellectual stimulation and may become routine experts. However, they will not be able to transfer their learning to new situations.

In the QuILT, students are presented with innovative tasks that strive to create a cognitive conflict. The QuILT then provides scaffolding aimed at resolving their cognitive conflict. For example, students are asked to consider conversations between hypothetical students in which one student makes an incorrect statement involving a common difficulty while other

students make statements that illuminate inconsistencies in the incorrect statement. They must decide which hypothetical students are correct and explain their reasoning. The goal is to create a cognitive conflict and have students realize that there is some inconsistency between their thoughts and the correct reasoning. After this when students want to resolve the conflict, further scaffolding is provided in order to resolve the inconsistencies and to help students reconcile their initial reasoning with the correct reasoning. Whether it be examples, hypothetical conversations, or calculations, the QuILT strives to help students develop a deeper understanding by actively working through the inquiry-based learning sequences. Student difficulties are incorporated in these examples and conversations to create a cognitive conflict in which they are then guided through future tasks designed to resolve these issues. Efficiency is addressed in the QuILT in several ways. First, the QuILT follows the sequence laid out in the cognitive task analysis. It is organized in a manner which attempts to build on the students' prior knowledge, and each section in the QuILT builds upon the previous section. Second, students are provided scaffolding designed to help address common difficulties, thus reducing the cognitive conflict. Third, the QuILT progressively reduces the scaffolding to help students solve problems without any assistance. Finally, as the students work through the different tasks, they develop more proficiency at identifying the concepts and answering the questions.

The development of the QuILT went through a cyclic, iterative process. The preliminary version was developed based upon the cognitive task analysis and knowledge of common student difficulties. Next, the QuILT underwent many iterations among the three researchers and then was iterated several times with three physics faculty members to ensure that they agreed with the content and wording. It was also administered to graduate and advanced undergraduate students in individual think-aloud interviews to ensure that the guided approach was effective, the questions were unambiguously interpreted, and to better understand the rationale for student responses. During these semi-structured interviews, students were asked to "think aloud" while answering the questions [86]. Students first read the questions on their own and answered them without interruptions except that they were prompted to think aloud if they were quiet for a long time (in order to not disrupt their thought processes). After students had finished answering a particular question to the best of their ability, they

were asked to further clarify and elaborate on issues that they had not clearly addressed earlier. The next step involved evaluating the impact of the QuILT on student learning and determining if the difficulties remained. Finally, modifications and improvements were made based upon the student and faculty feedback before it was administered to students in various QM courses.

### 6.5.2 Structure of the QuILT

The QuILT uses a guided inquiry-based approach to learning and actively engages students in the learning process. In an inquiry-based approach, students take an active role by answering questions throughout the task which requires that they work through problems and reflect upon the underlying concepts. A guided inquiry-based approach has these same features, but it also incorporates scaffolding based upon the expert and novice cognitive task analyses that provides students with support to help ensure they develop robust understanding while working on the task. It includes a pretest to be administered in class after traditional instruction in DPT. Then, students engage with the tutorial in small groups in class (or alone when using it as a self-paced learning tool in homework), and then a posttest is administered in class. As students work through the tutorial, they are asked to predict what should happen in a given situation. Then, the tutorial strives to provide scaffolding and feedback as needed to bridge the gap between their initial knowledge and the level of understanding that is desired. Students are also provided checkpoints to reflect upon what they have learned and make explicit connections between what they are learning and their prior knowledge. They are given an opportunity to reconcile differences between their predictions and the guidance provided in the checkpoints of the QuILT before proceeding further.

The DPT QuILT uses a blend of guided inquiry-based learning sequences involving both qualitative and quantitative reasoning to improve students' understanding. For example, the QuILT requires qualitative reasoning while students reason about hypothetical student conversations and quantitative reasoning to determine the matrix elements of the operators $\hat{H}'_{SO}$ and $\hat{H}'_{Z}$ in the coupled and uncoupled representations. The QuILT can be accessed via the link in ref. [27].

### 6.5.3 Addressing Student Difficulties Via Guided Learning Sequences in the QuILT

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples involving DPT in which they consider the terms $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs}$, $\hat{H}'_Z$, and $\hat{H}'_{fs} + \hat{H}'_Z$ as perturbations on $\hat{H}^0$ ($\hat{H}'_r$ is the relativistic correction term and $\hat{H}'_{SO}$ is the spin-orbit interaction term). In this manner, students focus on the fundamental concepts for determining a *good* basis for the fine structure and Zeeman corrections to the energy spectrum of the hydrogen atom. In particular, for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, students learn about (1) why DPT must be used, (2) why care must be taken to choose a *good* basis, and (3) how to determine a *good* basis using the two-step approximation method for the limiting cases of the strong and weak field Zeeman effects. Below, we discuss how the QuILT strives to address student difficulties and help them learn about the perturbative corrections to the energy spectrum of the hydrogen atom due to the strong and weak field Zeeman effects using the DPT.

Students first work through a warm-up for the tutorial that strives to help them identify the angular bases that diagonalize each of the operators $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs}$, and $\hat{H}'_Z$ for a given $n$. In addition, students also work through examples in which they must determine the matrix elements of each of the operators $\hat{H}'_{SO}$ or $\hat{H}'_Z$. For example, they calculate several diagonal and off-diagonal matrix elements of $\hat{H}'_{SO}$ and $\hat{H}_Z$ in both a basis consisting of states in the coupled representation and a basis consisting of states in the uncoupled representation for a fixed $n$. The warmup strives to help students learn the prerequisites for finding a *good* basis for the hydrogen atom in the limiting cases of the strong and weak field Zeeman effect in the context of DPT.

**Helping students identify $\hat{H}'_{weak}$ in the degenerate subspace of $\hat{H}^0_{strong}$:** In the QuILT, students are provided scaffolding that strives to help them develop systematic reasoning and build upon their prior knowledge for each step in the two-step approximation method of the DPT for the limiting cases of the strong and weak field Zeeman effects. In particular, students work through several guided inquiry-based sequences in which they must determine a *good* basis for step 1 and the corresponding first-order corrections to the energies.

Next, they are provided guidance and asked to identify a *good* basis for step 2. Students are then provided the matrices for the operators $\hat{H}^0_{strong}$ and $\hat{H}'_{weak}$ which allow them to identify degeneracy in the new unperturbed Hamiltonian $\hat{H}^0_{strong}$ and also identify $\hat{H}'_{weak}$ in each degenerate subspace of $\hat{H}^0_{strong}$. They can reconcile whether their initial choice of a *good* basis is correct and also determine the first-order corrections to the energy spectrum for step 2 if the given basis is a *good* basis.

For example, students work through a guided inquiry-based sequence for the strong field Zeeman effect in which they start by determining a *good* basis for the first step when the stronger perturbation $\hat{H}'_Z$ is treated as the only perturbation on the unperturbed Hamiltonian $\hat{H}^0$ (in this case the answer is exact for the first order correction since $\hat{H}^0$ and $\hat{H}'_Z$ commute and if the uncoupled representation is chosen as the basis, they are simultaneous eigenstates of both). Once the students identify a *good* basis for step 1, they engage with an inquiry-based sequence to identify $\hat{H}'_{weak} = \hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_Z$. The following is an example of a guided inquiry-based sequence students work through for the two-step approximation method in the context of the strong field Zeeman effect.

**Q4. <u>STEP 1:</u>**

*For the case $E'_Z \gg E'_{fs}$, we treat only $\hat{H}'_Z$ as the perturbation on $\hat{H}^0$.*

**Q4(a)** *For the case $E'_Z \gg E'_{fs}$, what is a good basis for step 1 when we ignore $\hat{H}'_{fs}$? Explain.*

**Q4(b)** *Write an expression for the first order corrections to the energies due to only the stronger perturbation $\hat{H}'_Z$ acting on the unperturbed Hamiltonian $\hat{H}^0$ (once you have found a good basis). Here the first order corrections are the exact results for the energies after STEP 1.*

**Q5. <u>STEP 2:</u>**

*In the strong field Zeeman effect when $E'_Z \gg E'_{fs}$, in step 2, the unperturbed Hamiltonian includes the Zeeman term and becomes*

$$\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m}B_{ext}(\hat{L}_z + 2\hat{S}_z). \tag{6.5}$$

*Is the $\hat{H}_Z^0$ matrix a diagonal matrix if the coupled representation or the uncoupled representation is chosen as the basis? Explain your reasoning.*

**Q6.** *Now for the $n = 2$ subspace, take a look at the $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ and $\hat{H}'_{fs}$ matrices given below in which $E_2 = -\frac{13.6eV}{4}$ and the basis vectors are chosen in the* **uncoupled representation** *($|l, m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$. Then answer questions Q6(a)-Q6(c) for the Strong field Zeeman effect.*

$$\hat{H_Z^0} = \begin{bmatrix} E_2+\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2-\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2+2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2+\beta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2-\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2-2\beta \end{bmatrix} \tag{6.6}$$

$$\hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192} \begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & 7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} \tag{6.7}$$

**Q6(a)** *Determine the degeneracy of the energy eigenvalues of the new unperturbed Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ after accounting for the stronger perturbation and circle the corresponding degenerate subspaces of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ (for $n = 2$ subspace) in the preceding*

*matrix representation.*

**Q6(b)** *Circle $\hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ and determine if $\hat{H}'_{fs}$ in any of these subspaces of $\hat{H}^0_Z$ is diagonal.*

**Q6(c)** *Determine whether the uncoupled representation chosen as the basis in question Q5 is a good basis for the unperturbed Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ and the perturbation $\hat{H}'_{fs}$. Explain how you made the determination.*

This guided inquiry-based sequence is designed to help students focus on the necessary requirements for a *good* basis in step 1 and step 2. For example, Q6(a) strives to help students realize that some of the degeneracy has been lifted after step 1 and that one needs to focus on the degeneracy of $\hat{H}^0_Z$. To determine whether a basis consisting of states in the uncoupled representation is a *good* basis for step 2, the students work to identify whether $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z$ in Q6(b). In Q6(c), the students are asked to describe whether a basis consisting of states in the uncoupled representation forms a *good* basis. Based upon their answers to Q6(a) and Q6(b), the QuILT strives to help students identify $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0_Z$ and find that a basis consisting of states in the uncoupled representation is a *good* basis for the strong field Zeeman effect. Students work through a similar guided inquiry-based sequence for the weak field Zeeman effect.

**Helping students realize that some of the degeneracy is broken after step 1 and that $\hat{H}'_{weak}$ need only be diagonal in each degenerate subspace of $\hat{H}^0_{strong}$:** It is also important that students realize that the utility of the two-step approximation lies in the fact that some of the degeneracy is broken in the first step, which allows for the weaker perturbation to be diagonal in the degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ in step 2. In the QuILT, students consider the following hypothetical students' statements in the context of the strong field Zeeman effect that are intended to help students realize that some of the degeneracy is broken after the first step and that in step 2, the weaker perturbation is diagonal in each degenerate subspace of $\hat{H}^0_Z$:

**Student 1:** *In step 1, when we only consider $\hat{H}'_Z$ as the perturbation on $\hat{H}^0$, we choose the uncoupled representation as the good basis. Once the uncoupled representation is chosen as the good basis, we are guaranteed to have off-diagonal matrix elements in the weaker fine*

*structure perturbation matrix $\hat{H}'_{fs}$. Thus the uncoupled representation is not a good basis in step 2.*

**Student 2:** *Actually, once we treat the stronger Zeeman perturbation $\hat{H}'_Z$ in the first step, we lift some of the degeneracy in the energy spectrum of $\hat{H}^0$. There is still degeneracy in the energy spectrum $E_n^0 = E_n + \mu_B B_{ext}(m_l + 2m_s)$ after the first step, but now the degeneracy is present in smaller subspaces of $\hat{H}^0$. For example, for the $n = 2$ subspace in step 2, $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ is*

*In the uncoupled representation, $\hat{H}'_{fs}$ is not diagonal in the entire $n = 2$ subspace, but it is diagonal in each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$. In the $\hat{H}'_{fs}$ matrix below, the elements in the degenerate subspace of $\hat{H}_Z^0$ corresponding to the degenerate energy $E_2 + \beta$ are boxed. We see $\hat{H}'_{fs}$ is diagonal in the $2 \times 2$ subspace corresponding to the degenerate energy $E_2 + \beta$.*

$$\hat{H}'_{fs} = \frac{(-13.6 \text{ eV})\alpha^2}{192} \begin{bmatrix} \boxed{15} & 0 & 0 & 0 & \boxed{0} & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ \boxed{0} & 0 & 0 & 4\sqrt{2} & \boxed{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} \tag{6.8}$$

*Similarly, $\hat{H}'_{fs}$ is diagonal in the degenerate subspace of $\hat{H}_Z^0$ for the degenerate energies $E_2$ and $E_2 - \beta$. Therefore, the uncoupled representation does form a good basis in this two-step process.*

In the preceding hypothetical conversation, Student 1 is correct in that the weaker perturbation $\hat{H}'_{fs}$ will have off-diagonal matrix elements if a basis consisting of states in the uncoupled representation is chosen. However, Student 1 does not realize that when using the two-step approximation method for the strong field Zeeman effect, $\hat{H}'_{fs}$ need only be diagonal in each degenerate subspace of $\hat{H}^0_Z$. Student 2's statement is designed to have students reflect upon the fact that some of the degeneracy is lifted after step 1 and as a result, the off-diagonal matrix elements of $\hat{H}'_{fs}$ are not in any of the degenerate subspaces of $\hat{H}^0_Z$. Thus, a basis consisting of states in the uncoupled representation is a *good* basis for the strong field Zeeman effect.

**Helping to connect the first order corrections to the energies in the intermediate field Zeeman effect to those found in the limiting cases using the two-step approximation method:** The QuILT strives to help students identify a *good* basis and determine the first-order corrections to the energy spectrum in the limiting cases of the strong and weak field Zeeman effects. Additionally, the QuILT strives to help students learn that the resulting first-order corrections to the energies in the two limiting cases are consistent with the first-order corrections to the energies in the intermediate field Zeeman effect when one takes the appropriate limit. In an effort to help students make these connections, the QuILT asks the following question:

**Q7.** *The splitting of the energy levels for the $n = 2$ states of the hydrogen atom in the intermediate field Zeeman effect are given in Table 48 below. Use the appropriate Taylor series expansion to check that the corrections to the energies in the intermediate field Zeeman effect are consistent with the corrections found in the limiting cases of the strong and weak field Zeeman effects earlier.* ($E_2 = \frac{-13.6\text{eV}}{4}$, $\gamma = \left(\frac{\alpha}{8}\right)^2 13.6$ eV, $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$, $\beta = \mu_B B_{ext}$ were defined previously in the QuILT.)

For example, in the strong field limit ($\gamma \ll \beta$), we have $\sqrt{4\gamma^2 \pm \frac{2}{3}\gamma\beta + \frac{1}{4}\beta^2} \approx \frac{1}{2}\beta \pm \frac{2}{3}\gamma$. Using the Taylor series expansion of the energy levels in the intermediate field Zeeman effect (see Table II) and taking the appropriate limit for the strong field Zeeman effect, one can show that the energy levels match those found using the two-step approximation method.

Students are also given an opportunity to make sense of a graph depicting the relationship

Table 17: Energy Levels in the Intermediate Field Zeeman Effect ($n = 2$)

$$
\begin{aligned}
\epsilon_1 &= E_2 - 5\gamma + \beta \\
\epsilon_2 &= E_2 - 5\gamma - \beta \\
\epsilon_3 &= E_2 - \gamma + 2\beta \\
\epsilon_4 &= E_2 - \gamma - 2\beta \\
\epsilon_5 &= E_2 - 3\gamma + \beta/2 + \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_6 &= E_2 - 3\gamma + \beta/2 - \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_7 &= E_2 - 3\gamma - \beta/2 + \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_8 &= E_2 - 3\gamma - \beta/2 - \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4}
\end{aligned}
$$

between the splitting of the energy levels and strength of the external magnetic field. They are asked to compare the results they obtained for the intermediate field Zeeman effect and the limiting cases of the strong and weak field Zeeman effect and discuss whether their results are consistent with the graph and whether the intermediate field expression yields the limiting values in the appropriate limits.

## 6.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in Ph.D. level and upper-level undergraduate quantum mechanics courses. Students in both Ph. D. level and upper-level undergraduate courses were given a pretest after traditional instruction in relevant concepts in DPT but before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The Ph. D. level students were given the tutorial as their only homework assignment for the week. After

Table 18: The percentage of students who answered the multiple-choice portion of Q1 correctly for the strong and weak field Zeeman effects on the pretest and posttest for undergraduates (number of students $N = 32$ for the pretest and $N = 31$ for the posttest) and Ph. D. level students ($N = 42$).

| | Undergraduate Students (%) | | Ph. D. level Students (%) | |
|---|---|---|---|---|
| Limiting Case | Pretest | Posttest | Pretest | Posttest |
| Strong Field | 41 | 84 | 39 | 83 |
| Weak Field | 31 | 87 | 33 | 81 |

working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

The pre/posttest results for Q1 (as shown in Section III) are summarized in Table 18 and suggest that the QuILT was helpful in reducing student difficulties with these concepts. In particular, over 80% of Ph. D. level students and undergraduate students were able to correctly identify that a basis consisting of states in the uncoupled representation is a *good* basis for the strong field Zeeman effect and a basis consisting of states in the coupled representation is a *good* basis for the weak field Zeeman effect.

Table 19 shows the performance of undergraduate and Ph. D. level students on the pretest and posttest. The average score includes both the answer for the multiple-choice question and the students' explanation for Q1. Table 19 also includes the average gain, $G$, and normalized gain [87], $g$. The normalized gain is defined as the (posttest percent - pretest percent)/(100 - pretest percent). Both undergraduate and Ph. D. level students struggled with this topic as can be seen by the scores on the pretest. However, both groups showed significant improvement after working through the QuILT.

Q1 was graded using a rubric which was developed by the researchers together. Each question was worth six points. A maximum of four points were awarded for the multiple-choice portion of Q1 and two points were awarded for their explanation. For example, when

grading the multiple-choice portion of Q1 for the weak field Zeeman effect, students were given four points for correctly choosing only the coupled representation (option i). If they chose the coupled representation (option i) and any arbitrary complete orthonormal linear combination of states in the coupled representation (option iii), they were given two out of four points for the multiple-choice portion of Q1. We found that some interviewed students correctly reasoned that the degeneracy in the energy spectrum of $\hat{H}'_{fs}$ allowed for linear combinations of states in the coupled representation with the same $n$, $l$, and $j$ to diagonalize $\hat{H}'_{fs}$. However, it is not the case that ANY linear combination of states in the coupled representation diagonalizes $\hat{H}'_{fs}$. in the degenerate subspace of $\hat{H}^0$ While these students did not show entirely correct reasoning, they were correctly thinking about issues caused by the degeneracy in the energy spectrum but incorrectly overgeneralized these concepts to reason that ANY linear combination of states in the coupled representation diagonalizes $\hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0$. Students were given one out of four points if they chose both the coupled and uncoupled representation (options i and ii) as a basis that diagonalizes $\hat{H}'_{fs}$. Some students incorrectly claimed that the operator $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ is diagonal in both the coupled and uncoupled representations because $\hat{H}'_{SO} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$. Although states in the coupled representation are eigenstates of the operators $\hat{J}^2$, $\hat{L}^2$, and $\hat{S}^2$, states in the uncoupled representation are eignestates of $\hat{L}_Z$ and $\hat{S}_Z$ but they are not eigenstates of the operators $\hat{L}_\pm$ and $\hat{S}_\pm$. Therefore, $\hat{H}'_{SO}$ is diagonal in the coupled representation but not diagonal in the uncoupled representation. Thus, $\hat{H}'_{SO}$ is diagonal in the coupled representation in the degenerate subspace of $\hat{H}^0$ but not diagonal in the uncoupled representation. This type of response shows some correct reasoning ($\hat{H}'_{fs}$ is diagonal in the degenerate subspace of $\hat{H}^0$ in the coupled representation) and was awarded partial credit. No points were awarded for any other combination of answers for the weak field Zeeman effect in Q1. The explanations that provided correct reasoning were awarded two points, responses with mostly correct reasoning were awarded one point, and responses with little or no correct reasoning were given zero points.

A subset of questions was graded separately by the researchers with a final inter-rater reliability of nearly 100%.

The following are written responses to Q1 for the weak field Zeeman effect ($\hat{H}'_Z \ll \hat{H}'_{fs}$)

Table 19: Average pretest and posttest scores for Q1 (including reasoning), gains ($G$) and normalized gains ($g$) for undergraduate students (number of students $N = 32$ for the pretest and $N = 31$ for the posttest) and Ph. D. level students ($N = 42$).

| Limit | Undergraduate Students | | | | Ph. D. level Students | | | |
|---|---|---|---|---|---|---|---|---|
| | Pre (%) | Post (%) | G (%) | g | Pre (%) | Post (%) | G (%) | g |
| Strong Field | 31 | 82 | +51 | 0.74 | 27 | 75 | +48 | 0.66 |
| Weak Field | 26 | 85 | +59 | 0.80 | 25 | 76 | +51 | 0.68 |

taken from two students' posttests who correctly chose a basis consisting of states in the coupled representation as a *good* basis: "Neither really form a *good* basis, but we can use a 2-step process. 1st considering only the $\hat{H}'_{fs}$ perturbation then some of the degeneracy is lifted. Then solve a simplified problem with $\hat{H}'_Z$ as a perturbation on $\hat{H}^0 + \hat{H}'_{fs}$." "2 step process: $\hat{H}' = \hat{H}'_{fs}$ is diagonal (in the $n = 2$ degenerate subspace of $\hat{H}^0$) in coupled representation. $\hat{H}'_Z$ diagonal in the degenerate subspace of $\hat{H}^0_{fs}$ (lifted degeneracy)." Student responses on the posttests were analogous in the context of the strong field Zeeman effect. These types of responses by students on the posttest demonstrate that they had learned to reason about how to find a *good* basis in the limiting cases of the strong and weak field Zeeman effect.

## 6.7 SUMMARY

Using the common difficulties of advanced students with finding the corrections to the energies of the hydrogen atom in the limiting cases of the strong and weak field Zeeman effects, we developed and evaluated a research-based QuILT which strives to help students learn to reason about and find a *good* basis for these limiting cases. In particular, the QuILT strives to help students learn that when the corrections to the energies due to either the Zeeman term $\hat{H}'_Z$ or the fine structure term $\hat{H}'_{fs}$ are much larger than the other, one can perform

DPT using a two-step approximation. The QuILT strives to help students learn about these limiting cases to determine when it is appropriate to use this two-step approximation and be able to reason that these results in the limiting cases are consistent with the corrections to the energies in the intermediate field Zeeman effect in the appropriate regimes. Students learn to reason that not only are the results in various limits consistent with the general case, but there is a benefit to using the two-step approximation method in that a *good* basis can be determined without explicitly diagonalizing the perturbation $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ by "brute force". The QuILT uses these limiting case examples to help students develop expert-like reasoning skills and help them learn to think like a physicist. In particular, learning to use limiting cases and understanding why the limits can be obtained from the general case (i.e., intermediate field Zeeman effect) can be useful for developing the problem-solving and meta-cognitive skills of an expert physicist. The QuILT strives to provide appropriate scaffolding and feedback using a guided inquiry-based approach to help students develop a functional understanding of relevant concepts. The evaluation shows that the QuILT is effective in improving students' understanding of the perturbative corrections to the energy spectrum of the hydrogen atom placed in an external magnetic field in the limiting cases of the strong and weak field Zeeman effect in the context of DPT.

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# 7.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: BASICS FOR A SYSTEM OF IDENTICAL PARTICLES

## 7.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. There have been a number of research studies aimed at investigating student reasoning in QM [14, 15, 16, 17, 18, 19, 20, 21] and improving student understanding of QM [22, 23, 24, 25, 26, 27]. For example, our group has focused on using the common student difficulties as a guide to develop research-based learning tools which include Quantum Interactive Learning Tutorials (QuILTs) [28, 29, 30, 31, 32, 33, 34, 35] which strive to improve student understanding of different QM concepts. However, there have been few investigations into student difficulties with fundamental concepts involving a system of identical particles.

Here, we discuss an investigation of student difficulties with fundamentals of a system of non-interacting identical particles and how that research was used as a guide in the development, validation, and in-class evaluation of a QuILT that strives to help students develop a good grasp of relevant concepts. Through researching students' understanding of and reasoning about a system of identical particles, we found common student difficulties that can hinder their development of a consistent and coherent knowledge structure pertaining to these concepts.

Below, we start with a brief background of relevant concepts and then describe the methodology for the investigation of student difficulties followed by the common difficulties

found. Then, we describe the methodology for the development, validation and in-class evaluation of the corresponding research-based QuILT that strives to help students develop a functional understanding of the fundamental concepts involving a system of identical particles.

## 7.2 BACKGROUND

In nature, there are two general types of fundamental or composite particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g., photons and mesons). A system of $N$ identical particles consists of $N$ particles of the same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in QM, identical particles are indistinguishable and there is no measurement that can be performed to distinguish these particles from one another. For example, if the coordinates of two identical particles are interchanged, there is no physical observable that would reflect this interchange. To account for the indistinguishability of these identical particles and make the properties of fermions and bosons consistent with observations, the wavefunction for a system of identical fermions must be completely antisymmetric and the wavefunction for a system of identical bosons must be completely symmetric with respect to exchange of two particles. Furthermore, one property that distinguishes these two types of particles is that two or more bosons can occupy the same single-particle state, but two or more fermions can never occupy the same single-particle state. The restriction for fermions is known as the Pauli exclusion principle and is consistent with a system of identical fermions having a completely antisymmetric wavefunction [80].

Here we focus on the many-particle Hamiltonian and stationary state wavefunctions that are solutions to the Time-Independent Schrödinger Equation (TISE) for a system of non-interacting identical particles. Unless otherwise stated, here we will refer to the stationary state wavefunction as the wavefunction. For a system of $N$ non-interacting identical particles,

the Hilbert space ($\mathscr{H}$) for the $N$-particle system in $M^N$ dimensions is

$$\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N \tag{7.1}$$

which is the direct product of the $M$-dimensional Hilbert space for each particle $\mathscr{H}_i$. The many-particle Hamiltonian for the system of $N$ non-interacting identical particles in the product space is

$$\begin{aligned} \hat{\mathbf{H}} &= \hat{H}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N + \hat{I}_1 \otimes \hat{H}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N \\ &\quad + \cdots + \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \hat{I}_{N-2} \otimes \hat{H}_{N-1} \otimes \hat{I}_N + \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{N-1} \otimes \hat{H}_N, \end{aligned} \tag{7.2}$$

where the single-particle Hamiltonian, $\hat{H}_i$, and the identity operator, $\hat{I}_i$, for the $i^{th}$ particle are in the $M$-dimensional Hilbert space $\mathscr{H}_i$.

We will use the following shorthand notation for the many-particle Hamiltonian

$$\hat{\mathbf{H}} = \sum_i \hat{\mathbf{H}}_i = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 + \cdots + \hat{\mathbf{H}}_N. \tag{7.3}$$

in which $\hat{\mathbf{H}}_i = \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{i-1} \otimes \hat{H}_i \otimes \hat{I}_{i+1} \cdots \otimes \hat{I}_N$ is the Hamiltonian of the $i^{th}$ particle in the $M^N$ dimensional product space. Thus, in the rest of this paper, all the boldface Hamiltonians are in the product space.

In order to determine the many-particle stationary state wavefunction for a system of non-interacting identical particles, one must first solve the single-particle TISE. The single-particle stationary state wavefunctions are solutions to the single-particle TISE, i.e., $\hat{H}_i \psi_{n_j}(x_i) = E_{n_j} \psi_{n_j}(x_i)$ for the $i^{th}$ particle in the state $\psi_{n_j}(x_i)$. Next, one should construct the many-particle stationary state wavefunction for a system of non-interacting identical particles that can be treated as distinguishable as the product of the single-particle stationary state wavefunctions (these product states can be used as basis states to construct the many-particle stationary state wavefunction for identical fermions or bosons). The basis states can be determined from all the permutations of the labels for the states or the coordinates in the products of the single-particle states. Here, for convenience, we will refer to all direct products of single-particle states as "basis states", regardless of their symmetry under exchange. Please note that for identical fermions, only completely antisymmetric linear combinations

of these basis states are allowed, while for bosons only completely symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed. The final step is to appropriately symmetrize the many-particle stationary state wavefunction for a system of non-interacting identical fermions or bosons using the basis states in the product space.

If we have a system of two non-interacting electrons in which one electron is in the single-particle state denoted by $\psi_{n_1}$ and the other electron is in the single-particle state denoted by $\psi_{n_2}$, then the wavefunction for the system of two electrons must be completely antisymmetric. Assuming $n_1 \neq n_2$ and ignoring spin, this normalized two-particle wavefunction in position representation is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\right]. \tag{7.4}$$

in which $x_1$ denotes the coordinate of the first electron and $x_2$ denotes the coordinate of the second electron. This completely antisymmetric wavefunction reflects the fact that one electron is in the single-particle state $\psi_{n_1}$ and the other electron is in the single-particle state $\psi_{n_2}$, but we cannot say which electron is in which single-particle state. It is consistent with Pauli's exclusion principle. For example, for a system of two fermions both in the same single-particle state $\psi_{n_1}$, the antisymmetric wavefunction (ignoring the spin) would be

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_1)\psi_{n_1}(x_2)\right] = 0. \tag{7.5}$$

Thus, there is no wavefunction for a system of two fermions in the same single-particle state and such a state is not possible.

The completely symmetric wavefunction (ignoring the spin) for two bosons in which one boson is in the single-particle state $\psi_{n_1}$ and the other boson is in the single-particle state $\psi_{n_2}$ is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\right]. \tag{7.6}$$

The two bosons can be in the same single-particle state. For example, the completely symmetric wavefunction for two bosons in the single-particle state $\psi_{n_1}$ is

$$\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2). \tag{7.7}$$

When considering the spin part of the wavefunction for a single-particle, we will use the notation $|s_i,\ m_{s_i}\rangle$ (in which $s_i$ and $m_{s_i}$ are the quantum numbers corresponding to the total spin and z-component of the spin for the $i^{th}$ particle, respectively). The states $|s_1,\ m_{s_1}\rangle$ are eigenstates of $\hat{S}_1^2$ and $\hat{S}_{1z}$ and the states $|s_2,\ m_{s_2}\rangle$ are eigenstates of $\hat{S}_2^2$ and $\hat{S}_{2z}$. We will use the following abbreviated notation for a spin-1/2 particle: $|\uparrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ 1/2\rangle_1$ and $|\downarrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ -1/2\rangle_1$ for electron 1 in the "spin up" and "spin down" state, respectively, and $|\uparrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ 1/2\rangle_2$, and $|\downarrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ -1/2\rangle_2$ for electron 2 in the "spin up" and "spin down" state, respectively.

When considering the spin part of the wavefunction for the two spin-1/2 particles in the "uncoupled" representation in the product space, we will use the notation $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, $|\downarrow\rangle_1|\uparrow\rangle_2$, and $|\downarrow\rangle_1|\downarrow\rangle_2$ for the basis states. We will also use the notation $|s,\ m_s\rangle$ for states in the "coupled" representation (in which the quantum numbers $s$ and $m_s$ correspond to the total spin angular momentum and the $z$ component of the total spin angular momentum including both spins, respectively). The states $|s,\ m_s\rangle$ in the coupled representation are eigenstates of $\hat{S}^2$ and $\hat{S}_z$ where $\vec{S} = \vec{S}_1 + \vec{S}_2$. For a system of two spin-1/2 particles ($s_1 = 1/2,\ s_2 = 1/2$), the quantum number $s = s_1 + s_2 = 1/2 + 1/2 = 1$ or $s = |s_1 - s_2| = |1/2 - 1/2| = 0$. If the total spin quantum number is $s = 1$ then the corresonding $m_s = -1, 0, 1$. If $s = 0$ then the corresponding $m_s = 0$. A complete set of states in the coupled representation for $1/2 \otimes 1/2$ is given by $|s, m_s\rangle = \{|1,\ 1\rangle, |1,\ 0\rangle, |1,\ -1\rangle, |0,\ 0\rangle\}$. We will use the following abbreviated notation for a complete set of normalized states for a system of two spin-1/2 particles in the coupled representation $|s,\ m_s\rangle$ written in terms of states in the uncoupled representation ($|s_1,\ m_{s_1}\rangle|s_2,\ m_{s_2}\rangle$):

$$\begin{array}{rcccl} |1,\ 1\rangle & = & |\uparrow\rangle_1|\uparrow\rangle_2 & = & |\uparrow\uparrow\rangle \\ |1,\ -1\rangle & = & |\downarrow\rangle_1|\downarrow\rangle_2 & = & |\downarrow\downarrow\rangle \\ |1,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |0,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right). \end{array} \tag{7.8}$$

One feature of the coupled basis states for two identical spin angular momenta, e.g., $|1,\ 1\rangle$, $|1,\ 0\rangle$, $|1,\ -1\rangle$, $|0,\ 0\rangle$, for two spin-1/2 particles in the coupled representation, is that they are either completely symmetric or completely antisymmetric with respect to exchange

of particles. For example, $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ are completely symmetric spin states for the two fermions and often refered to as the "triplet" states. It is important to note that any linear combination of these three symmetric spin states is also a completely symmetric spin state (i.e., $C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + C_3(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ is a completely symmetric normalized spin state in which $C_1$, $C_2$, and $C_3$ are constants such that $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$). The state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is the completely antisymmetric normalized spin state for the two fermions and often refered to as the "singlet" state.

## 7.3 INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with fundamental concepts involving a system of $N$ identical particles were first investigated using three years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight was gained concerning these difficulties from responses of 14 students during a total of 81 hours of individual interviews. A "think aloud" protocol was used during the interviews in which students were asked to think aloud as they answered the questions posed without being disturbed [86]. Once the students had answered each question to the best of their ability, we asked them to clarify their reasoning and probed deeper into certain difficulties to gain a better understanding of the cognitive mechanisms behind these difficulties. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates and 30 first-year physics graduate students in their respective QM courses. The QuILT included a pretest, the tutorial, and a posttest. Students were given the pretest after traditional, lecture-based instruction on identical particles. The pretests were not returned to the students. Students began working on the tutorial in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest, tutorial, and posttest were analyzed for understanding of fundamental concepts involving a system of identical particles. If

new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in our investigation, the identical particles were restricted to one spatial dimension for convenience. Initially, students were asked to consider the wavefunction of the many-particle system ignoring the spin part of the wavefunction. Later, students considered the completely symmetrized many-particle wavefunction consisting of both the spatial and spin parts of the wavefunction. In order to familiarize the students with the notation, in the QuILT, they were given that $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for particles in states $n_1$ and $n_2$ and with coordinates $x_1$ and $x_2$, respectively.

Below, we discuss student difficulties in response to questions that were posed either during individual interviews or as in-class clicker questions, open-ended questions on quizzes or exams, or as questions on the pretest of the QuILT. Additional insight into these difficulties was gleaned during the individual think-aloud interviews in which students were asked questions pertaining to these issues.

### 7.3.1 Difficulty realizing that the Hamiltonian for a system of $N$ non-interacting identical particles in the product-space should be written in terms of the sum of the single-particle Hamiltonians

To investigate students' understanding of the Hamiltonian for a system of $N$ non-interacting identical particles, question Q1 below was asked on both the pretest after traditional lecture-based instruction on relevant concepts and posttest after engaging with the QuILT. In particular, Q1 is intended to determine whether students could identify that the Hamiltonian for a system of non-interacting identical particles is expressed as the sum of the individual Hamiltonians in the product space as in Eq. (7.3):

**Q1.** *Write the Hamiltonian for a system of $N$ non-interacting identical particles in terms of the Hamiltonians for the $i^{th}$ particle ($i = 1, 2, \ldots, N$).*

Below, we discuss two types of common difficulties students had writing the many-particle

Hamiltonian for a system of $N$ non-interacting identical particles.

**Incorrectly writing the many-particle Hamiltonian as the sum of the single-particle Hamiltonians $\hat{H}_i$ in which $\hat{H}_i$ is in the Hilbert space of individual particles:** The Hamiltonian for a system of $N$ non-interacting identical particles is the sum of the $M^N$-dimensional individual Hamiltonians $\hat{\mathbf{H}}_i$ for each particle $i$ as in Eq. 7.3. Interviews suggest that many students struggled to correctly reason about the dimension of the many-particle Hamiltonian. In response to Q1, some interviewed students incorrectly claimed that the Hamiltonian for the system of $N$ non-interacting identical particles was $\sum \hat{H}_i$ (as opposed to $\sum \hat{\mathbf{H}}_i$). They did not realize that each term in the sum must be an element in the $M^N$ dimensional product space (instead of an $M$-dimensional Hilbert space). They had difficulty identifying that the single-particle Hamiltonian $\hat{H}_i$ only acts on the subspace of the $i^{th}$ particle and that the many-particle Hamiltonian $\hat{\mathbf{H}}_i$ must have the dimensionality of the product space and contain identity operators in the subspaces of the $N-1$ other particles as in Eq 7.2. For example, the Hamiltonian for a spin-1/2 particle can be represented as a $2 \times 2$ matrix in a given basis; and the Hamiltonian for a system of two identical spin-1/2 particles can be represented as a $4 \times 4$ matrix in the product space. However, students with this type of difficulty often claimed that the Hamiltonian for the two non-interacting spin-1/2 particles is a $2 \times 2$ matrix resulting from adding the two $2 \times 2$ matrices for each spin-1/2 particle since the particles are non-interacting. This type of difficulty in determining the dimensionality of an operator in the product space has been documented in other contexts [64, 54].

**Incorrectly writing the many-particle Hamiltonian as the direct product of the single-particle Hamiltonians:** Other students incorrectly claimed that the answer to Q1 is that the Hamiltonian for non-interacting particles is the direct product of the $M^N$-dimensional single-particle Hamiltonians. Some students incorrectly claimed that the many-particle Hamiltonian was $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 \bigotimes \hat{\mathbf{H}}_2 \bigotimes \hat{\mathbf{H}}_3 \bigotimes \ldots \bigotimes \hat{\mathbf{H}}_N$. Students with this type of difficulty did not realize that each single-particle Hamiltonian $\hat{\mathbf{H}}_i$ is $M^N$-dimensional, and that the direct product produces a $(M^N)^N$-dimensional many-particle Hamiltonian. Other students incorrectly claimed that the many-particle Hamiltonian for the non-interacting particles is $\hat{\mathbf{H}} = \hat{H}_1 \bigotimes \hat{H}_2 \bigotimes \hat{H}_3 \bigotimes \ldots \bigotimes \hat{H}_N$. One interviewed student stated that "since the

wavefunction of the many-particle system is the product of the single-particle wavefunctions, then the Hamiltonian for the system of $N$ non-interacting identical particles is also a product of the individual Hamiltonians." This student correctly claimed that the many-particle wavefunction for non-interacting particles is written in terms of the direct product of the single-particle wavefunctions, but incorrectly inferred that the Hamiltonian for the system of non-interacting particles is also written as the direct product (as opposed to the sum) of the individual single-particle Hamiltonians in the product space. This student and others with this type of response did not realize that for a system of non-interacting identical particles there is no entanglement between the single particle Hamiltonians $\hat{H}_i$.

### 7.3.2 Difficulty realizing that each indistinguishable particle should have its own unique coordinate

Many students had difficulty with the fact that each quantum particle in a system of identical particles is indistinguishable but each particle is still expressed with a unique coordinate. For example, for the many-particle wavefunction for a system of $N$ indistinguishable particles, the coordinates $x_1, x_2, x_3, \ldots, x_N$ can be used to label the particles. The symmetrization requirement of the many-particle wavefunction ensures indistinguishability and accounts for the fact that there is no way to determine which particle is in which single-particle state. To probe whether students are able to identify that each identical particle has a unique coordinate in the product making up one of the terms, question Q2 was posed on both the pretest and posttest for the QuILT:

**Q2.** *For a system of three non-interacting identical particles, write a three-particle wavefunction* **in position representation** *for which all three particles are in different single-particle states for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no possible three-particle wavefunction for the given system of three particles, state the reason.* **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

Table 20: The percentage of undergraduate (N=25) and graduate students (N=30) who displayed the given difficulty in Q2 after traditional instruction.

| Difficulty | Undergraduate Students (%) | Graduate Students (%) |
|---|---|---|
| Did not use unique coordinates for each particle | 32 | 43 |
| Wrote the wavefunction as the sum of the single-particle wavefunctions | 16 | 10 |

Regardless of the type of particle, there should be a unique coordinate for each identical particle in the three-particle wavefunction. However, many students with this type of difficulty claimed that since there is no way to determine which particle is in which single-particle state, there is no way to assign a distinct coordinate to each indistinguishable particle. For example, one interviewed student incorrectly claimed that "we must use the coordinate $x$ for all the indistinguishable particles since we don't know where each particle is." This student went on to claim that the many-particle wavefunction for a system of three indistinguishable particles in which one of the particles is in each of the single-particle stationary states labeled $\psi_{n_1}(x)$, $\psi_{n_2}(x)$, and $\psi_{n_3}(x)$ is $\psi_{n_1}(x)\psi_{n_2}(x)\psi_{n_3}(x)$. This type of reasoning was common among students. Table 20 summarizes the number of students who displayed this type of difficulty in question Q2 after traditional lecture-based instruction.

### 7.3.3 Difficulty realizing that the many-particle wavefunction must be written in terms of the product (NOT the SUM) of the single-particle wavefunctions

Many students struggled to write the basis states for the many-particle wavefunction for a system of non-interacting identical particles in terms of the product of the single-particle wavefunctions. Question Q2 was intended to probe whether students were able to identify that the wavefunction for a system of identical particles must be expressed in terms of the direct product (as opposed to the sum) of the single-particle wavefunctions since these form possible basis states for a many-particle system.

Regardless of the type of particle, the three-particle wavefunction for a system of identical particles in Q2 must be expressed in terms of the direct product of the single-particle wavefunction. For example, the three-particle wavefunction for a system of three fermions (assuming $n_1 \neq n_2 \neq n_3$) is

$$\frac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3)$$
$$+\psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) + \psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)].$$

In order to satisfy the symmetrization requirements, the three-particle wavefunction for a system of three fermions consists of six terms. However, each term is expressed as the direct product of the single-particle wavefunctions.

Some students with this type of difficulty incorrectly expressed the many-particle wavefunction in question Q2 in terms of the sum (as opposed to the direct product) of the single-particle wavefunctions, such as $\psi_{n_1}(x_1) + \psi_{n_2}(x_2) + \psi_{n_3}(x_3)$. For example, one interviewed student considered this issue before deciding that the many-particle wavefunction must be written in terms of the sum. This student incorrectly stated that "since the particles do not interact, the wavefunction will just be the sum of the (single-particle stationary state) wavefunctions." This student was later asked whether the wavefunction for a system of identical particles is always expressed as the sum he had written down or whether there are any situations in which the many-particle wavefunction must be written in terms of the direct product of the single-particle wavefunctions. After a moment of hesitation, the student stated that only "if the particles were interacting, then the many-particle wavefunction could be expressed as the product (of the single-particle) wavefunctions." However, regardless of whether the particles are interacting or non-interacting, the many-particle wavefunction can always be expressed in terms of the direct product of the single-particle wavefunction since the many-particle wavefunctions obtained from the product of the single-particle wavefunctions form a basis for the Hilbert space for a many-particle system. Table 20 shows the percentages of students who expressed the many-particle wavefunction as a sum of the single-particle wavefunctions (as opposed to terms involving the product of the single-particle wavefunctions) for question Q2.

The next question, Q3, involves both the spatial and spin parts of the wavefunction. The question considers the ground state of the Helium atom which has two "non-interacting" electrons (i.e., two identical spin-1/2 particles with $s_1 = 1/2$ and $s_2 = 1/2$ in which $s_i$ is the spin quantum number for the $i^{th}$ electron). Q3 probed students' proficiency at identifying the spatial part of the wavefunction that corresponds to the ground state of Helium and whether it is symmetric or anti-symmetric (students were asked to assume that the two electrons in the Helium atom are non-interacting) and also probed their understanding that the spin state of the two electrons must be such that the overall wavefunction is antisymmetric.

**Q3.** *If the electrons in a Helium atom are in the ground state, write down the spin state of the two electrons,* $|s,\ m_s\rangle$.

In Q3, the spatial part of the wavefunction for a system of two electrons in a Helium atom in the ground state is symmetric, and therefore, the spin part of the wavefunction must be antisymmetric. The spin part of the wavefunction is

$$|s,\ m_s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2).$$

When asked to write the spin part of the wavefunction for a system of two electrons in the ground state of a Helium atom in Q3, some students expressed the spin part of the wavefunction as the sum of spin states of the two electrons. For example, one student with this type of difficulty wrote the spin part of the wavefunction as

$$|s,\ m_s\rangle = \frac{1}{\sqrt{2}}(\uparrow + \uparrow).$$

This student and others with similar difficulties often incorrectly claimed that each electron was in the "spin up" state and also incorrectly claimed that the spin part of the two-particle wavefunction is the sum of the two spin states for each electron. Using the notation described earlier to identify the first electron as $|\uparrow\rangle_1$ and the second electron as $|\uparrow\rangle_2$, students with this type of difficulty wrote that the spin part of the wavefunction takes the form $|s,\ m_s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 + |\uparrow_2)$, which is not a valid spin state in the product space.

In summary, we find that many students had difficulty realizing that the many-particle wavefunction should be expressed in terms of a direct product of the single-particle wavefunctions. This type of difficulty was found for both the spatial part and spin part of the wavefunction.

### 7.3.4 Difficulty realizing how each term in a many-particle Hamiltonians would act on a many-particle state consisting of a product of single-particle states

The Hamiltonian for a system of non-interacting identical particles is expressed as the sum of the Hamiltonian for the individual particles. For example, for a system of three non-interacting, identical particles, the many-particle Hamiltonian is $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 = \hat{H}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 + \hat{I}_1 \otimes \hat{H}_2 \otimes \hat{I}_2 \otimes \hat{I}_3 + \hat{I}_1 \otimes \hat{I}_2 \otimes \hat{H}_3$, in which $\hat{I}_i$ is the identity operator in the Hilbert space for the wavefunction of the $i^{th}$ particle. Some students struggled to identify how each term in the Hamiltonian would act on a state consisting of a product of single-particle states. In particular, they had difficulty recognizing in the many-particle product state in the uncoupled representation that the operators in the Hilbert space of a given particle act only on the single-particle states of that particle. For example, students were asked to evaluate the following expression: $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]$ in which $\hat{\mathbf{H}}_1$ is the Hamiltonian for particle 1 in the two-particle system and the single-particle states $\psi_{n_1}$ and $\psi_{n_2}$ are stationary states for particles 1 and 2, respectively (i.e., $\hat{H}_i\psi_{n_j}(x_i) = E_{n_j}\psi_{n_j}(x_i)$) with energy $E_{n_1}$ and $E_{n_2}$, respectively. One interviewed student incorrectly claimed that "$\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = 0$, because $\hat{\mathbf{H}}_1$ only acts on $\psi_{n_1}(x_1)$ and $\hat{\mathbf{H}}_1\psi_{n_2}(x_2) = 0$". This student and others who provided similar responses struggled to realize that the operator $\hat{\mathbf{H}}_1$ is equivalent to $\hat{H}_1 \otimes \hat{I}_2$, in which $\hat{H}_1$ acts on the subset of the Hilbert space corresponding to particle 1 and the identity operator $\hat{I}_2$ acts on the subset of the Hilbert space corresponding to particle 2. Thus, the correct answer to the above question is $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2)$.

### 7.3.5 Incorrectly determining the symmetry based on the appearance of a +/- sign in the many-particle wavefunction

Nature demands that the many-particle wavefunction for a system of indistinguishable bosons be completely symmetric and the many-particle wavefunction for a system of indistinguishable fermions be completely antisymmetric. Therefore, in order to recognize and generate a many-particle wavefunction for a system of indistinguishable particles, students must be able to determine a completely symmetric/antisymmetric wavefunction involving both spatial and spin degrees of freedom.

Question Q4 was posed during the think aloud interviews to investigate students' proficiency at identifying whether the spin part of a wavefunction is a symmetric or antisymmetric wavefunction. Students were given Eq. (9.1) before this question and were familar with the shorthand notation used in Q4.

**Q4.** *For the spin part of the wavefunction of a two-particle system given below, identify whether the spin state is symmetric, antisymmetric, or neither symmetric nor antisymmetric with respect to exchange of the two particles. Explain your reasoning.*

(a) $|\uparrow\uparrow\rangle$

(b) $|\downarrow\downarrow\rangle$

(c) $|\uparrow\downarrow\rangle$

(d) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

(e) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

In Q4, options (a), (b), and (d) are symmetric spin states (triplet states) since exchanging the two particles results in the same wavefunction. Option (e) in Q4 is an antisymmetric spin state (singlet state) since exchanging the two particles results in the original wavefunction multiplied by -1. Option (c) in Q4 is neither a symmetric nor an antisymmetric spin state.

Some students incorrectly applied a heuristic by which they claimed that a wavefunction is symmetric if it is written in terms of a sum. These students simply looked for all "+" signs to determine that a wavefunction is symmetric. They claimed that any wavefunction written as terms added together is a symmetric wavefunction. By a similar logic, these same students looked for a "-" sign to determine whether a given wavefunction is antisymmetric.

Some claimed that any wavefunction that has at least one negative sign is antisymmetric. In particular, their determination of whether the wavefunction is antisymmetric did not depend on a complete antisymmetrization requirement and the number of terms that had a negative sign in the wavefunction (which is a necessary but not sufficient condition). They merely looked for the presence of at least one minus sign in the wavefunction to determine that the wavefunction is antisymmetric. For example, in response to question Q4(a) and (b), one interviewed student incorrectly claimed that the spin part of the wavefunction given by $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ is neither symmetric nor antisymmetric as "the wavefunction is not a sum so it can't be symmetric and there is not a minus sign, so it can't be antisymmetric." However, the spin part of the wavefunction given by $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ is completely symmetric as the exchange of the two particles results in the same wavefunction, thus there need not be a plus sign in order for a wavefunction to be symmetric. Other students with this type of response used similar reasoning when determining the symmetry of a wavefunction.

### 7.3.6 Difficulty realizing that a linear combination of the product of single-particle wavefunctions can be a many-particle stationary state wavefunction

The many-particle wavefunction for a system of indistinguishable fermions must be completely antisymmetric and the many-particle wavefunction for a system of indistinguishable bosons must be completely symmetric. In general, when expressing the many-particle wavefunction in terms of the single-particle wavefunctions, one must satisfy the symmetrization requirement through a linear combination of the direct products of the single-particle wavefunctions for each particle. However, many students struggled with the fact that the completely symmetric/antisymmetric wavefunction consisting of an appropriately chosen linear combination of the products of single-particle wavefunctions (with the coordinates permuted) is a many-particle stationary state wavefunction.

Question Q5 was posed during the think aloud interviews to probe students' proficiency in determining whether the following completely symmetric and antisymmetric wavefunctions are stationary state wavefunctions for a system of two non-interacting identical

particles (bosons and fermions, respectively, for Q5(a) and Q5(b)). Students were asked to rewrite the following expressions on the right-hand side without any operators, i.e., perform the operations:

**Q5.** *Answer the following questions for a system of two non-interacting identical particles, whose single-particle wavefunctions satisfy the Time Independent Schrödinger Equation (TISE), $\hat{H}_i\psi_{n_j}(x_i) = E_{n_j}\psi_{n_j}(x_i)$ for the $i^{th}$ particle with coordinate $x_i$. Assume $n_1 \neq n_2$*

(a) $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)] =$
(b) $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] =$

The correct answer to Q5(a) is

$$
\begin{aligned}
&(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\quad = E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_2}\psi_{n_2}(x_1)\psi_{n_1}(x_2) + E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_1}\psi_{n_2}(x_1)\psi_{n_1}(x_2) \\
&\quad = (E_{n_1} + E_{n_2})[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\quad = E[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)],
\end{aligned}
$$

in which $E = E_{n_1} + E_{n_2}$ is the total energy of the two particle system. Thus, ignoring spin, the completely symmetric wavefunction given in Q5(a) is a stationary state wavefunction for the two-particle system (e.g., two spinless bosons). Similarly, the completely antisymmetric wavefunction in Q5(b) is a stationary state wavefunction with total energy $E = E_{n_1} + E_{n_2}$ for the system of two non-interacting particles (e.g., two spinless fermions). Below, we discuss some student difficulties with Q5 related to the linear combination of the products of the single-particle states.

**Overgeneralizing a system with no degeneracy to incorrectly claim that a linear combination of many particle stationary states can not be an energy eigenstate for the many-particle system:** Many students struggled with the fact that each of the two terms in the wavefunction (products of single particle states) that are added or subtracted in parts (a) and (b) of Q5 have the same total energy for the two-particle Hamiltonian $\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ and hence the wavefunctions in parts (a) and (b) of Q5 satisfy the TISE for the two-particle system. One interviewed student correctly stated that "a linear combination of the ground state and first excited state for a one-dimensional infinite square well is not a stationary state". Then he incorrectly stated that "any linear combination (of stationary states) cannot be a stationary state" and hence the wavefunctions in parts (a) and (b) in Q5

do not satisfy the TISE when answering Q5 for the system of two non-interacting particles. However, this student was incorrectly overgeneralizing the behavior of a one-particle system in which there is no degeneracy in the single-particle energy spectrum to a case in which it is not applicable. For systems that possess degeneracy in their energy spectrum, any linear combination of energy eigenstates (stationary states) with the same energy is also an energy eigenstate.

This student and others with this difficulty struggled to recognize that an appropriately chosen linear combination of the products of the single-particle wavefunctions, e.g., those in Q5, are valid two-particle stationary state wavefunctions. For example, each term in the symmetric or antisymmetric many-particle stationary state wavefunction in Q5 (consisting of products of the single particle wavefunctions) has the same energy $E_{n_1}+E_{n_2}$ and therefore, their linear combination is an appropriately symmetrized two-particle stationary state with the same energy. However, each term in the two-particle state in Q5 (which is a basis state in the product space) is not itself a two-particle stationary state wavefunction for fermions or bosons since the two-particle stationary state wavefunction in these cases must also satisfy the symmetrization requirement for the given system of identical particles. In general, a many-particle stationary state wavefunction for bosons or fermions consists of a linear combination of the products of single-particle stationary state wavefunctions which are appropriately symmetrized for the given case.

**Making computational mistakes and not identifying the inconsistency:** Many students struggled to show that an appropriately chosen linear combination as in Q5 is the stationary state wavefunction for the many-particle system and satisfies the many-particle TISE. For example, for question Q5, some students had difficulty realizing that the two-particle wavefunction $\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)$ is a unnormalized two-particle stationary state wavefunction for the system of two non-interacting fermions with Hamiltonian $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ due to computational mistakes and how they interpreted their mistakes. For

example, the following is a student's written response to part (b) of question Q5:

$$
\begin{aligned}
&(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\quad = \hat{H}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] + \hat{H}_2[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\quad = (E_{n_1} - E_{n_2})[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\qquad +(E_{n_2} - E_{n_1})[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] \\
&\quad = 0.
\end{aligned}
\tag{7.9}
$$

This was a very common mistake and led to incorrect inferences by students. Below, we discuss incorrect reasoning related to interpretation of the computational mistake in Eq. 7.9.

Total energy of the system is zero even if the single-particle energies are not zero: Some students struggled to reconcile that the total energy for a system of non-interacting identical particles is the sum of the energies of all the individual particles. For example, if two identical particles are in the symmetrized state given in Q5 (b), then the total energy must be $E_{n_1}+E_{n_2}$, which cannot be zero unless $E_{n_1}+E_{n_2}=0$. Students with this type of difficulty claimed that the total energy is zero according to Eq. 7.9. Other students making this type of computational mistake (as in Eq. 7.9) who stated that the total energy in the state in Q5(b) is zero, initially questioned whether they had made a mistake as they had doubts that the expression in Q5(b) yields zero. However, they often chose to trust their mathematical manipulation rather than their intuition and claimed that obtaining zero in Q5 (b) implies that the energy of the two-particle system is zero. This type of over-reliance on the results of mathematical manipulation when a student's answer does not match his/her intuition has also been observed among introductory physics students [38]. The students with this type of difficulty often did not reflect on whether they had made a mathematical mistake. In other words, they did not engage in sufficient metacognition to evaluate the reasonability and consistency of their answer after arriving at the result in Eq. 7.9.

Incorrectly claiming that if the energy of the many-particle system is zero then the wavefunction is not a many-particle stationary state wavefunction: Some interviewed students who made the computational mistake described in Eq. 7.9 for Q5(b) by incorrectly stating that $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] = 0$ then incorrectly claimed that since

$\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ acting on the state yields zero then the state $\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)$ cannot be a many-particle stationary state wavefunction because the energy of the system cannot be zero. However, the value of the energy of the many-particle system as determined by the many-particle TISE in Eq. 7.9 does not dictate whether the given wavefunction is or is not a stationary state wavefunction. In particular, a total energy of zero for the many-particle system simply means the sum of single-particle energies is zero and does not mean that the wavefunction is not a many-particle stationary state wavefunction.

Incorrectly claiming that an antisymmetric many-particle wavefunction cannot be a many-particle stationary state wavefunction: Some students who obtained zero as in Eq. 7.9 incorrectly concluded that a symmetric linear combination of products of single particle states is a valid many-particle stationary state wavefunction but that an antisymmetric linear combination is not a valid many-particle stationary state wavefunction. For example, some students who made the computational mistake in Eq. 7.9 in the context of solving Q5(b) and obtained a zero on the right hand side correctly calculated the right hand side in Q5(a). These students determined the energy of the two-particle system to be $2(E_{n_1} + E_{n_2})$ for the symmetric linear combination $\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)$. They correctly stated that the symmetric linear combination in Q5(a) is a many-particle stationary state wavefunction. However, when they incorrectly determined that the right-hand side of the expression in Q5(b) is zero, they then incorrectly claimed that this meant that the antisymmetric linear combination $\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)$ is not a possible stationary state wavefunction. Some of these students then went on to incorrectly generalize their result in Eq. 7.9 and claim that a linear combination of the products of single-particle wavefunction is a stationary state wavefunction if the linear combination produces a completely symmetric wavefunction, but is not a stationary state wavefunction if it produces a completely antisymmetric wavefunction for a system of identical particles. Some of the confusion after obtaining zero on the right-hand-side was due to the fact that students had learned that two fermions cannot be in the same single particle state, consistent with Pauli's exclusion principle (due to the fact that the overall fermionic wavefunction is completely antisymmetric). In particular, if one tries to put two identical fermions in the same single particle state, one obtains zero for the wavefunction, which is not possible consistent with Pauli's exclusion principle. Some stu-

dents overgeneralized this fact to conclude that two fermions cannot have an antisymmetric wavefunction such as that in Q5(b) (even if they are in different single particles states) when they obtained zero on the right hand side in Q5(b) due to algebraic mistakes.

## 7.4 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 7.4.1 Development and Validation of the QuILT

Based upon our research of student difficulties with fundamental concepts involving systems of identical particles, we developed a QuILT that strives to build a consistent and coherent knowledge structure while at the same time addressing the common student difficulties. The development of the QuILT was guided by a cognitive task analysis [**?**] from both a physics expert perspective and a novice (or student) perspective which consisted of the requisite knowledge and skills necessary for a functional understanding of a system of identical particles. The initial analysis was conducted from an expert perspective in which the authors outlined the required knowledge and skills and the order in which they are useful in solving problems. This was iterated with members of the physics faculty at the University of Pittsburgh. However, in an effort of determine if there are additional areas student may struggle with that are not predicted by the experts (due to expert blindspot), we conducted individual student interviews.

The QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure that the content was appropriate and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that was incorporated in the next version of the QuILT. Once it was agreed upon by the faculty that the content was clear and correct, the QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording was unambiguous, the scaffolding was effective, and to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and pro-

vided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the entire section of the tutorial focusing on these issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and to determine whether there were any changes that needed to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and in subsequent interviews. During each step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback to help with the common difficulties. After it was deemed successful by faculty and students (who performed well in the posttest after engaging with the QuILT in one-on-one administration), the QuILT was then administered to students in various advanced quantum mechanics courses.

### 7.4.2 Structure of the QuILT

The QuILT strives to help students engage with active learning tasks by employing an inquiry-based approach which requires students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. It consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is administered in class during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, the students are given the tutorial and encouraged to work together in small groups in class. The tutorial can be used to guide in-class discussion. The tutorial can also be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, students submit the tutorial for grading and are then given the posttest (similar to the pretest). The posttest is administered in class as an individual assessment in which the students are not permitted any additional resources beyond what is provided in the posttest.

The QuILT incorporates guided inquiry-based learning sequences which consist of sev-

eral questions, each building upon the previous question(s), that require students to take a stand and actively engage with the them in the learning process. The QuILT also includes hypothetical student conversations in which they must analyze each hypothetical student's statement to determine whether they are correct and explain why they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify any inconsistencies in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the guided learning sequences in the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include portions that strive to present the students with a contradiction between the answers to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back to reconcile any remaining difference between the correct reasoning and their own reasoning before moving on to the next section.

### 7.4.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples focusing on fundamental concepts for a system of identical particles regarding the form of the Hamiltonian and many-particle wavefunction and identifying and generating appropriate symmetric/antisymmetric wavefunctions in a given situation. Below are examples from the QuILT of scaffolding support intended to help students with these concepts and address some of the common difficulties.

**Helping students realize that the Hamiltonian for a system of non-interacting**

**identical particles should be expressed as a sum of operators that act on states in the product space:** In a guided inquiry-based learning sequence in the QuILT, the students are asked to consider the following hypothetical student conversation regarding the form of the Hamiltonian. After considering each hypothetical students' statement, they are asked whether they agree or disagree with each statement and to provide their reasoning for doing so.

**Student 1:** *In an infinite square well, we are only permitted to have one-particle in the well. If the system has two non-interacting identical particles, we MUST have two infinite square wells in order to place each particle.*

**Student 2:** *I disagree. We can have two non-interacting identical particles in the same infinite square well. If the particles are non-interacting and confined to a well of width a, the Hamiltonian for each particle in the product space will be* $\hat{\mathbf{H}}_i = \frac{\hat{p}_i^2}{2m} + V(x_i)$*, in which*

$$V(x_i) = \begin{cases} 0 & \text{if} \quad 0 \leq x_i \leq a \\ \infty & \text{otherwise} \end{cases} \qquad (i = 1, 2).$$

*The Hamiltonian for the system of two non-interacting identical particles in the same well in the product space is* $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2$*, where* $\hat{H}_1$ *and* $\hat{H}_2$ *are the Hamiltonians in the subspaces for the individual particles.*

Student 1 is incorrect and Student 2 is correct in the preceding conversation. By using an explicit example that is familiar to the students and via additional scaffolding, the QuILT strives to help students learn that the Hamiltonian for a system of non-interacting identical particles should be expressed as a sum in the product space as in Eq. 7.2.

**Helping students realize that each identical particle should have its own unique coordinate:** The QuILT strives to help students realize that each identical particle should have its own unique coordinate even though each particle is indistinguishable from all the other particles in the system. The following is an excerpt from a hypothetical student conversation in the QuILT regarding whether the single-particle wavefunctions in a product should have the same or different coordinates to properly specify a three-particle wavefunction for a system of three non-interacting identical particles. The students must state which hypothetical student they agree with and why.

**Student 1:** *We must assign a different coordinate to each identical particle. The wavefunction will have terms such as* $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$.

**Student 2:** *No. I disagree with Student 1. When the particles are indistinguishable, we can't possibly distinguish their individual coordinates. So the wavefunction will have terms such as* $\psi_{n_1}(x)\psi_{n_2}(x)\psi_{n_3}(x)$

Student 1 is correct and Student 2 is incorrect in the preceding conversation. A unique coordinate should be assigned to each identical particle. Follow-up guided inquiry-based learning sequences in the QuILT strive to help students focus on the fact that the symmetry requirement for the many-particle wavefunction is due to the indistinguishability of the particles and that the indistinguishability is not represented by all particles having the same coordinate (but by how the many-particle wavefunction is written). The students are later asked to construct symmetric and antisymmetric many-particle wavefunctions for various systems of identical particles with different coordinates for each particle and are asked to reflect upon how those wavefunctions take into account the indistinguishability of the particles.

**Helping students realize that each term in the many-particle stationary state wavefunction should be expressed in terms of a direct product of single-particle wavefunctions:** In the QuILT, students are asked to construct many-particle stationary state wavefunctions for different systems and provided scaffolding support to help them realize that the many-particle stationary state wavefunction should be expressed in terms of the direct product of the single-particle stationary state wavefunctions. For example, they are asked to construct the many-particle stationary state wavefunction for a system of three indistinguishable particles (identical fermions, identical bosons, and identical particles that can be treated as distinguishable) in which the particles are in three different single particle stationary states (as in Q2). They are also asked to construct the many-particle stationary state wavefunction for a system in which two of the three indistinguishable particles are in the same single particle stationary state.

Additionally, students are asked to explicitly show that the wavefunction $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$ cannot be a two-particle stationary state wavefunction for the Hamiltonian $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ for a system of two non-interacting identical particles. Students reflect on whether the wavefunction given as the sum of the two single-particle wave-

functions satisfies the time-independent Schrödinger equation for a many-particle system $\hat{\mathbf{H}}\Psi(x_1, x_2) = E\Psi(x_1, x_2)$. Q6 is an excerpt from a guided inquiry-based learning sequence in the QuILT in which the students consider whether a wavefunction expressed as the sum or the product of the single-particle states satisfies the TISE for a two-particle system. In particular, Q6 below asks students to write the right hand side without any operator, if possible, in each case Q6(a)-Q6(f) and reason whether the wavefunction given in each case can be a possible basis state for the many-particle stationary state wavefunction (i.e., symmetrization of the wavefunction for fermions and bosons has not been accounted for in Q6):

**Q6.** *Write the right-hand side without operators, if possible, in the following questions for a system of two non-interacting identical particles, whose single-particle wavefunctions satisfy the Time Independent Schrödinger Equation (TISE),* $\hat{H}_i\psi_{n_j}(x_i) = E_{n_j}\psi_{n_j}(x_i)$ *for the* $i^{th}$ *particle with coordinate* $x_i$ *in the single-particle state given by* $n_j$*. Assume* $n_1 \neq n_2$*. If it is not possible to write the right-hand side without operators and without encountering difficulties or inconsistencies, explain why.*

*(a)* $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$

*(b)* $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$

*(c)* $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$

*(d)* $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] =$

*(e)* $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] =$

*(f)* $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) =$

*Based upon your response, explain which of the wavefunctions in Q6 (a)-(f) can be used as a basis state for the product space of a two-particle system.*

If the wavefunction is expressed as the sum of the single-particle wavefunctions as in Q6(a)-Q6(c), then it is not a possible basis state for writing a two-particle wavefunction since the sum of the single-particle states is not a two-particle state in the product space. For example, in Q6(a), in the term $\hat{\mathbf{H}}_1\psi_{n_2}(x_2)$, the single-particle Hamiltonian $\hat{H}_1$ can only act on the wavefunction in the part of the Hilbert space corresponding to particle one, but the wavefunction corresponding to particle one is "1." However, "1" is not a possible wavefunction since it is not normalizable. There are similar inconsistencies in Q6(b) and Q6(c) when the sum of the two single-particle stationary states is considered.

However, each of the wavefunctions expressed as the product of the single-particle wavefunctions in Q6 (d)-(f), satisfy the TISE for the two-particle system and these states can be used as basis states for a two-particle system. For example, in Q6(f), the correct answer is

$$\begin{aligned}
\hat{\mathbf{H}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= \hat{\mathbf{H}}_1\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \hat{\mathbf{H}}_2\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (\hat{H}_1 \otimes \hat{I}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) + (\hat{I}_1 \otimes \hat{H}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (\hat{H}_1\psi_{n_1}(x_1))(\hat{I}_2\psi_{n_2}(x_2)) + (\hat{I}_1\psi_{n_1}(x_1))(\hat{H}_2\psi_{n_2}(x_2)) \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_1)E_{n_2}\psi_{n_2}(x_2) \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (E_{n_1} + E_{n_2})\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= E\psi_{n_1}(x_1)\psi_{n_2}(x_2).
\end{aligned}$$

In the next guided inquiry-based learning sequence, students are asked to reflect upon two hypothetical student conversations regarding which of the wavefunctions in Q6 are possible basis states for two-particle wavefunctions. For example, below are excerpts from a hypothetical student conversation regarding whether the basis states for the two-particle stationary state wavefunction can be written in terms of the sum of the single-particle wavefunctions. The students must agree or disagree with each hypothetical student and explain their reasoning for doing so:

**Student 1:** *The basis state that can be used to construct the two-particle stationary state wavefunction for a system of two non-interacting identical particles can be written in terms of the sum of the single-particle wavefunctions,* $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$.

**Student 2:** *I disagree. The sum of the single-particle states* $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$ *is not in the Hilbert space of the two-particle system. When the two-particle Hamiltonian* $\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ *acts on the state* $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$*, there are inconsistencies. Consider terms of the type* $\hat{\mathbf{H}}_1\psi_{n_2}(x_2)$ *when* $\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ *acts on* $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$.

**Student 1:** *Isn't* $\hat{\mathbf{H}}_1\psi_{n_2}(x_2) = 0$*?*

**Student 2:** *No. The single-particle Hamiltonian* $\hat{H}_1$ *only acts on the wavefunction corresponding to particle one but for this wavefunction* $\psi_{n_2}(x_2) = 1 \cdot \psi_{n_2}(x_2)$*, the wavefunction*

*corresponding to particle one is "1", which is not normalizable.*

**Student 3:** *I agree with Student 2. The sum of the single-particle states* $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$ *cannot be a basis state for a two-particle system.*

Students 2 and 3 are correct while Student 1 is incorrect in the preceding conversation. Below is the subsequent hypothetical student conversation in which students are asked to reflect upon whether the basis states for the two-particle stationary state wavefunction can be written in terms of the product of the single-particle wavefunctions.

**Student 1:** *The basis states used to construct the two-particle stationary state wavefunctions for a system of two non-interacting identical particles can be written in terms of the product of the single-particle wavefunctions, such as* $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$.

**Student 2:** *I agree with Student 1. Also, if we consider terms of the type* $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ *in the wavefunction for a system of two non-interacting identical particles, then it satisfies the TISE, as follows:*

$$\begin{aligned}
\hat{\mathbf{H}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (\hat{H}_1 \otimes \hat{I}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) + (\hat{I}_1 \otimes \hat{H}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= [\hat{H}_1\psi_{n_1}(x_1)][\hat{I}_2\psi_{n_2}(x_2)] + [\hat{I}_1\psi_{n_1}(x_1)][\hat{H}_2\psi_{n_2}(x_2)] \\
&= [\hat{H}_1\psi_{n_1}(x_1)]\psi_{n_2}(x_2) + \psi_{n_2}(x_2)[\hat{H}_2\psi_{n_1}(x_1)] \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_1)E_{n_2}\psi_{n_2}(x_2) \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (E_{n_1} + E_{n_2})\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= E\psi_{n_1}(x_1)\psi_{n_2}(x_2),
\end{aligned}$$

*in which* $E = E_{n_1} + E_{n_2}$.

Both Student 1 and Student 2 are correct in the preceding conversation. After working through the inquiry-based learning sequences and hypothetical conversations, students are provided checkpoints to help them reconcile their initial ideas with the correct reasoning. One goal is to have students reflect upon their own responses to Q6 to determine that basis states for a many-particle stationary state wavefunction cannot be expressed as the sum of the single-particle wavefunctions as in Q6 (a)-(c). On the other hand, a many-particle

Table 21: The percentage of students who expressed the Hamiltonian for a system of non-interacting identical particles as the sum of the Hamiltonians for the individual particles for the undergraduate (number of students $N = 25$) and graduate students ($N = 30$).

| Hamiltonian as Sum/ Direct Product | Undergraduate Students(%) | | Graduate Students(%) | |
|---|---|---|---|---|
| | Pre | Post | Pre | Post |
| Sum | 88 | 100 | 83 | 90 |
| Direct Product | 0 | 0 | 10 | 3 |

wavefunction expressed as a product of the single-particle wavefunctions (e.g., with the basis states in Q6(d) and Q6(f)) satisfy the TISE and are possible basis states for writing a many-particle wavefunction. Students are provided further scaffolding support that strives to help them identify the form of the possible basis states for writing the many-particle wavefunction, e.g., that the basis states for the many-particle wavefunction must be expressed in terms of the product and not the sum of the single-particle wavefunctions.

**Helping students identify and generate symmetric/antisymmetric wavefunctions for systems of identical bosons or fermions:** The students work through several guided inquiry-based sequences in which they are asked to generate symmetric wavefunctions for a system of identical bosons and antisymmetric wavefunctions for a system of identical fermions. They initially reflect upon cases in which they must only consider the spatial part of the wavefunction (ignore spin part of the wavefunction completely) in order to help them focus on the appropriate symmetrization requirements for fermions and bosons. Then, they are asked to identify and construct both the spatial and spin parts of the many-particle wavefunction for a system of non-interacting identical bosons or fermions. Students are provided checkpoints at the end of each section to allow them to reconcile any discrepancies between their initial reasoning and the correct reasoning.

**Helping students realize that certain linear combinations of the products of the single-particle stationary state wavefunctions can be possible many-particle**

Table 22: The percentage of students who gave unique coordinates to each particle in Q2 for the undergraduate (number of students $N = 25$) and graduate students ($N = 30$).

| | Pre | Post |
|---|---|---|
| Undergraduate | 68 | 100 |
| Graduate | 57 | 90 |

**stationary state wavefunctions:** In the QuILT, students are asked to explicitly show that an appropriately chosen linear combination of the products of single-particle stationary state wavefunctions is a many-particle stationary state wavefunction. For example, as a follow up question to Q6 in the inquiry-based sequence, students are asked to determine whether an appropriately chosen linear combination of products of single-particle stationary states is a possible many-particle stationary state wavefunction as in Q5. They are asked to explicitly show that in a properly symmetrized wavefunction, a linear combination of the products of the single-particle stationary state wavefunctions satisfies the TISE with the many-particle Hamiltonian. The goal is to have students use their responses to questions Q6(d) and Q6(e) to help them evaluate and reflect upon linear combinations of the products of the single-particle states in this context (i.e., reflect upon an appropriately symmetrized wavefunction for identical fermions or bosons). Students are asked to summarize in their own words what they learned from these examples and are then provided with checkpoints which allow them to compare their initial reasoning to the correct reasoning and reconcile any differences.

## 7.5 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional, lecture-based instruction in relevant concepts in DPT but before working through the

Table 23: The percentage of students who expressed the many-particle stationary state wavefunction as a sum or direct product in Q2 on the pretest and posttest for undergraduates (number of students $N = 25$) and graduate students ($N = 30$).

| Wavefunction as Sum/ Direct Product | Undergraduate Students(%) | | Graduate Students(%) | |
|---|---|---|---|---|
| | Pre | Post | Pre | Post |
| Sum | 16 | 0 | 10 | 0 |
| Direct Product | 76 | 100 | 73 | 100 |

tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

Table 21 shows the precentage of students in response to Q1 who expressed the Hamiltonian for a system of non-interacting identical particles as the sum of the Hamiltonians $\hat{\mathbf{H}}_i$ of the $i^{th}$ particle ($i = 1, 2, \ldots, N$). All of the undergraduate students and nearly all of the graduate students answered Q1 correctly. These results are encouraging and suggest that the QuILT is effective in addressing the difficulty students had with the form of the Hamiltonian for the system of identical particles.

Table 22 shows the precentage of students in response to Q2 who labeled each particle with its own unique coordinate. These results are encouraging and suggest that the QuILT is effective at addressing the difficulty students had with incorrectly associating the indistinguishability of the particles with the same coordinate for all the particles.

Table 23 summarizes the pre/posttest results for Q2 and suggests that the QuILT was helpful in determining that the many-particle wavefunction should be expressed as a sum of the direct products (as opposed to a sum) of the single particle wavefunctions. Specifi-

Table 24: The percentage of students who expressed the many-particle stationary state wavefunctions in Q2 for a system of indistinguishable fermions as an antisymmetric linear combination of the products of the single-particle state wavefunctions and a system of indistinguishable bosons as a symmetric linear combination of the products of the single-particle stationary state wavefunctions on the pretest and posttest for undergraduates (number of students $N = 25$) and graduate students ($N = 30$).

| System | Undergraduate Students(%) | | Graduate Students(%) | |
|---|---|---|---|---|
| | Pre | Post | Pre | Post |
| Fermions | 60 | 100 | 60 | 87 |
| Bosons | 56 | 96 | 57 | 97 |

cally, every student stated that the many-particle stationary state wavefunction is expressed as the sum over permutation of the direct products of the single-particle stationary state wavefunctions.

Table e shows the percentage of students who expressed the many-particle stationary state wavefunction for a system of identical fermions as an antisymmetric linear combination of the products of the single-particle stationary state wavefunctions in response to Q2 on the pretest and posttest. Table e also shows the percentage of students who expressed the many-particle stationary state wavefunction for a system of identical bosons as a symmetric linear combination of the products of the single-particle stationary state wavefunctions in response to Q2 on the pretest and posttest. These results suggests that the QuILT helped students in constructing the many-particle stationary state wavefunctions for fermions and bosons as linear combinations of the products of the single-particle stationary state wavefunctions that satisfy appropriate symmetrization requirements. Specifically, over 87% of the graduate students and 96% of the undergraduate students expressed the many-particle stationary state wavefunctions in Q2 as terms in an appropriately symmetrized linear combination of products of the single-particle wavefunctions.

## 7.6 SUMMARY

Investigation of students' understanding of the basics of a system of identical particles helped to uncover many common student difficulties that were used a guide to develop and validate a QuILT. The QuILT strives to help students develop a coherent understanding of fundamental concepts for a system of non-interacting identical particles, e.g., the form of the Hamiltonian and the many-particle stationary state wavefunction for a system of identical particles and how to generate many-particle stationary state wavefunctions that satisfy a given symmetrization requirement. It strives to help students learn that the Hamiltonian for a system of non-interacting identical particles can be expressed as a sum in the product space and the many-particle stationary state wavefunction is expressed in terms of the sum of direct products of the single particle stationary state wavefunctions in which each indistinguishable particle should have its own unique coordinate. The QuILT strives to help students determine the completely symmetric/antisymmetric many-particle stationary state wavefunction by using all the permutations of the labels for the states or the coordinates in the products of the single-particle states with the appropriate symmetrization requirement. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding through a guided inquiry-based approach. The findings suggest that the QuILT is effective in improving students' understanding of the fundamental concepts necessary for a functional understanding of the basics for a system of identical particles.

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# 8.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: WRITING THE MANY-PARTICLE STATIONARY STATE WAVEFUNCTION (IGNORING SPIN)

## 8.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. There have been a number of research studies aimed at investigating student reasoning in QM [14, 15, 16, 17, 18, 19, 20, 21] and improving student understanding of QM [22, 23, 24, 25, 26]. In prior investigations, our group has used the common student difficulties as a guide to help develop research-based learning tools which include the Quantum Interactive Learning Tutorials (QuILTs) [27, 28, 29, 30, 31, 32, 33].

However, there have been relatively few investigations into student difficulties with fundamental concepts involving a system of identical particles. Through researching students' understanding and reasoning about a system of identical particles, we have found many common student difficulties that can hinder the development of a consistent and coherent knowledge structure pertaining to these concepts. Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of the individual who is solving the problem, Simon's framework of "bounded rationality and satisficing" posits that an individual will make decisions while solving problems based upon their current level of expertise, which may not be optimal [34]. Some students may be motivated to find an optimal solution to the QM problems posed by searching for many possible pathways in the problem space. However, if

students' level of expertise is not sufficient to solve the problem on their own and they have not been provided with appropriate guidance and scaffolding support, they may experience cognitive overload and may not be able to determine an optimal solution to the problems posed [34, 35].

Here, we discuss an investigation of student difficulties with concepts related to the many-particle stationary state wavefunction for a system of non-interacting identical fermions or bosons when the spin part of the wavefunction is ignored and how that research was used as a guide in the development, validation, and in-class evaluation of a research-based QuILT that makes use of student difficulties as a guide and strives to provide appropriate scaffolding support to help students develop a good grasp of relevant concepts.

## 8.2 BACKGROUND

In nature, there are two general types of particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g., photons and mesons). A system of $N$ identical particles consists of $N$ particles of the same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in quantum mechanics, identical particles are indistinguishable and there is no measurement that can be performed to distinguish these identical particles from one another. For example, if the coordinates of two identical particles are interchanged, there is no physical observable that would reflect this interchange. To reflect the indistinguishability of these identical particles and make the statistical properties of fermions and bosons consistent with observations, the wavefunction for a system of identical fermions must be completely antisymmetric and the wavefunction for a system of identical bosons must be completely symmetric. Furthermore, one property that distinguishes these two types of particles is that two or more bosons can occupy the same single-particle quantum state, but two or more fermions can never occupy the same single-particle quantum state. The restriction for fermions is known as the Pauli exclusion principle and is consistent with a system of fermions

having a completely antisymmetric wavefunction [36].

Here we focus on the many-particle stationary state wavefunction that is a solution to the Time-Independent Schrödinger Equation (TISE) for a system of non-interacting identical particles. Unless otherwise stated, we will refer to the stationary state wavefunction as the wavefunction. In order to determine the many-particle stationary state wavefunction for a system of non-interacting identical particles, one must first solve the single-particle TISE. The single-particle stationary state wavefunctions are solutions to the single-particle TISE, i.e., $\hat{H}_i\psi_{n_j}(x_i) = E_{n_j}\psi_{n_j}(x_i)$ for the $i^{th}$ particle in the state $\psi_{n_j}(x_i)$. Next, one should construct the many-particle stationary state wavefunction for a system of non-interacting identical particles that can be treated as distinguishable as the product of the single-particle stationary state wavefunctions (these product states can be used to construct the many-particle stationary state wavefunction for identical fermions or bosons). Here, for convenience, we will refer to all direct products of single-particle states as "basis states", regardless of their symmetry under exchange. Please note that for identical fermions, only antisymmetric linear combinations of these basis states are allowed, while for bosons only symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed. The final step is to appropriately symmetrize the many-particle stationary state wavefunction for a system of non-interacting identical fermions or bosons using the product states.

If we have a system of two non-interacting electrons in which one electron is in the single-particle state denoted by $\psi_{n_1}$ and the other electron is in the single-particle state denoted by $\psi_{n_2}$ (assuming $n_1 \neq n_2$), then the wavefunction for the system of two electrons must be completely antisymmetric. Ignoring spin, the normalized two-particle wavefunction in position representation is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\right] \tag{8.1}$$

in which $x_1$ denotes the coordinates of the first electron and $x_2$ denotes the coordinates of the second electron. This completely antisymmetric wavefunction reflects the fact that one electron is in the single-particle state $\psi_{n_1}$ and the other electron is in the single-particle state $\psi_{n_2}$, but we cannot say which electron is in which single-particle state. This wavefunction is also consistent with Pauli's exclusion principle. For example, for a system of two fermions

both in the same single-particle state $\psi_{n_1}$, the antisymmetric wavefunction (ignoring the spin) would be

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_1)\psi_{n_1}(x_2)\right] = 0. \tag{8.2}$$

Thus, there is no wavefunction for a system of two fermions in the same single-particle state and such a state is not possible.

The completely symmetric wavefunction (ignoring the spin) for two bosons in which one boson is in the single-particle state $\psi_{n_1}$ and the other boson is in the single-particle state $\psi_{n_2}$ is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\right]. \tag{8.3}$$

Two bosons can also be in the same single-particle state. For example, the completely symmetric wavefunction for two bosons in the single-particle state $\psi_{n_1}$ is

$$\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2). \tag{8.4}$$

## 8.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with determining the many-particle stationary state wavefunction for a system of identical fermions or bosons were first investigated using three years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight concerning these difficulties was gained from responses of 14 students during a total of 81 hours of individual "think-aloud" interviews [37]. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates and 30 first-year physics graduate students in their respective QM courses. The QuILT includes a pretest, the tutorial, and a posttest. Students were given the pretest after traditional, lecture-based instruction on identical particles. The pretest was not returned to the students. Students began working on the tutorial in class and completed the tutorial

as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest, tutorial, and posttest were analyzed to determine their understanding of concepts related to many-particle stationary state wavefunctions for a system of identical fermions or bosons. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in our investigation discussed here, the non-interacting identical particles were restricted to one spatial dimension for convenience. Students were asked to consider the wavefunction of the many-particle system ignoring the spin part of the wavefunction (we refer to these particles as "spinless"). Thus, we only consider the spatial part of the wavefunction to simplify the problem and to help students focus on fundamental concepts such as the symmetrization requirement, the number of terms in the many-particle wavefunction, the correct normalization constant, and the fact that each particle should have its own unique coordinate. In order to familiarize the students with the notation, they were given that the wavefunction of a system of two non-interacting identical particles has terms such as $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, where $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for particles in states $n_1$ and $n_2$ and coordinates $x_1$ and $x_2$, respectively.

We will discuss student responses to some questions that were posed either as in-class clicker questions or open-ended questions after traditional lecture-based instruction in relevant concepts. Additional insight into these difficulties was gleaned during the individual think-aloud interviews in which students were asked questions pertaining to these issues. To probe whether students are able to identify and generate a many-particle stationary state wavefunction, four questions Q1-Q4 were posed to the students. Questions Q1 and Q2 were posed on the pretest following traditional lecture-based instruction and the posttest following engagement with the QuILT on identical particles to 30 graduate students and 25 undergraduate students. Questions Q3 and Q4 were given as clicker questions in an undergraduate quantum mechanics course following instruction on identical particles to 17 undergraduate students.

Question Q1 was intended to probe whether the students were able to generate a many-particle wavefunction. Students were told that the particles are confined in one spatial

dimension and that $\psi_{n_1}$, $\psi_{n_2}$, etc. are the single-particle stationary state wavefunctions.

**Q1.** *For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction* **in position representation** *where all three particles are in different single-particle states for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason.* **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

In Q1, for a system of three fermions, the completely antisymmetric three-particle stationary state wavefunction in position representation (with $n_1 \neq n_2 \neq n_3$) is

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ &\quad +\psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) \\ &\quad +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)].\end{aligned} \tag{8.5}$$

In Q1, for a system of three bosons, the completely symmetric three-particle stationary state wavefunction in position representation ( with $n_1 \neq n_2 \neq n_3$) is

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) + \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ &\quad +\psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) \\ &\quad +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) + \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)].\end{aligned} \tag{8.6}$$

One possible answer to Q1 for a system of identical particles that could be treated as distinguishable is

$$\Psi(x_1,x_2,x_3) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3). \tag{8.7}$$

Question Q2 was posed to determine whether students were able to identify that two identical fermions cannot occupy the same single-particle state. Question Q2 is also intended to probe whether students can generate a many-particle wavefunction for a system

of identical bosons and identify the differences between a wavefunction for a system of identical bosons and a system of particles that can be treated as distinguishable. Students were told that the particles are confined in one spatial dimension and that $\psi_{n_1}$, $\psi_{n_2}$, etc. are the single-particle stationary state wavefunctions.

**Q2.** *For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction* **in position representation** *when two of the particles are in same single-particle state $\psi_{n_1}$ for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason.* **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

In Q2, it is not possible for two fermions to occupy the same single-particle state $\psi_{n_1}$ and therefore it is not possible to write a three-particle stationary state wavefunction. On the other hand, it is possible to have a system of three bosons in which two of the bosons are in the same single-particle state $\psi_{n_1}$. For Q2, the completely symmetric three-particle stationary state wavefunction for identical bosons in position representation (with $n_1 \neq n_2$) is

$$\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)+\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)+\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)]. \tag{8.8}$$

One possible many-particle wavefunction for a system of identical particles that could be treated as distinguishable in Q2 is

$$\Psi(x_1, x_2, x_3) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) \tag{8.9}$$

Question Q3 probes whether students can identify that the wavefunction for a system of identical bosons must be symmetric and that more than one boson can occupy the same single-particle state (in addition to whether the spin of a boson is an integer):

**Q3.** *Choose all of the following statements that are correct about bosons.*
*(1) The spin of a boson is an integer.*
*(2) The overall wavefunction of identical bosons can be anti-symmetric.*
*(3) Two bosons cannot occupy the same quantum state.*

Only option (1) is correct for question Q3. Option (2) is incorrect because the overall wavefunction for a system of identical bosons MUST be symmetric and option (3) is incorrect because two or more bosons can occupy the same quantum state.

Question Q4 focuses on the wavefunction for a system of non-interacting identical bosons in the ground state and first excited state of a one-dimensional infinite square well. We were interested in investigating whether students could identify that the many-particle wavefunction must be completely symmetric, regardless of whether it corresponds to the ground state or the first excited state and that the given wavefunction is not completely symmetric in the first excited state:

**Q4.** *There are three identical spinless bosons in a one-dimensional infinite square well. The single particle stationary states are* $\psi_n$ $(n = 1, 2, 3, \ldots)$. *Choose all of the following statements that are correct for the three-particle system. Ignore spin.*
*(1) The ground state of the three particle system is* $\psi_1(x_1)\psi_1(x_2)\psi_1(x_3)$.
*(2)* $\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)$ *is a first excited state of the three particle system.*
*(3) The degeneracy of the first excited state is 3.*

Only option (1) is correct for question Q4. Since the first excited state of the three-boson system must be completely symmetric, option (2) is incorrect. In particular, the three-boson first-excited state wavefunction consists of three terms. However, option (2) only includes one term in the wavefunction corresponding to the system in the first-excited state. Option (3) is incorrect in Q4 because the degeneracy of the first-excited state is one since $\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_1(x_1)\psi_1(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3) + \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)]$ is the only state with the first-excited energy.

Table 25: The percentages of graduate (N=30) and undergraduate (N=25) students who correctly answered question Q1 for the given system of indistinguishable particles after traditional lecture-based instruction in relevant concepts.

| Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Fermions | 33 | 24 |
| Bosons | 37 | 28 |
| Distinguishable | 40 | 40 |

## 8.4 STUDENT DIFFICULTIES

Many students struggled with concepts related to many-particle stationary state wavefunctions for a system of indistinguishable bosons and fermions. For example, Tables 25 and 26 show that less than 55% of the students were able to generate the correct many-particle wavefunctions in questions Q1 and Q2 correctly on the pretest for the QuILT after traditional lecture-based instruction.

Written responses and interviews suggest that there are a number of underlying difficulties students had that interfere with their ability to write the completely symmetric/antisymmetric many-particle stationary state wavefunction for a system of

Table 26: The percentages of graduate (N=30) and undergraduate (N=25) students who correctly answered question Q2 for the given system of indistinguishable particles after traditional lecture-based instruction in relevant concepts.

| Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Fermions | 40 | 44 |
| Bosons | 30 | 16 |
| Distinguishable | 53 | 36 |

non-interacting indistinguishable particles. Below, we discuss some of these difficulties.

### 8.4.1 Difficulty accounting for the indistinguishability of the particles when constructing a many-particle stationary state wavefunction for a system of identical fermions or bosons

There is no measurement that can distinguish one fermion from another fermion in a system consisting of all fermions of the same type (e.g., electrons). The same is true for a system of identical bosons. Below we discuss difficulties students have with writing a wavefunction or correctly identifying a wavefunction that accounts for the indistinguishability of identical particles.

**Using the same coordinate for each particle in the many-particle wavefunction:** Some students did not realize that each identical particle must have a unique coordinate and incorrectly generated a many-particle wavefunction in which the particles shared the same coordinate. For example, in Q1, for both systems of indistinguishable fermions or bosons, one student wrote $\psi_1(x)\psi_2(x)\psi_3(x)$. Many students with this type of difficulty claimed that since there is no way to determine which particle is in which single-particle state, there is no way to assign a distinct coordinate to each indistinguishable particle. For example, one interviewed student incorrectly claimed that "we must use the coordinate $x$ for all the indistinguishable particles since we don't know where each particle is." In addition to writing a many-particle wavefunction that did not satisfy the symmetrization requirements, students with this type of response did not realize that each particle should have its own unique coordinate.

**Claiming that the wavefunction for a system of indistinguishable particles is the same as that for a system of distinguishable particles since the particles are non-interacting:** Many students provided the same answer to Q1 and Q2 for a system of indistinguishable particles and a system of identical particles that can be treated as distinguishable. Table 27 summarizes the percentages of students who wrote the same many-particle wavefunction for a system of identical fermions or bosons as they wrote for a system of distinguishable particles.

Table 27: The percentages of graduate (N=30) and undergraduate (N=25) students who wrote the same many-particle wavefunction for the given system of identical particles as for a system of distinguishable particles for Q1 and Q2 on the pretest after traditional lecture-based instruction in relevant concepts.

| Question | Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|---|
| Q1 | Fermions | 20 | 24 |
| | Bosons | 20 | 20 |
| Q2 | Fermions | 3 | 16 |
| | Bosons | 20 | 20 |

One interviewed student jotted down the same many-particle wavefunction for a system of indistinguishable fermions, indistinguishable bosons, and a system of identical particles that can be treated as distinguishable. When answering Q1 for a system of identical bosons, this student stated "I don't ... understand how distinguishability would change the wavefunction if the particles are non-interacting." This student focused on the fact that the system of identical particles was non-interacting and incorrectly assumed that all systems of non-interacting particles have the same wavefunction. Individual discussions with students suggest that students with this type of difficulty sometimes had difficulty differentiating between "non-interacting particles" vs. "non-overlapping wavefunctions". In particular, the fact that when the wavefunctions of different particles do not overlap, the particles can be considered distinguishable was mistaken or overgeneralized to "non-interacting" particles being distinguishable.

**Not realizing that in some situations a system of indistinguishable bosons could have the same many-particle wavefunction as a system of particles that can be treated as distinguishable:** It is possible for all bosons in a system of indistinguishable bosons to occupy the same single-particle state. For such a system of indistinguishable bosons, the many-particle wavefunction would be the same as that of a system of identical particles that can be treated as distinguishable. For example, if

there are three indistinguishable bosons in the state $\psi_{n_1}$, the many-particle wavefunction is $\Psi(x_1, x_2, x_3) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$. However, some students claimed that this could not be the many-particle wavefunction for a system of indistinguishable bosons since it was the same wavefunction as that for the system of particles that can be treated as distinguishable.

**Overgeneralizing the case when a system of indistinguishable bosons has the same many-particle wavefunction as a system of particles that can be treated as distinguishable:** Many students correctly identified that if all the bosons are in the same single-particle state, the many-particle wavefunction is the same as that of a system of identical particles that can be treated as distinguishable. However, some students overgeneralized this case to incorrectly claim that the wavefunction for a system of indistinguishable bosons is always the same as a system of identical particles that can be treated as distinguishable and there is no need to symmetrize the many-particle wavefunction. Many of these same students claimed that one must only treat a system of identical particles as indistinguishable and worry about appropriate symmetrization of the wavefunction if it is a system of identical fermions. Students with this difficulty did not realize that a system of identical bosons must always have a completely symmetric many-particle wavefunction and that it is only true for the case when all the bosons are in the same single-particle state that the many-particle wavefunction is the same as that for a system of identical particles that can be treated as distinguishable.

### 8.4.2 Difficulty realizing that no wavefunction exists for a system in which two or more fermions occupy the same single-particle state

In Q2(a), students were asked to construct the many-particle wavefunction for a system of three fermions in which two of the fermions occupy the same single-particle state or state the reason for why such a wavefunction does not exist. Below, we discuss difficulties students had with identifying what type of particles obey Pauli's exclusion principle, applying the Pauli's exclusion principle correctly, or not making connections between Pauli's exclusion principle and the completely antisymmetric many-particle state for a system of identical fermions.

**Not realizing Pauli's exclusion principle applies to all fermions:** Some students knew that the Pauli exclusion principle applied to certain types of particle (e.g., electrons) and forbids two particles from occupying the same single-particle state, but did not know it applies to all fermions. For example, when answering Q2 for a system of indistinguishable fermions, one interviewed student initially hesitated briefly then stated, "I know Pauli's exclusion principle applies to two electrons in the same state, but does it apply to all (of the different types of) fermions? I will say it is not possible (for two fermions to be in the same single-particle state), but I don't know if that's true for all fermions." While this student correctly answered that it is not possible to write a many-particle wavefunction for a system in which two electrons are in the same single-particle state, he was unsure about the fact that the Pauli exclusion principle applies to all fermions (electrons being one type of fermion).

**Not applying Pauli's exclusion principle correctly:** In Q2(a), students are asked to write the many-particle stationary state wavefunction for a system of three indistinguishable fermions in which two are in the same single-particle state. Some students struggled to apply the Pauli exclusion principle correctly. In particular, some students had difficulty in realizing that even two out of three fermions cannot be in the same single-particle state (ignoring the spin degrees of freedom) and no wavefunction exists for this system. For example, one student did not provide a stationary state wavefunction in Q2(a) but instead stated: "... But it is not possible (to write a many-particle wavefunction) for all three (fermions) to be in the same (single-particle) state." Further discussion suggests that this student incorrectly reasoned that a system in which all the fermions are in the same single-particle state is the only case that is prohibited, but did not realize that the Pauli's exclusion principle forbids any many-particle system in which *two* or more fermions occupy the same single-particle state as in Q2. He struggled to realize that the Pauli exclusion principle applies to the system in Q2(a) and can be used as justification as to why it is not possible to write the many-particle stationary state wavefunction for a system in which two fermions are in the same single-particle state.

**Difficulty connecting the Pauli exclusion principle to the completely anti-symmetric many-particle stationary state wavefunction for a system of indistinguishable fermions:** During the interview, students were asked questions concerning the

possibility of two or more fermions occupying the same single-particle state. Some of the interviewed students quickly stated that two or more fermions could not occupy the same single particle state because of the Pauli exclusion principle. Additionally, students were asked if a possible wavefunction for a system of indistinguishable fermions could be such that two fermions are in the same single-particle state. Again, most of the interviewed students eliminated the wavefunctions in which two or more fermions were in the same single-particle state as possible many-particle wavefunctions. For example, if one attempts to construct a system of two indistinguishable fermions in the same single-particle state $\psi_i$, the resulting two-particle stationary state wavefunction is $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_i(x_1)\psi_i(x_2) - \psi_i(x_2)\psi_i(x_1)] = 0$. Thus, there is no wavefunction for the system, which is consistent with Pauli's exclusion principle statement that no two fermions can be in the same quantum state. However, when explicitly asked if Pauli's exclusion principle is consistent with a completely antisymmetric many-particle stationary state wavefunction, some students struggled in making any connections between the two. For example, one interviewed student said "the Pauli exclusion principle says that we can't have two fermions, or more (than two fermions) in the same state. Fermions must have an antisymmetric wavefunction. But I don't really see how those two things are related to one another." This student viewed the Pauli exclusion principle and the symmetrization requirement for a system of identical fermions as two disjointed facts. He did not realize that a system with a completely antisymmetric wavefunction in which two or more fermions are in the same single-particle state producing a wavefunction equal to zero (i.e., there is no wavefunction for such a system) and Pauli's exclusion principle, which states that no two fermions can be in the same single-particle state, are intimately connected.

Other students were able to apply the Pauli exclusion principle in one context but then failed to apply it in a different situation. In one question in the interview, some of the interviewed students correctly stated in response to one question that no two fermions can be in the same single-particle state due to Pauli's exclusion principle. However, these same students later attempted to generate a completely antisymmetric many-particle wavefunction for fermions in question Q2 (which asks about a system in which two of the fermions are in the same single-particle state) as opposed to stating that such a wavefunction is not possible.

In Q2, some of these students often went through the procedure to generate terms in the many-particle stationary state wavefunction by permuting the labels for either the states or the coordinates, but did not reflect upon the fact that the many-particle stationary state wavefunction that they generated was zero, and thus not a possible many-particle stationary state wavefunction. Such context dependence of student responses has also been found in introductory physics and suggests that students are not experts in these concepts and their expertise is evolving [38, 39, 40, 41, 42].

### 8.4.3 Difficulty with the symmetrization requirement for the many-particle stationary state wavefunction for a system of identical fermions or bosons

The many-particle stationary state wavefunction for a system of bosons must be completely symmetric and the many-particle stationary state wavefunction for a system of indistinguishable fermions must be completely antisymmetric. However, many students did not realize that the many-particle wavefunction for a system of indistinguishable particles must obey these symmetrization requirements and/or struggled to correctly identify the symmetrization requirement for the system of identical particles given. Table 28 shows the percentages of students who provided the same response to Q1 and Q2 for a system of indistinguishable fermions and a system of indistinguishable bosons after traditional lecture-based instruction. Below, we discuss two types of difficulties students had with the symmetrization requirement for the many-particle stationary state wavefunction.

**Not realizing that the wavefunction for fermions or bosons must obey a symmetrization requirement:** Many students struggled to identify that the many-particle wavefunction for a system of identical particles must obey a symmetrization requirement or could not recognize whether a given wavefunction was appropriately symmetrized. For example, in Q1 and Q2 for a system of identical fermions or bosons, some students incorrectly claimed that the many-particle stationary state wavefunction is expressed as the sum of the single-particle stationary states (as opposed to having terms consisting of the product of the single-particle states). For example, in Q1, some students incorrectly stated that the

Table 28: The percentages of graduate (N=30) and undergraduate (N=25) students who wrote the same many-particle wavefunction for a system of indistinguishable fermions as for a system of indistinguishable bosons for Q1 and Q2 on the pretest after traditional lecture-based instruction in relevant concepts.

| Question | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Q1 | 20 | 28 |
| Q2 | 7 | 24 |

Table 29: The percentages of graduate (N=30) and undergraduate (N=25) students who wrote a many-particle wavefunction that was neither completely symmetric nor completely antisymmetric for a system of three indistinguishable fermions or bosons for Q1 on the pretest after traditional lecture-based instruction in relevant concepts.

| Question | Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|---|
| Q1 | Fermions | 40 | 56 |
| | Bosons | 23 | 48 |

many-particle stationary state wavefunction for the system of three particles is

$$\Psi(x_1, x_2, x_3) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2) + \psi_{n_3}(x_3)$$

for at least one of the systems of identical particles and some gave this answer for all three systems. In Q1, after traditional instruction, 25% of the undergraduates and 10% of the graduate students provided a many-particle wavefunction written in terms of the sum of the single-particle states. However, the sum of the single-particle states does not form a basis state in the Hilbert space for the many-particle system.

Other students constructed a many-particle wavefunction that was neither symmetric nor antisymmetric. Students with this type of difficulty often wrote the following three-particle stationary state wavefunction for both a system of indistinguishable fermions and a system of indistinguishable bosons for question Q1:

$$\Psi(x_1, x_2, x_3) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3).$$

This many-particle stationary state wavefunction is neither symmetric nor antisymmetric. Table 29 summarizes the percentages of students who constructed a many-particle wavefunction in Q1 that was neither symmetric nor antisymmetric. Many of these same students also struggled to make a distinction between the wavefunction for a system of indistinguishable bosons and a system of identical particles that can be treated as distinguishable.

Additionally, in question Q4, 71% of the undergraduate students selected the wavefunction $\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)$ as the first excited state of the given three particle system (option (2)) as a correct answer when answering individually. These students were then given the opportunity to discuss Q4 with their peers and answer the question again. This peer discussion did not help students identify option (2) as incorrect as 71% of the students still selected option (2) as correct after peer discussion. The ineffectiveness of peer discussion further suggests that students struggled with the concept that the wavefunction for the first excited state of a system of three identical spinless bosons must be symmetrized. Interviews suggest that students are more likely to overlook the symmetrization requirement for the first-excited state as compared to the ground state. This may partly be an issue with the cognitive load of having to consider a number of concepts for the first-excited state, such

as determining the single-particle states that yield the correct energy for the many-particle first-excited state, considering the type of identical particle and identifying the appropriate symmetrization requirement. Since these students are still developing expertise in quantum mechanics, they may not have enough cognitive resources to consider each of these concepts and coordinate them appropriately while solving problems.

**Difficulty identifying the correct symmetrization requirement:** Some students were unable to correctly identify which type of symmetrization requirement corresponded to each type of particle. In Q1, some students attempted to generate a symmetric wavefunction for a system of identical fermions. In Q1, 25% of the undergraduates and 23% of the graduate students wrote a completely symmetric wavefunction for a system of identical fermions. For example, one student wrote the following as the many-particle stationary state wavefunction for a system of three fermions in Q1: $\psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + \psi_1(x_2)\psi_2(x_3)\psi_3(x_1) + \psi_1(x_3)\psi_2(x_1)\psi_3(x_2)$. This student had difficulty writing all of the terms of the wavefunction and also did not antisymmetrize the wavefunction for the fermions. Students also had difficulty with the fact that the many-particle wavefunction for a system of identical bosons must be completely symmetric. For example, in Q3, 43% of the undergraduate students incorrectly answered that the overall wavefunction of identical bosons can be antisymmetric (option (2)). Even after peer discussion, 31% again incorrectly selected option (2) as correct. It is possible that these students knew that the many-particle wavefunction for a system of identical particles (bosons or fermions) must obey a symmetrization requirement, but could not correctly identify which symmetrization requirement corresponds to which particle. For example, one interviewed student in response to questions Q1 and Q2 stated that "there is a symmetrization requirement for fermions and a different symmetrization requirement for bosons." But the student was unable to recognize the appropriate symmetrization requirement in each case and wrote the same symmetric wavefunction for both a system of indistinguishable fermions and indistinguishable bosons. In Q1, after traditional instruction, 10% of the graduate students wrote a completely antisymmetric many-particle wavefunction for a system of identical bosons.

### 8.4.4 Difficulty generating a completely symmetric/antisymmetric wavefunction

A number of students were able to identify that the many-particle stationary state wavefunction for a system of fermions must be completely antisymmetric and that the many-particle stationary state wavefunction for a system of bosons must be completely symmetric. However, many of these students had difficulty generating a completely symmetric wavefunction for a system of indistinguishable bosons and a completely antisymmetric wavefunction for a system of indistinguishable fermions.

**Claiming that the single-particle wavefunctions in their product used to construct basis states for many-particle wavefunctions do not commute:** Some students struggled to realize that the order in which the single-particle wavefunctions are written in the product of the single-particle states (used to construct the many-particle basis states) is irrelevant. For example, the following are all equivalent ways to express one of the basis states for a system of three non-interacting identical particles: $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$, $\psi_{n_2}(x_2)\psi_{n_1}(x_1)\psi_{n_3}(x_3)$, $\psi_{n_2}(x_2)\psi_{n_3}(x_3)\psi_{n_1}(x_1)$, $\psi_{n_3}(x_3)\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, and $\psi_{n_3}(x_3)\psi_{n_2}(x_2)\psi_{n_1}(x_1)$. Some students focused on the order in which the labels for the single-particles states or the coordinates appeared to determine whether the products of the single-particle wavefunction were different. For example, when comparing the terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ and $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$, students with this type of difficulty claimed that $n_2$ and/or $x_2$ appear in the second term in the first product and in the third term in the second product, so these must be different basis states for the many-particle wavefunction. For each of the terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$, particle 1 denoted by the coordinate $x_1$ is in the state $\psi_{n_1}$, particle 2 denoted by the coordinate $x_2$ is in the state $\psi_{n_2}$, and particle 3 denoted by the coordinate $x_3$ is in the state $\psi_{n_3}$. Thus, the terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ and $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$ are equivalent and do not represent distinctly different many-particle states. Students who struggled to realize that the single-particle wavefunctions in a basis state in the product space commute often had difficulty generating a many-particle wavefunction with the appropriate number of terms and difficutly determining the normalization constant. For example, students with this type of

difficulty often claimed that the many-particle wavefunction for a system of three identical bosons in which all bosons are in the same single-particle state is

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)+\psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)\\ &\quad +\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)]\end{aligned} \tag{8.10}$$

or

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)+\psi_{n_1}(x_1)\psi_{n_1}(x_3)\psi_{n_1}(x_2)\\ &\quad +\psi_{n_1}(x_2)\psi_{n_1}(x_1)\psi_{n_1}(x_3)+\psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)\\ &\quad +\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)+\psi_{n_1}(x_3)\psi_{n_1}(x_2)\psi_{n_1}(x_1)].\end{aligned} \tag{8.11}$$

They struggled to realize that all these terms in the sum of both these expressions are equivalent and can be simplified to a single term $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$. Additionally, they struggled to determine the correct normalization constant. For example, the expression

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)+\psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)\\ &\quad +\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)]\end{aligned} \tag{8.12}$$

reduces to $\sqrt{3}\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ which is not the properly normalized many-particle wavefunction for a system of three identical bosons in the single-particle state $\psi_{n_1}$.

**Omitting a term in the many-particle wavefunction:** A common mistake when generating many-particle stationary state wavefunctions for identical fermions or bosons was omitting at least one term in the wavefunction and thus not producing a completely symmetric/antisymmetric wavefunction. This also created an obstacle when students determined the normalization constant for the many-particle wavefunction. For example, in Q1 for a system of fermions, one student wrote $|\psi\rangle = \frac{1}{\sqrt{3}}[|\psi_1\rangle|\psi_2\rangle|\psi_3\rangle - |\psi_3\rangle|\psi_2\rangle|\psi_1\rangle - |\psi_2\rangle|\psi_3\rangle|\psi_1\rangle - |\psi_3\rangle|\psi_1\rangle|\psi_2\rangle]$. There are several mistakes in this student's response, but here we point out that the student omitted two of the terms in the many-particle wavefunction and the normalization constant is incorrect. This student's normalization constant is not the correct value of $\frac{1}{\sqrt{6}}$, but it is also not consistent with the number of terms he generated.

**Making a sign error in at least one of the terms of the many-particle wavefunction for fermions:** Another common mistake was writing a many-particle wavefunction for a system of indistinguishable fermions with the correct number of terms but making a mistake with the sign of at least one term. For example, in question Q1,

one student wrote the three-particle stationary state wavefunction for a system of three fermions in which all the fermions are in different single-particle states as

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ &\quad \oplus\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) \ominus \psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) \\ &\quad +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)].\end{aligned} \tag{8.13}$$

In this expression, the circled signs of the third and fourth terms are incorrect resulting in a wavefunction that is not antisymmetric. This is a common mistake that students made when generating terms in the many-particle stationary state wavefunction by starting with one term and then generating all the other terms by interchanging either the labels for the states ($n_1, n_2$, or $n_3$) or the labels for the coordinates ($x_1, x_2$, or $x_3$). For a system of indistinguishable fermions, each time there is an interchange of labels, the new term is multiplied by a minus sign. Thus, starting with the term $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, all the odd permutations of the labels for the states (or coordinates) yield a term with a minus sign and all the even permutations of the labels yield a term with a plus sign. Once all the permutations are determined, they are added together to produce the many-particle stationary state wavefunction. Some interviewed students made mistakes when generating a new term by not multiplying every term by a -1 when exchanging two labels. They made a mistake with the sign of at least one of the terms by not carefully keeping track of the sign of the previous term or not multiplying the new term by a -1.

**Incorrectly switching both the labels for the coordinates and the states:** When determining the many-particle wavefunction for fermions or bosons starting from one product space basis state, one is free to interchange either the labels for the states ($n_1, n_2$, or $n_3$) or the labels for the coordinates ($x_1, x_2$, or $x_3$) until all the permuations are obtained. However, interchanging BOTH the labels for the states and the coordinates will result in an incorrect many-particle wavefunction. Some students began to find the many-particle wavefunction by switching the labels for the coordinates. After finding several permutations, they interchanged the labels for the single-particle states which led to determining an incorrect

many-particle wavefunction. Students did not check their wavefunction to make sure it was completely symmetric or antisymmetric with respect to exchange of two particles.

**Incorrectly applying a sign heuristic to determine a symmetric/antisymmetric wavefunction:** Some students incorrectly applied a heuristic in which they claimed that a wavefunction is symmetric if the wavefunction is written in terms of a sum. These students simply looked for all "+" signs to determine that a wavefunction is symmetric. In particular, they claimed that any wavefunction written as terms added together is a symmetric wavefunction. By a similar logic, these same students looked for a "-" sign to determine whether a given wavefunction is antisymmetric. They often claimed that any wavefunction that has at least one negative sign is antisymmetric. Their determination of whether the wavefunction is antisymmetric did not depend on the number of terms that were subtracted in the wavefunction. They merely looked for the presence of at least one minus sign in the wavefunction to determine that the wavefunction is antisymmetric.

One interviewed student who incorrectly applied this sign heuristic claimed that every term in the many-particle wavefunction is negative with the exception of the starting term and every term generated by permuting the labels is negative. For example, in Q1, this student wrote $\psi_1(x_1)\psi_2(x_2)\psi_3(x_3) - \psi_1(x_2)\psi_2(x_3)\psi_3(x_1) - \psi_1(x_3)\psi_2(x_1)\psi_3(x_2)$ as the many-particle wavefunction for a system of fermions. In addition to not generating all the terms of the many-particle wavefunction, he incorrectly subtracted each term found by permuting the labels of the previous term. Here the student generated all the even permutations for the coordinates and all the terms listed should have been added while all the terms representing the odd permutations of the coordinates are missing. This student and others with this type of difficulty struggled to realize that each new term generated by permuting the labels should have the opposite sign of the term used to find the new term by exchanging two of the labels.

When answering Q1 for a system of indistinguishable fermions, one interviewed student said, "maybe use the alternating thingy." This student proceeded to jot down the following wavefunction:

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{3!}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)].\end{aligned} \tag{8.14}$$

Here the wavefunction does not contain all six terms, but this student also produced only terms that correspond to the even permutations of the coordinates $x_1$, $x_2$, and $x_3$. All the even permutations should have a positive sign, while the terms in the many-particle wavefunction that correspond to the odd permutations of the coordinates $x_1$, $x_2$, and $x_3$ should have a negative sign. This student was simply alternating the sign for each product of the single-particle wavefunctions rather than using a systematic reasoning to determine whether each product corresponded to an even or odd permutation of the labels.

### 8.4.5 Difficulty using the Slater determinant to write the many-particle stationary state wavefunction for a system of indistinguishable fermions

One method to help students write the completely antisymmetric wavefunction for a system of indistinguishable fermions is using the "Slater determinant." The method of the Slater determinant is shown below for a system of three indistinguishable fermions in the states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$.

$$\frac{1}{\sqrt{6}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_2}(x_1) & \psi_{n_3}(x_1) \\ \psi_{n_1}(x_2) & \psi_{n_2}(x_2) & \psi_{n_3}(x_2) \\ \psi_{n_1}(x_3) & \psi_{n_2}(x_3) & \psi_{n_3}(x_3) \end{vmatrix} = \begin{array}{l} \frac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ -\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) + \psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) \\ +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)]. \end{array} \tag{8.15}$$

Students had difficulty writing the Slater determinant and using it properly to determine the many-particle stationary state wavefunction. In order to produce the completely antisymmetric many-particle wavefunction, one must keep the labels for the states fixed for a given row and the labels for the coordinates fixed for a given column (or vice-versa) and ensure that each label appears along one column/row. However, some students changed both the labels for the states and the labels for the coordinates in the rows/columns of the matrix. For example, one student wrote the following when determining the three-particle stationary state wavefunction for a system of indistinguishable fermions in Q1 after traditional instruction in relevant concepts:

$$\frac{1}{\sqrt{6}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_2}(x_2) & \psi_{n_3}(x_3) \\ \psi_{n_2}(x_2) & \psi_{n_3}(x_3) & \psi_{n_1}(x_1) \\ \psi_{n_3}(x_3) & \psi_{n_1}(x_1) & \psi_{n_2}(x_2) \end{vmatrix}.$$

The above determinant produces terms such as $\psi_{n_1}(x_1)\psi_{n_1}(x_1)\psi_{n_1}(x_1)$, $\psi_{n_2}(x_2)\psi_{n_2}(x_2)\psi_{n_2}(x_2)$, and $\psi_{n_3}(x_3)\psi_{n_3}(x_3)\psi_{n_3}(x_3)$ which have the same label $x_1, x_2$ or $x_3$ in all terms in the product of the single-particle states which cannot be a basis state for the product space of the three fermions.

Other students did not change either the label for the state or the coordinate for a given row or column. For example, one student wrote the following for a system of fermions for Q1 after traditional instruction in relevant concepts:

$$\frac{1}{\sqrt{6}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_1) & \psi_{n_1}(x_1) \\ \psi_{n_2}(x_2) & \psi_{n_2}(x_2) & \psi_{n_2}(x_2) \\ \psi_{n_3}(x_3) & \psi_{n_3}(x_3) & \psi_{n_3}(x_3) \end{vmatrix}.$$

This student left the expression with the determinant as his final answer and did not expand the determinant to produce all the terms of the three-particle stationary state wavefunction. However, since the determinant of a matrix in which any rows/columns are identical is equal to zero, the determinant expression written above produces no wavefunction. This student and others with similar difficulty failed to identify issues involved with setting up the Slater determinant and wrote a determinant in which two or more rows/columns are identical resulting in a determinant of zero and no wavefunction.

## 8.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 8.5.1 Development and Validation of the QuILT

Based upon our research of student difficulties with fundamental concepts for systems of identical particles, we developed a QuILT that attempts to build a consistent and coherent knowledge structure while at the same time addressing the common student difficulties. The

development and structure of the QuILT was inspired by several influential learning theories. In particular, the QuILT strives to incorporate Vygotsky's zone of proximal development (ZPD) [43], Bransford and Schwartz's preparation for future learning (PFL) framework [44], and Piaget's "optimal mismatch" [45].

The QuILT is inspired by Vygotsky's ZPD in that it strives to give the students the requisite knowledge and skill sets by providing students with appropriate scaffolding. The desired tasks, which the students were often unable to perform successfully at the onset of the QuILT, are addressed using a guided inquiry-based approach to build the students' knowledge to the point that they develop self-reliance and are able to successfully complete the same task on their own after working through the QuILT.

Additionally, the QuILT strives to incorporate Bransford and Schwartz's PFL framework with a special focus on instruction that is both innovative and efficient. They view innovation and efficiency as two orthogonal components of instruction that must be balanced for effective instruction. One interpretation of this framework is that innovation refers to presenting students with novel tasks that are just beyond their current understand, allowing them to grow and strive for more robust content knowledge. Efficiency has been viewed as a characteristic of instruction that allows the students to practice what they are learning to allow them to become skilled and develop a functional understanding of the material. The framework suggests that instruction should attend to both aspects. The concern is that if instruction only focuses on one of these aspects there is danger that the students will become disconnected when instruction is too advanced beyond their current state (the instruction is too innovative without allowing for efficiency to develop) or when the instruction focuses too much on rote memorization and procedural redundancy (the instruction is too efficient without the creative nature associated with innovation).

Finally, the QuILT was developed with Piaget's "optimal mismatch" as a guiding principle. The key idea behind Piaget's "optimal mismatch" is to allow students to discover their mistakes on their own and allow them to correct the inconsistencies in their own knowledge structures. To achieve this, the QuILT strives to scaffold student learning using a guided inquiry-based approach which focuses on all the necessary skills and concepts to help the students develop a functional understanding of a system of identical particles. It also ad-

dresses and helps students reconcile many of the common difficulties students have with this topic. In particular, the QuILT incorporates hypothetical student conversations and sets of inquiry-based sequences designed to help them realize inconsistencies in their prior knowledge, and provide scaffolding to help students resolve these inconsistencies.

The development of the QuILT was guided by a cognitive task analysis [46] from both a physics expert perspective and a novice (or student) perspective which consisted of the requisite knowledge and skills necessary for a functional understanding of a system of identical particles. The initial analysis was conducted from an expert perspective in which the authors outlined the required knowledge and skills and the order in which they are useful in solving problems. The analysis was iterated with members of the physics faculty at the University of Pittsburgh. However, in an effort of determine whether there are additional areas students may struggle with that are not predicted by the experts (due to expert blindspot), we conducted individual student interviews.

The QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure that the content was appropriate and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that was incorporated in the next version of the QuILT. Once it was agreed upon by the faculty that the content was clear and correct, the QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording is unambiguous, the scaffolding is effective, and to be able to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and provided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the entire section of the tutorial focusing on the issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and to determine whether there were any necessary changes that needed to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and in subsequent interviews. During each

step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback to help with the common difficulties. After it was deemed successful by faculty and students (who performed well in the posttest after engaging with the QuILT in one-on-one administration), the QuILT was then administered to students in various advanced quantum mechanics courses.

### 8.5.2 Structure of the QuILT

The QuILT strives to transform the students into active learners by employing an inquiry-based approach which requires the students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. The QuILT consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is given in class during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, they are given the tutorial and encouraged to work together on it in small groups in class. The tutorial can be used to guide in-class discussion. The tutorial can also be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, the students submit the tutorial for grading and are then administered the posttest. The posttest is given in class as an individual assessment in which the students are not permitted any additional resources beyond what is provided in the posttest.

The QuILT incorporates guided inquiry-based learning sequences which consist of several questions, each building upon the previous question(s), that require the students to take a stand and actively engage in the learning process. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether they are correct and explain why they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify any inconsistencies in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these com-

mon difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning, provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include excerpts that strive to present the students with a contradiction between the answer to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining difference between the correct reasoning and their own reasoning before moving on the next section.

### 8.5.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples focusing on fundamental concepts for the many-particle wavefunction for a system of indistinguishable fermions or indistinguishable bosons. In particular, the QuILT strives to help students (1) understand the symmetrization requirements for a system of indistinguishable fermions or bosons, (2) account for the indistinguishability of the particles by symmetrizing the many-particle wavefunction, and (3) construct the many-particle wavefunction for a system of indistinguishable fermions or bosons. Below are some examples from the QuILT that show scaffolding support intended to help students with these concepts and address some of the common difficulties.

**Helping students realize that the many-particle stationary state wavefunction for a system of indistinguishable particles must obey a symmetrization requirement and that it is possible to write a many-particle stationary state wavefunction for both a bosonic and fermionic system in which all particles are in different single-particle states:** In the QuILT, students work through several guided inquiry-based sequences in which they are asked to construct the many-particle wavefunction for a variety of systems of identical particles and then are provided scaffolding that strives to help students reconcile any differences between their initial responses and the correct reasoning. For exam-

ple, they are asked to construct the many-particle wavefunction for a system of two identical fermions and then generalize it to a system of three identical fermions. Students are asked to determine the many-particle wavefunction for the system, if possible, and explain their reasoning if it is not possible. After constructing the many-particle wavefunction, they are asked to reflect upon the following conversation in which three hypothetical students discuss how to construct the many-particle wavefunction for a system of two non-interacting identical fermions. The students must state whether they agree or disagree with each statement and explain their reasoning for doing so.

**Student 1:** *For a system of two non-interacting indistinguishable fermions, the wavefunction describing the system is $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, in which $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for the two-particles.*

**Student 2:** *I disagree. If the system consists of two fermions, there is no way to distinguish which fermion is in the state labeled by $n_1$ and which is in the state labeled by $n_2$. The wavefunction must reflect this symmetry.*

**Student 3:** *I agree with Student 2. The wavefunction describing a system of non-interacting indistinguishable fermions must be completely antisymmetric. Therefore, the normalized wavefunction for a system of two non-interacting fermions must be $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.*

Student 1 is incorrect, while both Student 2 and Student 3 are correct in the preceding conversation. In particular, Student 2's statement is intended to help students who had difficulty identifying that it is possible to write a many-particle wavefunction for a system of identical fermions despite not knowing which fermion is in which single-particle state. Student 3 then provides reasoning as to how one takes into account the indistinguishability of the particles and provides a completely antisymmetric wavefunction for the two fermions. Further scaffolding support is provided to help students reconcile their initial ideas with the correct concepts. After working on a system of two identical fermions, students engage with several guided inquiry-based sequences for a system of three identical fermions.

Later, students consider systems of identical bosons and work through similar guided inquiry-based learning sequences that strive to help them learn to write the many-particle wavefunction for a system of identical bosons such that the wavefunction is completely

symmetric.

**Helping students connect the Pauli exclusion principle to the completely antisymmetric many-particle stationary state wavefunction for a system of indistinguishable fermions:** The QuILT strives to help students relate the Pauli exclusion principle to the fact that the many-particle stationary state wavefunction for a system of indistinguishable fermions must be antisymmetric. The following is an excerpt from a hypothetical conversation that attempts to help students make this connection. The students must decide whether they agree or disagree with Student 2's statement and then explain their reasoning.

**Student 1:** *I thought the Pauli exclusion principle states that no two fermions can be in the same single-particle state. How is that consistent with the wavefunctions being completely antisymmetric?*

**Student 2:** *Let's suppose we have two fermions in the same single-particle state. Then* $n_1 = n_2$ *and the wavefunction would be* $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)] = 0$. *Thus* $\Psi(x_1, x_2) = 0$ *is not a possible wavefunction.*

Student 2 is correct and her statement strives to help students reflect upon the fact that a completely symmetric wavefunction for two fermions in the same single-particle state does not exist, consistent with Pauli's exclusion principle. They then work through a guided inquiry-based sequence focusing on a system of three identical fermions that strives to help them generalize the case for two identical fermions and learn that the completely antisymmetric three-particle stationary state wavefunction is also consistent with the Pauli exclusion principle.

**Helping students determine all the terms in the symmetric/antisymmetric wavefunction:** The QuILT strives to help students develop systematic reasoning about the number of terms to expect in a symmetric or antisymmetric wavefunction. For example, the following hypothetical conversation is part of a guided inquiry-based learning sequence which strives to help students connect the number of permutations of the labels for the indistinguishable fermions to the number of terms in the antisymmetric many-particle wavefunction. In the following hypothetical conversation, the students must state whether

they agree or disagree with Student 2 and state their reasoning.

**Student 1:** *When constructing the completely antisymmetric wavefunction for a system of three indistinguishable fermions, how do I know that I have found all the possible permutations?*

**Student 2:** *In general, for a system of $N$ indistinguishable fermions, there are $N!$ permutations of the labels. For example, there are $N!$ permutations of the coordinates $x_1, x_2, \ldots, x_N$ or $N!$ permutations of the labels for the single-particle states $\psi_{n_1}, \psi_{n_2}, \ldots, \psi_{n_N}$. The normalization factor is $\frac{1}{\sqrt{N!}}$.*

Further scaffolding is provided to help students reflect upon the fact that Student 2 is correct. In particular, for a system of $N$ indistinguishable fermions, there are $N!$ permutations of the labels for either the states or the coordinates. Therefore, the antisymmetric many-particle wavefunction will have $N!$ terms.

**Helping students use the Slater determinant to write the many-particle stationary state wavefunction for a system of indistinguishable fermions:** In the QuILT, students are asked to construct the many-particle wavefunction for a system of two fermions in which the fermions are in different single-particle states. They are later asked to use the Slater determinant for this same system of two fermions and compare the wavefunction obtained using the Slater determinant method with the one obtained witthout it. Additionally, the students are asked to construct the Slater determinant for a system of two fermions in which the two fermions are in the same single-particle state and reflect upon the implication of what they find to whether two fermions can be in the same single-particle state. The Slater determinant for such a system is zero, consistent with Pauli's exclusion principle and there is no such wavefunction for this system. The following is a hypothetical student's statement from a learning sequence in the QuILT that strives to help students make this connection in which the students must state whether they agree or disagree with the student and why.

**Student 1:** *The Slater determinant yields a many-particle wavefunction which is consistent with the Pauli exclusion principle. For example, for a system of two fermions, if we put both*

*fermions in the same state, then*

$$\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) \\ \psi_{n_1}(x_1) & \psi_{n_1}(x_2) \end{vmatrix} = \psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_1}(x_1) = 0,$$

*which cannot be a possible wavefunction since zero represents the absence of a wavefunction.*

This type of reflection strives to help students focus on how to set up the Slater determinant correctly and also strives to help students recognize that an antisymmetric wavefunction given by the Slater determinant is consistent with the Pauli exclusion principle for a system of two identical fermions. Later the students engage with a guided inquiry-based sequence which begins by asking them to construct the many-particle stationary state wavefunction for a system of three identical fermions using the Slater determinant. Students are then provided further scaffolding support to help them reconcile their initial ideas with the correct reasoning.

## 8.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts for constructing the many-particle stationary state wavefunction. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

Table 30 summarizes the percentages of students who answered questions Q1 and Q2 correctly on the pretest and the posttest. In particular, on the pretest less than 30% of the undergraduate and less than half of the graduate students answered Q1 or Q2(b) correctly for

Table 30: The percentages of students who correctly answered questions Q1 and Q2 for the given system on the pretest and posttest for graduate students ($N = 30$) and undergraduates (number of students $N = 25$).

| Question | Type of Particle | Graduate | | Undergraduate | |
|---|---|---|---|---|---|
| | | Pre (%) | Post (%) | Pre (%) | Post (%) |
| Q1(a) | Fermions | 40 | 60 | 24 | 72 |
| Q1(b) | Bosons | 37 | 73 | 28 | 80 |
| Q1(c) | Distinguishable | 40 | 80 | 40 | 97 |
| Q2(a) | Fermions | 40 | 97 | 44 | 84 |
| Q2(b) | Bosons | 37 | 70 | 16 | 76 |
| Q2(c) | Distinguishable | 53 | 83 | 36 | 97 |

a system in which it is possible to write a many-particle wavefunction After working through the QuILT, over 70% of the undergraduates and 60% of the graduate students answered all the parts of Q1 and Q2 correctly on the posttest. The results are encouraging and suggest that the QuILT is effective in helping students construct the many-particle stationary state wavefunction for a system of identical fermions or bosons.

The open-ended questions Q1 and Q2 were graded using rubrics which were developed by the researchers together. A subset of questions was graded separately by them. After comparing the grading, they discussed any disagreements and resolved them with a final inter-rater reliability of better than 95%. Table 31 shows the performance of undergraduate and graduate students on the pretest and posttest. Table 31 also includes the average gain, $G$, and normalized gain [47], $g$. The normalized gain is defined as (posttest percent - pretest percent)/(100 - pretest percent). In particular, the undergraduates score less than 40% and the graduate students scored less than 50% on all parts of Q1 and Q2 on the pretest. After working through the QuILT, both undergraduate and graduate students scored over 80% on all the parts of Q1 and Q2 on the posttest. The posttest scores are significantly better than the pretest scores on all of these questions for both groups.

Table 31: Average pretest and posttest scores, gains ($G$) and normalized gains ($g$) for graduate students (number of students $N = 30$) and undergraduate students (number of students $N = 25$).

| | Graduate Students | | | | Undergraduate Students | | | |
|---|---|---|---|---|---|---|---|---|
| Question | Pre (%) | Post (%) | G (%) | g | Pre (%) | Post (%) | G (%) | g |
| Q1(a) | 45 | 93 | +48 | 0.87 | 34 | 88 | +54 | 0.82 |
| Q1(b) | 41 | 95 | +54 | 0.92 | 35 | 93 | +58 | 0.89 |
| Q1(c) | 44 | 96 | +52 | 0.93 | 61 | 99 | +38 | 0.97 |
| Q2(a) | 44 | 84 | +40 | 0.71 | 37 | 97 | +60 | 0.95 |
| Q2(b) | 30 | 95 | +65 | 0.93 | 35 | 87 | +52 | 0.80 |
| Q2(c) | 48 | 97 | +49 | 0.94 | 49 | 99 | +50 | 0.98 |

As a measure of retention, 12 of the upper-level undergraduate students in Year 2 of the study were asked the following question on their final exam two months after engaging with the QuILT:

**Q5.** *Suppose we have two non-interacting particles, both of mass $m$, in a one-dimensional infinite square well of width $a$ (well is between $x = 0$ and $x = a$). Wrtie down the first-excited state wavefunctions and energies for two-particle system (in terms of single-particle wavefunction and ground state energy $E_0$) if the particles are (a) distinguishable, (b) identical bosons, and (c) identical femrions.*

Of the 12 undergraduates, 10 answered the question completely correctly. One student answered the question correctly for the fermion and boson case but incorrectly determined that the first-excited energy for the system of two distinguishable particles was $E_{21} = \frac{(1+3^2)\pi^2\hbar^2}{2ma^2} = \frac{10\pi^2\hbar^2}{2ma^2} = 10E_0$ and the corresponding first-excited state wavefunction was $\frac{2}{a}\sin(\frac{\pi x_1}{a})\sin(\frac{3\pi x_2}{a})$. The other student who answered Q5 incorrectly omitted the energies for the first-excited states for all three system and incorrectly claimed that the first-excited state for a system of identical fermions was $\frac{1}{\sqrt{2}}[\frac{2}{a}\sin(\frac{\pi x_1}{a})\sin(\frac{2\pi x_2}{a}) - \frac{2}{a}\sin(\frac{\pi x_2}{a})\sin(\frac{2\pi x_1}{a})]$ (but provided the correct response for the wavefunction for a system of two bosons or distinguishable

particles). Apart from these mistakes by two of the students, all of the students provided wavefunctions in response to Q5 that had the correct symmetrization and each particle had a unique coordinate in the many-particle wavefunction for each system of identical particles. These results are encouraging and suggest that the QuILT was effective in helping students learn and retain these concepts.

## 8.7 SUMMARY

We described an investigation of student difficulties and the development and evaluation of the corresponding research-validated QuILT that strives to help students develop a functional understanding of the fundamental concepts involved in constructing the many-particle stationary state wavefunction for a system of identical particles. Investigating student understanding of a system of identical particles helped to uncover many common student difficulties. These difficulties were used as a guide to develop a research-based QuILT focused on helping students develop a robust understanding of many-particle stationary state wavefunctions for a system of identical particles, e.g., helping them learn that the wavefunction for a system of fermions must be antisymmetric and the wavefunction for a system of bosons must be symmetric and construct the many-particle stationary state wavefunction for a system of identical particles (fermions or bosons) consistent with the symmetrization requirements. Many of the student difficulties discussed here may be attributed in part to students' bounded rationality in that students are limited in their cognitive resources while solving problems since they are still developing expertise in this area of QM [34]. Since the paradigm of QM is novel, these issues become critical. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding support through a guided inquiry-based approach. The posttest results show that the QuILT is effective in improving students' understanding of fundamental concepts necessary for a functional understanding of the many-particle stationary state wavefunction for a system of identical particles.

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# 9.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: WRITING THE MANY-PARTICLE STATIONARY STATE WAVEFUNCTION (INCLUDING SPIN)

## 9.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. There have been a number of research studies aimed at investigating student reasoning in QM[15, 16, 17, 18, 19, 20, 21, 22, 23, 24] and improving student understanding of QM [25, 26, 27, 28, 29, 30, 31, 32, 33, 34]. For example, our group has focused on using the common student difficulties as a guide to develop research-based learning tools which include Quantum Interactive Learning Tutorials (QuILTs) [35, 36, 37, 38, 39, 40] which strive to improve student understanding of different QM concepts.

However, there have been relatively few investigations into student difficulties with fundamental concepts involving a system of identical particles. Through researching students' understanding and reasoning about a system of identical particles, we have found many common student difficulties that can hinder the development of a consistent and coherent knowledge structure pertaining to these concepts. Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of the individual who is solving the problem, Simon's framework of "bounded rationality" posits that an individual will make decisions while solving problems based upon their current level of expertise, which may not be optimal [41]. Some students may be motivated to find an optimal solution to the QM problems posed

by searching for many possible pathways in the problem space. However, if students' level of expertise is not sufficient to solve the problem on their own and they have not been provided with appropriate guidance and scaffolding support, they may experience cognitive overload and may not be able to determine an optimal solution to the problems posed [41, 42].

Other students may be motivated to find an optimal solution but if the students' level of expertise is not sufficient and they have not been provided with the appropriate scaffolding support, they may experience cognitive overload and not be able to determine the correct solution to the problem posed [42].

Below, we start with a brief background of relevant concepts and then describe the methodology for the investigation of student difficulties followed by the common difficulties found. Then we describe the methodology for the development, validation and in-class evaluation of the corresponding research-validated QuILT that strives to help students develop a functional understanding of the fundamental concepts involving a system of identical particles.

## 9.2 BACKGROUND

In nature, there are two general types of particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g., photons and mesons). A system of $N$ identical particles consists of $N$ particles of the same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in quantum mechanics, identical particles are indistinguishable and there is no measurement that can be performed to distinguish these identical particles from one another. For example, if the coordinates of two identical particles are interchanged, there is no physical observable that would reflect this interchange. Furthermore, one property that distinguishes these two types of particles is that two or more bosons can occupy the same single-particle quantum state, but two or more fermions can never occupy the same single-particle quantum state. The restriction for fermions is known as the Pauli exclusion principle and is consistent

with a system of fermions having a completely antisymmetric wavefunction [43]. To reflect the indistinguishability of these identical particles and make the statistical properties of fermions and bosons consistent with observations, the wavefunction for a system of identical fermions must be completely antisymmetric and the wavefunction for a system of identical bosons must be completely symmetric. Here we focus on the many-particle stationary state wavefunction that is a solution to the Time-Independent Schrödinger Equation (TISE) for a system of non-interacting identical particles. Unless otherwise stated, throughout, we will refer to the stationary state wavefunction as the wavefunction.

Even though the spatial and spin parts of the wavefunction can be entangled in many situations, we will only consider many-particle wavefunctions $\Psi(x_1, x_2, x_3, \ldots, m_{s_1}, m_{s_2}, m_{s_3}, \ldots)$ in one spatial dimension that can be written as the product of the spatial part of the wavefunction $\psi(x_1, x_2, x_3, \ldots)$ and the spin part of the wavefunction $\chi(m_{s_1}, m_{s_2}, m_{s_3}, \ldots)$,

$$\Psi(x_1, x_2, x_3, \ldots, m_{s_1}, m_{s_2}, m_{s_3}, \ldots) = \psi(x_1, x_2, x_3, \ldots)\chi(m_{s_1}, m_{s_2}, m_{s_3}, \ldots),$$

in which $x_i$ denotes the spatial coordinate of the $i^{th}$ particle and $m_{s_i}$ denotes the $z$-component of spin quantum number of the $i^{th}$ particle. The spatial part of the wavefunction of a system of two non-interacting identical particles has terms such as $\psi_{n_a}(x_i)\psi_{n_b}(x_j)$, where $\psi_{n_a}(x_i)$ and $\psi_{n_b}(x_j)$ are the single-particle wavefunction for the $i^{th}$ particle with coordinate $x_i$ in the state $n_a$ and the single-particle wavefunction for the $j^{th}$ particle with coordinate $x_j$ in the state $n_b$, respectively.

If we have a system of two non-interacting identical fermions, the two-particle stationary state wavefunction must be completely antisymmetric. There are two ways to construct a completely antisymmetric wavefunction: the spatial part of the wavefunction could be completely symmetric and the spin part of the wavefunction could be completely antisymmetric or the spatial part of the wavefunction could be completely antisymmetric and the spin part of the wavefunction could be completely symmetric. If we have a system of two non-interacting identical bosons, the two-particle stationary state wavefunction must be completely symmetric. There are two ways to construct a completely symmetric wavefunction: the spatial and spin parts of the wavefunction could both be completely symmetric or the

spatial and spin parts of the wavefunction could both be completely antisymmetric.

When considering the spin part of the wavefunction for a single-particle, we will use the notation $|s_i,\ m_{s_i}\rangle$ (in which $s_i$ and $m_{s_i}$ are the quantum numbers corresponding to the total spin and z-component of the spin for the $i^{th}$ particle, respectively). The states $|s_1,\ m_{s_1}\rangle$ are eigenstates of $\hat{S}_1^2$ and $\hat{S}_{1z}$ and the states $|s_2,\ m_{s_2}\rangle$ are eigenstates of $\hat{S}_2^2$ and $\hat{S}_{2z}$. We will use the following abbreviated notation for a spin-1/2 particle: $|\uparrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ 1/2\rangle_1$ and $|\downarrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ -1/2\rangle_1$ for electron 1 in the "spin up" and "spin down" state, respectively, and $|\uparrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ 1/2\rangle_2$, and $|\downarrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ -1/2\rangle_2$ for electron 2 in the "spin up" and "spin down" state, respectively.

When considering the spin part of the wavefunction for the two spin-1/2 particles in the uncoupled representation in the product space, we will use the notation $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, $|\downarrow\rangle_1|\uparrow\rangle_2$, and $|\downarrow\rangle_1|\downarrow\rangle_2$ for the basis states.

We will also use the notation in the coupled representation $|s,\ m_s\rangle$ in which the quantum numbers $s$ and $m_s$ correspond to the total spin angular momentum and the $z$ component of the total spin angular momentum including both spins, respectively (we will use the notation that a state in the coupled representation will not have a subscript whereas states in the uncoupled representation will have a subscript indicating the particle associated with each spin state). For a system of two spin-1/2 particles ($s_1 = 1/2 \otimes s_2 = 1/2$), the states $|s,\ m_s\rangle$ in the coupled representation are eigenstates of $\hat{S}^2$ and $\hat{S}_z$ where $\vec{S} = \vec{S}_1 + \vec{S}_2$. For a system of two spin-1/2 particles, the quantum number $s = s_1 + s_2 = 1/2 + 1/2 = 1$ or $s = |s_1 - s_2| = |1/2 - 1/2| = 0$. If the total spin quantum number is $s = 1$ then $m_s = -1, 0, 1$ and the states in the coupled representation are given by $|s, m_s\rangle = \{|1,\ 1\rangle, |1,\ 0\rangle, |1,\ -1\rangle\}$. If $s = 0$ then $m_s = 0$ and the state in the coupled representation is given by $|s, m_s\rangle = |0,\ 0\rangle$. We will use the following abbreviated notation for a complete set of normalized states for a system of two spin-1/2 particles in the coupled representation $|s\ m_s\rangle$ written in terms of states in the uncoupled representation ($|s_1,\ m_{s_1}\rangle|s_2,\ m_{s_2}\rangle$):

$$\begin{aligned}
|1,\ 1\rangle &= |\uparrow\rangle_1|\uparrow\rangle_2 &&= |\uparrow\uparrow\rangle \\
|1,\ -1\rangle &= |\downarrow\rangle_1|\downarrow\rangle_2 &&= |\downarrow\downarrow\rangle \\
|1,\ 0\rangle &= \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) &&= \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\
|0,\ 0\rangle &= \tfrac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right) &&= \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right).
\end{aligned} \tag{9.1}$$

Eq. (9.1) shows that one feature of the basis states for two identical spin angular momenta in the coupled representation, e.g., $|1,\ 1\rangle$, $|1,\ -1\rangle$, $|1,\ 0\rangle$, $|0,\ 0\rangle$ for two spin-1/2 particles, is that they are either completely symmetric or completely antisymmetric with respect to exchange of particles. For example, in the case of two spin-1/2 particles, $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ are completely symmetric spin states of the two-fermion wavefunction and often referred to as the "triplet" states. It is important to note that a linear combination of these three symmetric spin states is also a completely symmetric spin state (i.e., $C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + C_3(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ in which $C_1$, $C_2$, and $C_3$ are constants such that $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$). The state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is the completely antisymmetric normalized spin state of the two-fermion wavefunction and often refered to as the "singlet" state.

The following are examples of completely antisymmetric normalized many-particle stationary state wavefunctions for a system of two spin-1/2 fermions in which the spatial part of the wavefunction is antisymmetric and the spin part of the wavefunction is symmetric:

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|1,\ 1\rangle \\
&= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|\uparrow\rangle_1|\uparrow\rangle_2
\end{aligned}$$

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|1,\ -1\rangle \\
&= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|\downarrow\rangle_1|\downarrow\rangle_2
\end{aligned}$$

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|1,\ 0\rangle \\
&= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}\tfrac{1}{\sqrt{2}}\{|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\}
\end{aligned}$$

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}\{C_1|1,\ 1\rangle + C_2|1,\ -1\rangle \\
&\quad + C_3|1,\ 0\rangle\} \\
&= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}\{C_1|\uparrow\rangle_1|\uparrow\rangle_2 + C_2|\downarrow\rangle_1|\downarrow\rangle_2 \\
&\quad + C_3\tfrac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2)\}
\end{aligned}$$

in which $C_1$, $C_2$, and $C_3$ are constants such that $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

The following are examples of completely antisymmetric normalized many-particle stationary state wavefunctions for a system of two spin-1/2 fermions in which the spatial part

of the wavefunction is symmetric and the spin part of the wavefunction is antisymmetric (assume $n_1 \neq n_2$):

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)][|0,\ 0\rangle \\ &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)\tfrac{1}{\sqrt{2}}\{|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow_2\rangle\}\end{aligned}$$

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}|0,\ 0\rangle \\ &= \tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}\tfrac{1}{\sqrt{2}}\{|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow_1|\uparrow\rangle_2\}.\end{aligned}$$

For a spin-1 boson, $|s_i, m_{s_i}\rangle = \{|1,\ -1\rangle, |1,\ 0\rangle, |1,\ 1\rangle\}$ for each particle. When considering the spin part of the wavefunction for two spin-1 particles in the uncoupled representation in the product space ($3\times3 = 9$ dimensional), we will use the notation $|1,1\rangle_1|1,\ 1\rangle_2$, $|1,1\rangle_1|1,\ 0\rangle_2$, $|1,1\rangle_1|1,\ -1\rangle_2$, $|1,0\rangle_1|1,\ 1\rangle_2$, $|1,0\rangle_1|1,\ 0\rangle_2$, $|1,0\rangle_1|1,\ -1\rangle_2$, $|1,-1\rangle_1|1,\ 1\rangle_2$, $|1,-1\rangle_1|1,\ 0\rangle_2$, and $|1,-1\rangle_1|1,\ -1\rangle_2$ for the basis states.

For a system of two spin-1 particles ($s_1 = 1 \otimes s_2 = 1$) the state $|s,\ m_s\rangle$ in the coupled representation is such that the quantum numbers are $s = 2, 1, 0$. If the total spin quantum number is $s = 2$ then the corresponding $m_s = -2, -1, 0, 1, 2$ and the states in the coupled representation are given by $|s,\ m_s\rangle = \{|2,\ 2\rangle, |2,\ 1\rangle, |2,\ 0\rangle, |2,\ -1\rangle, |2,\ -2\rangle\}$. If $s = 1$ then the corresponding $m_s = -1, 0, 1$ and the states in the coupled representation are given by $|s,\ m_s\rangle = \{|1,\ -1\rangle, |1,\ 0\rangle, |1,\ -1\rangle\}$. If $s = 0$ then the corresponding $m_s = 0$ and the state in the coupled representation is given by $|s, m_s\rangle = |0,\ 0\rangle$. Table 32 lists the product states for two spin-1 bosons in the coupled representation and equivalently in the uncoupled representation. For example, the product state $|2,\ 2\rangle$ in the coupled representation can be written as $|2,\ 2\rangle = |1,\ 1\rangle_1|1,\ 1\rangle_2$ in the uncoupled representation. Exchanging the labels 1 and 2, we find no change in the spin state so this spin state is completely symmetric. A completely symmetric spin state can be constructed by taking a linear combination of symmetric states in Table 32. For example, the spin states in product space in the coupled representation $|2,\ 2\rangle$, $|2,\ 1\rangle$, $|2,\ 0\rangle$, $|2,\ -1\rangle$, $|2,\ -2\rangle$ and $|0,\ 0\rangle$ are all symmetric, and so the spin state $C_1|2,\ 2\rangle + C_2|2,\ 1\rangle + C_3|2,\ 0\rangle + C_4|2,\ -1\rangle + C_5|2,\ -2\rangle + C_6|0,\ 0\rangle$ in which $|C_1|^2 + |C_2|^2 + |C_3|^2 + |C_4|^2 + |C_5|^2 + |C_6|^2 = 1$ is also completely symmetric. Similarly,

the product state in the coupled representation $|1,\ 1\rangle = \frac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2 - |1,\ 0\rangle_1|1,\ 1\rangle_2)$ in the uncoupled representation and exchanging the labels 1 and 2 of the two particles leads to a change in the overall sign. Thus, this spin state is completely antisymmetric. A completely antisymmetric spin state can be constructed by taking a linear combination of antisymmetric states in Table 32. For example, the spin states in product space in the coupled representation $|1,\ 1\rangle$, $|1,\ 0\rangle$, and $|1,\ -1\rangle$ are all antisymmetric, and so the spin state $C_1|1,\ 1\rangle + C_2|1,\ 0\rangle + C_3|1,\ -1\rangle$ in which $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$ is also completely antisymmetric.

The wavefunction for a system of identical bosons must be completely symmetric. The spatial and spin parts of the many-particle stationary state wavefunction can either be both symmetric or both antisymmetric.

The following are examples of completely symmetric many-particle stationary state wavefunctions for a system of two spin-1 bosons in which both the spatial and spin parts of the wavefunction are symmetric:

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)|2,\ 2\rangle \\ &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)|1,\ 1\rangle_1|1,\ 1\rangle_2\end{aligned}$$

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)|2,\ 1\rangle \\ &= \psi_{n_1}(x_1)\psi_{n_1}(x_2)\tfrac{1}{\sqrt{2}}\{(|1,\ 1\rangle_1|1,\ 0\rangle_2 + |1,\ 0\rangle_1|1,\ 1\rangle_2)\}\end{aligned}$$

$$\Psi(x_1, x_2, m_{s_1}, m_{s_2}) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)\{C_1|2,\ 2\rangle + C_2|2,\ 1\rangle + C_3|2,\ 0\rangle\}$$

in which $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$

The following are examples of a completely symmetric many-particle stationary state wavefunctions for a system of two spin-1 bosons in which both the spatial and spin parts of

the wavefunction are antisymmetric (assume $n_1 \neq n_2$):

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_1)\psi_{n_2}(x_2)|1,\ 1\rangle \\ &= \tfrac{1}{\sqrt{2}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_1)\psi_{n_2}(x_2)\tfrac{1}{\sqrt{2}}\{|1,\ 1\rangle_1|1,\ 0\rangle_2 \\ &\quad -|1,\ 0\rangle_1|1,\ 1\rangle_2\}\end{aligned}$$

$$\begin{aligned}\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= \tfrac{1}{\sqrt{2}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_1)\psi_{n_2}(x_2)\{C_1|1,\ 1\rangle + C_2|1,\ 0\rangle \\ &\quad +C_3|1,\ -1\rangle\}\end{aligned}$$

in which $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

## 9.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with determining the many-particle stationary state wavefunction for a system of identical fermions or bosons were first investigated using three years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight concerning these difficulties was gained from responses of 14 students during a total of 81 hours of individual "think-aloud" interviews [44]. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates (12 in year 1 of the study and 13 in year 2 of the study) and 30 first-year physics graduate students in their respective QM courses. The QuILT included a pretest, the tutorial, and a posttest. Students were given the pretest after traditional lecture-based instruction on identical particles. The pretest was not returned to the students. Students began working on the tutorial in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest, tutorial, and posttest were analyzed for understanding of how to determine the many-particle stationary state wavefunction for a system of identical

fermions or bosons. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in our investigation, the non-interacting identical particles were restricted to one spatial dimension for convenience. The word "identical" in the tutorial and in this paper refers to one type of particle (all particles with the same properties). For example, all electrons are identical.

We discuss student responses to several questions that were posed either as in class clicker questions or as open-ended questions on the pretest or posttest of the QuILT. Additional insight into these difficulties was gleaned during the individual think-aloud interviews in which students were asked questions pertaining to these issues. To probe whether students are able to identify and generate a many-particle stationary state wavefunction including spin, the following four questions were posed to the students. Questions Q1 and Q2 were posed on the pretest following traditional instruction on concepts involving a system of identical particles. Questions Q3, Q4, and Q5 were posed on the posttest following completion of the QuILT. Q1, Q2, and Q4 were posed to 30 graduate students and 25 undergraduate students (12 in Year 1 and 13 in Year 2). Q3 was posed to 30 graduate students and 12 undergraduate students in Year 1. Q5 was posed to 13 undergraduate students in Year 2. Students were told that the particles are confined in one spatial dimension and that $\psi_{n_1}$, $\psi_{n_2}$, etc., are the single-particle stationary state wavefunctions. The graduate students were provided Eq. 9.1 which gives the spin states of two spin-1/2 particles in the coupled representation $|s,\ m_s\rangle$ written in terms of states in the uncoupled representation. After finding that the graduate students struggled to determine the spin state for two spin-1 bosons in Q3, the undergraduate students were provided Table 32, which gives the spin states for two spin-1 particles in the coupled representation $|s,\ m_s\rangle$ written in terms of states in the uncoupled representation, in addition to Eq. 9.1.

**Q1.** *Write one possible spatial part of the wavefunction for two indistinguishable spin-1 bosons if the spin part of the wavefunction (expressed in terms of the uncoupled representation) is* $\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|1\ 1\rangle_1|1\ 0\rangle_2 + |1\ 0\rangle_1|1\ 1\rangle_2]$. *If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write "not possible"*

*and state the reason.*

The overall wavefunction for the two indistinguishable bosons must be completely symmetric. Since the spin part of the wavefunction given in Q1 is symmetric, the spatial part of the wavefunction must also be symmetric to ensure that the overall wavefunction is completely symmetric. Two possible symmetric spatial states for the two spin 1 bosons are

$$\psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$$

and (assume $n_1 \neq n_2$)

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)].$$

**Q2.** *Write one possible spin part of the wavefunction for two electrons if the spatial part of the wavefunction is* $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. *If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write "not possible" and state the reason.*

The overall wavefunction for the two electrons must be completely antisymmetric. Since the spatial part of the wavefunction given in Q2 is symmetric, the spin part of the wavefunction must be antisymmetric to ensure that the overall wavefunction is completely antisymmetric. The antisymmetric spin state for the two spin-1/2 fermions is

$$\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle].$$

**Q3.** *Write one possible spin part of the wavefunction for two indistinguishable bosons with spin 1 if the spatial part of the wavefunction is* $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. *If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write "not possible" and state the reason.*

The overall wavefunction for the two indistinguishable bosons must be completely symmetric. Since the spatial part of the wavefunction given in Q3 is symmetric, the spin part

of the wavefunction must also be symmetric to ensure that the overall wavefunction is completely symmetric. There are six possible symmetric spin states for the two spin 1 bosons given in the table in the appendix. One such spin state is

$$|2,\ 1\rangle = \frac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2 + |1,\ 0\rangle_1|1,\ 1\rangle_2).$$

**Q4.** *Write the spatial part of the wavefunction for two indistinguishable spin-$\frac{1}{2}$ fermions if the spin part of the wavefunction is $\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$. If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write "not possible" and state the reason.*

The overall wavefunction for the two indistinguishable fermions must be completely antisymmetric. Since the spin part of the wavefunction given in Q4 is antisymmetric, the spatial part of the wavefunction must be symmetric to ensure that the overall wavefunction is completely antisymmetric. A symmetric spatial state for the two spin-1/2 fermions is

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)].$$

**Q5.** *Write one possible spin part of the wavefunction for two indistinguishable bosons with spin 1 if the spatial part of the wavefunction is $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$ with $n_1 \neq n_2$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write "not possible" and state the reason.*

The overall wavefunction for the two indistinguishable bosons must be completely symmetric. Since the spatial part of the wavefunction given in Q3 is antisymmetric, the spin part of the wavefunction must also be antisymmetric to ensure that the overall wavefunction is completely symmetric. There are several possible antisymmetric spin states for the two spin 1 bosons. For example, the following are examples of a completely antisymmetric spin state:

$$|s,\ m_s\rangle = |1,\ -1\rangle = \frac{1}{\sqrt{2}}(|1,\ 0\rangle_1|1,\ -1\rangle_2 - |1,\ -1\rangle_1|1,\ 0\rangle_2)$$

and

$$\begin{aligned} |s,\ m_s\rangle &= \tfrac{1}{\sqrt{3}}[|1,\ 1\rangle + |1,\ 0\rangle + |1,\ -1\rangle] \\ &= \tfrac{1}{\sqrt{6}}[|1,\ 1\rangle_1|1,\ 0\rangle_2 - |1,\ 0\rangle_1|1,\ 1\rangle_2 + |1,\ 1\rangle_1|1,\ -1\rangle_2 - |1,\ -1\rangle_1|1,\ 1\rangle_2 \\ &\quad |1,\ 0\rangle_1|1,\ -1\rangle_2 - |1,\ -1\rangle_1|1,\ 0\rangle_2]. \end{aligned}$$

Q5 was posed as an in-class clicker question to 16 undergraduate students in a junior/senior level undergraduate quantum mechanics course following instruction on identical particles. The students first answered the question individually and then answered the question a second time after discussing the question with their peers in small groups.

**Q6.** *Choose all of the following statements that are correct about bosons.*

(1) *The spin of a boson is an integer.*

(2) *The overall wavefunction of identical bosons can be anti-symmetric.*

(3) *Two bosons cannot occupy the same single-particle state.*

Only option (1) is correct for question Q6. Option (2) is incorrect because the overall wavefunction for a system of identical bosons MUST be symmetric and option (3) is incorrect because two or more bosons can occupy the same single-particle state.

Question Q7 was posed during the think aloud interview to investigate the students' proficiency at identifying whether the spin part of a wavefunction is a symmetric or antisymmetric wavefunction. The question focuses on a system of two spin-1/2 particles ($s_1 = 1/2$, $s_2 = 1/2$). The students were familiar with the shorthand notation $|\uparrow\uparrow\rangle = |\uparrow\rangle_1|\uparrow\rangle_2$, $|\uparrow\downarrow\rangle = |\uparrow\rangle_1|\downarrow\rangle_2$, $|\downarrow\uparrow\rangle = |\downarrow\rangle_1|\uparrow\rangle_2$, and $|\downarrow\downarrow\rangle = |\downarrow\rangle_1|\downarrow\rangle_2$.

**Q7.** *For the spin part of the wavefunction (spin state) of a two-particle system given below, identify whether the spin state is symmetric, antisymmetric, or neither symmetric nor antisymmetric with respect to exchange of the two particles. Explain your reasoning.*

(a) $|\uparrow\uparrow\rangle$

(b) $|\downarrow\downarrow\rangle$

(c) $|\uparrow\downarrow\rangle$

(d) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

(e) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

In Q7, options (a), (b), and (d) are symmetric spin states (triplet states) since exchanging the two particles results in the same state. Option (e) in Q7 is an antisymmetric spin state (singlet state) since exchanging the two particles results in the original state multiplied by -1. Option (c) in Q7 is a neither a symmetric nor antisymmetric spin state.

Additionally, students were asked to consider a Helium atom as a system and another system of identical particles made up entirely of Helium atoms. They had learned that the wavefunction for the two electrons in a Helium atom must be completely antisymmetric. They had also learned that a system of identical Helium atoms could be a system of identical bosons or fermions depending upon the total spin quantum number of the composite system. In particular, in one case, they considered a system of identical Helium-3 ($^3He$) atoms, which is an example of a system of identical fermions. In another case, they considered a system of identical Helium-4 ($^4He$) atoms. Since each $^4He$ atom consists of an even number of fermions (two protons, two neutrons, and two electrons), it is a boson. A system of $N$ identical $^4He$ atoms is an example of a system of $N$ identical bosons.

## 9.4 STUDENT DIFFICULTIES

Many students struggled to recgonize and generate the completely symmetric many-particle wavefunction for a system of indistinguishable bosons in question Q1 and the completely antisymmetric many-particle wavefunction for a system of indistinguishable fermions in question

Q2. Table 33 summarizes the percentage of students who answered questions Q1 and Q2 correctly for a system of two indistinguishable fermions and bosons on the pretest to the QuILT after traditional instruction.

There are number of underlying difficulties students had that interfered with their ability to write the completely symmetric/antisymmetric many-particle stationary state wavefunction for a system of indistinguishable particles. Some of these struggles are due to difficulties with concepts related to writing the many-particle wavefunction for a system of identical particles.

### 9.4.1 Difficulty applying Pauli's exclusion principle correctly for a system of identical fermions

Some students struggled to realize that Pauli's exclusion principle states that no two fermions can be in the same single-particle state. Students with this type of difficulty often incorrectly overgeneralized the Pauli exclusion principle to state that no two fermions can occupy the same spatial state or the same spin state, as opposed to two fermions cannot be in the same single-particle state made up of both the spatial and spin states. Often students had difficulty realizing that two fermions can be in the same spatial state if they are in different spin states or vice-versa, so that the overall wavefunction is antisymmetric. During the interview, several students incorrectly applied the Pauli exclusion principle when considering a separable many-particle stationary state wavefunction that can be expressed as the direct product of the spatial and the spin parts of the wavefunction. For example, one interviewed student correctly stated that no two fermions can be in the same single-particle state, but then went on to incorrectly claim that "this means two fermions could not exist in the same single-particle stationary state (pointing to a case in which they were in the same spatial state)." This student and others with this type of difficulty often had difficulty realizing that if the two spin-1/2 fermions are in different spin states then it is possible for the two fermions to be in the same single-particle spatial state, i.e. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is a possible spatial part of the two-fermion system.

By a similar argument, several students incorrectly claimed that two fermions could not

exist in the same spin state as this too would violate the Pauli exclusion principle. For example, some interviewed students claimed that $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ were not possible spin states for the system of two spin-1/2 fermions regardless of whether the two fermions were in different single-particle spatial states. These students did not consider the fact that the two fermions could be in different spatial states producing distinct single-particle states for the two fermions.

### 9.4.2 Difficulty with the symmetrization requirements for the overall many-particle stationary state wavefunction due to the fact that it is the product of the spatial and spin parts of the wavefunction

Nature demands that the many-particle wavefunction for a system of indistinguishable bosons be completely symmetric and the many-particle wavefunction for a system of indistinguishable fermions be completely antisymmetric. Therefore, in order to identify and generate a many-particle wavefunction for a system of indistinguishable particles, students must be able to determine a completely symmetric/antisymmetric wavefunction involving both spatial and spin degrees of freedom. However, some students struggled to correctly identify whether the spatial part of the wavefunction or the spin part of the wavefunction is symmetric or antisymmetric when considering each part of the wavefunction separately. As a result, students with this difficulty often were not able to correctly identify the symmetry of the overall wavefunction that included both the spatial and spin parts of the wavefunction.

Students also had difficulty identifying that the many-particle wavefunction for a system of identical bosons must be completely symmetric. For example, in Q6, 43% of the undergraduate students incorrectly answered that the overall wavefunction of identical bosons can be anti-symmetric (option (2)). Even after peer discussion, 31% again incorrectly selected option (2) as correct. Written explanations and interviews suggest that these students knew that the many-particle wavefunction for a system of identical particles (bosons or fermions) must obey a symmetrization requirement, but could not correctly identify which symmetrization requirement corresponds to which particle. In Q1 and Q3, some students attempted to generate a completely antisymmetric wavefunction for a system of identical bosons. In

Q2 and Q4, some students generated a completely symmetric wavefunction for a system of identical fermions. For example, one student wrote the following completely antisymmetric spin part of the many-particle stationary state wavefunction for a system of two bosons in Q3: $|1,\ 1\rangle = \frac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2 - |1,\ 0\rangle_1|1,\ 1\rangle_2)$. The product of the given symmetric spatial part of the wavefunction and the antisymmetric spin part of the wavefunction produces a completely antisymmetric wavefunction for the system of two bosons. Table 34 summarizes the percentage of students who provided a part of the wavefunction with the correct symmetry in Q1 and Q2 on the pretest (although the not necessarily a correct wavefunction as given in Table 33). Additionally, 67% of the undergraduates and 27% of graduate students incorrectly provided a symmetric spin part of the wavefunction in Q2 resulting in an overall symmetric many-particle wavefunction for the two electrons.

Identifying the correct symmetrization requirement for the overall many-particle stationary state wavefunction is challenging due in part to the fact that one must consider the symmetry of both the spatial and spin parts of the wavefunction before determining the overall symmetry of the many-particle stationary state wavefunction. Table 35 summarizes all the possible combinations of the spatial and spin parts of the wavefunction to produce an overall many-particle stationary state wavefunction with the appropriate symmetrization requirement. This can be confusing for students who simply memorized the appropriate combinations of the spatial and spin parts of the wavefunction rather than developing an understanding of how to determine the symmetry of a wavefunction comprised of two separate parts. Below, we discuss specific difficulties students had when attempting to write a completely symmetric/antisymmetric many-particle stationary state wavefunction.

**Difficulty identifying that the spatial and spin parts of wavefunction can both be antisymmetric for a system of identical bosons:** Some students had difficulty realizing that both the spatial and spin parts of the wavefunction can be antisymmetric to produce an overall symmetric wavefunction for a system of identical bosons. A number of students correctly reasoned that the overall many-particle wavefunction for a system of indistinguishable bosons must be completely symmetric. However, some of these students went on to incorrectly claim that both the spatial part and spin part of the wavefunction must be symmetric. These students did not realize that a many-particle stationary state

wavefunction in which both the spatial part and spin part are antisymmetric would result in an overall many-particle wavefunction that is symmetric.

For example, students were asked to construct the spin part of the two-particle stationary state wavefunction for two spin-1 bosons whose spatial part of the wavefunction is given by $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. One interviewed student incorrectly claimed that "it is not possible to write the spin part since the spatial part is antisymmetric. There is no way to make the whole wavefunction symmetric." This student and many others with this type of difficulty did not realize that by choosing an antisymmetric spin part of the wavefunction, the overall two-particle wavefunction would be completely symmetric. For example, the two-particle wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]\frac{1}{\sqrt{2}}[|1,\ 1\rangle_1|1,\ 0\rangle_2 - |1,\ 0\rangle_1|1,\ 1\rangle_2]$ is a completely symmetric wavefunction in which both the spatial and spin parts of the wavefunction are antisymmetric.

**Difficulty identifying that the spatial part is antisymmetric and the spin part is symmetric (or vice versa) for the wavefunction for a system of identical fermions:** Some students correctly identified that the many-particle stationary state wavefunction for a system of identical fermions must be completely antisymmetric, but incorrectly claimed that both the spatial and spin parts of the wavefunction must be completely antisymmetric. For example, in Q4, some students incorrectly claimed that the spatial part of the wavefunction is $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. They struggled to realize that the product of two completely antisymmetric wavefunctions is a completely symmetric wavefunction.

**Confusion due to difficulty discerning that a system of identical bosons may consist of bosons which are made of two or more fermions:** In some situations, e.g., a system consisting of $^4$He atoms, some students struggled to identify whether it was a system of identical bosons or identical fermions and therefore whether the overall wavefunction for the system of $^4$He atoms should be completely symmetric or completely antisymmetric in terms of the single-particle wavefunctions of each $^4$He atom. The students were confused because each $^4$He atom in this system is a boson and is a composite of fermions. Students with this type of difficulty struggled to correctly identify the symmetrization requirement for the system. In particular, a system of identical $^4$He atoms which consists entirely of

spin-1/2 fermions (protons, neutrons, and electrons) is a system of identical bosons. Some students focused only on the fact that the $^4$He atoms are made up of spin-1/2 fermions and incorrectly claimed that a system consisting of identical $^4$He atoms is a system of identical fermions so that the many-particle wavefunction is a completely antisymmetric wavefunction made from the single-particle wavefunctions of $^4$He. The confusion was partly due to the fact that the electronic wavefunction of one Helium atom is completely antisymmetric with respect to the exchange of the two electrons (in this case the Helium atom is the system under consideration, consisting of two non-interacting indistinguishable electrons)

### 9.4.3 Difficulty writing the spin part of the many-particle stationary state wavefunction taking into account the symmetrization requirement

Previous studies have shown that students struggle with concepts involving addition of angular momentum [29]. In order to determine the spin state for a system of identical particles, one must be comfortable with determining the total spin angular momentum. Additionally, in order to generate a completely symmetric or antisymmetric overall many-particle stationary state wavefunction, one needs to know how to generate a completely symmetric or antisymemetric spin part of the wavefunction. However, many students struggled in identifying and generating the spin part of the wavefunction with the appropriate symmetrization requirement. Below, we discuss three specific difficulties students had with identifying the spin states and the symmetry of the spin states for a system of identical particles.

**Incorrectly determining the symmetry based on the appearance of a +/- sign in the many-particle wavefunction:** Some students incorrectly applied a heuristic by which they claimed that a wavefunction is symmetric if the wavefunction is written in terms of a sum. These students simply looked for all "+" signs to determine that a wavefunction is symmetric. They claimed that any wavefunction written as terms added together is a symmetric wavefunction. By a similar logic, these same students looked for a "-" sign to determine whether a given wavefunction is antisymmetric. Some claimed that any wavefunction that had at least one negative sign was antisymmetric. In particular, their determination of whether the wavefunction is antisymmetric did not depend on whether the

wavefunction is completely antisymmetric and the number of terms that have a negative sign in the wavefunction. They merely looked for the presence of at least one minus sign in the wavefunction to determine that the wavefunction is antisymmetric. For example, in response to question Q7(a), one interviewed student incorrectly claimed that the spin part of the wavefunction given by $|\uparrow\uparrow\rangle$ iss neither symmetric nor antisymmetric as "the wavefunction is not a sum so it can't be symmetric and there is not a minus sign, so it can't be antisymmetric." However, the spin part of the wavefunction given by $|\uparrow\uparrow\rangle$ is completely symmetric as the exchange of the two particles results in the same wavefunction, thus there need not be a plus sign in order for a wavefunction to be symmetric. Other students used similar reasoning when determining the symmetry of the spin part of the wavefunction.

Students with this type of difficulty often struggled to write the overall many-particle stationary state wavefunction for a system of identical particles with the appropriate symmetrization requirement. For example, many students who incorrectly claimed that the spin part of the wavefunction $|\uparrow\uparrow\rangle$ is neither symmetric nor antisymmetric went on to incorrectly claim that it is not possible to write a many-particle stationary state wavefunction for two fermions with this spin state.

**Difficulty identifying the spin state for two identical particles:** For all questions, the undergraduate students were provided separate tables corresponding to the possible two-particle spin states for a system of two spin-1/2 fermions and two spin-1 bosons (the tables provided to the students are given in the appendix). After traditional lecture-based instruction, students had difficulty using the tables to correctly identify the spin part of the wavefunction for two spin-1/2 fermions and two spin-1 bosons. For example, in question Q3, in which students were asked to write one possible spin part of the wavefunction for two indistinguishable bosons with spin 1 for a given spatial part of the wavefunction, many students wrote a spin part of the wavefunction corresponding to two spin-1/2 particles. The following were written responses from students to question Q3 after traditional instruction: $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$, $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$, and $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. The antisymmetric singlet state $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ is also problematic in that it is an antisymmetric spin part of the wavefunction. In Q3, the given spatial part of the wavefunction is symmetric and therefore the spin part of the wavefunction must also be symmetric.

## 9.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 9.5.1 Development and Validation of the QuILT

Based upon our research of student difficulties with fundamental concepts with systems of identical particles, we developed a QuILT that attempts to build a consistent and coherent knowledge structure while at the same time addressing the common student difficulties.

As noted in [34], the development of the QuILT was also guided by a cognitive task analysis [48] from both an expert perspective and a novice perspective which consisted of all the requisite knowledge and skills necessary for a functional understanding for a system of identical particles. The initial cognitive task analysis was conducted from an expert perspective in which the researchers outlined the required knowledge and skills and the order in which they are useful in solving problems. This cognitive task analysis was iterated with members of the physics faculty members. However, in an effort of determine if there are additional areas student may struggle with that are not predicted by the experts (expert blindspot) we conducted the student interviews. The cognitive task analysis was then expanded to include these areas in which students needed additional scaffolding support.

As noted in [34], the QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure that the content is correct and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that was incorporated in the next version of the QuILT. Once it was agreed upon by the faculty that the content was clear and appropriate, the QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording was unambiguous, the scaffolding was effective, and to be able to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and provided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the

entire section of the tutorial focusing on these issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and determine whether there were any necessary changes that needed to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and in subsequent interviews. During each step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback and responses to help students with the common difficulties and improve the ability of the students to build a consistent and coherent knowledge structure. After it was deemed successful, the QuILT was next administered to students in various advanced quantum mechanics courses.

### 9.5.2 Overview of the QuILT

As noted in [34], the QuILT strives to transform the students into active learners by employing an inquiry-based approach which requires the students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. The QuILT consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is given in class, during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, they are given the tutorial and encouraged to work together on it in small groups in class. The tutorial can also abe used to guide in-class discussion. As an alternative, the tutorial can be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, the students submit the tutorial for grading and are then administered the posttest. The posttest is given in class as an individual assessment in which the students are not permitted any additional resources beyond what is provided in the posttest.

As noted in [34], the QuILT incorporates guided inquiry-based learning sequences which consist of several questions, each building upon the previous question(s), that require the students to take a stand and actively engage with the material. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether they are correct and explain why they agree or

disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify an inconsistency in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include excerpts that strive to present the students with contradictions between the answers to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining differences between the correct reasoning and their own reasoning before moving on the next section.

### 9.5.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples focusing on fundamental concepts for the many-particle wavefunction for a system of indistinguishable fermions or indistinguishable bosons. In particular, the QuILT strives to help students identify the symmetrization requirements for a system of indistinguishable fermions or bosons and construct the many-particle wavefunction for a system of indistinguishable fermions or bosons. Below are several examples from the QuILT that show scaffolding support intended to help students with these fundamental concepts and address some of the common difficulties.

**Helping students recognize that a given wavefunction is completely symmetric/antisymmetric:** The students work through several guided inquiry-based sequences in which they are asked to focus on the fact that the wavefunction for a system of iden-

tical bosons must be completely symmetric and the wavefunction for a system of identical fermions must be completely symmetric. They engage with examples in which they are asked to determine the symmetry of the wavefunction in which they only consider the spatial part of the wavefunction (ignore spin part of the wavefunction completely) in order to help them focus on the appropriate symmetrization requirements. Then, they are asked to identify and construct both the spatial and spin parts of the many-particle wavefunction for a system of identical particles.

The following is a hypothetical student conversation that is part of a guided inquiry-based learning sequence aimed at helping students identify symmetric and antisymmetric spin states for a system of two spin-1/2 fermions. The students must provide reasoning as to why they agree or disagree with each student.

**Student 1:** *In the uncoupled representation, the two-particle spin states* $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\downarrow\rangle_1|\downarrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, *and* $|\downarrow\rangle_1|\uparrow\rangle_2$ *are all appropriate choices for the spin part of the wavefunction to satisfy the symmetrization requirement.*

**Student 2:** *I disagree with Student 1. In order to satisfy the symmetrization requirement of the wavefunction, we must choose spin states which are either symmetric or antisymmetric. In the uncoupled representation, the two-particle spin states* $|\uparrow\rangle_1|\downarrow\rangle_2$ *and* $|\downarrow\rangle_1|\uparrow\rangle_2$ *are neither symmetric nor antisymmetric. For example, the product of the spin state* $|\uparrow\rangle_1|\downarrow\rangle_2$ *with the spatial part of the wavefunction will not produce a wavefunction that is completely antisymmetric. The same is true for the spin state* $|\downarrow\rangle_1|\uparrow\rangle_2$.

**Student 3:** *I agree with Student 2. The two-particle spin states* $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, *and* $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ *in the coupled representation expressed in terms of states in the uncoupled representation, are symmetric. The two-particle spin state* $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ *is antisymmetric. Therefore, the two-particle spin states* $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, *and* $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ *are all appropriate choices for the spin part of the two-particle wavefunctions to be combined with suitable spatial wavefunctions to satisfy the symmetrization requirement.*

Student 1 is incorrect while Students 2 and 3 are correct in the preceding conversation. The two-particle spin states $|\uparrow\rangle_1|\downarrow\rangle_2$ and $|\downarrow\rangle_1|\uparrow\rangle_2$ are neither symmetric nor antisymmetric. One can create a spin part of the wavefunction with the appropriate symmetry by taking a

linear combination of these two spin states. Students are also asked to reflect upon the fact that a completely symmetric spin state can be constructed from a linear combination of the symmetric triplet states (i.e., that $C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + C_3\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ is a completely symmetric normalized spin state in which $C_1$, $C_2$, and $C_3$ are constants such that $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$)

After working through the guided inquiry-based learning sequences, students are provided checkpoints at the end of each section to allow them to reconcile any discrepancies between their initial reasoning and the correct reasoning.

**Helping students identify the proper symmetry of the wavefunction for a system of identical fermions or bosons:** The students engage with several guided inquiry-based sequences that strive to help them identify that the many-particle stationary state wavefunction for a system of identical fermions must be completely antisymmetric and the many-particle stationary state wavefunction for a system of identical bosons must be completely symmetric. Initially, they work through examples in which they only consider the spatial part of the many-particle stationary state wavefunction in an effort to have them focus on identifying the symmetrization requirements for a system of identical bosons or fermions. Next, students consider the symmetry of the possible spin states involved in a system of identical spin-1/2 fermions and for a system of spin-1 bosons. After engaging with examples focusing on the spatial and spin parts of the wavefunction separately, they work through guided inquiry-based sequences that strive to help them identify all the possible combinations of spatial and spin parts of the many-particle wavefunction for a system of identical fermions or bosons that satisfy the appropriate symmetrization requirement.

**Helping students realize that two fermions in different spin states can occupy the same spatial state:** In the QuILT, students consider various systems of identical fermions and construct the completely antisymmetric stationary state wavefunctions for these systems. For example, in one guided inquiry-based learning sequence students construct the ground state and first-excited state wavefunctions for a system of two fermions placed in a one-dimensional harmonic oscillator potential energy well in response to the following question.

**Q8.** *Two identical non-interacting spin-1/2 fermions are placed in a one-dimensional har-*

*monic oscillator potential energy well with Hamiltonian* $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$. *The single-particle energies are given by*

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

*Construct the spatial part of the two-particle ground state and first-excited state for two non-interacting particles in the one-dimensional harmonic oscillator potential energy well if the particles are*

(a) *Indistinguishable fermions with spin-1/2 in a total spin* $s = 0$ *state.*

(b) *Indistinguishable fermions with spin-1/2 in a total spin* $s = 1$ *state.*

For the following questions, you can denote the spatial state of the $i^{th}$ particle in the ${n_i}^{th}$ single-particle state of the oscillator by $\psi_{n_i}(x_i)$.

In Q8(a), the total spin $s = 0$ state is the antisymmetric singlet state and therefore, the spatial part of the wavefunction must be symmetric. The ground state wavefunction is $\Psi_{00} = \psi_0(x_1)\psi_0(x_2)$ and the spatial part of the first-excited state wavefunction is $\Psi_{01} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2))$. In Q8(b), the total spin $s = 1$ state is one of the symmetric triplet states and thus, the spatial part of the ground state wavefunction must be antisymmetric. The spatial part of ground state wavefunction is $\Psi_{01} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2))$ and the spatial part of the first-excited state wavefunction is $\Psi_{02} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_0(x_2))$.

In the guided inquiry-based learning sequence, students are provided scaffolding support that strives to help them identify that the spatial part of the ground state wavefunction when both fermions are in the same single-particle state is $\psi_0$. For example, the following excerpt is from a hypothetical student conversation designed to help students reflect upon the fact that two fermions can both be in the same single-particle state as is the case for the spatial part of the ground state wavefunction in Q8(a).

**Student 1:** *The two fermions cannot both be in the same single-particle spatial state* $\psi_0$. *For the two-particle ground state, one fermion is in the lowest single-particle spatial state* $\psi_0$ *and the other fermion is in the first-excited single-particle spatial state* $\psi_1$, *so* $n_1 = 0$ *and*

$n_2 = 1$ *or* $n_1 = 1$ *and* $n_2 = 0$. *The two-particle ground state energy is* $E_{10} = 2\hbar\omega$.

**Student 2:** *I disagree with Student 1. You are forgetting about the spin degrees of freedom. For a system of indistinguishable fermions, the overall two-particle state must be antisymmetric. Since the fermions are in the total spin* $s = 0$ *antisymmetric singlet state* $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, *the spatial part of the many-particle state must be symmetric. Two fermions in the same single-particle spatial state* $\psi_0$ *correspond to the symmetric spatial state* $\psi_0(x_1)\psi_0(x_2)$.

Student 1 is incorrect and Student 2 is correct in the preceding conversation. The overall two-particle ground state including both spatial and spin parts is $\Psi_{00} = [\psi_0(x_1)\psi_0(x_2)]$ $[\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)]$. In the total spin $s = 0$ state, the two fermions can be in the same single-particle spatial state $\psi_0$ since the fermions are in different spin states with the two-particle spin-state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ being antisymetric.

**Helping students generate a completely symmetric/antisymmetric wavefunction:** In the QuILT, students engage with several guided inquiry-based learning sequences in which they must write the overall wavefunction for a system of fermions or bosons. For example, students are asked to write all the possible two-particle stationary state wavefunctions including spin for a system of two non-interacting indistinguishable spin-1/2 fermions in different single-particle spatial states labeled by $n_1$ and $n_2$. After answering this question, students are provided scaffolding support that strives to help them identify that the overall wavefunction for the two fermions is antisymmetric so that the spatial part of the wavefunction is symmetric and the spin part of the wavefunction is antisymmetric, or vice versa. The following is an excerpt from a hypothetical student conversation that strives to help them reflect upon how to construct the completely antisymmetric wavefunction for the two fermions:

**Student 1:** *We must only ensure that the spatial part of the two-particle stationary state wavefunction is antisymmetric. The spatial part of the two-particle stationary state wavefunction must be* $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$. *The spin part of the two-particle stationary state wavefunction can be either the antisymmetric singlet state* $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ *or one of the three symmetric triplet states* $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\}$.

**Student 2:** *I agree with Student 1 that the spatial part of the two-particle stationary state wavefunction must be antisymmetric. However, we must also choose the antisymmetric singlet state as the spin part of the two-particle stationary state wavefunction.*

**Student 3:** *I disagree with both Student 1 and Student 2. The overall two-particle stationary state wavefunction must be antisymmetric. If the spatial part of the two-particle stationary state wavefunction is symmetric* $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$*, the spin part of the two-particle stationary state wavefunction must be the antisymmetric singlet state* $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

**Student 4:** *I agree with Student 3. Additionally, the spatial part of the two-particle stationary state wavefunction could be antisymmetric* $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ *which would imply that the spin part of the two-particle stationary state wavefunction can be one of the symmetric triplet states* $\{|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle,\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\}$*. In either case, the product of one symmetric and one antisymmetric wavefunction produces an overall antisymmetric two-particle stationary state wavefunction.*

**Student 3:** *I agree with Student 4. However, remember that a linear combination of the triplet states such as* $C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + C_3(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ *is a completely symmetric spin state where* $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

Students 1 and Students 2 are incorrect while Student 3 and Student 4 are correct in the preceding conversation. Either the spatial part or the spin part must be antisymmetric and the other is symmetric to produce an overall antisymmetric many-particle wavefunction. Further scaffolding is provided to help students develop a good grasp of relevant concepts.

In the QuILT, students are asked to construct the many-particle stationary state wavefunction for general system (e.g., one particle in state $n_1$ and the other particle in state $n_2$) as well as for specific systems. For example, students construct the ground state and first-excited state wavefunctions for a system of two identical particles in a one-dimensional infinite square well potential energy and two identical particles in a one-dimensional harmonic oscillator potential energy well. The next question, Q9, focuses on two identical spin-1 bosons placed in a one-dimensional harmonic oscillator potential energy well and asks students to write the many-particle ground state and many-particle first-excited state wavefunctions for the two bosons.

**Q9.** *Two identical non-interacting spin 1 bosons ($s_1 = 1, s_2 = 1$) are placed in a one-dimensional harmonic oscillator potential energy well with Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$. The single-particle energies are given by*

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

*For the following questions, you can denote the spatial state of the $i^{th}$ particle in the $n_i{}^{th}$ single-particle state of the oscillator by $\psi_{n_i}(x_i)$.*

*Construct at least two possible overall two-particle ground state and at elast two possible first-excited state (including both spatial and spin parts) wavefunctions for two non-interacting particles in the one-dimensional harmonic oscillator potential energy well if the particles are indistinguishable bosons with spin 1.*

After reflecting upon this question, students are provided scaffolding support that strives to help them identify the possible spin states for the two bosons, identify that the overall many-particle stationary state wavefunction must be symmetric, and generate a many-particle stationary state wavefunction. The following is an excerpt from a hypothetical student conversation regarding how to construct a two-particle ground state in Q9 with which the students must state whether they agree or disagree with and explain their reasoning:

**Student 1:** *The two-particle ground state for a system of two indistinguishable bosons with spin 1 ($s_1 = 1 \otimes s_2 = 1$) must be symmetric. There are two possibilities for the two-particle ground state: both the spatial part and the spin part are symmetric or both the spatial part and spin part are antisymmetric.*

**Student 2:** *While that is generally the case, the two-particle ground state must be a state with the lowest energy. The lowest energy occurs when both bosons are in the same single-particle spatial state $\psi_0$. Therefore, the spatial part of the two-particle ground state is $\psi_0(x_1)\psi_0(x_2)$. The two-particle ground state energy is $E_{00} = \hbar\omega$.*

**Student 3:** *I agree with Student 2. Since the spatial part of the two-particle ground state is symmetric, the spin part of the two-particle ground state must also be symmetric. Six possible symmetric combinations for the spin part of the many-particle state for two indistinguishable*

*bosons both with spin 1 ($s_1 = 1, s_2 = 1$) in the coupled representation are $|2,\ 2\rangle$, $|2,\ 1\rangle$, $|2,\ 0\rangle$, $|0,\ 0\rangle$, $|2,\ -1\rangle$, and $|2,\ -2\rangle$. One possible overall two-particle ground state including both spatial and spin parts is $\Psi_{00} = \psi_0(x_1)\psi_0(x_2)|2,\ 2\rangle$.*

**Student 2:** *I agree with Student 3. We can also construct a completely symmetric spin state by taking a linear combination of these symmetric states $C_1|2,\ 2\rangle + C_2|2,\ 1\rangle + C_3|2,\ 0\rangle + C_4|0,\ 0\rangle + C_5|2,\ -1\rangle + C_6|2,\ -2\rangle$, where $|C_1|^2 + |C_2|^2 + |C_3|^2 + |C_4|^2 + |C_5|^2 + |C_6|^2 = 1$ will yeild a normalized state.*

Students 2 and 3 are correct in the preceeding conversation, while Student 1's statement is true in general, but it is not true for the ground state in Q9 that both the spatial and spin part are antisymmetric. The spatial part of the ground state must be $\psi_0(x_1)\psi_0(x_2)$ and therefore, the spin part of the ground state must also be symmetric. Next, the students consider the following hypothetical student conversation regarding how to construct the two-particle first-excited state in Q9 in response to which they must explain why they agree or disagree with each student:

**Student 1:** *If the two-particle first-excited state energy is $E_{01} = 2\hbar\omega$, one boson is in the single-particle spatial state $\psi_0$ and the other boson is in the single-particle spatial state $\psi_1$. The spatial part of the two-particle first-excited state MUST be $\frac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2)]$ since the overall wavefunction must be symmetric. Therefore, the spin part of the two-particle first-excited state must be a symmetric spin state.*

**Student 2:** *The spatial part of the two-particle first-excited state can also be $\frac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2)]$ in which case the spin part of the two-particle first-excited state must be an antisymmetric spin state.*

Student 1 is correct that both the spatial and spin part of the two-particle stationary state wavefunction can be symmetric to produce an overall symmetric first-excited state wavefunction for the two bosons. However, it is also possible that both the spatial and spin parts of the two-particle stationary state wavefunction can be antisymmetric resulting in an overall symmetric first-excited state wavefunction for the two , as stated by Student 2.

After working through these guided inquiry-based learning sequences, students are asked to summarize what they have learned and are provided checkpoints that allow them to reconcile their initial reasoning with the correct reasoning.

## 9.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts for constructing the many-particle stationary state wavefunction for a system of identical particles before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

Questions Q1 and Q2 were posed on the pretest of the QuILT after traditional lecture-based instruction on relevant concepts for a system of identical particles. Questions Q3, Q4, and Q9 were posed on the posttest of the QuILT. Questions Q3 and Q4 were posed to all the graduate students and to 12 of the undergraduate students in Year 1. Question Q9 was posed to 13 undergraduate students in Year 2.

Questions Q1, Q3, and Q9 are similar in that students must identify the overall symmetrization requirement for a system of identical bosons and generate either the spatial or spin part of the wavefunction so that the product of the spatial and spin parts is completely symmetric. Questions Q2 and Q4 are similar in that students must identify the overall symmetrization requirement for a system of identical fermions and generate either the spatial or spin part of the wavefunction so that the product of the spatial and spin parts is completely antisymmetric.

We note that in Year 1, the graduate students were given the QuILT prior to the undergraduate students. The graduate students were not given Table 32 for the two spin-1 bosons on the pretest or the posttest. Many of the graduate students provided a symmetric spin state in response to Q3; however many of them provided a spin state that was consistent with a system of two spin-1/2 fermions. The goal of the QuILT was to have the students be

able to identify and construct the many-particle stationary state wavefunction for a system of identical particles with the correct symmetry. After observing the difficulty that the graduate students had in generating the spin states for two spin-1 bosons on the posttest, Table 32 was added to the pretest and posttest in later implementations with the undergraduate students. Despite the fact that the undergraduate students were given the tables listed in the appendix, they still struggled to correctly write the spin part of the wavefunction for a system of two bosons in Q3 on the posttest. Many of these undergraduate students provided similar responses to those of the graduate students in that they listed a symmetric spin part of the wavefunction consistent with a system of two spin-1/2 particles. Table 36 gives the percentages of students who provided part of the wavefunctions in Q1-Q4 with the correct symmetry. Although identifying the correct spin state for two bosons in Q3 proved to be challenging for students even when they were provided with Table 36, the majority of the students were able to correctly identifying the necessary symmetry. This is an area to improve upon in future refinements and implementations of the QuILT to address these difficulties more effectively.

Table 37 summarizes the percentage of students who answered correctly on the pretest and the posttest and Table 38 provides the average student score on the pretest and posttest. The average score was determined using a rubric which was developed by the researchers together. For each question, the students were awarded 4 points for the correct answer and two points for incorrect answers that had the correct symmetry. A subset of student responses was graded separately by the researchers with a final inter-rater reliability of nearly 100%. The results are encouraging and suggest that the QuILT is effective in helping students identify the symmetrization requirements for the spatial and spin parts of the many-particle stationary state wavefunction for a system of identical fermions. While there is a significant improvement in the number of students who correctly identified the correct symmetrization requirement for the spatial and spin parts of the many-particle stationary state wavefunction, many students struggled to generate a correct spin part of the wavefunction in Q3 or Q5 on the posttest. Focusing on identifying and generating the spin part of the wavefunction for a system of identical bosons is an area to improve upon in future refinements and implementations of the QuILT to help students develop a better understanding of a system

of identical particles.

As a measure of retention, the undergraduate students in the first year of the study were asked Q2 on their midterm examination four weeks after completing the QuILT. The percentage of students who answered Q2 correctly on the midterm examination. Here we find students improved on this question in the exam compared to the pretest of the QuILT. Additionally, the student performance on Q2 on the exam four weeks after completing the QuILT is comparable to their performance on Q4 on the posttest (the group of students in Year 1 scored 8% points lower on the midterm exam compared to the posttest). This suggests that the QuILT helped students gain a better understanding of identifying and generating the many-particle stationary state wavefunction for a system of identical fermions. This also suggests that the QuILT was effective in helping students retain this understanding.

## 9.7 SUMMARY

Investigation of students' understanding of a system of identical particles helped to uncover many common student difficulties that were used as a guide to develop a research-validated QuILT that strives to help students construct the many-particle stationary state wavefunction for a system of non-interacting identical particles. The QuILT focuses on helping students learn that the wavefunction for a system of fermions must be antisymmetric and the wavefunction for a system of bosons must be symmetric and construct the many-particle stationary state wavefunction for a system of non-interacting identical particles (fermions or bosons) consistent with the symmetrization requirements. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding through a guided inquiry-based approach. The results show that the QuILT is effective in improving students' understanding of concepts necessary for a functional understanding of the many-particle stationary state wavefunction for a system of non-interacting identical particles.

## 9.8 ACKNOWLEDGEMENTS

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Table 32: The product states for spin degrees of freedom in the coupled representation $|s,\ m_s\rangle$ (left) are given in terms of linear combinations of product states in the uncoupled representation $|s_1,\ m_{s_1}\rangle_1|s_2,\ m_{s_2}\rangle_1$ (right) using the Clebsch-Gordon table for the case $s_1 = 1 \otimes s_2 = 1$.

| Product states in Coupled Representation $\|s,\ m_s\rangle$ | Written in terms of product states in Uncoupled Representation $\sum_{m_{s_1}+m_{s_2}=m_s} C^{s_1,s_2,S}_{m_{s_1},m_{s_2},m_s}\|s_1,\ m_{s_1}\rangle_1\|s_2,\ m_{s_2}\rangle_2$ |
|---|---|
| $\|2,\ 2\rangle$ | $\|1,\ 1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 + \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|1,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 - \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|2,\ 0\rangle$ | $\frac{1}{\sqrt{6}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 + \sqrt{\frac{2}{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2$ $+\frac{1}{\sqrt{6}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|1,\ 0\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 1\rangle_2)$ |
| $\|0,\ 0\rangle$ | $\frac{1}{\sqrt{3}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \frac{1}{\sqrt{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2$ $+\frac{1}{\sqrt{3}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 + \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|1,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|2,\ -2\rangle$ | $\|1,\ -1\rangle_1\|1,\ -1\rangle_2$ |

Table 33: The percentages of graduate ($N = 30$) and undergraduate ($N = 25$) students who correctly answered questions Q1 and Q2 for the given system of indistinguishable particles for the pretest.

| Question | Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|---|
| Q1 | Bosons | 33 | 48 |
| Q2 | Electrons | 30 | 44 |

Table 34: The percentages of graduate ($N = 30$) and undergraduate ($N = 25$) students who provided a symmetric spatial part of the wavefunction in Q1 and an antisymmetric spin part of the wavefunction in Q2 for the given system of indistinguishable particles for the pretest.

| Question | Type of Particle | Part of the Wavefunction | Graduate (%) | Undergraduate (%) |
|---|---|---|---|---|
| Q1 | Bosons | Spatial | 33 | 48 |
| Q2 | Electrons | Spin | 30 | 44 |

Table 35: All the possible combinations of the spatial and spin parts of the wavefunction to yield an overall many-particle stationary state wavefunction with the appropriate symmetrization requirement.

| Type of Particle | Spatial Part of the Wavefunction | Spin part of the Wavefunction | Complete Wavefunction |
|---|---|---|---|
| Indistinguishable Fermions | Symmetric | Antisymmetric | Antisymmetric |
| | Antisymmetric | Symmetric | |
| Indistinguishable Bosons | Symmetric | Symmetric | Symmetric |
| | Antisymmetric | Antisymmetric | |

Table 36: The percentages of graduate ($N = 30$) and undergraduate ($N = 12$ in Year 1 and $N = 13$ in Year 2) students who provided a part of the wavefunction with the correct symmetry in Q1 and Q2 on the pretest and Q3, Q4, and Q9 on the posttest.

| Question | Type of Particle | Part of the Wavefunction | Graduate | | | Undergraduate | | |
|---|---|---|---|---|---|---|---|---|
| | | | N | Pre (%) | Post (%) | N | Pre (%) | Post (%) |
| Q1 | Bosons | Spatial | 30 | 33 | - | 25 | 48 | - |
| Q2 | Electrons | Spin | 30 | 30 | - | 25 | 44 | - |
| Q3 | Bosons | Spin | 30 | - | 97 | 12 | - | 92 |
| Q4 | Fermions | Spatial | 30 | - | 87 | 25 | - | 80 |
| Q5 | Bosons | Spin | - | - | - | 13 | - | 69 |

Table 37: The percentages of students who answered questions Q1 and Q2 correctly for the given system on the pretest and Q3, Q4, and Q9 correctly for the given system on the posttest for graduate students ($N = 30$) and undergraduates ($N = 12$ in Year 1 and $N = 13$ in Year 2).

| Question | Type of Particle | Graduate | | | Undergraduate | | |
|---|---|---|---|---|---|---|---|
| | | N | Pre (%) | Post (%) | N | Pre (%) | Post (%) |
| Q1 | Bosons | 30 | 33 | - | 25 | 48 | - |
| Q2 | Electrons | 30 | 20 | - | 25 | 36 | - |
| Q3 | Bosons | 30 | - | 10 | 12 | - | 17 |
| Q4 | Fermions | 30 | - | 87 | 25 | - | 80 |
| Q5 | Bosons | - | - | - | 13 | - | 53 |

Table 38: The average student score on questions Q1 and Q2 for the given system on the pretest and Q3, Q4 and Q9 for the given system on the posttest for graduate students ($N = 30$) and undergraduates ($N = 12$ in Year 1 and $N = 13$ in Year 2).

| Question | Type of Particle | Graduate | | | Undergraduate | | |
|---|---|---|---|---|---|---|---|
| | | N | Pre (%) | Post (%) | N | Pre (%) | Post (%) |
| Q1 | Bosons | 30 | 34 | - | 25 | 51 | - |
| Q2 | Electrons | 30 | 29 | - | 25 | 36 | - |
| Q3 | Bosons | 30 | - | 52 | 12 | - | 54 |
| Q4 | Fermions | 30 | - | 88 | 25 | - | 80 |
| Q5 | Bosons | - | - | - | 13 | - | 53 |

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# 10.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: COUNTING THE NUMBER OF DISTINCT MANY-PARTICLE STATES FOR A SYSTEM WITH A FIXED NUMBER OF AVAILABLE SINGLE-PARTICLE STATES

## 10.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. There have been a number of research studies aimed at investigating student reasoning in QM [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] and improving student understanding of QM [27, 28, 29, 30, 31, 32, 33, 34, 35]. For example, our group has focused on using the common student difficulties as a guide to develop research-based learning tools which include Quantum Interactive Learning Tutorials (QuILTs) [36, 37, 38, 39, 40, 41, 42] which strive to improve student understanding of different QM concepts. However, there have been few investigations into student difficulties with fundamental concepts involving a system of identical particles.

Here, we discuss an investigation of student difficulties with the number of distinct many-particle stationary states for a system of non-interacting identical particles and how that research was used as a guide in the development, validation, and in-class evaluation of a QuILT that strives to help students develop a good grasp of relevant concepts pertaining to the number of distinct many-particle states. Through researching students' understanding of and reasoning about a system of identical particles, we found common student difficulties that can hinder their development of a consistent and coherent knowledge structure pertaining to these concepts.

Students must have a good understanding of quantum mechanical properties of a system of identical particles as well as a strong background in combinatorics to be proficient in determining the number of distinct many-particle states. However, it has been found in a number of different contexts in introductory physics that students struggle to apply mathematics correctly in the context of physics even if they can solve similar mathematics problems without the physics context [43, 44, 45, 46]. Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of the individual who is solving the problem, Simon's framework of "bounded rationality" posits that an individual will make decisions while solving problems based upon their current level of expertise, which may not be optimal depending on their experise [47]. In particular, students often only look for a solution that appears satisfactory to them in which they see no inconsistencies rather than searching for additional pathways in the problem space which may yield more productive solutions. Some students may be motivated to find an optimal solution but if the students' level of expertise is not sufficient and they have not been provided with the appropriate scaffolding support, they may experience cognitive overload and not be able to determine the correct solution to the problem posed [48].

Below, we start with a brief background of relevant concepts and then describe the methodology for the investigation of student difficulties followed by the common difficulties found. Then we describe the methodology for the development, validation and in-class evaluation of the corresponding research-based QuILT that strives to help students develop a functional understanding of the fundamental concepts involved in determining the number of many-particle states for a system of identical particles.

## 10.2 BACKGROUND

In nature, there are two general types of particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g., photons and mesons). A system of $N$ identical particles consists of $N$ particles of the

same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in quantum mechanics, identical particles are indistinguishable and there is no measurement that can be performed to distinguish these identical particles from one another. For example, if the coordinates of two identical particles are interchanged, there is no physical observable that would reflect this interchange. For a system of identical fermions, it is not possible for two or more fermions to occupy the same single-particle state. On the other hand, it is possible for two or more bosons to occupy the same single-particle state.

Here, we will consider a system of identical particles in which the total number of particles is fixed. Also, for these systems considered here, the energy of the system is not constant but there are only a fixed number of single-particle states available for the particles to occupy and there is no degeneracy in the single-particle energies.

In order to construct a many-particle stationary state for a system of fermions (ignoring spin degrees of freedom), there must be at least as many available spatial single-particle states as the number of identical fermions. If this condition is satisfied, one must determine the number of ways to arrange the identical fermions into the available single-particle states such that each single particle state has either zero or one fermion until all the fermions have been placed into a single-particle state. The number of ways to arrange $N$ identical objects among $M$ available slots ($M \geq N$) is $\binom{M}{N} = \frac{M!}{N!(M-N)!}$. Thus, for a system of $N$ fermions with $M$ available single-particles states, the number of distinct many-particle states is

$$\begin{cases} \binom{M}{N} & M \geq N \\ 0 & M < N. \end{cases} \tag{10.1}$$

One technique for determining the number of ways to arrange the identical bosons among the available single-particle states is often referred to as the "bin and divider" method. In particular, we can treat the single-particle states as bins to be filled with bosons and dividers to separate the different single-particle states, or bins. The number of distinct many-particle states can be found by determining the number of distinct arrangements of the identical bosons and diviiders. For a system of $N$ identical bosons and $M$ available single-particle states, there are $M-1$ identical dividers separating the single-particle states.

This gives $N + M - 1$ objects from which to arrange the $N$ identical bosons and the $M - 1$ identical dividers. Thus, the number of distinct many-particle states for a system of $N$ indistinguishable bosons with $M$ available single-particle states is

$$\binom{N+M-1}{N} = \binom{N+M-1}{M-1} = \frac{(N+M-1)!}{N!(M-1)!}. \tag{10.2}$$

As a contrasting case, if identical particles could be treated as distinguishable, then one can determine which particle is in which single-particle state and there is no restriction on the number of particles in each single-particle state. For a system of $N$ identical particles that can be treated as distinguishable and $M$ available single-particle states, each particle can be placed in any of the $M$ single-particle states. The number of distinct $N$-particle states for a system of $N$ identical particles if they could be treated as distinguishable with $M$ available single-particle states is

$$M^N. \tag{10.3}$$

Determining the number of distinct many-particle states for a system in which the number of single-particle states is fixed is an important concept for students to help prepare them, e.g., for quantum mechanics leading to quantum statistical mechanics.

## 10.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with determining the number of distinct many-particle states for a system of identical fermions or bosons were first investigated using three years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight was gained concerning these difficulties from responses of 14 students during a total of 81 hours of individual think-aloud interviews. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates and 30 first-year physics graduate students in their respective QM courses. The QuILT included a pretest, the tutorial, and a posttest. Students were given the pretest after traditional

lecture-based instruction on identical particles. The pretest was not returned to the students. Students began working on the tutorial in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest, tutorial, and posttest were analyzed for their understanding of how to determine the number of distinct many-particle states for a system of identical particles in which the number of single-particles states is fixed. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in our investigation, the non-interacting identical particles were restricted to one spatial dimension for convenience. Students were asked to consider the spatial part of the wavefunction to simplify the problem (i.e., students were asked to ignore the spin degrees of freedom) and to help them focus on fundamental concepts involved in determining the number of distinct many-particle states for system of identical particles.

To probe whether students are able to determine the number of distinct many-particle states for a given system, the following two questions were posed to the students. Question Q1 was posed during the individual interviews as well as on the pretest for the QuILT after traditional instruction in relevant topics. Q2 was posed on the posttest following traditional instruction on identical particles as well as after students engaged with the QuILT. Q1 and Q2 were posed to 30 graduate students and 25 undergraduate students.

**Q1.** For a system of three non-interacting identical particles, there are four distinct single-particle states $\psi_{n_1}(x)$, $\psi_{n_2}(x)$, $\psi_{n_3}(x)$, and $\psi_{n_4}(x)$ available to each particle. How many different three-particle states can you construct if the particles are

a. Fermions? (Ignore spin).

b. Bosons? (Ignore spin).

c. Distinguishable particles? (Ignore spin).

In Q1(a), for a system of three identical fermions, there are four distinct single-particle states in which to place the three fermions. Since no single-particle state can have more than two fermions and there are $\binom{4}{3} = \frac{4!}{3!(4-3)!} = 4$ distinct three-particle states in Q1(a). For the system of three identical bosons, a single-particle state can have more than one boson. In

Q1(b), there are $\binom{4-1+3}{3} = \binom{6}{3} = \frac{6!}{3!(6-3)!} = 20$ distinct three-particle states for a system of three identical bosons. In Q1(c), for the contrasting case of identical particles that can be treated as distinguishable, each particle can be placed in any of the four single-particle states. Since there is no symmetrization requirement and the particles are distinguishable, each three-particle state is distinct. There are $4^3 = 64$ distinct three-particle states for a system of three identical particles that can be treated as distinguishable.

**Q2.** For a system of two non-interacting identical particles, there are five distinct single-particle states $\psi_{n_1}(x)$, $\psi_{n_2}(x)$, $\psi_{n_3}(x)$, $\psi_{n_4}(x)$, and $\psi_{n_5}(x)$ available to each particle. How many different two-particle states can you construct if the particles are

a. Fermions? (Ignore spin).

b. Bosons? (Ignore spin).

c. Distinguishable particles? (Ignore spin).

In Q2(a), there are $\binom{5}{2} = \frac{5!}{2!(5-2)!} = 10$ distinct two-particle states. In Q2(b), for a system of identical bosons, a single-particle state can have more than one boson. There are $\binom{6}{2} = \frac{6!}{2!(6-2)!} = 15$ distinct two-particle states for a system of two identical bosons in Q2(b). In Q2(c), for the contrasting case of identical particles that can be treated as distinguishable, there are $5^2 = 25$ distinct two-particle states for a system of two identical particles that can be treated as distinguishable.

## 10.4 STUDENT DIFFICULTIES

Many students struggled to determine the number of distinct many-particle states for a system of identical particles. Table 39 summarizes the percentages of students who answered question Q1 correctly for a system of three identical particles after traditional lecture-based instruction. We will discuss several categories of student difficulties that interfered with their ability to determine the number of distinct many-particle states for a system of non-interacting identical particles. These categories include (1) conceptual difficulties, (2) reliance on memorized formulas, (3) difficulty with procedural knowledge, and (4) difficulty

Table 39: The percentages of graduate (N=30) and undergraduate (N=25) students who correctly answered question Q1 for the given system of indistinguishable particles after traditional instruction.

| Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Fermions | 40 | 48 |
| Bosons | 17 | 16 |
| Distinguishable | 17 | 20 |

with mathematical sense-making in the context of physics. Some of the difficulties discussed here may be placed in several categories, but we have placed them into a particular category in an effort to illustrate these broader categories with explicit examples. Some students provided the same incorrect answer to Q1 but reasoned about it differently based upon different underlying difficulties, and therefore the same incorrect answer may be placed in different categories based upon the reasoning provided by the students (note that the categories are not mutually exclusive)

### 10.4.1 Conceptual difficulties with indistinguishability pertaining to a system of identical particles

A system of identical fermions or bosons consists of indistinguishable particles and one must be careful not to count the number of distinct many-particle states for these particles as if they are distinguishable particles. For example, if two identical fermions are in the single-particle states labeled by $\psi_{n_1}$ and $\psi_{n_2}$, then there is no way to distinguish the system in which the first fermion is in the single-particle state $\psi_{n_1}$ and the second fermion is in the single-particle state $\psi_{n_2}$ with the system in which the first fermion is in the single-particle state $\psi_{n_2}$ and the second fermion is in the single-particle state $\psi_{n_1}$. These two arrangements of the fermions make up the different terms of a two-particle stationary state wavefunction and are not two distinct two-particle states. Assuming $n_1 \neq n_2$, the completely

antisymmetric two-particle wavefunction for this system (ignoring spin degrees of freedom) is $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.

Many students struggled to identify how the number of distinct many-particle states for a system of indistinguishable particles differs from that of a system of identical particles that can be treated as distinguishable. Some students claimed that the number of distinct many-particle states in Q1 is the same for a system of indistinguishable fermions or bosons and a system of identical particles that can be treated as distinguishable. Table 40 shows the percentages of students who incorrectly determined the same number of distinct many-particles states in Q1 for a system of indistinguishable fermions or bosons as for a system of identical particles that can be treated as distinguishable.

For a system of identical fermions, the most common incorrect answer to Q1(a) was $4 \cdot 3 \cdot 2 = 24$ distinct many-particle states. Students with this response claimed that there were 4 single-particle states available to place the first particle, 3 available single-particle states for the second particle, and 2 remaining available single-particle states for the last particle. One interviewed student with this type of response claimed that "there are four states for the first fermion, three for the second (fermion) since it cannot be in the same state as the first (fermion), and two left for the last one." This student and others with similar reasoning correctly tried to apply Pauli's exclusion principle but did not take into account the fact that these three fermions are indistinguishable. By way of example, if the three fermions occupy the single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$ there is no way to detect which fermion is in which single-particle state. Assuming $n_i \neq n_j \neq n_k$, the many-particle stationary state wavefunction for this system is $\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}}[\psi_{n_i}(x_1)\psi_{n_j}(x_2)\psi_{n_k}(x_3) - \psi_{n_i}(x_1)\psi_{n_k}(x_2)\psi_{n_j}(x_3) + \psi_{n_j}(x_1)\psi_{n_k}(x_2)\psi_{n_i}(x_3) - \psi_{n_j}(x_1)\psi_{n_i}(x_2)\psi_{n_k}(x_3) + \psi_{n_k}(x_1)\psi_{n_i}(x_2)\psi_{n_j}(x_3)$
$-\psi_{n_k}(x_1)\psi_{n_j}(x_2)\psi_{n_i}(x_3)]$. There are 4 ways to choose the labels $n_i, n_j$, and $n_k$ from the available states labeled by $n_1, n_2, n_3$, and $n_4$. If the particles could be treated as distinguishable, each of the six terms in this completely antisymmetric many-particle stationary state would be six distinct many-particle states producing a total of 24 distinct many-particle states, which is what the students in Q1(a) reasoned was the case for fermions.

For a system of identical bosons, many students struggled to identify how the number of distinct many-particle states would differ from that of a system of identical particles

Table 40: The percentages of graduate (N=30) and undergraduate (N=25) students who incorrectly answered question Q1 the same for the given system of indistinguishable particles as for a system of identical particles that can be treated as distinguishable.

| Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Fermions | 23 | 8 |
| Bosons | 23 | 12 |

that can be treated as distinguishable. In Q1(b), students who claimed that there were $4^3 = 64$ distinct many-particle states for a system of indistinguishable bosons often stated that since bosons can occupy the same single-particle state, there are 4 available single-particle states for each boson and thus, $4 \cdot 4 \cdot 4 = 64$ distinct many-particle states. However, these students were not taking into account the fact that the bosons are indistinguishable and therefore some states that are distinct for a system of distinguishable particles are not distinct for a system of indistinguishable bosons. Some of these distinct states for distinguishable particles are terms in the completely symmetric many-particle stationary state wavefunction for a system of indistinguishable bosons. For example, students with this type of reasoning were incorrectly counting the many-particle states $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)$, $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)$ and $\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ as distinct many-particle states in Q1(b). However, these three states correspond to the three terms in a completely symmetric many-particle stationary state wavefunction $\frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)]$ and are not three distinct many-particle states for the system of indistinguishable bosons.

In addition, some students struggled to determine the number of distinct many-particle states in part because they had difficulty realizing that the order in which the single-particle wavefunctions are expressed in the product of the single-particle states in the many-particle basis states is irrelevant. Here, for convenience, we will refer to all direct products of single-particle states as "basis states", regardless of their symmetry under exchange. Please note that for identical fermions, only antisymmetric linear combinations

of these basis states are allowed, while for bosons only symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed. For example, the following are all equivalent ways to express the basis state for a system of three non-interacting identical particles: $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$, $\psi_{n_2}(x_2)\psi_{n_1}(x_1)\psi_{n_3}(x_3)$, $\psi_{n_2}(x_2)\psi_{n_3}(x_3)\psi_{n_1}(x_1)$, $\psi_{n_3}(x_3)\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, and $\psi_{n_3}(x_3)\psi_{n_2}(x_2)\psi_{n_1}(x_1)$ where the coordinates $x_1, x_2$, and $x_3$ refer to particles 1, 2, and 3, respectively. However, in Q1, students with this type of difficulty counted each of these equivalent products of the single-particle states as if it were a distinct many-particle state for the system or distinct basis states for the many-particle wavefunction. Some students focused on the order in which the labels for the single-particle states or the coordinates appeared to determine whether the products of the single-particle wavefunction were different. For example, when comparing $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ and $\psi_{n_1}(x_1)\psi_{n_3}(x_3)\psi_{n_2}(x_2)$, they claimed that $n_2$ and/or $x_2$ appear in the second place in the first product and in the third place in the second product, so these must be different terms in the many-particle wavefunction.

### 10.4.2 Reliance on memorized formulas

**Using a memorized formula as opposed to systematic reasoning:** Some interviewed students struggled to calculate the number of distinct many-particle states in Q1 and they used a memorized formula for the number of many-particle states rather than formulating a systematic reasoning for the given system. In some cases, students recalled one or more expressions which were correct for a particular type of system but applied these expressions to the wrong system of identical particles. For example, in the interview, some students answered Q1(a) in a manner which would have been correct for a system of identical bosons and Q1(b) in a manner that would have been correct for a system of identical fermions. Interviews suggest that these students often wrote the formula for the number of many-particle states from memory and did not reflect upon whether the formula was appropriate for the given system.

Moreover, whether a student would reason about a given situation to find the number of distinct many-particle states conceptually or use memorized knowledge depended on the

context. Some students could identify that two or more fermions could not occupy the same single-particle state in one context but not in a different situation. For example, during the interview, students were asked to write all of the possible many-particle stationary state wavefunctions for a system of three indistinguishable fermions in two distinct single-particle states and then later asked to determine the number of distinct many-particle states for this same system. It is not possible to have three fermions in only two single-particle states. However, some students incorrectly provided at least one many-particle stationary state and/or calculated a non-zero number of distinct many-particle states for this system. In particular, these students generally either determined that there are zero distinct many-particle states for a system in which two or more fermions are in the same single-particle state or that the many-particle stationary state wavefunction does not exist for such a system, but then answered the other related question as though such a system does exist. One interviewed student with this difficulty correctly stated that "we can't write a many-particle stationary state wavefunction for a system that has two fermions in the same state." But this same student later in the interview incorrectly calculated that there are $\binom{3}{2} = 3$ distinct many-particle states for the system of three indistinguishable fermions in two single-particle states. Interviews suggest that students with this type of difficulty often used the formula $\binom{M}{N}$ from memory to find the number of distinct ways to arrange the $N$ identical objects among $M$ total objects, but they did not do a reasonability check for whether this formula should be used for the given situation and correctly identify what $N$ and $M$ in $\binom{M}{N}$ represent. For example, upon questioning by the interviewer, this interviewed student incorrectly identified $M$ as the number of identical fermions as opposed to the number of available single-particle states and incorrectly identified $N$ as the number of available single-particle states as opposed to the number of identical fermions. He did not detect the inconsistency in his two responses. The lack of sufficient sense-making to recognize that different responses for the same physical situation are inconsistent is common in introductory physics but has also been observed in prior research related to student understanding of Dirac notation in QM [14]. One reason for the difficulty in metacognition is that students' working memory is constrained by the demands of the problem since they are still developing expertise in these concepts and must do mathematical sense-making in a given context. Therefore, the cognitive overload makes

it difficult to do metacognition and ensure that different responses are consistent with each other [48].

For a system of identical bosons in Q1(b), some of the interviewed students who answered that there are $3^4 = 81$ distinct many-particle states were incorrectly recalling the formula for a system of identical particles that can be treated as distinguishable and also incorrectly applying this formula to a system of identical bosons. For example, some students during the interview debated whether the number of distinct many-particle states for a system of identical particles that can be treated as distinguishable for a system of $N$ particles and $M$ available single-particle states is $M^N$ or $N^M$ without explicitly reasoning about what it should be given $N$ particles and $M$ available single-particle states. Students with this type of difficulty often did not engage in sufficient sense-making to ensure that their answers were reasonable. For example, one can check the reasonability of the formulas $M^N$ or $N^M$ for a system with a small number of particles and available single-particle states. One could consider a system of one particle and two available single-particle states. In this case, the particle can be in either of the two single-particle states and there are two distinct many-particle states and thus, $M^N = 2^1 = 2$ gives the correct answer. However, using the formula $N^M = 1^2 = 1$, one incorrectly obtains only one distinct many-particle state for the system.

**Incorrectly multiplying (as opposed to dividing) by the number of indistinguishable combinations:** Many students attempted to determine the number of distinct many-particle states for a system of indistinguishable particles by determining the number of arrangements of identical particles in the single-particle states and then adjusting this number based upon the number of indistinguishable permutations. However, in Q1(a) and Q1(b), some students incorrectly multiplied the number of distinct many-particle states by the number of permutations of the indistinguishable particles (as opposed to dividing it). One interviewed student considered about whether to multiply or divide by the number of permutations of the indistinguishable particles and ultimately decided to multiply. He did not explicitly reason about whether indistinguishability should give rise to more or less many-particle states compared to the case when particles are distinguishable.

For a system of identical fermions in Q1(a), one interviewed student incorrectly determined that there are $4! \cdot 3!$ distinct many-particle states for the system of three indistinguish-

able fermions in four single-particle states. When asked, this student stated how he obtained 4! by noting that "we can put the first fermion in any of the four states. The second fermion can go in any of the three states that the first fermion didn't go in. And the third fermion can be in either of the two remaining states." The student then went on to try to account for the indistinguishability of the three fermions. "Then we need to multiply by the number of arrangements that are the same for these three identical fermions. There are 3! ways to arrange these three fermions so we need to multiply by this factor." The student then jotted down his answer as $4! \cdot 3!$. This student used rote memory to multiply rather than divide and claimed that there are more distinct states when taking into account the indistinguishability of the fermions. However, there are fewer distinct many-particle states for the system of indistinguishable fermions than there are for a system of three distinguishable particles all in different single-particle states. For example, there are $\binom{4}{3} = \frac{4!}{3!1!} = 4$ distinct ways to arrange the three indistinguishable fermions among the four single-particle states.

**Incorrectly determining the number of distinct many-particle states for a different case in which the number of particles in the system was not fixed:** Some students focused on the number of particles that could occupy a given single-particle state without realizing that the number of identical particles for a given system was specified in the problem. Interviews suggest that students may have been attempting to recall an example they had seen in class in which the number of particles in the system was not fixed and instead they were asked to determine the number of distinct many-particle states for the system with different conditions specified by the problem. Below, we give two such examples.

For a system of identical fermions in Q1(a), one interviewed student correctly stated that "each single-particle state can have either zero or one fermion, so there are two possibilities for the first single-particle state, two for the second, and two for the third and fourth. There are $2 \times 2 \times 2 \times 2 = 2^4 = 16$ distinct many-particle states." This student and others with this type of response failed to realize that the system in Q1 had three indistinguishable fermions and instead calculated all the possible many-particle states for fermions in these four single-particle states ranging from zero to four fermions.

For a system of identical particles that can be treated as distinguishable in Q1(c), one interviewed student incorrectly claimed that "there are three particles that can be put in

the first state, three particles that can be put in the second state, three in the third, and three in the fourth." The student then wrote $3^4 = 81$ as the total number of distinct three particle states. This student failed to realize that his method for counting the total number of distinct states was not consistent for a system of only three particles. If there are three identical particles that can be treated as distinguishable in the first single-particle state, then there are none remaining to be placed in the other single-particle states. For a system in which there are three particles in each of the four single-particle states, the system would have 12 particles not 3. However, this student and others with this type of reasoning failed to realize that they were not determining the number of distinct many-particle states for systems restricted to only the specified number of particles.

### 10.4.3 Difficulties with procedural knowledge

Interviews suggest that some students had the correct conceptual understanding but struggled to connect their conceptual knowledge with the procedure for determining the number of distinct many-particle states correctly. Many of these students struggled with systematic reasoning for determining the number of distinct many-particle states. In particular, some students had difficulty determining the number of distinct many-particle states for a system with a small number of particles and available single-particle states while others had difficulty generalizing to a system with a large number of particles and available single-particle states. Below are several difficulties students had formulating a systematic approach for determining the number of distinct many-particle states.

**Attempting to explicitly list all of the possible many-particle states but omitting at least one possible combination:** Nearly all the interviewed students began by attempting to list all of the possible many-particle states for a system of indistinguishable bosons in Q1(b). Most of the students continued to list as many of the distinct many-particle states as they could. However, some of them omitted at least one of the possible many-particle states partly because they were not systematic. For example, in Q1(b), some students began by listing several states in one type of arrangement (e.g., all the bosons in the same single-particle state) and then moved on to listing states in another type of

arrangement (e.g., all the bosons in different single-particle states) without listing all the many-particle states in each arrangement before moving on to the next arrangement. They would often continue to list states in various arrangements and then stop when they could not identify any new many-particle states that they had not already listed. In general, many students missed at least one of the three-particle states in Q1(b) in which two of the bosons are in one single-particle state and one boson is in a different single-particle state.

**Incorrectly deducing the total number of distinct many-particle states after determining the first few many-particle states:** Other students used their intuition and deductive reasoning after determining the first few distinct many-particle states to calculate the total number of distinct many-particle states. This was particularly true for a system of indistinguishable bosons in Q1(b). In general, students were able to correctly calculate all the distinct three-particle states when the three bosons were in the same single-particle state. Then they explicitly listed the first few distinct three-particle states when all the three bosons were in different single-particle states and attempted to identify a pattern to enable them to calculate the total number of distinct many-particle states. Often, students applied a similar tactic to determine the total number of three-particle states when two of the bosons are in one single-particle state and one boson is in a different single-particle state. However, some students incorrectly generalized their pattern and miscounted the total number of distinct three-particle states in Q1(b). Other students who answered Q1(b) correctly had difficulty generalizing to a system with a large number of particles and available single-particle states. They were able to explicitly list all of the possible many-particle states for systems in which there were few identical particles and a small number of available single-particle states but then struggled to generalize the method to systems with a large number of identical particles and a large number of available single-particle states. In general, they were able to explicitly list all of the possible many-particle states for a system with relatively few particles and available states, but struggled to recognize a pattern to generalize the results. For a system with a large number of particles and a large number of available single-particle states, these students could not list every possible many-particle state and were not able to calculate the number of distinct many-particle states.

**Claiming that the single-particle wavfunctions do not commute in their product used to construct basis states for many-particle wavefunctions:** Students who claimed that the single-particle wavefunctions of different particles in the basis states in the product space do not "commute" had difficulty generating a many-particle wavefunction with the appropriate number of terms and in determining the normalization constant. For example, students with this type of difficulty often claimed that the many-particle wavefunction for a system of three identical bosons in which all the bosons are in the same single-particle state is $\frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)+\psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)+\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)]$ or $\frac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)+\psi_{n_1}(x_1)\psi_{n_1}(x_3)\psi_{n_1}(x_2)+\psi_{n_1}(x_2)\psi_{n_1}(x_1)\psi_{n_1}(x_3)$ $+\ \psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)+\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)+\psi_{n_1}(x_3)\psi_{n_1}(x_2)\psi_{n_1}(x_1)]$. They struggled to realize that all terms in both expressions are equivalent and can be simplified to a single term $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$. Additionally, they struggled to correctly determine the normalization constant. For example, the expression $\frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)\ +$ $\psi_{n_1}(x_2)\psi_{n_1}(x_3)\psi_{n_1}(x_1)+\psi_{n_1}(x_3)\psi_{n_1}(x_1)\psi_{n_1}(x_2)]$ reduces to $\sqrt{3}\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$, which is not the properly normalized many-particle wavefunction for a system of three identical bosons in the single-particle state $\psi_{n_1}$.

Another interviewed student in Q1(b) claimed that there are $4^3 \times 3!$ distinct many-particle states for a system of three indistinguishable bosons in four single-particle states. The student incorrectly multiplied $4^3$ by 3! to account for number of ways to arrange the single-particle states in each basis state.

**Difficulty with the bin and divider method for determining the number of distinct many-particle states for a system of identical bosons:** One approach for determining the number of distinct many-particle states for a system of indistinguishable bosons is the "bin and divider" method. In this method, the indistinguishable bosons can be placed into any of the single-particle states which can be thought of as bins to hold the bosons. The number of distinct many-particle states is given in Eq. 12.5.

Many students who used the bin and divider method had difficulty realizing that one should be using the number of dividers (number of available single-particle states minus 1) as opposed to the number of bins (number of available single-particle states) to determine the number of distinct states for a system of identical bosons. One interviewed student

incorrectly claimed that "we can either count the number of ways to arrange the bosons or the states" among the total number of indistinguishable objects. This student and others with this type of difficulty incorrectly claimed that the number of distinct many-particle states was $\binom{N+M}{N}=\binom{N+M}{M}=\frac{(N+M)!}{N!M!}$.

### 10.4.4 Difficulty with mathematical sense-making in the context of determining the number of distinct many-particle states

Students must integrate physics and mathematics concepts correctly in order to determine the number of distinct many-particle states for a system of identical particles. This requires students to have a strong understanding of the combinatorics which deals with how to count objects with different properties (e.g., whether the particles are distinguishable vs indistinguishable) and restrictions on the ways in which these objects can be arranged and be able to apply combinatorics correctly in the context of quantum mechanics. Below, we discuss some difficulties students had in determining the number of distinct many-particle states due to difficulty in applying an underlying mathematical concept correctly in the quantum mechanical context.

**Incorrectly adding the number of available single-particle states for each identical particle:** Some students stated that each indistinguishable particle can be placed in any of the available single-particle states and that the total number of distinct many-particle states is the sum of the number of available single-particle states for each boson.

For a system of identical fermions in Q1(a), one interviewed student incorrectly claimed that there are $4+3+2=9$ distinct many-particle states for a system of three fermions and four available single-particle states. Interviews suggest that at least some students with this type of response correctly applied Pauli's exclusion principle and determined the number of distinct many-particle states such that no two fermions are in the same single-particle state, but incorrectly added the number of ways to arrange the fermions in each single-particle state rather than multiplying. This is an interesting way of incorrectly applying the Pauli exclusion princple or justifying the procedure for determining the number of distinct many-particle states.

For a system of identical bosons in Q1(b), one interviewed student stated that "there are four available (single-particle) states for the first boson to go in and there are four available (single-particle) states for the second, since bosons can occupy the same (single-particle) state. The same for the third. So there are four (available single-particle states) for the first (boson), four (available single-particle states) for the second (boson), and four (available single-particle states) for the third (boson)." The student then jotted down $4 + 4 + 4 = 12$ and claimed there were 12 distinct three-particle states for Q1 for a system of identical bosons.

**Difficulty counting the different arrangements correctly for a system of indistinguishable bosons:** In Q1, for a system of three identical bosons and four available single-particle states, many students attempted to determine the number of ways: (1) all three particles could be arranged in the same single particle state, (2) two bosons could be in the same state and the other boson is in a different state, (3) all three bosons could be in different single-particle states to determine the total number of distinct many particle states. For example, one common incorrect response in Q1 was $\binom{4}{1}+\binom{4}{2}+\binom{4}{3} = 4+6+4 = 14$. One interviewed student with this response stated that "when all the bosons are in the same state, there are four states and we need to choose which one has the bosons. There are $\binom{4}{1}$ ways to arrange all the bosons in one state. If two of the bosons are in the same state and one is in another, then we need to choose which two states have the bosons. That makes $\binom{4}{2}$ ways to arrange the bosons. And then, if all three bosons are in different states, then we need to choose which three states have the bosons. There are $\binom{4}{3}$ ways to do that." The student then jotted down that the total number of distinct many-particle states in Q1(b) was $\binom{4}{1} + \binom{4}{2} + \binom{4}{3} = 4 + 6 + 4 = 14$.

## 10.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 10.5.1 Development and Validation of the QuILT

Based upon our research of student difficulties with fundamental concepts with systems of identical particles, we developed a QuILT that attempts to build a consistent and coherent knowledge structure while at the same time addressing the common student difficulties.

As noted in [37], the development of the QuILT was also guided by a cognitive task analysis [49] from both an expert perspective and a novice (or student) perspective which consisted of all the requisite skills and concepts necessary for a functional understanding of a system of identical particles. The initial cognitive task analysis was conducted from an expert perspective in which the researchers outlined the required knowledge and skills and the order in which they are useful in solving problems. This cognitive task analysis was iterated with physics faculty members. However, in an effort to determine if there are additional areas student may struggle with that are not predicted by the experts (expert blindspot) we conducted the student interviews. The cognitive task analysis was then expanded to include these areas in which students needed additional scaffolding support.

As noted in [37], the QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure content was correct and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that were incorporated in the next version. Once it was agreed upon by the faculty that the content was clear and appropriate, the QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording was unambiguous, the scaffolding was effective, and to be able to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and provided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the entire section

of the tutorial focused on the issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and determine whether there were any necessary changes that needed to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and for subsequent interviews. During each step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback and responses to help students address many of the common difficulties and improve the ability of the students to build a consistent and coherent knowledge structure. After it was deemed successful, the QuILT was next administered to students in various advanced quantum mechanics courses.

### 10.5.2 Structure of the QuILT

As noted in [37], the QuILT strives to transform the students into active learners by employing an inquiry-based approach which requires the students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. The QuILT consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is given in class, during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, the students are given the tutorial and encouraged to work on it together in small groups in class. The tutorial can also be used to guide in-class discussion. As an alternative, the tutorial can be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, the students submit the tutorial for grading and are then administered the posttest. The posttest is given in class as an individual assessment in which the students are not permitted any additional resources beyond what is provided in the posttest.

As noted in [37], the QuILT incorporates guided inquiry-based learning sequences which consist of several questions, each building upon the previous question(s) that require the students to take a stand and actively engage them in the learning process. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether they are correct and explain why

they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify an inconsistency in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include excerpts that strive to present the students with contradictions between the answers to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining differences between the correct reasoning and their own reasoning before moving on the next section.

### 10.5.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples focusing on concepts in a given situation, e.g., how to determine the number of distinct many-particle states in a given situation. In particular, the QuILT strives to help students develop a systematic approach for determining the number of many-particle states for a system of identical particles and connect the number of distinct many-particle states to the possible number of many-particle stationary state wavefunctions. In the QuILT, students consider the systems of identical particles in the following order: (1) indistinguishable fermions, (2) indistinguishable bosons, and (3) identical particles that can be treated as distinguishable. For each system, students begin by determining the number of distinct many-particle states for a system of two identical particles. They then consider a system of three identical particles and determine the number of distinct many-particle states. Finally,

students are presented with systems in which the number of particles becomes very large and they are provided guidance and support in learning to determine the number of distinct many-particle states. For the systems of indistinguishable fermions and indistinguishable bosons, students also work with diagrammatic representations for the system that strives to help students recognize why care must be taken to ensure that one is determining these particles as indistinguishable particles. These diagrammatic representations are intended to help them develop a systematic reasoning for determining the number of distinct many-particle states for a system with a large number of particles and available single-particle states. Below are several examples from the QuILT that strives to provide scaffolding support intended to help students with these fundamental concepts and address some of the common difficulties.

**Helping students determine the number of distinct many-particle states for a system of fermions:** There were several common difficulties students had with determining the number of distinct many-particle states for a system of fermions that the QuILT strives to address via the guided inquiry-based learning sequences. We wanted students to be able to identify that a system of identical fermions is made up of indistinguishable particles and one must be careful to only count distinct many-particle stationary states. The QuILT also strives to help students learn that the many-particle states for a system of indistinguishable fermions are consistent with the Pauli exclusion principle. One consequence of the Pauli exclusion principle is that a system cannot have more fermions than the number of available single-particle states.

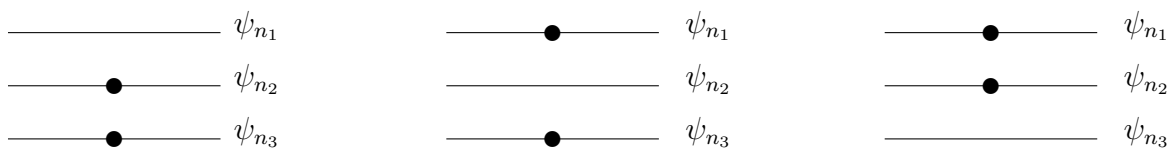
The following is an example of a hypothetical student conversation from the QuILT that focuses on providing an opportunity for reflection of some common difficulties in which students must consider each statement and explain why they agree or disagree with each. This conversation is part of a guided inquiry-based learning sequence that strives to help students determine the number of distinct two-particle states for a system of two indistinguishable fermions and three distinct single-particle states while not overcounting states by treating the particles as distinguishable.

**Student 1:** *For a system of two fermions and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$, there are three available single-particle states for the first fermion. That leaves two single-particle states for the second fermion since the second fermion cannot occupy the same*

*single-particle state as the first fermion. The number of two-particle states is* $3 \times 2 = 6$.

**Student 2:** *I disagree with Student 1. Since the fermions are indistinguishable, we cannot distinguish which fermion is in which single-particle state. For example, we can only tell that one fermion is in single-particle state* $\psi_{n_2}$ *and another fermion in single-particle state* $\psi_{n_3}$. *But, there is no way to tell which fermion is in which single-particle state. This indistinguishability is reflected in the antisymmetrized wavefunction.*

**Student 3:** *I agree with Student 2. Here is the diagrammatic representation for the 3 distinct two-particle states:*




Student 1 is not correct while Students 2 and 3 are correct in the preceding conversation. This conversation is designed to help students reflect upon the fact that the fermions are indistinguishable. After considering this hypothetical conversation, as part of the guided inquiry-based sequence, students are asked to write all the possible stationary state wavefunctions for a system of two fermions and three available single-particles states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$ for the case when the two fermions are in the same single-particle state and when the two fermions are in different single-particle states. The students are then asked to reflect upon the number of distinct many-particle states and the number of possible many-particle stationary state wavefunctions. Further scaffolding is provided that strives to help students realize that the number of distinct many-particle states is the same as the number of possible many-particle stationary state wavefunctions for a given system.

The following statement is an excerpt from a hypothetical conversation between students that strives to help them reflect upon how to determine the number of distinct many-particle states and connect this reasoning to a mathematical expression for counting the states. Students are asked to explain why they agree or disagree with each student such as the following:

**Student 2:** *There are three distinct single-particle states available to the fermions and we must choose any two for the fermions to occupy. The number of distinct two-particle*

*states for a system of two indistinguishable fermions and three distinct single-particle states is* $\binom{3}{2}=\frac{3!}{2!(3-2)!}=3$.

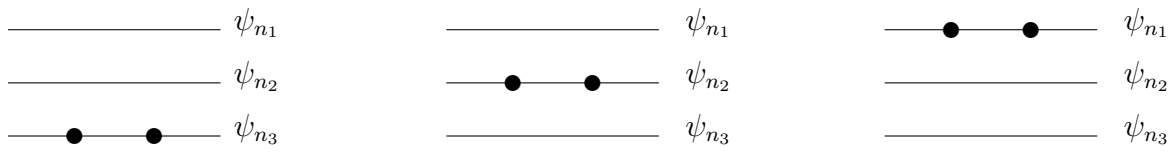
Student 2 is correct. After students consider these types of examples of determining the number of distinct two-particle states for a system of two fermions, they then work through guided inquiry-based sequences for a system of three identical fermions. Then, they consider systems for a large number of fermions and a large number of available single-particle states. Students are provided further scaffolding support that strives to help them generalize the results from the systems of two and three fermions and become proficient in determining the number of distinct many-particle states for a system with a large number of fermions.

**Helping students determine the number of distinct many-particle states for a system of bosons:** The QuILT strives to help students learn that a system of identical bosons must be treated as a system of indistinguishable particles and develop a systematic approach for determining the number of distinct many-particle states in a given situation.

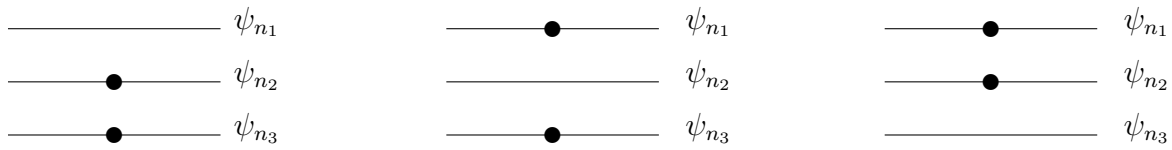
The following hypothetical conversation is part of a guided inquiry-based learning sequence that aims to help students with the fact that a system of identical bosons cannot be treated as a system of distinguishable particles and provides a diagrammatic representation to help them reflect upon the distinct many-particle states. In this conversation, students consider a system of two indistinguishable bosons and three distinct single-particle states and are asked to explain why they agree or disagree with each:

**Student 1:** *For a system of two bosons and three distinct single-particle states* $\psi_{n_1}$, $\psi_{n_2}$, *and* $\psi_{n_3}$, *there are three available states for the first boson and three available states for the second boson. The number of two-particle states is* $3 \times 3 = 9$.

**Student 2:** *I disagree with Student 1. You are overcounting since you are not taking into account the fact that bosons are indistinguishable. If the bosons are in the same single-particle state, there are three possibilities as follows:*



*But, if the bosons are in different single-particle states, there are three possibilities since bosons are indistinguishable and swapping the two bosons in the two single-particle states in each of the following situations does not produce a new two-particle state:*




*There are 6 distinct two-particle states for a system of two bosons and three distinct single-particle states.*

Student 1 is inccorect and Student 2 is correct in the preceding conversation. If one treats the identical bosons as distinguishable, as Student 1 has, then one is overcounting the case in which the two identical bosons are in different single-particle states. Student 2's statement regarding the particles being indistinguishable under the exchange of the particles strives to draw students' attention to the fact that these two bosons cannot be distinguished. After considering this hypothetical conversation, as part of the guided inquiry-based sequence, students are asked to write all of the possible stationary state wavefunctions for a system of two bosons and three available single-particles states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. The students are then asked to reflect upon the number of distinct many-particle states and the number of possible many-particle stationary state wavefunctions. Further scaffolding is provided that strives to help students realize that one must obtain the same number of distinct many-particle states from the combinatorics as the number of possible many-particle stationary state wavefunctions for a given system.

The next hypothetical conversation in the guided inquiry-based learning sequence strives to help students learn a method for determining the number of distinct ways two indistinguishable bosons can be arranged in the three distinct single-particle states by introducing the bin and divider method.

**Student 1:** *For a system of two bosons, there can be more than one boson in a given single-particle state. We can treat the single-particle states as bins to be filled with bosons and*

*dividers to separate the different single-particle states or bins. For example, if the system had two bosons in the first single-particle state then the first bin would have two bosons. For a system with three single-particle states available, we would need two dividers between the three single-particle states. In the case of three single-particle states and two bosons, we must find the number of possible arrangements of the two bosons and two dividers.*

**Student 2:** *I agree with Student 1. Furthermore, since the two dividers cannot be distinguished from one another and the bosons cannot be distinguished from one another, we can permute the indistinguishable dividers with the indistinguishable bosons to find all the possible ways to permute two bosons in the three single-particle states as follows:*

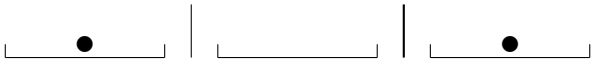
*Two Bosons in the First State*

*Two Bosons in the Second State*

*Two Bosons in the Third State*

*One Boson in the First State and One Boson in the Second State*

*One Boson in the First State and One Boson in the Third State*



*One Boson in the Second State and One Boson in the Third State*

**Student 3:** *The number of distinct many-particle states comes from the number of ways the two bosons and two dividers can be permuted. We have a total of four objects (two bosons and two dividers) and we can find the number of ways to permute the two bosons or equivalently the number of ways to permute the two dividers among the four objects. The number of distinct two-particle states is* $\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$.

All three students in the preceding conversation are correct. Student 1 is describing the bin and divider method and Student 2 is providing a diagrammatical representation of different arrangements of the two bosons in the bins representing the single-particle states. Student 3 provides a mathematical expression for the total number of distinct two-particle states.

After students consider examples that strive to help them learn how to determine the distinct two-particle states for a system of two bosons, they then work through several guided inquiry-based sequences for a system of three identical bosons. Then, they consider systems for a large number of bosons and a large number of available single-particle states. Students are provided scaffolding support that strives to help them generalize the results from the systems of two and three bosons to be able to determine the number of distinct many-particle states for a system with a large number of bosons. The following is a hypothetical student conversation aimed at helping students develop a systematic approach for determining the number of distinct ways $N$ indistinguishable bosons can be arranged in the $M$ distinct single-particle states.

**Student 1:** *Using the bin and divider method, there are* $N + M - 1$ *total objects that should be permuted, out of which* $N$ *bosons are indistinguishable from each other and the* $M - 1$ *dividers are indistinguishable from each other. We must calculate the number of distinct arrangements.*

**Student 2:** *When we choose the number of ways to place the* $M - 1$ *indistinguishable di-*

*viders between the N bosons, we get* $\binom{N+M-1}{M-1} = \frac{(N+M-1)!}{(M-1)![(N+M-1)-(M-1))]!} = \frac{(N+M-1)!}{(M-1)!N!}$. *If instead we choose the number of ways to place the N bosons between* $M-1$ *dividers, we get* $\binom{N+M-1}{N} = \frac{(N+M-1)!}{N![(N+M-1)-N)]!} = \frac{(N+M-1)!}{N!(M-1)!}$. *Either way it is the same!*

Both students in the previous conversation are correct and are drawing attention to the fact that one must focus on the number of bosons and the number of dividers (as opposed to the number of available single-particle states).

The QuILT also asks students to reflect upon and compare the number of distinct many-particle states for a system of indistinguishable fermions, indistinguishable bosons, and identical particles that could be treated as distinguishable. In particular, they are asked to rank the number of distinct many-particle states for each system with the same number of particles and the same number of single-particle states. The goal is to have students understand that for the same number of particles and available single-particle states a system of distinguishable particles has the largest number of distinct many-particle states and that the indistinguishability of the identical fermions and bosons results in fewer distinct states (unless the system of identical bosons has only one available single-particle state, in which case this system will have the same number of distinct many-particle states as a system of distinguishable particles). A system of identical fermions must satisfy the Pauli exclusion principle which reduces the number of possible many-particle states compared to identical bosons. The QuILT strives to help students learn that the number of distinct many-particles states for a given number of particles and available single-particle states increase by particle type in the order: indistinguishable fermions, indistinguishable bosons, and identical particles that can be treated as distinguishable and be able to reason why that is the case.

## 10.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level un-

Table 41: Average pretest and posttest scores for Q1 and Q2 for the given system on the pretest and posttest for undergraduates (number of students $N = 25$) and graduate students ($N = 30$).

| Question | Type of Particle | Graduate | | Undergraduate | |
|---|---|---|---|---|---|
| | | Pre (%) | Post (%) | Pre (%) | Post (%) |
| Q1 | Fermions | 48 | - | 56 | - |
| | Bosons | 28 | - | 27 | - |
| | Distinguishable | 28 | - | 39 | - |
| Q2 | Fermions | - | 100 | - | 100 |
| | Bosons | - | 92 | - | 96 |
| | Distinguishable | - | 93 | - | 86 |

dergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts for constructing the many-particle stationary state wavefunction for a system of identical particles before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

The open-ended questions Q1 and Q2 were graded using rubrics which were developed by the researchers together. A subset of questions was graded separately by them. After comparing the grading, they discussed any disagreements and resolved them with a final inter-rater reliability of better than 95%. Table 41 shows the performance of undergraduate and graduate students on the pretest and posttest. The results are encouraging and suggest that the QuILT is effective in helping students count the number of distinct many-particle states for systems of identical fermions or bosons, as well as the contrasting case in which

Table 42: The percentages of undergraduate students who answered questions Q1(a) and Q1(b) correctly for the given system on the midterm examination four weeks after completing the Quantum Interactive Learning Tutorial (number of students $N = 12$).

| Question | Type of Particle | Answered Correctly (%) |
|---|---|---|
| Q1(a) | Fermions | 75 |
| Q1(b) | Bosons | 75 |

the identical particles could be treated as distinguishable. Q2 was given on the posttest and was intended to be a similar question to Q1 on the pretest. There are a different number of identical particles and available single-particle states in the two questions. Overall, the students did very well with more than 80% of the graduate students and 75% of the undergraduates answering all three parts of Q2 correctly for the given system of identical particles.

As a measure of retention, the students in the first year were given questions Q1(a) and Q1(b) on their midterm examination four weeks after completing the posttest. Table 42 summarizes the percentages of students who determined the number of distinct many-particle states in Q1(a) and Q1(b) correctly on the midterm examination.

## 10.7 SUMMARY

Investigating students' understanding of a system of identical particles helped to uncover many common student difficulties that were used as a guide to develop a research-based QuILT that strives to help students learn to reason and determine the number of distinct many-particle states for a system of identical particles. The QuILT strives to help students (1) realize that a system of identical fermions or bosons consists of indistinguishable particles (2) develop a systematic approach for determining the number of distinct many-particle states and (3) determine the number of distinct many-particle states from lowest to highest

for a system of indistinguishable fermions, indistinguishable bosons, and identical particles that could be treated as distinguishable for systems containing the same number of particles and the same number of single-particle states. Many of the student difficulties discussed here may be attributed in part to students' bounded rationality in that they are limited in their cognitive resources so they may not be able to solve problems correctly if they are not provided appropriate guidance and scaffolding support [47]. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding through a guided inquiry-based approach. The results suggest that the QuILT is effective in improving students' understanding of fundamental concepts necessary for determining the number of distinct many-particle states for a system of identical particles.

## 10.8 ACKNOWLEDGMENTS

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# 11.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: COUNTING THE NUMBER OF DISTINCT MANY-PARTICLE STATES FOR A SYSTEM WITH A FIXED TOTAL ENERGY

## 11.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. There have been a number of research studies aimed at investigating student reasoning in QM [14, 15, 16, 17, 18, 19, 20, 21] and improving student understanding of QM [22, 23, 24, 25, 26, 27]. For example, our group has focused on using the common student difficulties as a guide to develop research-based learning tools which include Quantum Interactive Learning Tutorials (QuILTs) [28, 29, 30, 31, 32, 33, 34] which strive to improve student understanding of different QM concepts. However, there have been few investigations into student difficulties with fundamental concepts involving a system of identical particles with fixed total energy.

Here, we discuss an investigation of student difficulties with the number of distinct many-particle stationary states for a system of non-interacting identical particles and how that research was used as a guide in the development, validation, and in-class evaluation of a QuILT that strives to help students develop a good grasp of relevant concepts pertaining to the number of distinct many-particle states. Through researching students' understanding of and reasoning about a system of identical particles, we found common student difficulties that can hinder their development of a consistent and coherent knowledge structure pertaining to these concepts.

Students must have a good understanding of quantum mechanical properties of a system of identical particles as well as a background in combinatorics to be proficient in determining the number of distinct many-particle states, whether a total energy is possible for the system under given constraints, and the possible outcomes of an energy measurement and the probability of obtaining a particular energy if we randomly measured the energy of one particle in a system of non-interacting identical particles. However, prior research suggests that students struggle in mathematical sensemaking in the context of physics even if they can answer similar mathematics questions not involving physics context in a number of different introductory physics contexts [35, 36, 37, 38]. Since the QM paradigm is novel, student difficulties in mathematical sense-making in the context of QM has also been observed in prior studies.

Below, we start with a brief background of relevant concepts and then describe the methodology for the investigation of student difficulties followed by the common difficulties found. Then, we describe the methodology for the development, validation and in-class evaluation of the corresponding research-based QuILT that strives to help students develop a functional understanding of the fundamental concepts involved in determining the number of distinct many-particle states for a system of identical particles with a fixed total energy, the possible outcomes of an energy measurement and the probability of obtaining a particular energy if we randomly measured the energy of one particle in a system of non-interacting identical particles.

## 11.2 BACKGROUND

In nature, there are two general types of particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g., photons and mesons). A system of $N$ identical particles consists of $N$ particles of the same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in quantum mechanics, identical particles are indistinguishable and there is

no measurement that can be performed to distinguish these identical particles from one another. For example, if the coordinates of two identical particles are interchanged, there is no physical observable that would reflect this interchange. Here we focus on systems of identical particles in which the total energy of the many-particle system is fixed. For a system of identical fermions, it is not possible for two or more fermions to occupy the same single-particle state. In order to construct a many-particle wavefunction for fermions satisfying the given constraint on the total energy of the system, there must be at least one combination of the single-particle states with the specified total energy for which all the particles are in different single-particle states. For a system of identical bosons, it is possible for two or more bosons to occupy the same single-particle state so satisfying the constraint on the total energy of the many-particle system is generally easier and there are many more possibilities, in general, than for the corresponding case for fermionic systems. As a contrasting case, if identical particles could be treated as distinguishable, there is no restriction on the number of particles that can be placed in a single-particle state so there are generally more many-particle states for the distinguishable particles with the same constraint on the total energy compared to a system of indistinguishable particles of both types.

For a system of $N$ non-interacting identical particles each in a $M$-dimensional Hilbert space, the $M^N$-dimensional Hilbert space ($\mathscr{H}$) for the many-particle ($N$-particle) system is

$$\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N, \tag{11.1}$$

which is the direct product of the $M$-dimensional Hilbert spaces for each particle $\mathscr{H}_i$. The many-particle Hamiltonian for the system of $N$ non-interacting identical particles in the product space is

$$\begin{aligned} \hat{\mathbf{H}} \;=\; & \hat{H}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N + \hat{I}_1 \otimes \hat{H}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N + \cdots + \\ & \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \hat{I}_{N-2} \otimes \hat{H}_{N-1} \otimes \hat{I}_N + \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{N-1} \otimes \hat{H}_N, \end{aligned} \tag{11.2}$$

where the single-particle Hamiltonian, $\hat{H}_i$, and the identity operator, $\hat{I}_i$, for the $i^{th}$ particle are in the $M$-dimensional Hilbert space $\mathscr{H}_i$.

We will use the following shorthand notation for the many-particle Hamiltonian

$$\hat{\mathbf{H}} = \sum_i \hat{\mathbf{H}}_i = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 + \cdots + \hat{\mathbf{H}}_N \tag{11.3}$$

in which $\hat{\mathbf{H}}_i = \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{i-1} \otimes \hat{H}_i \otimes \hat{I}_{i+1} \cdots \otimes \hat{I}_N$ is the Hamiltonian of the $i^{th}$ particle in the $M^N$ dimensional product space. All the Hamiltonians in boldface will refer to a Hamiltonian in the $M^N$ dimensional product space.

In all the questions in this investigation discussed here, the non-interacting identical particles are restricted to one spatial dimension for convenience. Students were asked to consider the wavefunction of the many-particle system ignoring the spin part of the wavefunction (we refer to these particles as "spinless"). As an example of such a quantum system, we consider non-interacting identical particles of mass $m$ in a one-dimensional infinite square well of width $a$ ($0 \leq x \leq a$). For a system of $N$ non-interacting identical particles, the total energy of the many-particle system can be written in terms of the single-particle energies as

$$\begin{aligned} E &= E_{n_1} + E_{n_2} + E_{n_3} + \cdots + E_{n_N} \\ &= (n_1^2 + n_2^2 + n_3^2 + \cdots + n_N^2)\left(\tfrac{\pi^2\hbar^2}{2ma^2}\right) \\ &= (n_1^2 + n_2^2 + n_3^2 + n_N^2)E_1. \end{aligned} \tag{11.4}$$

Here $n_1, n_2, n_3, \ldots, n_N$ are positive integers (quantum numbers) that label the single-particle states in which the $N$ particles are placed and $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$ is the ground state energy for one particle in the one-dimensional infinite square well.

For example, let's suppose that the total energy of the many-particle system for three non-interacting identical particles of mass $m$ in the one-dimensional infinite square well of width $a$ is $E = 243\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 243E_1$. We note that the only possible integers, quantum numbers, $n_1, n_2$, and $n_3$ whose squares sum to 243 are

$$\begin{aligned} 243 &= 1^2 + 11^2 + 11^2 \\ 243 &= 3^2 + 3^2 + 15^2 \\ 243 &= 5^2 + 7^2 + 13^2 \\ 243 &= 9^2 + 9^2 + 9^2. \end{aligned} \tag{11.5}$$

Here we will use the notation $(n_i, n_j, n_k)$ to denote the combination in which the quantum numbers $n_i, n_j$, and $n_k$ refer to the single-particle states, i.e., particle 1 is in the single-particle state labeled by $n_i$, particle 2 is in the single-particle state labeled by $n_j$, and particle 3 is in the single-particle state labeled by $n_k$. In the example, the combination $(5, 7, 13)$ means that particle 1 is in the single-particle state $\psi_5$, particle 2 is in the single-particle state $\psi_7$ and particle 3 is in the single-particle state $\psi_{13}$. For a system of indistinguishable particles, one cannot determine which particle is in which single-particle state. The many-particle stationary state wavefunction for a system of three non-interacting identical particles will consist of basis states of the form $\psi_i(x_1)\psi_j(x_2)\psi_k(x_3)$ where $x_m$ is the coordinate of the $m^{th}$ particle. Here, for convenience, we will refer to all direct products of single-particle states as "basis states", regardless of their symmetry under exchange. Please note that for identical fermions, only antisymmetric linear combinations of these basis states are allowed, while for bosons only symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed. In order to satisfy the symmetrization requirements for a system of identical fermions or bosons, a linear combination of all permutations of these basis states with correct symmetrization is required. For example, the combinations $(5, 7, 13)$, $(5, 13, 7)$, $(7, 5, 13)$, $(7, 13, 5)$, $(13, 5, 7)$, $(13, 7, 5)$ in Eq. 11.5 with constraints on the total energy do not yield six distinctly different states for a system of identical bosons or fermions but correspond to terms in a many-particle stationary state wavefunction that satisfy the appropriate symmetrization requirement. These six combinations, for a system of identical fermions, correspond to the completely antisymmetric three-particle stationary state wavefunction

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_5}(x_1)\psi_{n_7}(x_2)\psi_{n_{13}}(x_3) - \psi_{n_5}(x_1)\psi_{n_{13}}(x_2)\psi_{n_7}(x_3) \\ &\quad +\psi_{n_7}(x_1)\psi_{n_{13}}(x_2)\psi_{n_5}(x_3) - \psi_{n_7}(x_1)\psi_{n_5}(x_2)\psi_{n_{13}}(x_3) \\ &\quad +\psi_{n_{13}}(x_1)\psi_{n_5}(x_2)\psi_{n_7}(x_3) - \psi_{n_{13}}(x_1)\psi_{n_7}(x_2)\psi_{n_5}(x_3)],\end{aligned}$$

and interchanging the coordinates of any two particles in each term only introduces an overall minus sign. For a system of identical bosons, these six combinations correspond to the completely symmetric three-particle stationary state wavefunction

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_5}(x_1)\psi_{n_7}(x_2)\psi_{n_{13}}(x_3) + \psi_{n_5}(x_1)\psi_{n_{13}}(x_2)\psi_{n_7}(x_3) \\ &\quad +\psi_{n_7}(x_1)\psi_{n_{13}}(x_2)\psi_{n_5}(x_3) + \psi_{n_7}(x_1)\psi_{n_5}(x_2)\psi_{n_{13}}(x_3) \\ &\quad +\psi_{n_{13}}(x_1)\psi_{n_5}(x_2)\psi_{n_7}(x_3) + \psi_{n_{13}}(x_1)\psi_{n_7}(x_2)\psi_{n_5}(x_3)]\end{aligned}$$

and interchanging the coordinates of any two particles in each term returns the same wavefunction.

Since no two fermions can occupy the same single-particle state, only the combinations in which each fermion is in a different single-particle state, in this case only the set $\psi_5$, $\psi_7$, and $\psi_{13}$ are possible for a system of identical fermions with constraint on the total energy given in Eq. 11.5. The combinations $(5, 7, 13)$, $(5, 13, 7)$, $(7, 5, 13)$, $(7, 13, 5)$,$(13, 5, 7)$, $(13, 7, 5)$ all correspond to the terms in the completely antisymmetric stationary state wavefunction and thus, there is only one distinct many-particle state corresponding to the six term for a system of identical fermions.

There are four distinct many-particle states for a system of identical bosons with the constraint given in Eq. 11.5: the combination $(9, 9, 9)$ in which all the bosons are in the single-particle state $\psi_9$, the combinations $(3, 3, 15)$, $(3, 15, 3)$, and $(15, 3, 3)$ in which two bosons are in the single-particle state $\psi_3$ and one boson is in the single-particle state $\psi_{15}$, the combinations $(1, 11, 11)$, $(11, 1, 11)$, and $(11, 11, 1)$ in which two bosons are in the single-particle state $\psi_{11}$ and one boson is in the single-particle state $\psi_1$, or the combination $(5, 7, 13)$, $(5, 13, 7)$, $(7, 5, 13)$, $(7, 13, 5)$, $(13, 5, 7)$, and $(13, 7, 5)$ in which one boson is in each of the single-particle states $\psi_5$, $\psi_7$, and $\psi_{13}$. As in all of the questions posed to the students, we will assume that each of these four many-particle states is equally likely.

For the constraint given in Eq. 11.5, there are 13 distinct many-particle states for a system of identical particles that can be treated as distinguishable. The combinations $(9, 9, 9)$, $(3, 3, 15)$, $(3, 15, 3)$, $(15, 3, 3)$, $(1, 11, 11)$, $(11, 1, 11)$, $(11, 11, 1)$, $(5, 7, 13)$, $(5, 13, 7)$, $(7, 5, 13)$, $(7, 13, 5)$, $(13, 5, 7)$, and $(13, 7, 5)$ all correspond to distinct many-particle states. As in all of the questions posed to the students, we will assume that each of these thirteen many-particle states is equally likely.

## 11.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with determining the number of distinct many-particle states for a system of identical fermions or bosons were first investigated using three years of data involving

responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight was gained concerning these difficulties from responses of 14 students during a total of 81 hours of individual "think-aloud" interviews [41]. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates and 30 first-year physics graduate students in their respective QM courses. The QuILT included a pretest, the tutorial, and a posttest. Students were given the pretest after traditional lecture-based instruction on identical particles. The pretest was not returned to the students. Students began working on the tutorial in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial after working through it. Student responses on the pretest, tutorial, and posttest were analyzed for their understanding of how to determine the number of distinct many-particle states for a system of identical particles. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in this investigation, the non-interacting identical particles were restricted to one spatial dimension for convenience. Initially students were asked to consider the wavefunction of the many-particle system ignoring the spin part of the wavefunction. Later they considered the completely symmetrized many-particle wavefunction consisting of both the spatial and spin parts of the wavefunction. We began by only considering the spatial part of the wavefunction to simplify the problem (asking students to ignore the spin degrees of freedom) and to help students focus on fundamental concepts involved in determining the number of distinct many-particle states for a system of identical particles, determining whether a specified total energy is possible for the system of identical particles under the given constraint, finding the possible outcomes of an energy measurement, and determining the probability of measuring a given energy when the energy of one particle is measured randomly.

To probe whether students were able to determine the possible outcomes of an energy measurement and the probability of measuring a particular energy when one particle is

measured at random in a given situation, the following question was posed to 30 graduate students and 25 undergraduate students on the pretest of the QuILT after traditional lecture-based instruction.

**Q1.** *For a system of two non-interacting identical particles in a one-dimensional infinite square well, the total energy of the two particle system is* $E_{n_1,n_2} = (n_1^2 + n_2^2)E_1$*, in which* $E_1$ *is the ground state energy for one particle. The total energy of the system is* $E = 338E_1$*. Assume all the possible combinations are equally probable. Note: The only pairs of integers* $n_1$ *and* $n_2$ *whose squares sum to 338 are given below.*

$$\begin{aligned} 338 &= 7^2 + 17^2 \\ &= 13^2 + 13^2 \end{aligned}$$

*(a) If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

*(b) If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

*(c) If the particles are distinguishable and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

Since two fermions cannot occupy the same single-particle state (when we ignore the spin of the fermions which students were asked to do), the combination (13,13) in Q1(a) is not possible. Only the combinations (7,17) and (17,7) are possible for the two fermions. The combinations $(7, 17)$ and $(17, 7)$ together correspond to the completely antisymmetric two-fermion wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_7}(x_1)\psi_{n_{17}}(x_2) - \psi_{n_{17}}(x_1)\psi_{n_7}(x_2)]$. Therefore, the probability of measuring a particle with energy $7^2E_1$ is 1/2 and the probability of measuring a particle with energy $17^2E_1$ is 1/2.

Two bosons can occupy the same single-particle state. Thus, in Q1(b), the combinations (7, 17), (17,7) and (13,13) are possible for a system of two bosons. These three combinations correspond to two distinct two-boson wavefunctions, $\frac{1}{\sqrt{2}}[\psi_{n_7}(x_1)\psi_{n_{17}}(x_2) + \psi_{n_{17}}(x_1)\psi_{n_7}(x_2)]$ and $\psi_{n_{13}}(x_1)\psi_{n_{13}}(x_2)$. By the assumption that each distinct arrangement is equally probable, there is a probability of 1/2 of both bosons being in the single-particle state with energy

$13^2E_0$ and a probability of 1/2 of one boson being the in the single-particle state with energy $7^2E_1$ and one boson being in the single-particle state with energy $17^2E_1$. Therefore, the probability of measuring a particle with energy $7^2E_1$ is (1/2)(1/2)=1/4, the probability of measuring a particle with energy $17^2E_1$ is (1/2)(1/2)=1/4, and the probability of measuring a particle with energy $13^2E_1$ is (1/2)(1)=1/2.

If the identical particles can be treated as distinguishable, in Q1(c), there are three distinct combinations (7, 17), (17,7), and (13,13). There is an equal probability of 1/3 of measuring each of the energies $7^2E_0$, $17^2E_0$, and $13^2E_0$.

To probe whether students were able to determine the number of distinct many-particle states, identify whether a total energy is possible for a system of identical fermions or bosons, and determine the probability of measuring a given energy when the energy of one particle is measured at random in a given situation, the following two questions were posed as in-class clicker questions to 16 undergraduate students. In these two questions, students were told to ignore the spin degrees of freedom and consider the particles as "spinless." The questions were posed after traditional lecture-based instruction in relevant topics.

**Q2.** *We have three non-interacting particles in a one-dimensional infinite square well. The total energy for the three particle system is* $E_{(n_1,n_2,n_3)} = (n_1^2 + n_2^2 + n_3^2)E_0$*, in which* $E_0$ *is the ground state energy for a single particle system. If the total energy is* $E = 27E_0$ *and the particles are identical, choose all of the following statements that are correct. Note: The combinations of three positive numbers, the sum of whose squares give 27, are (1,1,5), (1,5,1), (5,1,1) and (3,3,3).*

(1) *The particles can be either bosons or fermions.*
(2) *If the particles are spinless bosons, there are 4 distinct states in this system.*
(3) *If the particles are bosons, when we measure the energy of one particle at random, the probability of obtaining* $9E_0$ *is 1/2.*

The correct answer to Q2 is option (3) only. Option (1) is incorrect due to the fact that the total energy of $27E_0$ requires at least two of the particles to be in the same single-particle state (either two in the single-particle state $\psi_1$ or all three in the single-particle state $\psi_3$).

If the particles are spinless bosons, there are 2 distinct many-particle states in the system (not 4 as in option (2)). The three combinations of the numbers 1, 1, and 5 correspond to one completely symmetric many-particle wavefunction and make up one many-particle state. There are only two distinct combinations: all three bosons are in the single-particle state $\psi_3$ or there are two bosons in the single-particle state $\psi_1$ and one boson in the single-particle state $\psi_5$

**Q3.** *We have three non-interacting particles in a one-dimensional infinite square well. The energy of particle* $i(i = 1, 2, 3)$ *is* $E_i = n_i^2 E_0$. *If the total energy* $E = 75E_0$ *and the particles are identical, choose all of the following statements that are correct. Note: The combinations of three positive numbers, the sum of whose squares give 75, are (5,5,5), (1,5,7), (5,1,7), (7,1,5), (1,7,5), (5,7,1), (7,5,1).*

(1) *If the particles are spinless bosons, there are seven distinct three-particle states in this system with this energy.*

(2) *If the particles are spinless bosons, when we measure the energy of one particle at random, the probability of obtaining* $25E_0$ *is 1/2.*

(3) *If the particles are spinless bosons, when we measure the energy of one particle at random, the probability of obtaining* $49E_0$ *is 1/6.*

In Q3, option (3) is the only correct answer. Option (1) is incorrect. If the particles are spinless bosons, there are two distinct three-particle states with a total energy of $75E_0$. The combinations (1,5,7), (5,1,7), (7,1,5), (1,7,5), (5,7,1), (7,5,1) together correspond to a completely symmetric many-particle wavefunction when one boson is in each of the single-particle states $\psi_1$, $\psi_5$, and $\psi_7$. Option (2) is incorrect as the probability of obtaining an energy of $25E_0$ when measuring the energy of one particle at random is 2/3.

## 11.4 STUDENT DIFFICULTIES

Many students struggled to identify whether a given total energy is possible for a specified system of identical particles and determine the number of distinct many-particle states for a

Table 43: The percentage of graduate (N=30) and undergraduate (N=25) students who correctly determined the energies and their probabilities in question Q1 for the given system of indistinguishable particles after traditional instruction.

| Type of Particle | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Fermions | 27 | 36 |
| Bosons | 30 | 48 |
| Distinguishable | 3 | 12 |

system of identical particles in which the total energy of the system is fixed. Some students also struggled to determine the possible outcomes of an energy measurement and the probability of obtaining a particular energy if we randomly measured the energy of one particle in a system with a certain fixed total energy. Table 43 summarizes the percentage of students who answered question Q1 correctly after traditional lecture-based instruction for a system of three identical particles on the pretest to the QuILT.

Below, we discuss some of the common student difficulties with a system of identical particles in which the total energy of the many-particle system is fixed.

### 11.4.1 Difficulty determining the number of distinct many-particle states for a system of identical particles

When asked to determine the number of distinct many-particle states for a system of identical particles for which the total energy of the system is fixed, some students struggled to determine the distinct many-particle states correctly. In particular, many students incorrectly identified indistinguishable combinations as distinct many-particle states for a system of identical fermions or bosons. For example, some interviewed students incorrectly claimed that there are two distinct many-particle states corresponding to the combinations $(7, 17)$ and $(17, 7)$ in Q1 for a system of identical fermions and bosons. One interviewed student claimed "we just count all the combinations $((5, 5), (7, 17)$, and $(17, 7))$ for identical bosons

Table 44: The percentage of graduate (N=30) and undergraduate (N=25) students who incorrectly determined the possible outcomes of an energy measurement as $7E_1$, $17E_1$, or $13E_1$ for all three systems of identical particles in question Q1 after traditional lecture-based instruction.

| Difficulty | Graduate (%) | Undergraduate (%) |
|---|---|---|
| Incorrectly determined the possible outcomes of an energy measurement as $7E_1$, $17E_1$, or $13E_1$ for all three systems of identical particles (neglecting to square the $n_i$) | 23 | 32 |
| Incorrectly claimed that two fermions can be in the single-particle state $\psi_{13}$ | 27 | 20 |
| Incorrectly claimed that the energies obtained and the corresponding probabilities would be the same for a system of identical bosons and a system of identical particles which can be treated as distinguishable | 23 | 48 |

(to determine the number of distinct many-particle states). For fermions, we throw out the combination $(5, 5)$ where two fermions are in the same (single-particle) state and count what's left $(7, 17)$ and $(17, 7)$." He incorrectly counted the combinations $(7, 17)$ and $(17, 7)$ as corresponding to two distinct many-particle states for fermions. Students struggled to determine the number of distinct many-particle states in Q2 and Q3 that were posed as in class clicker questions. For example, in Q2, 25% of the students incorrectly claimed that there are four distinct states for the given system (option (2)). In response to Q3, 14% of the students incorrectly claimed that there are seven distinct many-particle states of the given system (option (1)). Interviews suggest that students with these types of responses were often determining all of the combinations as distinct many-particle states for a system of identical bosons rather than considering the combinations that correspond to indistinguishable arrangements of the identical particles together as one many-particle state.

### 11.4.2 Difficulty correctly identifying possible outcomes of energy measurements

Some students had difficulty determining the possible outcomes of an energy measurement when the energy of one particle is measured at random. For example, in Q1, some students claimed that the randomly measured energies could be $7E_1$ or $17E_1$ (instead of $7^2E_1$ or $17^2E_1$) for a system of identical fermions. Most of these students also incorrectly claimed that the randomly measured energies could be $7E_1$, $17E_1$, or $13E_1$ (instead of $7^2E_1$, $17^2E_1$, or $13^2E_1$) for a system of identical bosons or a system of identical particles that can be treated as distinguishable. As given in Table 44, roughly one-third of the undergraduates and one-fourth of the graduate students provided this type of response for all three systems of identical particles in Q1 after traditional lecture-based instruction for which the total energy of the system was not consistent with the total energy specified in the problem. Interviews suggest that this is at least in some cases not due to a lack of conceptual understanding, but an issue with metacognition and the fact that students often did not reflect upon their responses to ensure that they make sense. All the questions posed were for a system in which the total energy of the system was fixed. In questions similar to Q1 in which students were asked to determine the possible outcomes of an energy measurement when the energy of one particle is measured at random, many students did not verify that the energies must add up to the total fixed energy of the system. The interviewed students often did not check that the energies from the different combinations add up to the total energy of the system. For example, one interviewed student determined that the total energy of the system is $7E_1 + 17E_1 = 24E_1$ for a system of fermions and $13E_1 + 13E_1 = 26E_1$ for a system of bosons. When prompted to check that these energies are consistent with the total energy of the many-particle system, he identified that there was an inconsistency with his responses for the single-particle energies to Q1. The student was then able to trace back his mistake and realized that the single-particle energies should be $7^2E_1$, $17^2E_1$, or $13^2E_1$. Students with this type of difficulty incorrectly determined a total energy that was different depending on which combination corresponded to the single-particle state the particles were in (e.g., the interviewed student determined the energy to be $24E_1$ in one combination and $26E_1$ in

another). Students with this type of response also determined a total energy of the system that was not the given total energy of $338E_1$. Other interviewed students who made similar mistakes were able to identify and reconcile their mistakes only after explicit prompting. Discussion with students suggest that they often struggled with self-monitoring and did not check whether their responses were consistent with the given situation unless prompted explicitly by the interviewer.

### 11.4.3 Difficulty realizing that two fermions cannot occupy the same single-particle state

Some students did not apply Pauli's exclusion principle to a system of indistinguishable fermions and instead incorrectly answered questions consistent with two or more fermions occupying the same single-particle state. For example, in Q2, students struggled to identify that the given system was not possible for identical spinless fermions. In Q2, the only combinations require placing two of the particles in the single-particle state $\psi_1$ or all three particles in the single-particle state $\psi_3$. Therefore, in Q2 it is not possible for a system of three identical fermions to have the total energy $27E_0$. However, in Q2, 44% of the students individually chose option (i), thereby incorrectly identifying that the system with total energy of $27E_0$ is possible for a system of identical fermions. After answering Q2 individually, the students discussed the question in small group and answered again. After group discussion, 33% of the students still incorrectly chose option (i) as correct.

In Q1, some students incorrectly claimed that if the energy of one particle is measured at random, it is possible to obtain an energy corresponding to a combination in which the spinless fermions are in the same spatial single-particle state. As summarized by Table 44, one-fifth of the undergraduate students and roughly one-quarter of the graduate students incorrectly claimed that the combination $(13, 13)$ in which both fermions are in the single-particle state $\psi_{13}$ was possible in Q1, after traditional lecture-based instruction.

### 11.4.4 Difficulty determining the probability of obtaining a specific energy when the energy of one particle is measured at random

Some students struggled to correctly calculate the probability of measuring a specified energy when the energy of one particle is measured at random. This is particularly true for students who had difficulty correctly determining the number of distinct many particle states described earlier. Below, we discuss one general difficulty and two specific difficulties students had with determining the probability of obtaining a particular energy when the energy of one boson is measured at random.

**Incorrectly claiming that the outcomes are the same for all three systems of identical particles:** Some students answered all the parts in Q1 the same. In Q1 on the pretest after traditional lecture-based instruction, 16% of the undergraduate students and 3% of the graduate students incorrectly claimed that one obtains the energies $7^2E_1$, $17^2E_1$, and $13^2E_1$ for all three systems. All of these students incorrectly claimed that one obtains the following energies and probabilities: $7^2E_1$ with probability 1/4, $17^2E_1$ with probability 1/4, and $13^2E_1$ with probability 1/2. Students with this type of response were treating the combinations $(7, 17)$ and $(17, 7)$ as indistinguishable combinations. They were incorrectly determining the combination $(13, 13)$ as a possible combination for a system of identical fermions. The stated energies and probabilities are correct for a system of identical bosons, but not for a system of identical fermions or a system of identical particles that can be treated as distinguishable. These students' responses have a complete disconnect with Pauli's exclusion principle or other constraints on the states. In other words, determining the number many-particle states was treated totally differently than determining the many-particle stationary state wavefunction for a system of identical particles. However, you need the wavefunction in order to determine the probabilities of obtaining a given energies when the energy of one particle is measured at random.

**Difficulty realizing that each energy is not equally probable for a system of identical bosons:** Some students incorrectly claimed that the probability of measuring each single-particle energy for the two bosons in Q1(b) was the same. Students with this type of difficulty were treating the indistinguishable bosons as if they were distinguishable

particles. For example, in Q1 after traditional instruction, 4% of the undergraduate students and 13% of the graduate students incorrectly claimed that measuring the energies $7^2E_1$, $17^2E_1$, and $13^2E_1$ is equally likely (each with probability 1/3). One interviewed student with this response incorrectly claimed that for a system of identical bosons "there are three combinations $(7, 17)$, $(17, 7)$ and $(13, 13)$. Since each is equally likely, the probability of each is 1/3. So that means there is a 1/3 probability of measuring $13^2E_1$ and 1/3 times 1/2 probability of measuring $7^2E_1$ in the first combination and the same (1/3 times 1/2) in the second combination which gives 1/3 (probability of measuring $7^2E_1$). Then (the probability of measuring) $17^2E_1$ is the same as (the probability of measuring) $7^2E_1$, so it's 1/3 too." This student and others with this type of difficulty struggled to realize that the combinations $(7, 17)$ and $(17, 7)$ are not distinct many-particle states. Students with this difficulty often struggled to realize that it is equally probable that one has the combination in which both bosons are in the single-particle state $\psi_{13}$ or one boson is the state $\psi_7$ and the other boson is in the state $\psi_{17}$.

**Difficulty realizing that the probability for obtaining each energy for a system of identical bosons is different than for a system of identical particles that can be treated as distinguishable:** Many students provided the same answer to questions Q1(b) and Q1(c). In Q1 on the pretest, roughly half of the undergraduate students and one-fourth of the graduate students incorrectly claimed that the energies obtained and the corresponding probabilities are the same for a system of identical bosons and a system of identical particles which can be treated as distinguishable, as listed in Table 44. All of these students incorrectly claimed that one obtains the following energies and probabilities: $7^2E_1$ with probability 1/4, $17^2E_1$ with probability 1/4, and $13^2E_1$ with probability 1/2. Students with this type of response were treating the distinguishable particles as if they were indistinguishable bosons. Interviews suggest that these students incorrectly determined the number of distinct many-particle states for a system of identical particles that can be treated as distinguishable. For example, one interviewed student claimed "the combinations $(7, 17)$ and $(17, 7)$ are the same so there are two possibilities...". He claimed that there are two distinct many-particle states and that one of these many-particle states corresponds to the indistinguishable combinations $(7, 17)$ and $(17, 7)$. This student did not realize that if the

particles can be treated as distinguishable, the combination $(7, 17)$ in which particle 1 is in the single-particle state $\psi_7$ and particle 2 is in the single-particle state $\psi_{17}$ is different than the combination $(17, 7)$ in which particle 1 is in the single-particle state $\psi_{17}$ and particle 2 is in the single-particle state $\psi_7$. He reasoned about the system of identical particles that can be treated as distinguishable in exactly the same manner as he did about the system of identical bosons.

## 11.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 11.5.1 Development and Validation of the QuILT

The development of the QuILT was guided by a cognitive task analysis [45] from both an expert perspective and a novice (or student) perspective which consisted of all the requisite knowledge and skills necessary for a functional understanding of a system of identical particles. The initial cognitive task analysis was conducted from an expert perspective in which the researchers outlined the required knowledge and skills and the order in which they are useful in solving problems. This cognitive task analysis was iterated with physics faculty members at the University of Pittsburgh. However, in an effort of determine if there are additional areas students may struggle with that are not predicted by the experts, we conducted student interviews. The cognitive task analysis was then expanded to include areas in which students needed additional scaffolding support.

The QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure that the content was appropriate and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that was incorporated in the next version of the QuILT. Once it was agreed upon by the faculty that the content was clear and correct, the QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording

is unambiguous, the scaffolding is effective, and to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and provided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the entire section of the tutorial focusing on the issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and determine whether there were any changes that needed to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and in subsequent interviews. During each step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback and responses to help students with the common difficulties and to build a consistent and coherent knowledge structure. After it was deemed successful, the QuILT was next administered to students in various advanced quantum mechanics courses.

### 11.5.2 Overview of the QuILT

The QuILT strives to transform the students into active learners by employing an inquiry-based approach which requires the students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. The QuILT consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is given in class during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, the students are given the tutorial and encouraged to work together in small groups in class. The tutorial can be used to guide in-class discussion. The tutorial can also be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, the students submit the tutorial for grading and are then administered the posttest. The posttest is given in class as an individual assessment in which the students are not permitted

any additional resources beyond what is provided in the posttest.

The QuILT incorporates guided inquiry-based learning sequences which consist of several questions, each building upon the previous question(s), that require the students to take a stand and actively engage them in the learning process. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether it is correct and explain why they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify any inconsistencies in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an inconsistency with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include portions that strive to present the students with a contradiction between the answer to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining difference between the correct reasoning and their own reasoning before moving on to the next section.

### 11.5.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples of a system of identical particles in a one-dimensional infinite square well (with boundaries between $x = 0$ and $x = a$) with a fixed total energy for the many-particle system. They initially focus on systems with only two or three particles in order to reflect upon the major concepts rather than working through problems with many particles with

algebraic complexities. In all problems, students are provided all the possible sets of integers whose squares sum to obtain the total energy of the system. They are asked to determine the number of distinct many-particle states, write all the possible many-particle stationary state wavefunctions, and determine the energies and probabilities of obtaining these energies when the energy of one particle is measured at random. In the QuILT, students consider the systems of identical particles in the following order: indistinguishable fermions, indistinguishable bosons, and identical particles that can be treated as distinguishable. After each section, students are provided further scaffolding and checkpoints to help them reconcile any differences between their initial responses and the correct reasoning.

**Helping students determine the number of distinct many-particle states for a system of identical particles:** In the QuILT, as part of a guided inquiry-based learning sequence, students are asked to list the possible combinations resulting from the provided sets of integers whose squares sum to obtain the total energy of the system. They are then asked to determine the number of distinct many-particle states that can be constructed with the specified fixed energy (they must determine the combinations of quantum numbers denoting the single-particle states that are possible and those that are distinctly different for the given system of identical particles for a system of identical fermions or bosons). Students engage with the following example in the QuILT for a system of three identical fermions, identical bosons, or identical particles that can be treated as distinguishable:

*Let's consider three non-interacting spinless identical particles of mass m in a one-infinite square well of width "a". Recall that the total energy of the many-particle system can be written in terms of the single-particle energies as*

$$\begin{aligned} E &= E_{n_1} + E_{n_2} + E_{n_3} = (n_1^2 + n_2^2 + n_3^2)\left(\frac{\pi^2\hbar^2}{2ma^2}\right) \\ &= (n_1^2 + n_2^2 + n_3^2)E_1. \end{aligned}$$

*Here $n_1, n_2, n_3$ are positive integers that label the different single-particle states in which the three particles can be placed. Suppose the total energy is $E = 243\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 243E_1$.*

*Note: The only possible integers $n_1, n_2$, and $n_3$ whose squares sum to 243 are given below:*

$$\begin{aligned} 243 &= 1^2 + 11^2 + 11^2 \\ 243 &= 3^2 + 3^2 + 15^2 \\ 243 &= 5^2 + 7^2 + 13^2 \\ 243 &= 9^2 + 9^2 + 9^2. \end{aligned} \tag{11.6}$$

Students begin by working through a guided inquiry-based learning sequence focusing on the number of distinct many-particle states for a system of identical fermions. The QuILT strives to help them recognize that any combination in which two or more fermions occupy the same single-particle state is not possible for a system of identical fermions. It also strives to help students do sense making pertaining to the combinations that make up a completely antisymmetric wavefunction and that these combinations should only be counted as one distinct many-particle state (not each permutation of the quantum numbers denoting the single-particle states in the combination counting as a distinct many-particle state as would be the case for distinguishable particles). The following is a hypothetical student conversation in which students must explain why they agree or disagree with each student:
**Student 1:** *There are four disinct three-particle states for the three spinless fermions:* $\psi_1(x_1)\psi_{11}(x_2)\psi_{11}(x_3)$, $\psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3)$, $\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3)$, *and* $\psi_9(x_1)\psi_9(x_2)\psi_9(x_3)$.
**Student 2:** *There cannot be more than one fermion in each single-particle state. The combination* $(9, 9, 9)$ *corresponds to a system with three spinless fermions in the state* $\psi_9$. *The combinations* $(3, 3, 15)$, $(3, 15, 3)$, *and* $(15, 3, 3)$ *have two spinless fermions in the state* $\psi_3$ *and the combinations* $(1, 11, 11)$, $(11, 1, 11)$, *and* $(11, 11, 1)$ *have two spinless fermions in the state* $\psi_{11}$. *None of these are possible for spinless fermions.*

Student 1 is incorrect and Student 2 is correct in the preceding conversation. The combinations in which two or more fermions are in the same single-particle state are not possible for a system of identical fermions. There is only one distinct three-particle state that corresponds to the case in which one fermion is in each of the single particle states $\psi_5$, $\psi_7$, and $\psi_{13}$. After reflecting upon each student's statement in the preceding conversation, students are asked to construct the three-particle stationary state wavefunction for the system of

identical fermions with the constraint given in Eq 11.6.

Next, the students work through several guided inquiry-based learning sequences focusing on determining the number of distinct many-particle states for a system of identical bosons and a contrasting case of a system of identical particles that can be treated as distinguishable. They focus on the system discussed earlier in which there are three non-interacting identical particles in a one-dimensional infinite square well with a total energy of the many-particle system of $243E_1$. The QuILT strives to help students reflect upon and learn that all of the combinations in Eq. 11.6 are distinct many-particle states for a system of identical particles that can be treated as distinguishable. However, not all these combinations correspond to distinct many-particle states for a system of identical bosons since the bosons are indistinguishable and the many-particle stationary state wavefunction must be completely symmetric.

**Helping students determine the energies and corresponding probabilities of measuring the energies if the energy of one particle is measured at random:** In the QuILT, students engage with the following example as part of a guided inquiry-based learning sequence that strives to help them determine the energies and corresponding probabilities of measuring the energies if the energy of one particle is measured at random:

**Q5.** *Suppose that for a system of two non-interacting identical particles in a one-dimensional infinite square well, the total energy of the two-particle system is* $E_{n_1,n_2} = (n_1^2 + n_2^2)E_1$, *in which* $E_1$ *is the ground state energy for the single-particle system. The total energy of the two-particle system is* $E = 50E_1$. *Assume all of the possible combinations are equally probable. Note: The only possible integers* $n_1$ *and* $n_2$ *whose squares sum to 50 are given below:*

$$\begin{aligned} 50 &= 1^2 \quad +7^2 \\ &= 5^2 \quad +5^2. \end{aligned}$$

The students are asked to determine the single-particle energies one might obtain and their probabilities if you randomly measure the energy of one particle for a system of identical fermions, identical bosons, and a system of identical particles that can be treated as distinguishable. They are then provided scaffolding support that strives to help them identify the possible energies and the corresponding probabilities for a system of identical particles.

The following is an excerpt from a hypothetical student conversation that strives to help students reflect upon the fact that any combination in which two fermions are in the same single-particle state is not possible and determine the possible energies and the corresponding probabilities for measuring the energy of one particle at random. The students must explain whether they agree or disagree with each statement.

**Student 1:** *The fermions could have the combination* $(5, 5)$ *in which both fermions are in the single-particle state* $\psi_5$*. Therefore, if you randomly measure the energy you could obtain the energies* $E_1$*,* $49E_1$*, or* $25E_1$ *with equal probability 1/3.*

**Student 2:** *I disagree with Student 1. The fermions cannot be in the same single-particle state* $\psi_5$*. One fermion must be in the single-particle state* $\psi_1$ *and one fermion must be in the single-particle state* $\psi_7$*. If you randomly measure the energy, you could obtain the energy* $E_1$ *or* $49E_1$ *with equal probability of 1/2.*

Student 1 is incorrect and Student 2 is correct in the preceding conversation. The two fermions cannot be in the same single-particle state $\psi_5$ and therefore, one cannot obtain the energy $25E_1$ when the energy of a particle is measured at random. Thus, it is equally probable that the energy of one particle measured randomly is $E_1$ or $49E_1$.

The following conversation strives to help students determine the possible outcomes if one measures the energy of a single particle at random and the corresponding probability if the particles are indistinguishable bosons. This conversation also aims to help students differentiate between a system of identical bosons and a system of identical particles that can be treated as distinguishable. After reflecting upon the hypothetical conversation, the students must state whether they agree or disagree with each statement and explain their reasoning.

**Student 1:** *The combinations* $(1, 7)$ *and* $(7, 1)$ *correspond to the completely symmetric state* $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_7(x_2) + \psi_7(x_1)\psi_1(x_2)]$*. The probability of the bosonic system having the combination* $(5, 5)$ *is 1/2 and the probability of having the combinations* $(1, 7)$ *and* $(7, 1)$*, which correspond to one two-particle state* $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_7(x_2) + \psi_7(x_1)\psi_1(x_2)]$ *is 1/2. The probability of obtaining* $E_1$ *is* $(1/2)\times(1/2) = 1/4$*, the probability of obtaining* $49E_1$ *is* $(1/2)\times(1/2) = 1/4$*, and the probability of obtaining* $25E_1$ *is* $(1/2) \times 1 = 1/2$*.*

**Student 2:** *I disagree with Student 1. Since the three combinations are equally likely,*

*the probability that the system has the combination* $(1,7)$*,* $(7,1)$*, or* $(5,5)$ *is 1/3. For the combination* $(1,7)$*, the probability of obtaining* $1^2E_1$ *is* $1/2$*. Similarly, the probability of obtaining* $E_1$ *for the combination* $(7,1)$ *is 1/2. Therefore, the probability of obtaining* $E_1$ *is* $(1/3)\times(1/2)+(1/3)\times(1/2)=1/3$*. By the same reasoning, the probability of obtaining* $49E_1$ *is* $2\times(1/3)\times(1/2)=1/3$*. The probability of the system being in the combination* $(5,5)$ *is 1/3. For bosons with the combination* $(5,5)$*, the probability of being in state* $\psi_5$ *is 1. Thus, the probability of obtaining* $25E_1$ *is* $(1/3)\times 1=1/3$*.*

Student 1 is correct in the preceding conversation since we are assuming the combinations $(5,5)$, $(1,7)$, and $(7,1)$ corresponding to the two distinct two-boson wavefunctions $\psi_{n_5}(x_1)\psi_{n_5}(x_2)$ and $\frac{1}{\sqrt{2}}[\psi_{n_7}(x_1)\psi_{n_1}(x_2)+\psi_{n_1}(x_1)\psi_{n_7}(x_2)$ are equally likely with probability $1/2$.

After reflecting upon this conversation, students are provided further scaffolding support in the guided inquiry-based learning sequence that strives to help them understand the differences between these issues for a system of identical bosons and identical particles that can be treated as distinguishable.

## 11.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional lecture-based instruction in relevant concepts for constructing the many-particle stationary state wavefunction for a system of identical particles before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

The following two questions were posed on the posttest of the QuILT,. Students were told to ignore the spin degrees of freedom and consider the particles as "spinless" in both questions. Q6 was given to all 30 graduate students and 12 undergraduate students in year 1 of the study. Q7 was given to 13 undergraduate students in year 2 of the study.

**Q6.** *For a system of two non-interacting identical particles in a one-dimensional infinite square well, the total energy of the two particle system is* $E_{n_1,n_2} = (n_1^2 + n_2^2)E_1$*, in which* $E_1$ *is the ground state energy for one particle. The total energy of the system is* $E = 450E_1$*. Assume all the possible combinations are equally probable. Note: The only possible integers* $n_1$ *and* $n_2$ *whose squares sum to 450 are given below:*

$$\begin{aligned} 450 &= 3^2 + 21^2 \\ &= 15^2 + 15^2. \end{aligned}$$

(a) *If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

(b) *If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

(c) *If the particles are distinguishable and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

**Q7.** *For a system of three non-interacting identical particles in a one-dimensional infinite square well, the total energy of the three particle system is* $E_{n_1,n_2,n_3} = (n_1^2 + n_2^2 + n_3^2)E_1$*, in which* $E_1$ *is the single-particle ground state energy. The total energy of the system is* $E = 75E_1$*. Assume all the possible three-particle states with this total energy* $75E_1$ *are equally probable.*

*Note: The only possible integers* $n_1$*,* $n_2$ *and* $n_3$ *whose squares sum to 75 are given below.*

$$\begin{aligned} 75 &= 1^2 + 5^2 + 7^2 \\ 75 &= 5^2 + 5^2 + 5^2 \end{aligned}$$

(a) *If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

(b) *If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

(c) *If the particles are distinguishable and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?*

In Q6(a), there is an equal probability of 1/2 of measuring the energies $3^2E_1$ and $21^2E_1$. In Q6(b), by the assumption that each combination is equally probable, there is a probability of 1/2 of both bosons being in the single-particle state with energy $15^2E_1$ and a probability of 1/4 of one boson being in the single-particle state with energy $3^2E_1$ or $21^2E_1$. If the particles are identical particles that can be treated as distinguishable as in Q6(c), there is an equal probability of 1/3 of measuring each of the energies $3^2E_1$, $21^2E_1$, and $15^2E_1$.

In Q7(a), there is an equal probability of 1/3 of measuring the energies $E_1$, $5^2E_1$, and $7^2E_1$. In Q7(b), by the assumption that each combination is equally probable, there is an equal probability of 1/6 of measuring the energy $E_1$ or $7^2E_1$ and a probability of 2/3 of measuring the energy $5^2E_1$. If the particles are identical particles that can be treated as distinguishable as in Q7(c), there is an equal probability of 2/7 of measuring the energy $E_1$ or $7^2E_1$ and a probability of 3/7 of measuring the energy $5^2E_1$

The open-ended questions Q1, Q6, and Q7 were graded using rubrics which were developed by the researchers together. A subset of questions was graded separately by them. After comparing the grading, they discussed any disagreements and resolved them with a final inter-rater reliability of better than 95%. Tables 45 and 46 show the performance of undergraduate and graduate students on the pretest and posttest.

The results are encouraging and suggest that the QuILT is effective in helping students determine the number of distinct many-particle states for systems of identical fermions or bosons, as well as the contrasting case in which the identical particles could be treated as distinguishable. Question Q6 was intended to be a similar problem to Q1 in that both particles can be in the same single-particle state or in different single-particle states. Interviews suggest that after traditional instruction, some students had simply memorized the probabilities of obtaining a particular energy when the energy of one particle is measured at random for a system of two particles such as in Q1 and Q6. Therefore, in year 2, students were asked Q7 on the posttest in which they cannot obtain the correct answer simply from memorization

Table 45: Average pretest and posttest scores for Q1 and Q6 for the given system for graduate students ($N = 30$).

| Question | Type of Particle | Graduate | |
|---|---|---|---|
| | | Pre (%) | Post (%) |
| Q1 | Fermions | 54 | |
| | Bosons | 49 | |
| | Distinguishable | 26 | |
| Q6 | Fermions | | 99 |
| | Bosons | | 98 |
| | Distinguishable | | 89 |

of examples of two particles in which both particles can be in the same single-particle state or in different single-particle states as in Q1 and Q6.

One area in which the students struggled on the posttest was related to determining the energies consistent with the fixed total energy of the system (difficulty B). Here all the students correctly identified the combinations that were possible in Q6, however some students provided energies whose sum was not $450E_1$. In particular, most of the students who did not answer Q6 correctly claimed that the energies of the single particles would be $3E_1, 15E_1$, and $21E_1$. Interviews suggest this was often an issue with students not reflecting upon whether their answers made sense more than due to conceptual difficulties identifying the correct energies. Roughly one-third of the undergraduates and one-tenth of the graduate students provided an answer to Q6 or Q7 on the posttest for which the miscalculated energies of the particles did not add up to the total energy given in the question. Addressing this difficulty more effectively is an area to improve upon in future refinements of the QuILT.

In general, students did well identifying the energies and corresponding probabilities for a system of fermions in Q6(a) and Q7(a) on the posttest. Nearly all of the students on the posttest correctly identified that the two fermions cannot be in the same single-particle state.

Table 46: Average pretest and posttest scores for Q1, Q6, Q7 for the given system for undergraduates (number of students $N = 25$, in Year 1 $N = 12$ and in Year 2 $N = 13$).

| Question | Year | Type of Particle | Undergraduate | |
|---|---|---|---|---|
| | | | Pre (%) | Post (%) |
| Q1 | 1 & 2 | Fermions | 60 | |
| | | Bosons | 73 | |
| | | Distinguishable | 30 | |
| Q6 | 1 | Fermions | | 93 |
| | | Bosons | | 75 |
| | | Distinguishable | | 47 |
| Q7 | 2 | Fermions | | 96 |
| | | Bosons | | 91 |
| | | Distinguishable | | 73 |

## 11.7 SUMMARY

Investigation of students' understanding of a system of identical particles helped to uncover many common student difficulties that were used as a guide to develop a QuILT that strives to help students learn how to determine whether a system with a specified total energy for a system containing a specified number of identical particles, determine the number of distinct many-particle states for a system of identical particles, and determine all of the possible energies and their corresponding probabilities if the energy of one particle is measured at random. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding through a guided inquiry-based approach. We find that the QuILT is effective in improving students' understanding of these fundamental concepts.

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# 12.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A SYSTEM OF IDENTICAL PARTICLES: COUNTING THE NUMBER OF DISTINCT MANY-PARTICLE STATES FOR A SYSTEM WITH DEGENERACY IN THE SINGLE-PARTICLE ENERGY SPECTRUM AND CONSTRAINTS ON THE NUMBER OF PARTICLES IN THE DIFFERENT SINGLE-PARTICLE STATES

## 12.1 INTRODUCTION

Quantum mechanics (QM) is a particularly challenging subject for upper-level undergraduate and graduate students in physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. There have been a number of research studies aimed at investigating student reasoning in QM [17, 18, 19, 20, 21, 22, 23, 24, 25] and improving student understanding of QM [26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]. For example, our group has focused on using the common student difficulties as a guide to develop research-based learning tools which include Quantum Interactive Learning Tutorials (QuILTs) [38, 39, 41, 37, 40, 42] which strive to improve student understanding of different QM concepts. However, there have been relatively few investigations into student difficulties with fundamental concepts involving a system of identical particles.

Here, we discuss an investigation of student difficulties with concepts related to determining the number of distinct many-particle states for a system when there is degeneracy in the single-particle energy spectrum and there are constraints on the number of particles in different single-particle states with a certain energy. We also discuss how that research was used as a guide in the development, validation, and in-class evaluation of a research-based

QuILT that makes use of student difficulties as a guide and strives to help students develop a good grasp of relevant concepts.

Students must have a good understanding of quantum mechanical properties of a system of identical particles as well as a strong background in combinatorics to be proficient in determining the number of distinct many-particle states. However, it has been found in a number of different contexts in introductory physics that students struggle to apply mathematics correctly in the context of physics even if they can solve similar mathematics problems without the physics context [43, 44, 45, 46]. Since human working memory while solving a problem is restricted to a limited number of "chunks" and the size of a chunk in the working memory depends on the expertise of the individual who is solving the problem, Simon's framework of "bounded rationality posits that individuals will make decisions while solving problems based upon their current level of expertise, which may not be optimal depending on their experise [47]. Some students may be motivated to find an optimal solution but if the students' level of expertise is not sufficient and they have not been provided with the appropriate scaffolding support, they may experience cognitive overload and may not be able to determine the correct solution to the problem posed [48].

Below, we start with a brief background of relevant concepts and then describe the methodology for the investigation of student difficulties followed by the common difficulties found. Then we describe the methodology for the development, validation and in-class evaluation of the corresponding research-based QuILT that strives to help students develop a functional understanding of the fundamental concepts involved in determining the number of distinct many-particle states for a system of identical particles when there is degeneracy in the single-particle energy spectrum and a fixed number of particles in different single-particle states with a certain energy.

## 12.2 BACKGROUND

In nature, there are two general types of particles: fermions with a half-integer spin quantum number (e.g., electrons and protons) and bosons with an integer spin quantum number (e.g.,

photons and mesons). A system of $N$ identical particles consists of $N$ particles of the same type (e.g., electrons). For a system of identical particles in classical mechanics (e.g., five identical tennis balls), each particle can be distinguished from all the other particles. In contrast, in quantum mechanics, identical particles are indistinguishable and there is no measurement that can be performed to distinguish these identical particles from one another. For example, if the coordinate of two identical particles is interchanged, there is no physical observable that would reflect this interchange. For a system of identical fermions for which the many-particle wavefunction is completely antisymmetric, it is not possible for two or more fermions to occupy the same single-particle state. For a system of identical bosons for which the many-particle wavefunction is completely symmetric, it is possible for two or more bosons to occupy the same single-particle state.

Here, we consider a system of identical particles in which there is degeneracy in the single-particle energy spectrum and there are constraints on the number of particles in different single-particle states with a certain energy. We will focus on the spatial part of the wavefunction and ignore the spin degrees of freedom (assume particles are spinless for simplicity). We will consider a group of degenerate states together and the arrangement $(N_1, N_2, N_3, \ldots, N_n, \ldots)$ is such that for all of the single-particle states with energy $E_i$, the total number of particles is $N_i$ in which the energies $E_i$ are indexed in order of increasing energy. We will use the notation $Q(N_1, N_2, N_3, \ldots, N_n, \ldots)$ to represent the number of distinct many-particle states for a given arrangement $(N_1, N_2, N_3, \ldots, N_n, \ldots)$. If there are no particles with energy greater than $E_m$, then for the arrangement $(N_1, N_2, N_3, \ldots, N_i, \ldots)$, we only list the number of particles $(N_m)$ up to and including the highest occupied energy $E_m$. For example, $(3, 4)$ denotes that there are three particles in the single-particle states with the lowest energy $E_1$, four particles in the single-particle states with the first-excited state energy $E_2$, and zero particles in the single-particle states with higher energy. We will use the symbol $d_i$ to represent the degeneracy corresponding to the energy level $E_i$. For example, if $d_i = 5$ then there are five degenerate single-particle states with energy $E_i$.

In order to construct a many-particle state for a system of fermions, there must be at least as many available spatial single-particle states as the number of identical fermions. If this condition is satisfied, one must determine the number of ways to arrange the identical

fermions into the available spatial single-particle states such that each single particle state has either zero or one fermion until all the fermions have been placed into an available single-particle state. The arrangement of the identical fermions must be consistent with the constraint on the number of particles in different single-particle states with a certain energy. The number of ways to arrange $N$ identical objects among $M$ available slots ($M \geq N$) is $\binom{M}{N} = \frac{M!}{N!(M-N)!}$. Thus, for a system of $N$ fermions with $M$ available single-particles states, the number of distinct many-particle states is

$$\begin{cases} \binom{M}{N} & M \geq N \\ 0 & M < N. \end{cases} \tag{12.1}$$

For a system of identical fermions with degeneracy in the single-particle energy spectrum and constraints on the number of particles in different single-particle states with a certain energy, one can determine the number of ways to arrange the $N_i$ fermions among the $d_i$ degenerate single-particle states with energy $E_i$. Applying Eq. 12.1 to all the single-particle states with energy $E_i$ and degeneracy $d_i$ gives $\binom{d_i}{N_i}$. Taking the product of all these possibilities, we find that the number of distinct many-particle states for a system of identical fermions is

$$\binom{d_1}{N_1}\binom{d_2}{N_2}\binom{d_3}{N_3}\cdots = \prod_n \frac{d_n!}{N_n!(d_n - N_n)!}. \tag{12.2}$$

One technique for determining the number of ways to arrange the identical bosons among the available single-particle states is often referred to as the "bin and divider" method. In particular, we can treat the single-particle states as bins to be filled with bosons and dividers to separate the different single-particle states, or bins. The number of distinct many-particle states can be found by determining the number of distinct arrangements of the identical bosons among the different single-particle states. For a system of $N$ identical bosons and $M$ available single-particle states, there are $M - 1$ identical dividers separating the single-particle states. We must determine the number of distinct arrangements of the $N$ identical bosons among the $M$ available single-particle states. Thus, the number of distinct many-particle states for a system of $N$ indistinguishable bosons with $M$ available single-particle

states is

$$\binom{N+M-1}{N} = \binom{N+M-1}{M-1} = \frac{(N+M-1)!}{N!(M-1)!}. \tag{12.3}$$

For a system of identical bosons with degeneracy in the single-particle energy spectrum and constraints on the number of particles in different single-particle states with certain energies, one can determine the number of ways to arrange the $N_i$ bosons among the $d_i$ degenerate single-particle states with energy $E_i$. Applying the "bin and divider" method (Eq. 12.3) to all of the single-particle states in which there are $N_i$ bosons with energy $E_i$ and degeneracy $d_i$ gives $\binom{N_i+d_i-1}{d_i-1}$. Taking the product of all these degenerate states, we find that the number of distinct many-particle states for a system of identical bosons is

$$\binom{N_1+d_1-1}{d_1-1}\binom{N_2+d_2-1}{d_2-1}\binom{N_3+d_3-1}{d_3-1}\cdots \tag{12.4}$$

$$= \prod_n \frac{(N_n+d_n-1)!}{N_n!(d_n-1)!}. \tag{12.5}$$

As a contrasting case, if identical particles could be treated as distinguishable, then one can determine which particle is in which single-particle state and there is no restriction on the number of particles in each single-particle state. For a system of $N$ identical particles that can be treated as distinguishable and $M$ available single-particle states, each particle can be placed in any of the $M$ single-particle states. The number of distinct $N$-particle states for a system of $N$ identical particles if they could be treated as distinguishable with $M$ available single-particle states is

$$M^N. \tag{12.6}$$

For a system of identical particles that can be treated as distinguishable with degeneracy in the single-particle energy spectrum and constraints on the number of particles in different single-particle states with a certain energy, one must choose which of the distinguishable particles are in each of the available single-particle states with the same energy and the number of ways to arrange the particles among the $d_i$ degenerate single-particle states. The

number of distinct many-particle states for a system of identical particles that can be treated as distinguishable is

$$\left[\binom{N}{N_1} d_1^{N_1}\right] \cdot \left[\binom{N-N_1}{N_2} d_2^{N_2}\right] \cdot \left[\binom{N-N_1-N_2}{N_3} d_3^{N_3}\right] \cdots \tag{12.7}$$

$$= N! \prod_n \frac{d_n^{N_n}}{N_n!}. \tag{12.8}$$

We note that Eq. 12.8 does not divide by $N!$ to take into account the Gibb's Paradox.

For a system with degeneracy in the single-particle energy spectrum and constraints on the number of particles with each single-particle energy, the degeneracy of the many-particle states is the number of distinct many-particle states that have the same total energy of the system specified in the problem. Thus, Eqs. 12.2, 12.5, and 12.8 yield the degeneracy in the energy spectrum of the many-particle system.

## 12.3 METHODOLOGY FOR INVESTIGATING STUDENT DIFFICULTIES

Student difficulties with determining the number of distinct many-particle states for a system of identical particles in which the total energy of the system is fixed and there is degeneracy in the single-particle energy spectrum were first investigated using three years of data involving responses to open-ended and multiple-choice questions administered after traditional instruction in relevant concepts from 57 upper-level undergraduate students in a junior/senior level QM course and 30 graduate students in the second semester of the graduate core QM course. Additional insight was gained concerning these difficulties from responses of 14 students during a total of 81 hours of individual think-aloud interviews. Moreover, after the development and validation of the QuILT, it was administered to 25 upper-level undergraduates (12 in year 1 of the study and 13 in year 2 of the study) and 30 first-year physics graduate students in their respective QM courses. The QuILT included a pretest, the tutorial, and a posttest. Students were given the pretest after traditional lecture-based instruction on identical particles. The pretest was not returned to the students. Students began working on the tutorial

in class and completed the tutorial as their weekly homework assignment. The posttest was administered after the students submitted the tutorial. Student responses on the pretest, tutorial, and posttest were analyzed for their understanding of how to determine the number of distinct many-particle states for a system of identical particles in which the total energy of the system is fixed and there is degeneracy in the single-particle energy spectrum. If new difficulties were discovered during the interviews or on the pretest, tutorial, or posttest, the difficulties were addressed in later versions of the QuILT.

In all the questions in our investigation, the non-interacting identical particles were restricted to one spatial dimension for convenience. We begin by only considering the spatial part of the wavefunction to simplify the problem (asking students to ignore the spin degrees of freedom) and to help students focus on fundamental concepts involved in determining the number of distinct many-particle states for a system of identical particles. The word "identical" in the tutorial and in this paper refers to one type of particle (all particles with the same properties) and does not necessarily imply that the particles are indistinguishable.

To investigate student understanding and reasoning related to the degeneracy in the single-particle energy spectrum for a system of identical particles, question Q1 was given as clicker question in an undergraduate quantum mechanics course following traditional, lecture-based instruction on identical particles to 17 undergraduate students (we ignore the spin degrees of freedom and call these particles "spinless" which students were asked to do).

**Q1.** *There are three identical spinless bosons in a one-dimensional infinite square well. The single particle stationary states are* $\psi_n$ $(n = 1, 2, 3, \ldots)$. *Choose all of the following statements that are correct for the three particle system.*

(a) *The ground state of the three particle system is* $\psi_1(x_1)\psi_1(x_2)\psi_1(x_3)$.

(b) $\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)$ *is a first excited state of the three particle system.*

(c) *The degeneracy of the first excited state is 3.*

Option (a) is the only correct answer for question Q1. Option (b) is incorrect since the first-excited state is $\frac{1}{\sqrt{3}}[\psi_1(x_1)\psi_1(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3) + \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)]$. Option (c) is incorrect as there is only one many-particle first-excited state for a system of

three identical spinless bosons in a one-dimensional infinite square well.

To probe whether students are able to determine the number of distinct many-particle states for a system of identical particles when there is degeneracy in the single-particle energy spectrum and a fixed number of particles in different single-particle states with a certain energy, the following two questions were posed to the students. Questions Q2 and Q3 were posed during the individual interviews as well as on the pretest and/or posttest for the QuILT. The pretest for the QuILT was given after traditional lecture-based instruction on relevant topics for a system of identical particles. The posttest was given after students had engaged with the QuILT and submitted it as a homework assignment. Q2 and Q3 were posed to 30 graduate students and 25 undergraduate students.

**Q2.** *Suppose a system with nine single-particle states contains 8 particles. The degeneracy of the lowest energy states with energy $E_1$ is $d_1 = 5$ and the degeneracy of the first-excited states with energy $E_2$ is $d_2 = 4$. If the total energy of the system is such that 3 particles are in the lowest energy states and 5 particles are in the first-excited states, what is the number of distinct eight-particle states $Q(3, 5)$ corresponding to this particular arrangement $(3, 5)$:*

(a) *if the particles are indistinguishable fermions?*

(b) *if the particles are indistinguishable bosons?*

(c) *if the particles are distinguishable?*

In Q2(a), the specified arrangement of the particles with the two single-particle energies is not possible for a system of identical fermions when the degeneracy of $E_1$ is $d_1 = 5$ and the degeneracy of $E_2$ is $d_2 = 4$. In particular, it is not possible to have 5 fermions in the 4 first-excited states. In Q2(b), for a system of identical bosons, there are $\binom{7}{3}\binom{8}{5} = 1960$ distinct eight-particle states. In Q2(c), for a system of identical particles that can be treated as distinguishable, there are $\binom{8}{3}5^3 \cdot 4^5 = 7,168,000$ distinct nine-particle states.

**Q3.** *Suppose a system with eleven single-particle states contains 7 particles. The degeneracy of the lowest energy states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited states with energy $E_2$ is $d_2 = 7$. If the total energy of the system is such that 3 particles are in the lowest energy states and 4 particles are in the first-excited states, what is the number of distinct seven-particle states $Q(3, 4)$ corresponding to this particular arrangement $(3, 4)$:*

(a) *if the particles are indistinguishable fermions?*

(b) *if the particles are indistinguishable bosons?*

(c) *if the particles are distinguishable?*

In Q3(a), for a system of identical fermions, there are $\binom{4}{3}\binom{7}{4} = 140$ distinct seven-particle states. In Q3(b), for a system of identical bosons, there are $\binom{6}{3}\binom{10}{4} = 4200$ distinct seven-particle states. In Q3(c), for a system of identical particles that can be treated as distinguishable, there are $\binom{7}{3}4^3 \cdot 7^4 = 5,378,240$ distinct seven-particle states.

## 12.4 STUDENT DIFFICULTIES

As discribed in the preceding chapters, determining the number of distinct many-particle states for a system of identical particles is a challenging task for many students when there is no degeneracy in the single-particle energy spectrum. In particular, many students relied on memorized formulas and struggled to reason systematically to determine the number of distinct many-particle states for a system of identical particles. Here we found several common student difficulties that are consistent with the previous studies in which the total energy of the system was fixed and there was no degeneracy in the single-particle energies. Here we focus on difficulties in determining the number of distinct many-particle states when there is degeneracy in the single-particle energy spectrum and constraints on the number of particles with each single-particle energy. Less than 10% of students answered questions Q2 and Q3 completely correctly for a system of three identical particles on the pretest to the QuILT after traditional instruction. Below, we discuss some of the student difficulties found.

### 12.4.1 Difficulty recognizing that it is not possible for a system to have more fermions than available single-particle states

The Pauli exclusion principle states that no two fermions can occupy the same single-particle state. Thus, the number of available single-particle states must be greater than or equal to the number of identical fermions. Some students had difficulty recognizing that the degeneracy $d_i$ of the single-particle energy states with energy $E_i$ must be greater than or equal to the number of particles in the single-particle states with energy $E_i$. For example, some students

struggled to recognize that the given arrangement of fermions in Q2(a) is not possible. In Q2(a), the total energy of the eight-particle system is such that three fermions are in the lowest energy single-particle states and five fermions are in the first-excited single-particle states. However, since the degeneracy of the first-excited states with energy $E_2$ is four, it is not possible to have five fermions occupy the four single-particle states with the first-excited state energy $E_2$.

Interviews suggest that determining the number of distinct many-particle states for a system of identical particles in which there is degeneracy in the single-particle energy spectrum and constraints on the number of particles in the degenerate single-particle states with a given energy is a more challenging task for students than determining the number of distinct many-particle states when each single-particle state has a different energy and there are no constraints on the total energy of the system. In particular, determining the number of distinct many-particle states when there is degeneracy in the single-particle energy spectrum and constraints on the number of particles in the different single-particle states is difficult because this requires students to determine the number of ways to arrange the particles among each of the degenerate single-particle states and then combine each of these arrangements for all of the different single-particle energies. Additionally, some students struggled to determine the number of distinct many-particle states when there is a constraint on the numbers of particles in the degenerate single-particle particle states with a given energy due to the fact that they must ensure they are only determining the number of many-particle states consistent with the given constraints. In this context, applying the Pauli exclusion principle correctly became more difficult for some students than the case in which there is no degeneracy in the single-particle energies and no constraint on the total energy of the system. Here students must consider the constraints on the number of particles in degenerate single-particle states with a given energy and ensure that there are more single-particle states than the number of particles to be placed in each single-particle state consistent with the constraints on the system, i.e., $d_i \geq N_i$. During the interviews, students were asked to determine the number of distinct many-particle states for systems in which there is no degeneracy in the single-particle energy spectrum and for systems in which there is degeneracy in the single-particle energy spectrum. For example, in some problems that students

were posed, there were more fermions than available single-particle states for these two cases. Some of the interviewed students correctly recognized that it is not possible to have a system of identical fermions in which there are more fermions than available single-particle states when there is no degeneracy in the single-particle energy spectrum, but then struggled to identify that such a system is not possible when there is degeneracy in the single-particle energy spectrum. One possibility is that the additional consideration of the degeneracy in the single-particle energies creates cognitive overload for many students so that they do not have resources available to engage in metacognition and reflect upon their answers or reconcile any inconsistencies in different parts of their reasoning [48]. Below, we discuss two types of student responses in which students struggled to identify that a system of identical fermions is not possible for a system when there is degeneracy in the single-particle energies and a fixed number of particles in different single-particle states with a fixed energy.

In Q2(a), one interviewed student identified that it is not possible to have five fermions in the first-excited states, but he still determined a non-zero number of distinct eight-particle states. He stated that "we have three fermions with the lowest energy and five with the first-excited energy. The degeneracy of the lowest energy states is five, so we have five choose three from the lowest energy. The first-excited states have degeneracy of four, so that gives us five choose four." After writing out the expressions $\binom{5}{3} = \frac{5!}{3!(5-3)!}$ and $\binom{4}{5} = \frac{4!}{5!(4-5)!}$, he identified tthat there was a problem. He said "wait, there are more fermions than states" as he pointed to the expression $\frac{4!}{5!(4-5)!}$. "This is impossible." However, he then went on to claim that the number of distinct eight-particles states in Q2(a) is $\binom{5}{3} = \frac{5!}{3!(5-3)!} = 10$ and said "we only get something from the lowest energy states." He did not realize that if it is not possible to have five fermions in the first-excited energy states then it is not possible for a system of identical fermions to be in the given state and therefore, there are zero distinct many-particle states in Q2(a). He went back and forth between memorized formulas and systematic reasoning about the problem, but in the end provided reasoning that relied on memorized formulas and attempted to make his expression consistent and meaningful for the given formula. This type of approach to problem solving has been observed in prior research in introductory physics in which students went back and forth between different problem solving strategies and often relied on memorized formulas over their own physical intuition

[45].

Some students provided a written response to Q2(a) after traditional instruction in which they wrote $\binom{5}{3} \cdot \binom{4}{5}$ and circled this expression to indicate that it was their final answer. Interviews suggest that often times students used Eq. 12.2 to find an expression for the number of distinct many-particle states, but they did not always check that these expressions are sensible. For example, one interviewed student claimed that the total number of distinct many-particle states in Q2(a) is $\binom{5}{3} \cdot \binom{4}{5}$. After he had finished the problem, he was asked to reflect upon his answer and work out the numerical value for the expression $\binom{5}{3} \cdot \binom{4}{5}$. He correctly evaluated the expression $\binom{5}{3} = \frac{5!}{3!2!} = 10$. Next, he evaluated the expression $\binom{4}{5}$. He initially wrote down $\binom{4}{5} = \frac{4!}{5!(4-5)!} = \frac{4!}{5!(-1)!}$, but after seeing the (-1)! in the denominator stated, "Oh, I must have made a mistake with the labels." He then changed his expression to $\binom{5}{4} = \frac{5!}{4!(5-4)!} = 5$. Instead of reflecting upon the physical situation and the fact that his initial response produced a contradiction, this student instead chose to alter his calculation to resolve this contradiction. This student and others with this type of difficulty often relied on the mathematics and equations rather than reflecting upon the physical situation in an attempt to resolve their incorrect reasoning. This type of reliance on mathematics over physical intuition has been observed in introductory physics. For example, when solving a conservation of energy problem, some students make an error with the sign of at least one of the terms and calcuate the speed $v$ to be the square root of a negative number. To resolve this issue, some students simply remove the minus sign from the number under the square root and claim the answer is the square root of the positive value [53]. For example, in one problem, students who determined that $v^2 = 2gh$ and then obtained $v = \sqrt{2(-9.8)23}$, when solving for the numerical value of the speed, dropped the minus sign and claimed that $v = 21.2$ m/s. Another example from introductory physics is from a study in which students were asked to write a mathematical expression for the electric field and plot the electric field as a function of the distance from the center of a sphere [45]. Students often relied upon a mathematical expression rather than their correct physical intuition. For example, one student correctly stated that the electric field inside a solid conducting spherical shell of inner radius $b$ and outer radius $c$ is zero, but then later when asked for a mathematical expression for the electric field wrote the expression $E = -4\pi c^2 + 4\pi b^2$ which is nonzero since

$b \neq c$. Students in this study often used quantitative reasoning in writing the mathematical expression for the electric field and used qualitative reasoning when plotting the electric field. As a result, students often provided contradictory solutions to the same problem via the two approaches without realizing that there was inconsistency between different responses.

### 12.4.2 Difficulty determining the degeneracy of the many-particle states

Some students struggled to identify the degeneracy in the many-particle energy spectrum for a system of identical particles. For a system in which there is degeneracy in the energy spectrum of both the single-particle states and the many-particle states, some students had difficulty realizing how these are different and how to consider the single-particle degeneracy when determining the number of many-particle states with the same energy (i.e., the degeneracy in the many-particle energy). Below, we discuss three types of difficulties students had with determining the degeneracy of the many-particle states.

Incorrectly claiming that the degeneracy of the many-particle states is the sum or product of the degeneracies of the single-particle states: During the interviews, students were asked to determine the degeneracy in the energy spectrum of the many-particle system under the given constraints on the number of particles in different single-particle states after working through questions Q2 and Q3. Some students simply added or multiplied the degeneracy of the lowest and first-excited single-particle states to determine the degeneracy in the energy of the many-particle system. For example, in Q3, the two most common incorrect answers were $4 + 7 = 11$ and $4 \cdot 7 = 28$ for all three systems of identical particles. Students with this type of reasoning often incorrectly claimed that the degeneracy of both the many-particle state and the single-particle states is $4 + 7 = 11$.

Difficulty differentiating between the degeneracy of the single-particle states and degeneracy of the many-particle states: Some students struggled to determine the degeneracy in the many-particle energy spectrum and had difficulty differentiating between degeneracy in the single-particle energy spectrum and degeneracy in the many-particle energy spectrum. The degeneracy in the energy spectrum of the many-particle system is the number of distinct many-particle states that have the fixed total energy specified in the problem. Thus, the

answers to Q2 and Q3 for the three different systems yield the degeneracy in the energy spectrum of the many-particle system. In Q2 and Q3, the degeneracy in the single-particle energy spectrum is specified in the problem.

Some students claimed that the degeneracy of the many-particle states must be due to the degeneracy of the single-particle states. However, it is possible that there is degeneracy in the many-particle energy spectrum when there is no degeneracy in the single-particle energy spectrum. For example, for a system of two identical particles in a one-dimensional infinite square well with a total energy of $E = 65E_1$ in which $E_1$ is the single-particle ground state energy. The single-particle energies could be $1^2E_1$ and $8^2E_1$ such that $65E_1 = 1^2E_1 + 8^2E_1$ or the single-particle energies could be $4^2E_1$ and $7^2E_1$ such that $65E_1 = 4^2E_1 + 7^2E_1$. Thus, the many-particle energy spectrum is two-fold degenerate while there is no degeneracy in the single-particle energy spectrum.

Difficulty differentiating between degeneracy of the many-particle states for indistinguishable and distinguishable particles: Some students incorrectly claimed that the number of terms in the many-particle stationary state wavefunction determines the degeneracy of the many-particle system with a fixed total energy (as opposed to the number of distinct many-particle stationary state wavefunctions with the same total energy). For example, in Q1, some students incorrectly chose option (c) as a correct answer. The question was given as an in-class clicker question to 17 students in a junior/senior level quantum mechanics course. The students first answered the question individually and then discussed the question in small groups and answered the question again. In Q1, when answering individually, 35% of the students selected option (3) as a correct answer. After group discussion, 24% of the students chose option (c) as a correct answer, which implies that the group discussion led to fewer students selecting the correct answer. In Q1, the first excited state for a system of three identical spinless bosons in a one-dimensional infinite square well is $\frac{1}{\sqrt{3}}[\psi_1(x_1)\psi_1(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3) + \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)]$. This is the only first-excited state of the three-particle bosonic system and therefore, has a degeneracy of 1. During the interviews, some students incorrectly claimed that the number of terms in the many-particle first-excited state wavefunction determine the degeneracy of the many-particle state. However, in Q1, the three terms in the first-excited state of the three-particle bosonic

system are the terms in the completely symmetric many-particle first-excited state wavefunction and not three distinct many-particle states with the same energy. For a system of three identical particles that can be treated as distinguishable particles, the many-particle states $\psi_1(x_1)\psi_1(x_2)\psi_2(x_3), \psi_1(x_1)\psi_2(x_2)\psi_1(x_3)$, and $\psi_2(x_1)\psi_1(x_2)\psi_1(x_3)$ are distinct many-particle states with the same energy. Thus, the degeneracy of the many-particle energy spectrum for a system of three identical particles that can be treated as distinguishable is three when two of the particles are in the state $\psi_1$ and one particle is in the state $\psi_2$. Some students struggled to differentiate distinctly different many-particle states for a system of indistinguishable particles from a system of identical particles that can be treated as distinguishable and could not determine the degeneracy of the many-particle system with a given total energy.

### 12.4.3 Incorrectly adding (as opposed to multiplying) the number of ways to arrange the particles in the states with a given energy to the number of ways to arrange the particles in various single-particle energy states with a different energy

Some students argued that the number of distinct many-particle states is the sum of the number of ways to arrange each particle. For example, in Q3(b), one interviewed student claimed that the number of distinct seven-particle states for a system of identical bosons is $4 \cdot 3 + 7 \cdot 4$. He incorrectly reasoned that "in the lowest energy states, there are four states for the three bosons. And in the first-excited (energy) states, there are seven states for the four bosons. For the bosons in the lowest energy states, there are four states for each boson, so there are $4 \cdot 3$ ways to arrange them. For the bosons in the first-excited (energy) states, there are seven states for each boson. That makes $7 \cdot 4$ ways to arrange those bosons. So, in total, we get $4 \cdot 3 + 7 \cdot 4 = 40$ (distinct seven-particle states)." This student made several mistakes including treating the bosons as distinguishable particles, but also incorrectly added the number of ways to arrange each particle.

Some students correctly found the number of arrangements among the degenerate single-particle states with the same energy, but then incorrectly added the total number of arrangements of the particles in the lowest and first-excited energy states. For example, in Q3(a),

one interviewed student correctly determined that the number of ways to arrange the identical fermions in the lowest energy state is $\binom{4}{3}$ and also correctly determined that the number of ways to arrange the identical fermions in the first-excited energy states is $\binom{7}{4}$. However, this student then incorrectly stated that "the total number of (distinct seven-particle) states is the sum of ones from the lowest energy and the first-excited state (energy). So the answer is 4 choose 3 plus 7 choose 4." After evaluating the expression, he determined the number of distinct seven-particle states in Q3(a) to be $4 + 35 = 39$.

These interviewed students and others with this type of reasoning struggled to realize that one should multiply the number of ways to arrange each identical particle when determining the number of distinct many-particle states.

### 12.4.4 Not taking into account the constraints on the many-particle system

In Q2 and Q3, many students struggled to realize that the total number of particles in each single-particle state is given and that one must determine the number of distinct many-particle states consistent with the given constraints. For example, in Q3, many students determined the number of ways to arrange the seven identical particles among the eleven total single-particle states. The two most common incorrect responses for students with this type of difficulty were $\binom{11}{7}$ distinct seven-particle states for a system of identical fermions or bosons and $11^7$ distinct seven-particle states for a system of identical particles that can be treated as distinguishable.

In Q1 (a), the answer $\binom{11}{7}$ would be the correct number of distinct seven-particle states for a system of identical fermions if there were no energy constraints on the system. However, since the energy of the system is such that three particles are in the lowest energy states and four particles are in the first-excited states, one must only count states that satisfy this constraint.

In Q1(c), the students who incorrectly claimed that there are $11^7$ distinct seven-particle states for a system of identical particles that can be treated as distinguishable were determining the number of distinct many-particle states correctly for a system with no constraint on the number of particles in different single-particle states with the same energy. They

incorrectly claimed that there are 11 single-particle states available to each particle.

### 12.4.5 Memorization of formulas rather than using systematic reasoning

Many interviewed students attempted to recall the formula (Eq. 12.2, 12.5, or 12.8) for determining the number of distinct many-particle states for a given system of identical particles rather than using systematic reasoning to generate it. Often times students would omit at least one of the terms in the formulas or did not have the appropriate symbols in the appropriate place in the formula. For example, common mistakes in Q3(c) were to use the expression $\prod_n d_n^{N_n}$ or $N! \prod_n d_n^{N_n}$ instead of the correct expression given in Eq. 12.8. Other students switched the number of degenerate single-particle states and the number of particles with the specified degenerate energy in Eq. 12.8. For example, in Q3(c), some students incorrectly wrote the formula for determining the number of distinct many-particle states in terms of $N_n^{d_n}$ as opposed to $d_n^{N_n}$ in Eq. 12.8.

In some cases, students recalled a correct formula but used it for the incorrect system of identical particles. For example, some students correctly recalled Eq. 12.2, but used it to calculate the number of distinct many-particle states for a system of identical bosons.

Moreover, some students who recalled a formula correctly did not use it correctly. During the interview and on written responses after traditional lecture-based instruction, students with this type of difficulty often struggled to correctly recognize the meaning of each symbol in the equation. For example, in Q3, some students used the total number of particles $N$ in the formulas for $N_n$ instead of the occupation number for the particles in the single-particle states with a given energy $E_n$.

### 12.4.6 Difficulty accounting for the indistinguishability of the identical particles

Some students struggled to account for the fact that for a system of identical fermions or bosons, the identical particles are indistinguishable. Below, we discuss student difficulties in determining the number of distinct many-particle states for a system of indistinguishable particles in which students incorrectly determined the number of ways to arrange the identical particles among the degenerate single-particle states consistent with the constraints on the

number of particles with each single-particle energy.

In Q3, some students determined the number of distinct seven-particle states by calculating the number of ways to choose the particles to occupy the lowest energy states and the first-excited energy states. For example, in Q3, for both a system of identical fermions and bosons, one interviewed student claimed that "we have seven identical particles. Three must go in the lowest energy states and four must go in the first-excited energy states. So there are 7 choose 3 different combinations for the lowest energy (states) and 7 choose 4 combinations for the first-excited (energy) states." He then jotted down that there are $\binom{7}{3}\binom{7}{4}$ distinct seven-particle states in Q3 for both a system of identical fermions and bosons. In Q3, after traditional lecture-based instruction, some students wrote that there are $\binom{7}{3}\binom{4}{4} = \binom{7}{3} \cdot 1$ distinct seven-particle states. Students with this type of reasoning were making two mistakes. First, they were treating the indistinguishable fermions and bosons as distinguishable particles by first choosing three of the seven indistinguishable particles to place in the lowest energy single-particle state and then determining which of the four particles to place into the first-excited energy single-particle states. Second, they determined the number of ways to choose the particles to be placed in the lowest and first-excited energy single-particle states, but they did not determine the number of ways these particles can be distinctly arranged among the four-fold degenerate lowest energy states or the seven-fold degenerate first-excited energy states.

Many students struggled with the fact that there are constraints on the number of particles with each single-particle energy is fixed and that one must only determine distinct many-particle states that satisfy the specified arrangement given in the problem. In particular, since there is degeneracy in the single-particle energy spectrum, one must make sure that the single-particle states with the same energy have the appropriate number of particles in addition to determining the number of ways these identical particles can be arranged among these degenerate single-particle states. When determining the number of distinct many-particle states for a system of identical particles that can be treated as distinguishable, one must determine the number of arrangements of the specified number of identical particles among the degenerate single-particle states. However, for a system of indistinguishable particles, choosing different particles to be placed in the different single-particle states does not

make up a distinctly different many-particle state.

## 12.5 METHODOLOGY FOR THE DEVELOPMENT AND VALIDATION OF THE QUILT

### 12.5.1 Development and Validation of the QuILT

Based upon our research of student difficulties with fundamental concepts with systems of identical particles, we developed a QuILT that attempts to build a consistent and coherent knowledge structure while at the same time addressing the common student difficulties. The development and structure of the QuILT was inspired by several influential learning theories. In particular, the QuILT strives to incorporate Vygotsky's zone of proximal development (ZPD) [49], Bransford and Schwartz's preparation for future learning (PFL) framework [50], and Piaget's "optimal mismatch" [51].

The QuILT is inspired by Vygotsky's ZPD in that it strives to give the students the requisite knowledge and skill sets by providing students with appropriate scaffolding. The desired tasks, which the students were often unable to perform successfully at the onset of the QuILT, are addressed using a guided inquiry-based approach to build the students' knowledge to the point that they develop self-reliance and are able to successfully complete the same task on their own after working through the QuILT.

Additionally, the QuILT strives to incorporate Bransford and Schwartz's PFL framework with a special focus on instruction that is both innovative and efficient. They view innovation and efficiency as two orthogonal components of instruction that must be balanced for effective instruction. One interpretation of this framework is that innovation refers to presenting students with novel tasks that are just beyond their current understanding that allow them to grow and strive for more robust content knowledge. Efficiency has been viewed as a characteristic of instruction that allows the students to practice what they are learning to enable them to become skilled and develop a functional understanding of the material. The framework suggests that instruction should attend to both aspects. The concern is that if instruction only focuses on one of these aspects there is danger that the students will become

disconnected when instruction is too advanced beyond their current state (the instruction is too innovative without allowing for efficiency to develop) or when the instruction focuses too much on rote memorization and procedural redundancy (the instruction is too efficient without the creative nature associated with innovation).

Finally, the QuILT was developed with Piaget's "optimal mismatch" as a guiding principle. The key idea behind Piaget's "optimal mismatch" is to allow students to discover their mistakes on their own and correct the inconsistencies in their own knowledge structures. To achieve this, the QuILT strives to scaffold student learning using a guided inquiry-based approach which focuses on all the necessary skills and concepts to help the students develop a functional understanding of a system of identical particles. It also addresses and helps students reconcile many of the common difficulties students have with this topic. In particular, the QuILT incorporates hypothetical student conversations and sets of inquiry-based sequences designed to help them realize inconsistencies in their prior knowledge, and provides scaffolding to help students resolve these inconsistencies.

The development of the QuILT was also guided by a cognitive task analysis [52] from both an expert perspective and a novice perspective which consisted of all the requisite knowledge and skills necessary for a functional understanding of a system of identical particles. The initial cognitive task analysis was conducted from an expert perspective in which the researchers outlined the required knowledge and skills and the order in which they are useful in solving problems. This cognitive task analysis was iterated with members of the physics faculty. However, in an effort of determine if there are additional areas students may struggle with that are not predicted by the experts (expert blindspot), we conducted the student interviews. The cognitive task analysis was then expanded to include these concepts or tasks in which students needed additional scaffolding support.

The QuILT was iterated many times among the three researchers and at several points during the development it was iterated with three physics faculty members at the University of Pittsburgh to ensure that the content was appropriate and they agreed with the wording. During this cyclical iterative process, faculty members provided feedback regarding the current version of the QuILT that was incorporated or addressed in the next version of the QuILT. Once it was agreed upon by the faculty that the content was clear and correct, the

QuILT was administered to 14 graduate students in "think aloud" interviews to ensure that the wording was unambiguous, the scaffolding was effective, and to further investigate any student difficulties. During these semi-structured interviews, the students worked through the QuILT and provided their rationale for each question in the pretest, the guided inquiry-based tutorial, and the posttest. The students were not interrupted as they answered the questions and worked through the tutorial. They were asked follow up questions or asked to clarify any unclear statements only upon completion of the pretest, the entire section of the tutorial focusing on the issues discussed here, or the posttest. After each interview, the student's responses were analyzed to measure the effectiveness of the tutorial and determined whether there were any necessary changes to be made to the QuILT. These changes were incorporated in subsequent versions of the QuILT and in subsequent interviews. During each step in the cyclically iterative process, the QuILT was adjusted to incorporate the faculty suggestions as well as the students' feedback and responses to help students with the common difficulties and improve the ability of the students to build a consistent and coherent knowledge structure. After it was deemed successful, the QuILT was next administered to students in various advanced quantum mechanics courses.

### 12.5.2 Structure of the QuILT

The QuILT strives to transform the students into active learners by employing an inquiry-based approach which requires the students to build their own knowledge structure by answering questions, analyzing the validity of given statements, and reflecting upon what they have learned. The QuILT consists of three parts: the pretest, a guided inquiry-based tutorial, and the posttest. The pretest is administered to the students after traditional, lecture-based instruction covering systems of identical particles. The pretest is administered in class during which the students completed it individually with no additional resources other than what is provided in the pretest itself. After completing the pretest, they are given the tutorial and encouraged to work together in small groups in class. The tutorial can be used to guide in-class discussion. The tutorial can also be administered as a self-paced learning tool that the students work on as part of their weekly homework assignment. Upon completion, the students submit the tutorial for grading and are then administered the posttest. The posttest is given in class as an individual assessment in which the students are not permitted

any additional resources beyond what is provided in the posttest.

The QuILT incorporates guided inquiry-based learning sequences which consist of several related questions, each building upon the previous question(s), that require the students to take a stand and actively engage with the learning process. The QuILT also includes hypothetical student conversations in which the students must analyze each hypothetical student's statement to determine whether they are correct and explain why they agree or disagree with each student. Many of the common student difficulties were used as a guide when constructing these hypothetical conversations and inquiry-based sequences with the goal being that students would identify any inconsistency in their reasoning and then use the provided support to reconcile these inconsistencies. For example, there are a number of hypothetical student conversations in which one or more students make statements reflecting these common difficulties and provide incorrect reasoning mirroring those given by actual students. Other students in these hypothetical conversations disagree with their incorrect reasoning and provide correct reasoning and often note an issue with the incorrect statement(s). As the students work through the QuILT, they must consider each student's argument and reflect upon their own reasoning in order to determine which student(s) are correct. Similarly, the guided inquiry-based sequences often include portions that strive to present the students with a contradiction between the answer to the questions in the sequence and their prior knowledge that they must then reconcile. Checkpoints are provided at the end of each section that allow the students to go back and reconcile any remaining difference between the correct reasoning and their own reasoning before moving on the next section.

### 12.5.3 Addressing Student Difficulties

In the guided inquiry-based learning sequences in the QuILT, students actively engage with examples focusing on concepts in a given situation, e.g., how to determine the number of distinct many-particle states for a system with degeneracy in the single-particle energy spectrum and a fixed number of particles in each group of degenerate single-particle states with a certain energy. In particular, the QuILT strives to help students develop a systematic ap-

proach for determining the number of many-particle states for a system of identical particles. In the QuILT, students consider the systems of identical particles in the following cases: (1) indistinguishable fermions, (2) indistinguishable bosons, and (3) identical particles that can be treated as distinguishable. We begin with the following example that is part of a guided inquiry-based sequence students engage with in the QuILT.

**Q4.** *Suppose that a system with ten single-particle states has 4 particles. The degeneracy of the lowest single-particle stationary state with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$. If the total energy of the system is such that 2 particles are in the lowest energy states and 2 particles are in the first-excited states, what is the number of distinct four-particle states $Q(2, 2)$ corresponding to this particular arrangement (2,2):*

(a) *if the particles are indistinguishable fermions?*

(b) *if the particles are indistinguishable bosons?*

(c) *if the identical particles can be treated as distinguishable?*

In Q4(a), for a system of indistinguishable fermions, there are $\binom{4}{2} \cdot \binom{6}{2} = 6 \times 15 = 90$ distinct four-particle states. In Q4(b), for a system of indistinguishable bosons, there are $\binom{4+2-1}{2} \cdot \binom{6+2-1}{2} = \binom{5}{2} \cdot \binom{7}{2} = 10 \times 21 = 210$ distinct four-particle states. In Q4(c), for a system of identical particles that can be treated as distinguishable, there are $\left[\binom{4}{2} \cdot 4^2\right] \left[\binom{4-2}{2} \cdot 6^2\right] = 96 \times 36 = 3456$ distinct four-particle states.

Below, we discuss how this guided inquiry-based sequence strives to provided scaffolding support intended to help students with these concepts involved in determining the number of distinct many-particle states and address some of the common difficulties.

**Helping students recognize that two fermions cannot occupy the same single-particle state:** Students begin by working through several guided inquiry-based learning sequences focusing on the number of distinct many-particle states for a system of identical fermions. One of these guided inquiry-based sequences in the QuILT strives to help them identify that any arrangement in which two or more fermions occupy the same single-particle state is not possible for a system of identical fermions.

**Helping students realize that one should multiply (not add) the number of**

**ways to arrange the identical particles in different single-particle states:** Another guided inquiry-based learning sequence aims to help students do sensemaking of the combinatorics in this quantum physics context and realize that one should multiply the number of ways to arrange the identical particles in different groups of states with the same single-particle energies (e.g., the ground and first-excited energies). In order to help students reflect upon relevant issues, the following is a hypothetical student conversation regarding whether one should add or multiply the number of arrangements of the identical fermions in the lowest energy states and the first-excited energy states in Q4(a). After considering the validity of each statement, the students must explain why they agree or disagree with each student:
**Student 1:** *Since there are 6 ways to arrange two indistinguishable fermions among the four degenerate single-particle states with energy $E_1$ and 15 ways to arrange two indistinguishable fermions among the six degenerate single-particle states with energy $E_2$, there are a total of* $6 + 15 = 21$ *distinct four-particle states corresponding to the arrangment of two fermions in the lowest energy states and two fermions in the first-excited energy states.*
**Student 2:** *I disagree with Student 1. The total number of distinct four-particle states* $Q(2, 2)$ *corresponding to the arrangement of two fermions in the lowest energy states and two fermions in the first-excited energy states is the product of the number of ways to arrange the indistinguishable fermions in the four degenerate states with energy $E_1$ and the six degenerate states with energy $E_2$, not the sum. The number of distinct four-particle states corresponding to the arrangement of two fermions in the lowest energy states and two fermions in the first-excited energy states for the system is* $6 \times 15 = 90$.

Student 1 is incorrect and Student 2 is correct in the preceding conversation. Students are provided further scaffolding that strives to help them learn that the number of distinct many-particle states for a system of identical particles is expressed as the product (as opposed to the sum) of the number of ways to arrange the particles in the lowest energy states and the first-excited energy states.

**Helping students realize that one must be careful to determine the many-particle states consistent with the constraints on the number of particles in single-particle states with a given energy:** For a system with constraints on the number of particles in single-particle states with a given energy, one must ensure that this energy

constraint is satisfied when determining the number of distinct many-particle states. The following is a hypothetical student conversation regarding Q4 that focuses on arranging the particles such that the number of particles in single-particle states with a given energy is consistent with the given constraint. After reflecting upon each statement in the hypothetical conversation, the students must explain why they agree or disagree with each student:

**Student 1:** *In the given example, since the lowest energy single-particle states with energy $E_1$ have degeneracy $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$, there are a total of 10 available single-particle states. We must determine all the permutations of the four particles among the 10 single-particle states.*

**Student 2:** *I agree with Student 1 only in the case in which there is no constraint on the total energy of the system. However, in this example, the permutations of the four particles must be consistent with the fixed total energy of the system. Therefore, only two particles with energy $E_1$ and two particles with energy $E_2$ are permitted.*

Student 1 is incorrect and Student 2 is correct, since the only many-particle states that should be counted are those with the specified total energy and the arrangement stated in Q4. The students are provided further scaffolding aimed at helping them determine the number of ways to arrange the particles in different single-particle states consistent with the given arrangement and total energy of the many-particle system.

## 12.6 EVALUATION OF THE QUILT

Once the researchers determined that the QuILT was successful in one-on-one implementation using a think-aloud protocol, it was administered in graduate and upper-level undergraduate classes. Both undergraduate and graduate students were given a pretest after traditional instruction in relevant concepts for constructing the many-particle stationary state wavefunction for a system of identical particles before working through the tutorial. The pretests were not returned to the students after grading. The undergraduates worked through the tutorial in class for two days and were asked to work on the remainder of the

Table 47: Average pretest and posttest scores for Q2 and Q3 for the given system on the pretest and posttest for undergraduates (number of students $N = 25$) and graduate students ($N = 30$).

| Question | Type of Particle | Graduate | | Undergraduate | |
|---|---|---|---|---|---|
| | | Pre (%) (number of students) | Post (%) (number of students) | Pre (%) (number of students) | Post (%) (number of students) |
| Q2 | Fermions | - | 93 (30) | 46 (13) | 83 (12) |
| | Bosons | - | 64 (30) | 34 (13) | 74 (12) |
| | Distinguishable | - | 61 (30) | 20 (13) | 64 (12) |
| Q3 | Fermions | 8 (30) | - | 15 (12) | 85 (13) |
| | Bosons | 4 (30) | - | 2 (12) | 92 (13) |
| | Distinguishable | 10 (30) | - | 8 (12) | 80 (13) |

tutorial as homework. The graduate students were given the tutorial as their only homework assignment for the week. After working through and submitting the completed tutorial, both groups were given the posttest in class. Students were given enough time in class to work through the pretest and posttest.

The QuILT was administered to 30 graduate students in one year of a second semester graduate level QM course and to 25 undergraduate students over two years in a second semester upper-level undergraduate QM course. There were 12 undergraduate students in the first year of the study and 13 undergraduate students in the second year of the study. In Year 1, both the undergraduates and graduate students were given question Q3 on the pretest and Q2 on the posttest. In Year 2, the undergraduate students were given question Q2 on the pretest and Q3 on the posttest. Q2 and Q3 were intended to be similar questions with minor changes in the number of identical particles and degenerate single-particle states in the two energy levels.

Overall, there was a significant improvement in the student performance on the posttest questions compared to the pretest questions. Table 47 summarizes the student performance on questions Q2 and Q3. In particular, over 80% of the undergraduates and over 90% of the graduate students correctly identified that no system of identical fermions is possible if

there are more fermions than available single-particle states in Q2 on the posttest in Year 1. The graduate students scored 64% on the posttest for a system of identical bosons in questions Q2. The undergraduate students scored over 74% on the posttest for a system of identical bosons in questions Q2 and Q3. The results are encouraging and suggest that the QuILT is effective in helping students determine the number of distinct many-particle states for systems of identical fermions or bosons when the total energy of the system is fixed and there is degeneracy in the single-particle energy spectrum.

## 12.7 SUMMARY

Investigation of students' understanding of a system of identical particles helped to uncover many common student difficulties that were used as a guide to develop a research-validated QuILT that strives to help students learn how to determine the number of distinct many-particle states for a system of identical particles when there is degeneracy in the single-particle energy spectrum and constraints on the number of particles in different single-particle states with a certain energy. Many of the student difficulties discussed here may be attributed in part to students' bounded rationality in that they are limited in their cognitive resources since they are still developing expertise in these concepts [47]. Since the paradigm of QM is novel, these issues become critical. The QuILT strives to place the students in the role of active learners while providing an appropriate level of scaffolding through a guided inquiry-based approach. The results show that the QuILT is effective in improving students' understanding of concepts necessary for determining the number of distinct many-particle states for a system of identical particles with degeneracy in the single-particle energy spectrum and constraints on the number of particles in different single-particle states with a certain energy.

## 12.8 ACKNOWLEDGMENTS

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# 13.0 FUTURE OUTLOOK

The study on investigating and improving student difficulties with Degenerate Perturbation Theory was only carried out in the context of time-independent perturbation theory. The study can be extended to include Time-Dependent Perturbation Theory (TDPT). In this case, a time-dependent potential energy allows for transitions to occur between different unperturbed energy levels if the time-dependent perturbation acts for a certain time. One application of TDPT is in the emission or absorption of electromagnetic radiation by an atom.

The study on investigating and improving student difficulties with a System of Identical Particles focused on writing the many-particle stationary state wavefunction and counting the number of distinct many-particle states for a system of identical particles. This study can be extended to focus on additional concepts in quantum statistical mechanics. In particular, at finite temperatures, one can investigate student difficulties in determining the most probable configuration, the density of states, the Maxwell-Boltzmann distribution, the Fermi-Dirac distribution, and the Bose-Einstein distribution.

# APPENDIX A

# DEGENERATE PERTURBATION THEORY QUANTUM INTERACTIVE LEARNING TUTORIAL

## A.1 DEGENERATE PERTURBATION THEORY PRETEST/POSTTEST

# Degenerate Perturbation Theory Pretest/Posttest

NOTE : For the matrix representation of a Hermitian operator $\hat{Q}$ in a given basis, we will use "=" or "is equal to" instead of "$\doteq$" or "is represented by" as in the notation below

$$\hat{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \quad \text{is equivalent to} \quad \hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}$$

with $Q_{ij} = (Q_{ji})^*$. Here $^*$ denotes the complex conjugate.

The Hamiltonian of the hydrogen atom placed in an external magnetic field is

$$\hat{H} = \hat{H}^0 + \hat{H}'_r + \hat{H}'_{SO} + \hat{H}'_Z = \hat{H}^0 + \hat{H}'_{fs} + \hat{H}'_Z \tag{A.1}$$

in which (all notations are standard)

- $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$ only accounts for the interaction of the electron with the nucleus via Coulomb attraction

- $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term
- $\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{r^3}\hat{\vec{S}} \cdot \hat{\vec{L}}$ is the spin-orbit interaction term
- $\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r$ is the fine structure term
- $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ is the Zeeman term.

The unperturbed energy for the hydrogen atom with $\hat{H}^0$ only is $-\frac{13.6 \text{ eV}}{n^2}$ for a given value of $n$.

* We will use the following notations interchangeably to write states in the uncoupled representation (in which basis states are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{L}_Z$, and $\hat{S}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ m_l\ m_s\rangle$
  - $|l,\ m_l\rangle|s,\ m_s\rangle$ (if $n$ is fixed)
  - $|l,\ m_l,\ m_s\rangle$ (if $n$ and $s$ are fixed)
* $\vec{J} = \vec{L} + \vec{S}$
* We will use the following notations interchangeably to write states in the coupled representation (in which basis vectors are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ j\ m_j\rangle$
  - $|l,\ s,\ j,\ m_j\rangle$ (if $n$ is fixed)
  - $|l,\ j,\ m_j\rangle$ (if $n$ and $s$ are fixed)
* Assume that for all questions that follow, the radial part of the basis corresponds to $R_{nl}(r)$, found by solving the radial part of the time-independent Schrödinger equation for the unperturbed Hamiltonian $\hat{H}^0$.
* Assume that for all cases, the principal quantum number is fixed to $n = 2$ and the spin quantum number is fixed to $s = 1/2$.

The following equations may be helpful (all notations are standard).

$$\hat{S}^2|s\ m_s\rangle = \hbar^2 s(s+1)|s\ m_s\rangle \qquad \hat{S}_z|s\ m_s\rangle = \hbar m_s|s\ m_s\rangle$$

$$\hat{S}_\pm|s\ m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1))}|s\ m_s \pm 1\rangle$$

$$\hat{L}^2|l\ m_l\rangle = \hbar^2 l(l+1)|l\ m_l\rangle \qquad \hat{L}_z|l\ m_l\rangle = \hbar m_l|l\ m_l\rangle$$

$$\hat{L}_\pm|l\ m_l\rangle = \hbar\sqrt{l(l+1) - m_l(m_l \pm 1))}|l\ m_l \pm 1\rangle$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$\hat{J}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 j(j+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{J}_z|l,\ s,\ j\ m_j\rangle = \hbar m_j|l,\ s,\ j,\ m_j\rangle$$

$$\hat{S}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 s(s+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{L}^2|l,\ s,\ j\ m_j\rangle = \hbar^2 l(l+1)|l,\ s,\ j,\ m_j\rangle$$

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$$

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$$

$$|\psi_n^1\rangle = \sum_{m\neq n}\frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle$$

In the following table, the states for $n = 2$ are listed in the coupled representation (left), and each state in the coupled representation is given in terms of a linear combination of states in the uncoupled representation (right) using the Clebsch-Gordon table.

| | Coupled Representation $\lvert l,\ j,\ m_j\rangle$ | Uncoupled Representation $\lvert l,\ m_l\rangle\lvert s,\ m_s\rangle$ |
|---|---|---|
| $\lvert\psi_1\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_2\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_3\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{3}{2}\right\rangle$ | $\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_4\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{3}{2}\right\rangle$ | $\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_5\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{1}{2}\right\rangle$ | $\sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_6\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $-\sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_7\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{1}{2}\right\rangle$ | $\sqrt{\frac{1}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_8\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $-\sqrt{\frac{2}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |

1. Evaluate the following matrix elements useful for the matrix elements of $\hat{H}'_{SO}$, in which the states are written in the coupled representation $|n\ l\ s\ j\ m_j\rangle$ ($C$ is a constant to make the dimensions of $\hat{H}'_{SO}$ that of energy). **In order to receive credit you must show your work or explain your reasoning.**

   a. $C\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\frac{1}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}\ \frac{3}{2}\frac{1}{2}\rangle$

   b. $C\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\frac{3}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}\ \frac{3}{2}\ -\frac{1}{2}\rangle$

2. Evaluate the following matrix elements useful for the matrix elements of $\hat{H}'_{SO}$, in which the states are written in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$ ($C$ is a constant to make the dimensions of $\hat{H}'_{SO}$ that of energy). **In order to receive credit you must show your work or explain your reasoning.**

   a. $C\langle 2\ 1\ \frac{1}{2}\ 1\ \frac{1}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}1\ \frac{1}{2}\rangle$

   b. $C\langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}\ 1\ \ -\frac{1}{2}\rangle$

3. Evaluate the following matrix elements useful for the matrix elements of $\hat{H}'_{Z}$, in which the states are written in the coupled representation $|n\ l\ s\ j\ m_j\rangle$ ($C$ is a constant to make the dimensions of $\hat{H}'_{Z}$ that of energy). **In order to receive credit you must show your work or explain your reasoning.**

   a. $C\langle\psi_3|(\hat{L}_z+2\hat{S}_z)|\psi_3\rangle = C\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{3}{2}|(\hat{L}_z+2\hat{S}_z)|2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle$

b. $C\langle\psi_5|(\hat{L}_z + 2\hat{S}_z)|\psi_6\rangle = C\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{1}{2}|(\hat{L}_z + 2\hat{S}_z)|2\ 1\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle$

4. Evaluate the following matrix elements useful for the matrix elements of $\hat{H}'_Z$, in which the states are written in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$, ($C$ is a constant to make the dimensions of $\hat{H}'_Z$ that of energy). **In order to receive credit you must show your work or explain your reasoning.**

   a. $C\langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|(\hat{L}_z + 2\hat{S}_z)|2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}\rangle$

   b. $C\langle 2\ 1\ \frac{1}{2}\ 1\ \frac{1}{2}|(\hat{L}_z + 2\hat{S}_z)|2\ 1\ \frac{1}{2}\ -1\ -\frac{1}{2}\rangle$

5. For each of the following operators in parts (a)-(j), circle **ALL** of the bases which make the operator diagonal in the $n = 2$ subspace of $\hat{H}^0$ and explain your reasoning. Assume that for all cases the principal quantum number $n = 2$.

   a. The unperturbed Hamiltonian $\hat{H}^0$

      i. Coupled representation

      ii. Uncoupled representation

      iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      v. Neither coupled nor uncoupled representation

   b. Explain your reasoning.

   c. The spin-orbit interaction term $\hat{H}'_{SO}$

      i. Coupled representation

      ii. Uncoupled representation

      iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      v. Neither coupled nor uncoupled representation

   d. Explain your reasoning.

e. The relativistic correction term $\hat{H}'_r$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

f. Explain your reasoning.

g. The fine structure term $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

h. Explain your reasoning.

i. The Zeeman term $\hat{H}'_Z$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

j. Explain your reasoning.

6. In parts (1)-(a) of the following questions, a perturbation $\hat{H}'$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For each of the following perturbations, circle **ALL** of the representations that form a "good" basis and explain your reasoning. Assume that for all cases the principal quantum number is fixed to a particular value, e.g., $n = 2$. ($C$ is a constant which makes the dimensions of $\hat{H}'$ that of energy in each case.)

   a. $\hat{H}' = C\delta(r)$

      i. Coupled representation

      ii. Uncoupled representation

      iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      v. Neither coupled nor uncoupled representation

   b. Explain your reasoning.

   c. $\hat{H}' = \hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$

      i. Coupled representation

      ii. Uncoupled representation

      iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

      v. Neither coupled nor uncoupled representation

   d. Explain your reasoning.

e. $\hat{H}' = \hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right) \frac{1}{m^2c^2r^3} \ \vec{L} \cdot \vec{S}$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

f. Explain your reasoning.

g. $\hat{H}' = \hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

h. Explain your reasoning.

i. $\hat{H}' = \hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

j. Explain your reasoning.

k. $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $E'_Z \gg E'_{fs}$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

l. Explain your reasoning.

m. $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $E'_{fs} \gg E'_Z$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

n. Explain your reasoning.

o. $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $E'_Z \approx E'_{fs}$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

p. Explain your reasoning.

7. In a Hydrogen atom, for $n = 2$, what is the degeneracy due only to the Coulomb interaction between the electron and nucleus (without considering the effect of any perturbation)? Explain your answer.

8. Consider the strong field Zeeman effect ($E'_Z \gg E'_{fs}$) in a hydrogen atom, for $n = 2$, (after accounting for the Zeeman term in the first step but not yet accounting for the fine structure term).
   a. What are the first order corrections to the unperturbed energy $E^0$ (after accounting for the Zeeman term in the first step but not yet accounting for the fine structure term)? You must show your reasoning to receive credit.

   b. For $n = 2$, write down each of the states that correspond to each first order correction to the unperturbed energy $E^0$ (after accounting for the Zeeman term in the first step but not yet accounting for the fine structure term). You must explain your answer to receive credit.

9. For $n = 2$, in the strong field Zeeman effect ($E'_Z \gg E'_{fs}$) in a hydrogen atom, after accounting for the Zeeman perturbation (but not accounting for the fine structure term), the unperturbed energies including the Zeeman term are $E^0_Z = E_2 + \mu_B B_{ext}(m_l + 2m_s)$. Explain why you agree or disagree with the following student. (The basis is chosen to be $|n\ l\ m_l\ m_s\rangle$.)

   **Student:** The off-diagonal matrix element $\langle 2\ 1\ 1\ -\frac{1}{2}|\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z|2\ 1\ -1\ \frac{1}{2}\rangle$ is NON-ZERO.

10. Consider the unperturbed Hamiltonian

$$\hat{H}^0 = V_0 \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 7 \end{bmatrix}.$$

Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis does NOT form a "good" basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use $\epsilon$ as a small parameter. **In addition to writing the $\hat{H}'$ matrix, you must explain your reasoning to receive full credit.**

11. Consider the unperturbed Hamiltonian

$$\hat{H}^0 = V_0 \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 7 \end{bmatrix}.$$

Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis forms a "good" basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use $\epsilon$ as a small parameter. **In addition to writing the $\hat{H}'$ matrix, you must explain your reasoning to receive full credit.**

12. Given

$$\hat{H} = \hat{H}^0 + \epsilon\hat{H}' = V_0 \begin{bmatrix} 2 & 0 & -2\epsilon \\ 0 & 2-2\epsilon & 0 \\ -2\epsilon & 0 & 3+3\epsilon \end{bmatrix} \qquad (\epsilon \ll 1),$$

determine the first order corrections to the energies. **In order to receive credit you must show your work or explain your reasoning.**

13. Given

$$\hat{H} = \hat{H}^0 + \epsilon \hat{H}' = V_0 \begin{bmatrix} 3 & \epsilon & \epsilon \\ \epsilon & 2 & \epsilon \\ \epsilon & \epsilon & 2 \end{bmatrix} \qquad (\epsilon \ll 1),$$

determine the first order corrections to the energies. **In order to receive credit you must show your work or explain your reasoning.**

## A.2 BASICS OF DEGENERATE PERTURBATION THEORY - FINITE DIMENSIONAL SPACES TUTORIAL

Basics of Degenerate Perturbation Theory - Finite Dimensional Spaces

## A.3 DEFINITION

For a given $\hat{H}^0$ and $\hat{H}'$, a **"good"** basis consists of a set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ (keeping $\hat{H}^0$ diagonal everywhere).

- Once you have a "good" basis for a given $\hat{H}^0$ and $\hat{H}'$, you can use the same expressions that you use in non-degenerate perturbation theory for the perturbative corrections to the energies and energy eigenstates.

## A.4 NOTES FOR THIS TUTORIAL ON DEGENERATE PERTURBATION THEORY:

* A Hermitian operator $\hat{Q}$ must satisfy the property $Q_{ij} = (Q_{ji})^*$. Here $^*$ denotes the complex conjugate.
* For the matrix representation of a Hermitian operator $\hat{Q}$ in a given basis, we will use "$=$" or "is equal to" instead of "$\doteq$" or "is represented by" as in the notation below

$$\hat{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \quad \text{is equivalent to} \quad \hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}.$$

* Since both $\hat{H}^0$ and $\hat{H}'$ correspond to physical observables, $\hat{H}^0$ and $\hat{H}'$ must be Hermitian. For the matrix representations of the unperturbed Hamiltonian $\hat{H}^0$ and perturbing

Hamiltonian $\hat{H}'$ in a given basis, we have

$$\hat{H}^0 = V_0 \begin{pmatrix} a & b & c \\ b^* & e & f \\ c^* & f^* & i \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} a' & b' & c' \\ b'^* & e' & f' \\ c'^* & f'^* & i' \end{pmatrix}.$$

* In this tutorial, "degeneracy" denotes degeneracy in the energy eigenvalue spectrum, i.e., the fact that more than one distinct energy eigenstate can have the same energy eigenvalue. For example, if

$$\hat{H}^0|\psi_a\rangle = E_1|\psi_a\rangle \qquad \text{and} \qquad \hat{H}^0|\psi_b\rangle = E_1|\psi_b\rangle,$$

  $|\psi_a\rangle$ and $|\psi_b\rangle$ are degenerate eigenstates for the Hamiltonian $\hat{H}^0$ since they correspond to the same energy $E_1$.

* Assume that the initially chosen basis states $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$ are always eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ whether or not they are "good" basis states for a given pair $\hat{H}^0$ and $\hat{H}'$.

* Assume that all basis states are orthonormal (normalized and orthogonal).

## A.5 OBJECTIVES

**Upon completion of this tutorial, you should be able to do the following:**

1. For a given $\hat{H}^0$ and $\hat{H}'$, describe why the expressions may fail for finding corrections to the energies and energy eigenstates from non-degenerate perturbation theory when there is degeneracy in the unperturbed energy if the basis states are not chosen correctly.
   a. For a given $\hat{H}^0$ and $\hat{H}'$, describe the problem that may occur when the expressions from non-degenerate perturbation theory are used if the basis states are not chosen carefully and how the problem can be addressed by choosing a "good" basis.
   b. Identify the degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$.
   c. Show that the off-diagonal matrix elements of $\hat{H}'$ must be zero in the degenerate subspace of $\hat{H}^0$ when "good" basis states are chosen.
2. For a given $\hat{H}^0$ and $\hat{H}'$, determine "good" states for finding corrections to the unperturbed energy.
   a. Show that in the subspace in which $\hat{H}^0$ does not have a degeneracy, the originally chosen basis states are "good" basis states since the eigenstates of $\hat{H}^0$ are unique in the subspace in which there is no degeneracy.
   b. Show that the basis states in the subspace in which $\hat{H}^0$ has degeneracy may or may not be "good" basis states for a given $\hat{H}'$.
      i. Show that if $\hat{H}'$ is already diagonal in the degenerate subspace of $\hat{H}^0$, the initially chosen energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ already are "good" states.
      ii. Show that if $\hat{H}'$ is NOT diagonal in the degenerate subspace of $\hat{H}^0$, the initially chosen energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ are NOT "good" states.
         A. Demonstrate that linear combinations of the eigenstates of $\hat{H}^0$ are still eigenstates of $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$ and we can make use of this fact to diagonalize both $\hat{H}^0$ and $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.
         B. Find "good" basis states by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

C. Show that in a "good" basis (in which $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$), $\hat{H}^0$ remains diagonal.

D. Explain why it is necessary to choose a basis that keeps the unperturbed Hamiltonian $\hat{H}^0$ diagonal (basis states are eigenstates of $\hat{H}^0$, i.e. we need to find perturbative corrections to the energies using a basis in which $\hat{H}^0$ is diagonal).

c. Calculate corrections to the unperturbed energies and energy eigenstates when $\hat{H}^0$ has degeneracy.

d. Describe why we must diagonalize $\hat{H}'$ only in the degenerate subspace of $\hat{H}^0$ (instead of diagonalizing the entire $\hat{H}'$ matrix).

i. Demonstrate that diagonalizing the entire $\hat{H}'$ matrix makes the $\hat{H}^0$ matrix non-diagonal if $\hat{H}^0$ and $\hat{H}'$ don't commute (we cannot find a complete set of simultaneous eigenstates of $\hat{H}^0$ and $\hat{H}'$ when they don't commute).

- Note that if two operators commute, in the basis consisting of a complete set of simultaneous eigenstates of both, each operator is diagonal (however, if there is degeneracy in the eigenvalue spectrum of one or both operators then all eigenstates of one operator may not be eigenstates of another and both operators may not be diagonal in that basis, but it is possible to find a complete set of simultaneous eigenstates of both).

## A.6 REVIEW OF NON-DEGENERATE PERTURBATION THEORY

In perturbation theory, for the case in which the unperturbed Hamiltonian $\hat{H}^0$ has NO degeneracy:

- the first order corrections to the energies are

$$E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle \tag{A.2}$$

- the first order corrections to the energy eigenstates are

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle \tag{A.3}$$

in which $\{|\psi_n^0\rangle\}$ is the set of energy eigenstates of the unperturbed Hamiltonian $\hat{H}^0$.

## A.7 DEGENERATE PERTURBATION THEORY

### A.7.1 Degeneracy in the Eigenvalue Spectrum of $\hat{H}^0$ Requires Finding a "GOOD" Basis to Determine Corrections to the Energies and Energy Eigenstates

If there is degeneracy in the eigenvalue spectrum of $\hat{H}^0$, are equations (A.2) and (A.3) still valid for a given perturbation $\hat{H}'$? If so, in which situations are they valid? Explain any constraints on the basis states.

Use the following two examples to help answer these questions.

### A.7.1.1 CASE 1: First Order Corrections to the Energy when $\hat{H}'$ IS DIAGONAL IN THE DEGENERATE SUBSPACE of $\hat{H}^0$

**EXAMPLE 1:** Consider the following example, in which the Hilbert space is three dimensional and $\epsilon$ is a small parameter ($\epsilon \ll 1$). Answer questions 1-6.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} \epsilon & 2\epsilon & 0 \\ 2\epsilon & \epsilon & 0 \\ 0 & 0 & 3\epsilon \end{pmatrix} \tag{A.4}$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.5}$$

1. The basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ are eigenstates of
   (A) $\hat{H}^0$ only
   (B) $\hat{H}'$ only
   (C) Both $\hat{H}^0$ and $\hat{H}'$
   (C) Neither $\hat{H}^0$ nor $\hat{H}'$
   Explain your reasoning.

2. Does $\hat{H}^0$ have degeneracy? Why or why not?

3. Choose one of the following options to fill in the blank. In the degenerate subspace of $\hat{H}^0$, the matrix representation of $\hat{H}^0$ is _____ and the matrix representation of $\hat{H}'$ is _____, respectively.

(A)
$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \qquad V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$$

(B)
$$V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \qquad V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$$

(C)
$$V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}, \qquad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

(D)
$$V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}, \qquad V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

4. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a "good" basis? Explain.

Consider the following conversation regarding whether the initially chosen basis is a "good" basis in EXAMPLE 1.

**Student 1:** In EXAMPLE 1, in the degenerate subspace of $\hat{H}^0$, the perturbing Hamiltonian $\hat{H}'$ is $V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$. So we can use equations (A.2) and (A.3) from non-degenerate perturbation theory to find the corrections to the energies and energy eigenstates.

**Student 2:** How can we use equation (A.3) when the unperturbed energies are degenerate with $E_2^0 = E_3^0 = 2V_0$? In equation (A.3), the first order corrections to the energy eigenstates $|\psi_2^0\rangle$ and $|\psi_3^0\rangle$ is undefined as the denominator is zero!

**Student 3:** Since $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ in equation (A.4), we can use equations (A.2) and (A.3). Since $\langle\psi_2^0|\hat{H}'|\psi_3^0\rangle = 0$ and $\langle\psi_3^0|\hat{H}'|\psi_2^0\rangle = 0$, the undefined terms that "blow up" do not appear in equation (A.3).[1]

Explain why you agree or disagree with each student.

5. The first order corrections to the energies are
   (A) $E_1^1 = \epsilon V_0, E_2^1 = \epsilon V_0$, and $E_3^1 = 3\epsilon V_0$.
   (B) $E_1^1 = \epsilon V_0, E_2^1 = 2\epsilon V_0$, and $E_3^1 = 0$.
   (C) $E_1^1 = 2\epsilon V_0, E_2^1 = \epsilon V_0$, and $E_3^1 = 3\epsilon$.
   (D) $E_1^1 = 0, E_2^1 = 0$, and $E_3^1 = 0$.
   (E) None of the above

6. The first order corrections to the energy eigenstates are
   (A) $|\psi_1^1\rangle = 2\epsilon V_0|\psi_2^0\rangle + 0|\psi_3^0\rangle, |\psi_2^1\rangle = 2\epsilon V_0|\psi_1^0\rangle + \epsilon V_0|\psi_3^0\rangle$, and $|\psi_3^1\rangle = 0|\psi_1^0\rangle + \epsilon V_0|\psi_2^0\rangle$.
   (B) $|\psi_1^1\rangle = -2\epsilon|\psi_2^0\rangle + 0|\psi_3^0\rangle, |\psi_2^1\rangle = 2\epsilon|\psi_1^0\rangle + 0|\psi_3^0\rangle$ and $|\psi_3^1\rangle = 0$.
   (C) $|\psi_1^1\rangle = 0$, $|\psi_2^1\rangle = 0$, and $|\psi_3^1\rangle = \epsilon V_0|\psi_1^0\rangle$.
   (D) None of the above.

[1] Please note that once we have a good basis, we do not have 0/0 terms present in Eq. A.3.

*** Check your answers to questions 1-6 in EXAMPLE 1. ***

1. A ($|\psi_3^0\rangle$ is an eigenstate of both $\hat{H}^0$ and $\hat{H}'$, however $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are only eigenstates of $\hat{H}^0$.)
2. Yes. $\hat{H}^0|\psi_2^0\rangle = 2V_0|\psi_2^0\rangle$ and $\hat{H}^0|\psi_3^0\rangle = 2V_0|\psi_3^0\rangle$.
3. B
4. Yes.
5. A
6. B

If your answers to questions 1-6 do not match with the checkpoint for EXAMPLE 1, go back and reconcile any differences.

### A.7.2 Checkpoint

- In order to find the first order corrections to the energies and energy eigenstates using equations (A.2) and (A.3), **the basis set $|\{\psi_n^0\rangle\}$ in equations (A.2) and (A.3) must be "good" states** ($\hat{H}^0$ is diagonal everywhere since the basis states are eigenstaes of $\hat{H}^0$ and $\hat{H}'$ must be diagonal in the degenerate subspace of $\hat{H}^0$ in that basis).
- If $\hat{H}'$ **is already diagonal in the degenerate subspace of** $\hat{H}^0$:
  - The initially chosen basis states make up a "good" basis.
  - The expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ CAN be used to find corrections to the energies since $\{|\psi_n^0\rangle\}$ are "good" states.
  - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$ CAN be used to find the first order corrections $|\psi_n^1\rangle$ to the energy eigenstates $|\psi_n^0\rangle$ since $\{|\psi_n^0\rangle\}$ are "good" states and the divergent terms (that "blow up") do not appear in equation (A.3).

#### A.7.2.1 CASE 2: Corrections to the Energies and Energy Eigenstates when $\hat{H}'$ is not Diagonal in the Degenerate Subspace of $\hat{H}^0$

**EXAMPLE 2:** Consider a second example, in which $\epsilon$ is a small parameter ($\epsilon \ll 1$), and answer questions 7-10:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & -4\epsilon \\ \epsilon & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix} \tag{A.6}$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.7}$$

7. The basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ are eigenstates of
   (A) $\hat{H}^0$ only
   (B) $\hat{H}'$ only
   (C) Both $\hat{H}^0$ and $\hat{H}'$
   (C) Neither $\hat{H}^0$ nor $\hat{H}'$
   Explain your reasoning.

8. Does $\hat{H}^0$ have degeneracy? Why or why not?

9. Choose one of the following options to fill in the blank. In the degenerate subspace of $\hat{H}^0$, the matrix representation of $\hat{H}^0$ is _____ and the matrix representation of $\hat{H}'$ is _____, respectively.

(A)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}. \qquad V_0 \begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}$$

(B)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$$

(C)

$$V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}, \qquad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(D)

$$V_0 \begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}, \qquad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

10. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a "good' basis? Explain.

Consider the following conversation regarding whether the initially chosen basis is or is not a "good" basis in EXAMPLE 2.

**Student 1:** In EXAMPLE 2, we can use equations (A.2) and (A.3) obtained from non-degenerate perturbation theory.

**Student 2:** We cannot use equation (A.3) when the unperturbed states are degenerate with $E_1^0 = E_2^0 = V_0$. In the degenerate subspace of $\hat{H}^0$, the perturbing Hamiltonian $\hat{H}'$ is $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$. The first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ "blow up" because the denominators are zero! However, we can use equation (A.2) to calculate the corrections to the energies since nothing in that equations "blows up."

**Student 3:** If $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$, we can neither use equation (A.2) nor (A.3) in the chosen basis $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$. The initially chosen basis is not a "good" basis. We need to find a "good" basis in order to use equations (A.2) and (A.3).

**Student 4:** Student 3 is right. The first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ "blow up", we cannot use these basis states to find even the first order corrections to the energies using equation (A.2).

Explain why you agree or disagree with each student.

*** Check your answers to questions 7-10 in EXAMPLE 2. ***

7. A
8. Yes. $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$.
9. B
10. No.

If your answers to questions 7-10 do not match with the checkpoint for EXAMPLE 2, go back and reconcile any differences.

**EXAMPLE 2 Revisited**

For the following four conversations, consider Example 2 again in which equations (A.2) and (A.3) could not be used with the initial basis states $|\psi_1^0\rangle, |\psi_2^0\rangle$, and $|\psi_3^0\rangle$. Recall that in EXAMPLE 2, the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ was given by:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & -4\epsilon \\ \epsilon & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix} \tag{A.8}$$

and the basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, for which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.9}$$

Consider the following conversation regarding whether the basis states are "good" in EXAMPLE 2.

**Student 1:** In this case, we can calculate the first order corrections to the energies as $E_1^1 = \langle\psi_1^0|\hat{H}'|\psi_1^0\rangle = 0$ and $E_2^1 = \langle\psi_2^0|\hat{H}'|\psi_2^0\rangle = 2\epsilon V_0$.

**Student 2:** I disagree. $\hat{H}^0$ has a two-fold degeneracy, since $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$. We cannot use the basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ to calculate even the first order corrections to the energies because $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$. $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not "good" basis states.

**Student 1:** I see. If $\hat{H}^0$ has a degenerate eigenvalue spectrum, the expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ requires that the chosen basis states are "good" basis states, which is not the case for the initially chosen eigenstates $\{|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle\}$ of $\hat{H}^0$.

Explain why you agree or disagree with the students.

Consider the following conversation regarding finding the corrections to energy eigenstates using "good" basis states in EXAMPLE 2.

**Student 1:** In EXAMPLE 2, $\hat{H}^0$ has a two-fold degeneracy since $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$. We cannot calculate the first order corrections to the energy eigenstates using $|\psi_1^0\rangle$, $|\psi_2^0\rangle$ or $|\psi_3^0\rangle$ in equation (A.3).

**Student 2:** I agree that we cannot calculate first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. The first order corrections to the energy eigenstates in equation (A.3) "blow up", i.e.,

$$|\psi_1^1\rangle = \frac{\langle\psi_2^0|\hat{H}'|\psi_1^0\rangle}{(E_1^0 - E_2^0)}|\psi_2^0\rangle + \frac{\langle\psi_3^0|\hat{H}'|\psi_1^0\rangle}{(E_1^0 - E_3^0)}|\psi_3^0\rangle = \frac{\epsilon V_0}{0}|\psi_2^0\rangle + \frac{-4\epsilon V_0}{-V_0}|\psi_3^0\rangle$$

and

$$|\psi_2^1\rangle = \frac{\langle\psi_1^0|\hat{H}'|\psi_2^0\rangle}{(E_2^0 - E_1^0)}|\psi_1^0\rangle + \frac{\langle\psi_3^0|\hat{H}'|\psi_2^0\rangle}{(E_2^0 - E_3^0)}|\psi_3^0\rangle = \frac{\epsilon V_0}{0}|\psi_1^0\rangle + \frac{0}{-V_0}|\psi_3^0\rangle.$$

**Student 3:** I agree with both Student 1 and Student 2. But we can calculate the first order corrections to the energy eigenstates if we first select "good" basis states. $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not "good" states since the $\hat{H}'$ matrix is not diagonal in the degenerate subspace of $\hat{H}^0$. So $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ cannot be used to find the first order corrections to the energy eigenstates using equation (A.3). We need to first choose a different basis that is "good" so terms that "blow up" in the corrections $|\psi_1^1\rangle$ and $|\psi_2^1\rangle$ are not present.

Explain why you agree or disagree with each student.

Summarize in one to three sentences what you learned from the previous two conversations.

Consider the following conversation regarding whether one can trust the corrections to the non-degenerate eigenvalues of $\hat{H}^0$ if some of the basis states are not "good" basis states in EXAMPLE 2.

**Student 1:** What about the first order correction to $E_3$ in EXAMPLE 2? Can we trust $E_3^1 = \langle\psi_3^0|\hat{H}'|\psi_3^0\rangle$ even if $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$?

**Student 2:** No, we cannot trust it because $\hat{H}^0$ has degeneracy in EXAMPLE 2. We must find a "good" basis first before finding any corrections to any of the energies.

**Student 3:** Actually, in EXAMPLE 2 we can trust $E_3^1 = \langle\psi_3^0|\hat{H}'|\psi_3^0\rangle = 2\epsilon V_0$ to yield the first order correction to energy $E_3 = 2V_0$. Since $|\psi_3^0\rangle$ corresponds to the non-degenerate subspace of $\hat{H}^0$, it is unique. $|\psi_3^0\rangle$ must already be a "good" state.

Do you agree with Student 2 or Student 3? Explain.

Consider the following conversation regarding first order corrections to the energy eigenstates in the non-degenerate subspace.

**Student 1:** For EXAMPLE 2, can we use the expression $|\psi_3^1\rangle = \frac{\langle\psi_1^0|\hat{H}'|\psi_3^0\rangle}{(E_3^0 - E_1^0)}|\psi_1^0\rangle + \frac{\langle\psi_2^0|\hat{H}'|\psi_3^0\rangle}{(E_3^0 - E_2^0)}|\psi_2^0\rangle = \frac{-4\epsilon V_0}{V_0}|\psi_1^0\rangle + \frac{0}{V_0}|\psi_2^0\rangle$ from non-degenerate perturbation theory to find the correction $|\psi_3^1\rangle$?

**Student 2:** Yes, that is correct. However, we can also determine the first order correction $|\psi_3^1\rangle$ by determining a "good" basis and using the "good" basis states in Eq. A.3 to find the first order correction to the energy eigenstate.**Student 3:** I agree with Student 2. In EXAMPLE 2, "good" basis states in the degenerate subspace of $\hat{H}^0$ will be the non-degenerate state $|\psi_3^0\rangle$ and two linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. So a "good" basis will be

$$|\phi_1^0\rangle = \alpha_1|\psi_1^0\rangle + \alpha_2|\psi_2^0\rangle, \quad |\phi_2^0\rangle = \beta_1|\psi_1^0\rangle + \beta_2|\psi_2^0\rangle, \quad \text{and} \quad |\phi_3^0\rangle = |\psi_3^0\rangle$$

in which $\alpha_1, \alpha_2, \beta_1$, and $\beta_2$ are the coefficients for obtaining a "good" orthonormal basis states which diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. $\{|\phi_n^0\rangle\}$ are still eigenstates of $\hat{H}^0$.

**Student 4:** I agree with Student 2 and Student 3. To find first order corrections to $|\phi_3^0\rangle = |\psi_3^0\rangle$, we must use a "good" basis. $|\psi_3^0\rangle$ is a "good" basis state. However, $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not "good" basis states. We must find "good" basis states $|\phi_1^0\rangle$ and $|\phi_2^0\rangle$ by diagonalizing the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ to calculate the first order correction to $|\psi_3^0\rangle$. Once we have the "good" basis, we use equation (A.3) to find the first order correction to $|\psi_3^0\rangle$:

$$|\psi_3^1\rangle = \frac{\langle\phi_1^0|\hat{H}'|\phi_3^0\rangle}{(E_3^0 - E_2^0)}|\phi_1^0\rangle + \frac{\langle\phi_2^0|\hat{H}'|\phi_3^0\rangle}{(E_3^0 - E_1^0)}|\phi_2^0\rangle.$$

Explain why you agree or disagree with Student 2, Student 3, and Student 4.

Summarize in one to three sentences what you learned from the previous two conversations.

Summarize why care should be exercised in using perturbation theory if the unperturbed Hamiltonian $\hat{H}^0$ possesses degeneracy in the eigenvalue spectrum.

Describe the procedure to deal with the difficulty that arises when we can't use the initially chosen basis states to find perturbative corrections. What must we ensure about $\hat{H}^0$ and $\hat{H}'$ to find the corrections to the energies (including first order corrections to the energies for the cases in which the given basis is not good even though the first order correction to the energies do not "blow up")?

### A.7.3 Checkpoint

- If the first-order corrections to the energy eigenstates "blow up," we cannot even trust the first order corrections to the energies because the basis states are not "good."

- If $\hat{H}'$ **is NOT diagonal in a degenerate subspace of** $\hat{H}^0$:
  - The initially chosen basis states do not make up a "good" basis (even though they are eigenstates of $\hat{H}^0$).

  - The expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ **CANNOT** be used to find the corrections to energies if $|\psi_n^0\rangle$ is **NOT** a "good" basis state.

  - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$ **CANNOT** be used in the degenerate subspace to find corrections to energy eigenstates if $\{|\psi_n^0\rangle\}$ are **NOT** "good" basis states.

**A.7.3.1 A "good" basis depends on both $\hat{H}^0$ and $\hat{H}'$.** Consider the following conversation regarding whether choosing a "good" basis requires consideration of both $\hat{H}^0$ and $\hat{H}'$.

**Student 1:** In degenerate perturbation theory, for a given $\hat{H}'$, "good" basis states must be the eigenstates of the unperturbed Hamiltonian, $\hat{H}^0$.

**Student 2:** I disagree. A "good" basis should diagonalize the $\hat{H}'$ matrix but $\hat{H}^0$ need not be diagonal in that basis. The diagonal elements of the $\hat{H}'$ matrix in a "good" basis give us the first order corrections to the energies.

**Student 3:** Actually, we need to consider both $\hat{H}^0$ and $\hat{H}'$ when determining a "good" basis. A "good" basis will diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ while simultaneously keeping $\hat{H}^0$ diagonal. The entire $\hat{H}^0$ matrix must be diagonal in a "good" basis since the basis states must be eigenstates of $\hat{H}^0$.

Explain why you agree or disagree with each student.

In the following example, note that the unperturbed Hamiltonian $\hat{H}^0$ is the same as the $\hat{H}^0$ given in EXAMPLE 2. However, the perturbing Hamiltonian $\hat{H}'$ is not the same as the $\hat{H}'$ given in EXAMPLE 2.

**EXAMPLE 3:** Consider the following example in a three dimensional Hilbert space, in which $\epsilon$ is a small parameter ($\epsilon \ll 1$):

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} \epsilon & 0 & 2\epsilon \\ 0 & -3\epsilon & \epsilon \\ 2\epsilon & \epsilon & -3\epsilon \end{pmatrix} \tag{A.10}$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.11}$$

Now consider the following conversation about EXAMPLE 3 focusing on the Degenerate Subspace of $\hat{H}^0$.

**Student 1:** In EXAMPLE 3, the $\hat{H}^0$ matrix is the same as in EXAMPLE 2, so we will not be able to use equation (A.2) with the initial basis states $\{|\psi_n^0\rangle\}$ that are given to find the first order corrections to the energies. We also cannot use equation (A.3) to find the first order corrections to the energy eigenstates.

**Student 2:** I disagree. Actually, you must consider both $\hat{H}^0$ and $\hat{H}'$ before deciding whether the basis is good and whether we can use equations (A.2) and (A.3) with that basis. Since $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ in EXAMPLE 3, equations (A.2) and (A.3) can be used with the given basis to find the first order corrections to the energies and energy eigenstates, respectively. This is just like EXAMPLE 1!

Do you agree with Student 1 or Student 2? Why?

11. What are the first order corrections to the unperturbed energies in EXAMPLE 3? (HINT: Refer to EXAMPLE 1.)

*** Check your results to question 11 in EXAMPLE 3: ***

11. $E_1^1 = \epsilon V_0$, $E_2^1 = -3\epsilon V_0$, and $E_3^1 = -3\epsilon V_0$

If your first order corrections to the energies do not match the checkpoint for EXAMPLE 3, go back and reconcile any differences you may have.

### A.7.4 Checkpoint

- When determining a "good" basis, we need information about **both** $\hat{H}^0$ **and** $\hat{H}'$.
  - A "good" basis is one that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ while keeping $\hat{H}^0$ diagonal.

SUMMARY: To Find Corrections to the Energies and Energy Eigenstates You Must Choose a "Good" Basis

- If the first-order corrections to the eigenstates "blow up," we cannot even trust the first order corrections to the energies because the basis states may not be "good."

- Choosing a "good" basis requires information about **both** $\hat{H}^0$ **and** $\hat{H}'$.

- In order to find the first order corrections to the energies and energy eigenstates using equations (A.2) and (A.3), **the basis set** $|\{\psi_n^0\rangle\}$ **used in equations (A.2) and (A.3) must be "good" states** (in such a basis, $\hat{H}'$ must be diagonal in a degenerate subspace of $\hat{H}^0$ and $\hat{H}^0$ must be entirely diagonal).

CASE 1: $\hat{H}'$ IS DIAGONAL IN THE DEGENERATE SUBSPACE OF $\hat{H}^0$ IN THE INITIAL BASIS.

- If $\hat{H}'$ **is already diagonal in the degenerate subspace of** $\hat{H}^0$:
  - The initial basis states make up a "good" basis (note that since we choose basis states to be eigenstates of $\hat{H}^0$, $\hat{H}^0$ is diagonal in the basis everywhere).

  - The expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ **CAN** be used to find corrections to energies since all $\{|\psi_n^0\rangle\}$ are "good" states.

  - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$ **CAN** be used to find the first order corrections to the energy eigenstates $|\psi_n^0\rangle$ as all $\{|\psi_n^0\rangle\}$ are "good" states.

CASE 2: $\hat{H}'$ IS NOT DIAGONAL IN THE DEGENERATE SUBSPACE OF $\hat{H}^0$ IN THE INITIAL BASIS.

- If $\hat{H}'$ **is NOT diagonal in the degenerate subspace of** $\hat{H}^0$:
  - The initially chosen basis states do not make up a "good" basis (even though they are eigenstates of $\hat{H}^0$).
  - The expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ **CANNOT** be used to find corrections to energies associated with the degenerate states since $\{|\psi_n^0\rangle\}$ does **NOT** form a complete set of "good" basis states.
  - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$ **CANNOT** be used to find corrections to energy eigenstates associated with the degenerate states since $\{|\psi_n^0\rangle\}$ is **NOT** a "good" set of basis states.
  - We must first choose a "good" basis!
- As you will demonstrate shortly, in the degenerate subspace of $\hat{H}^0$, "good" basis states will be made up of linear combinations of the initially chosen eigenstates of $\hat{H}^0$ that diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

### A.7.5 Ensuring a "good" basis and determining corrections to the energies and energy eigenstates.

#### A.7.5.1 CASE 1: First Order Corrections to the Energies when $\hat{H}'$ IS DIAGONAL IN THE DEGENERATE SUBSPACE of $\hat{H}^0$ EXAMPLE 4:

Answer the following questions for this example:

$$\hat{H}^0 = V_0 \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 0 & 2\epsilon \\ 0 & -\epsilon & 3\epsilon \\ 2\epsilon & 3\epsilon & 0 \end{pmatrix} \quad (\epsilon \ll 1) \tag{A.12}$$

and the basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.13}$$

12. Does $\hat{H}^0$ have degeneracy? If so, circle the part of $\hat{H}^0$ and $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

13. Use your answer to the previous part to explain whether the basis states chosen in equation (A.13), which are used to write $\hat{H}^0$ and $\hat{H}'$ in equation (A.12), are "good" basis states or not.

14. If the given basis is not a "good" basis, find a "good" basis.

15. Determine the first order corrections to the unperturbed energies.

16. Find the first order corrections to the unperturbed energy eigenstates.

Consider the following conversation regarding $\hat{H}'$ already being diagonal in the degenerate subspace of $\hat{H}^0$ in EXAMPLE 4.

**Student 1:** If we are given an $\hat{H}'$ matrix that is already diagonal in the degenerate subspace of $\hat{H}^0$ as in equation (A.12), the basis is already "good." We can simply read off the matrix elements of $\hat{H}'$ along the diagonal in the degenerate subspace of $\hat{H}^0$ to obtain the first order corrections to the degenerate energies.

**Student 2:** I disagree. You must still diagonalize $\hat{H}'$ in equation (A.12) in the degenerate subspace of $\hat{H}^0$ to find the first order corrections to the energies.

**Student 3:** It does not make sense to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ if $\hat{H}'$ is already diagonal in that subspace. You would be doing unnecessary work. Since $\hat{H}'$ is already diagonal in that subspace, if you choose to diagonalize $\hat{H}'$, you would simply obtain the same matrix back with the same eigenvalues as long as you didn't make any mistakes along the way.

**Student 1:** I agree with Student 3. And when $\hat{H}'$ is also diagonal in the degenerate subspace of $\hat{H}^0$ as in equation (A.12), "good" basis states are the initially chosen energy eigenstates of $\hat{H}^0$, i.e., the basis states used to write $\hat{H}^0$ and $\hat{H}'$ in equation (A.12)).

Explain why you agree or disagree with each student.

*** Check your answers to questions 12-16 pertaining to EXAMPLE 4.***

12. $\hat{H}^0$ has a two-fold degeneracy. In the degenerate subspace of $\hat{H}^0$, $\hat{H}^0$ is $V_0 \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$ and the perturbation $\hat{H}'$ is $V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & -\epsilon \end{pmatrix}$

13. Since $\hat{H}'$ is already diagonal in the degenerate subspace of $\hat{H}^0$, the set of initially chosen energy eigenstates of $\hat{H}^0$ in equation (A.12) form a "good" basis.

14 "Good" basis states are the initially chosen eigenstates of $\hat{H}^0$, $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

15. The first order corrections to the energies are $E_1^1 = -\epsilon V_0$, $E_2^1 = -\epsilon V_0$, and $E_3^1 = 0$.

16 The first order corrections to the energy eigenstates are $|\psi_1^1\rangle = \frac{2}{3}\epsilon|\psi_3^0\rangle$, $|\psi_2^1\rangle = \epsilon|\psi_3^0\rangle$, and $|\psi_3^1\rangle = -\frac{2}{3}\epsilon|\psi_1^0\rangle - \epsilon|\psi_2^0\rangle$.

If your "good" basis states and first order corrections to the energies and energy eigenstates for EXAMPLE 4 do not match with the checkpoint answers, go back and reconcile any difference you may have.

For the case in which $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ and basis states are eigenstates of $\hat{H}^0$, summarize in one to two sentences why we can simply use equations (A.2) and (A.3) to find the first order corrections to the energies and energy eigenstates.

Consider the following conversation regarding whether the first order corrections to the energies will remove all the degeneracy in the eigenvalue spectrum of $\hat{H}^0$.

**Student 1:** If $\hat{H}^0$ has a degenerate energy spectrum, the perturbation $\hat{H}'$ will always remove the degeneracy when we find the first order corrections to the energies. The energy levels will split into distinct energy levels.

**Student 2:** This may be true for some $\hat{H}^0$ and $\hat{H}'$ but not necessarily true for all cases. The symmetry of the unperturbed Hamiltonian $\hat{H}^0$ and the perturbing Hamiltonian $\hat{H}'$ will dictate whether all the degeneracies will be removed in first order.

**Student 3:** I agree with Student 2. Consider EXAMPLE 4 in which the perturbing Hamiltonian was already diagonal in the degenerate subspace of $\hat{H}^0$. We found the energies including the first order corrections to be $E_1 = 4V_0 - \epsilon V_0$ and $E_2 = 4V_0 - \epsilon V_0$. Sometimes, even a higher order correction to the energy may not lift a degeneracy.

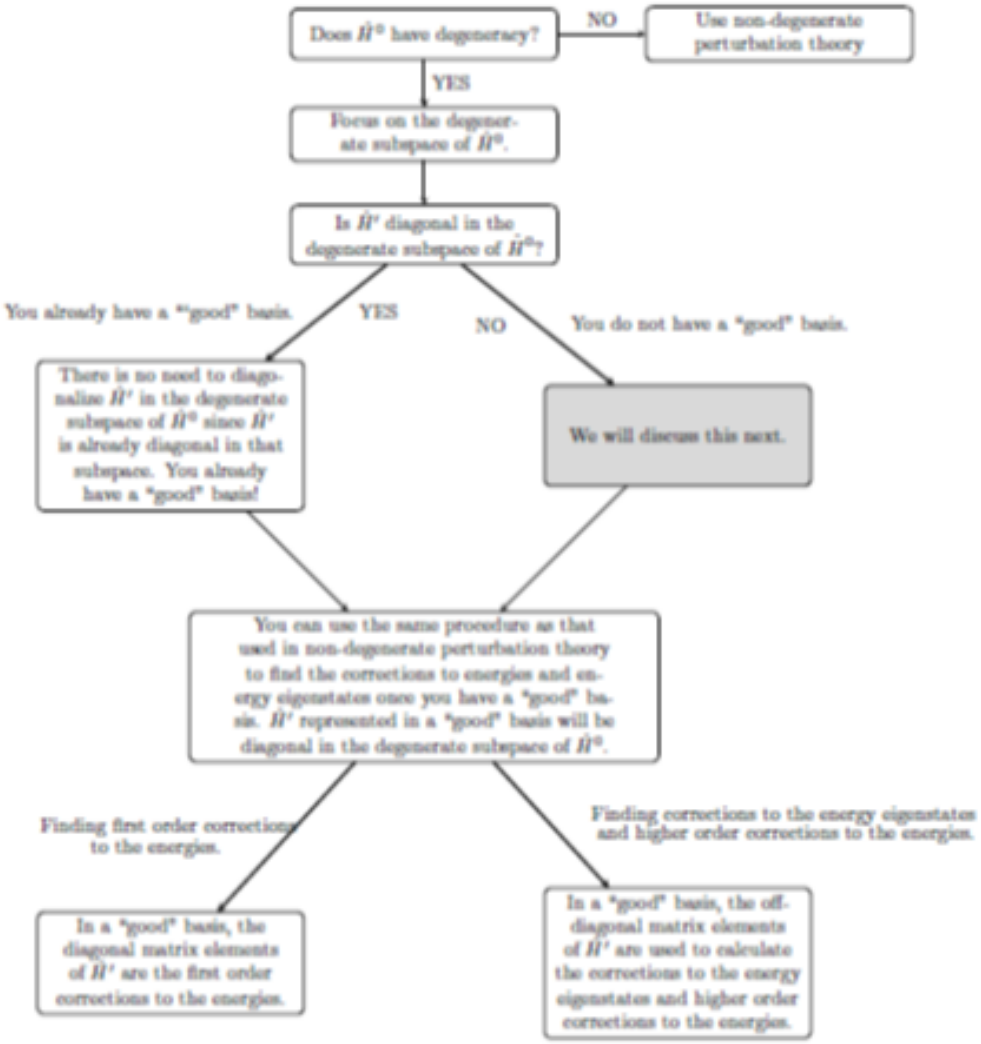
Explain why you agree or disagree with each student.

### A.7.6 Checkpoint - Finding a "good" basis for Case 1

- If $\hat{H}'$ **is already diagonal in a degenerate subspace of** $\hat{H}^0$ **(and basis states are eigenstates of** $\hat{H}^0$**)**:
  - The initially chosen basis states make up a "good" basis.
  - The expression $E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$ **CAN** be used to find corrections to the energies since $\{|\psi_n^0\rangle\}$ are "good" basis states.
    - These first order corrections to the energies correspond to the diagonal matrix elements of $\hat{H}'$ in a "good" basis.
  - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$ **CAN** be used to find the first order corrections to the energy eigenstates $\{|\psi_n^0\rangle\}$ as $\{|\psi_n^0\rangle\}$ are "good" basis states.
    - For a given $\hat{H}^0$ and $\hat{H}'$, these first order corrections to the energy eigenstates can be determined making use of equation (A.3) using the off-diagonal matrix elements of $\hat{H}'$ in a "good" basis.
- Calculating the first order corrections to the energies may not be enough to lift all the degeneracy in many cases.

Review the flowchart for the steps to determine the corrections to the energies and energy eigenstates ˇ**when $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$.**

# Finding First Order Corrections to the Energies and Energy Eigenstates



### A.7.6.1 CASE 2: Corrections to the Energies and Energy Eigenstates when $\hat{H}'$ is not Diagonal in the Degenerate Subspace of $\hat{H}^0$

- If $\hat{H}'$ is not diagonal in the degenerate subspace of $\hat{H}^0$ then the initially chosen set of eigenstates of $\hat{H}^0$ does **NOT** form a complete set of "good" basis states.
- In this case, we must find a "good" basis first. To find "good" basis states, we must choose a basis that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ and simultaneously keeps $\hat{H}^0$ diagonal everywhere.
- Since the "good" basis states are still eigenstates of $\hat{H}^0$, $\hat{H}^0$ will remain diagonal in a "good" basis.

Consider the following conversation regarding diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ when $\hat{H}^0$ and $\hat{H}'$ don't commute.

**Student 1:** I thought we cannot simultaneously diagonalize $\hat{H}^0$ and $\hat{H}'$ unless they commute.

**Student 2:** Yes that's true! The entire $\hat{H}^0$ and $\hat{H}'$ matrices cannot be diagonalized simultaneously unless they commute. But in the degenerate subspace of $\hat{H}^0$, we can always diagonalize both $\hat{H}^0$ and $\hat{H}'$ simultaneously.

Do you agree with Student 2? Explain your reasoning.

17. Can we find a linear combination of the eigenstates of $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in that subspace? If so, will a linear combination of eigenstates of $\hat{H}^0$ in the degenerate subspace remain an eigenstate of $\hat{H}^0$? Explain your reasoning.

Use the following example to help check your answers to question 17.

**EXAMPLE 5:** Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ in which

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \qquad (\epsilon \ll 1) \tag{A.14}$$

and the normalized eigenstates of $\hat{H}^0$ given by $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, are

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.15}$$

18. Fill in the blanks using equations (A.14) and (A.15).

$$\hat{H}^0|\psi_1^0\rangle = \_\_\_\_\_$$

$$\hat{H}^0|\psi_2^0\rangle = \_\_\_\_\_$$

$$\hat{H}^0|\psi_3^0\rangle = \_\_\_\_\_$$

$$\hat{H}^0(a\ |\psi_1^0\rangle + \ b\ |\psi_2^0\rangle) = \_\_\_\_\_$$

$$\hat{H}^0(e\ |\psi_1^0\rangle + \ f\ |\psi_3^0\rangle) = \_\_\_\_\_$$

19. Is $a\ |\psi_1^0\rangle + \ b\ |\psi_2^0\rangle$ a normalized eigenstate of $\hat{H}^0$, where $a$ and $b$ are arbitrary complex numbers that satisfy $|a|^2 + |b|^2 = 1$? Explain.

20. Can $\hat{H}^0$ still be diagonal if $a\ |\psi_1^0\rangle + b\ |\psi_2^0\rangle$ and $c\ |\psi_1^0\rangle + d\ |\psi_2^0\rangle$ are used as new basis states instead of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$? Suppose that $a, b, c$ and $d$ are chosen such that $a\ |\psi_1^0\rangle + b\ |\psi_2^0\rangle$ and $c\ |\psi_1^0\rangle + d\ |\psi_2^0\rangle$ are orthonormal and $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$, is $\hat{H}^0$ diagonal if these new basis states are chosen? Explain.

21. Is $e\,|\psi_1^0\rangle + f\,|\psi_3^0\rangle$ a normalized eigenstate of $\hat{H}^0$, where $e$ and $f$ are arbitrary complex numbers that satisfy $|e|^2 + |f|^2 = 1$?

a. Will the $\hat{H}^0$ matrix remain diagonal if $e\,|\psi_1^0\rangle + f\,|\psi_3^0\rangle$ is chosen as one of the basis states to write the $\hat{H}^0$ matrix? Explain your answer.

b. Based upon whether your answer to the preceding question is yes or no, can $e\,|\psi_1^0\rangle + f\,|\psi_3^0\rangle$ be used as a basis state to calculate corrections to the energies and energy eigenstates in perturbation theory? Explain.

Consider the following conversation regarding whether a linear combination of energy eigenstates of $\hat{H}^0$ that includes non-degenerate eigenstates of $\hat{H}^0$ (in EXAMPLE 5 in equation (A.14) is an energy eigenstate of $\hat{H}^0$.

**Student 1:** I don't see why we cannot have $e\ |\psi_1^0\rangle + f\ |\psi_3^0\rangle$ as a basis state for using perturbation theory.

**Student 2:** I disagree. $\hat{H}^0$ is not diagonal if $e\ |\psi_1^0\rangle + f\ |\psi_3^0\rangle$ is one of the basis states because the $\hat{H}^0$ matrix can only be diagonal if all basis states are eigenstates of $\hat{H}^0$. As we showed in questions 18 and 21, since $\hat{H}^0$ acting on $e\ |\psi_1^0\rangle + f\ |\psi_3^0\rangle$ does not return a number times the same state $e\ |\psi_1^0\rangle + f\ |\psi_3^0\rangle$, this state is not an eigenstate of $\hat{H}^0$.

Explain why you agree with Student 1 or Student 2.

Consider the following conversation regarding choosing orthonormal linear combinations of eigenstates of $\hat{H}^0$ that diagonalize the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ as basis states for EXAMPLE 5.

**Student 1:** We showed in question e that any linear combination of eigenstates of $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$, such as $a\ |\psi_1^0\rangle + b\ |\psi_2^0\rangle$ and $c\ |\psi_1^0\rangle + d\ |\psi_2^0\rangle$, remains an eigenstate of $\hat{H}^0$. Can we choose any two linear combinations of the eigenstates of $\hat{H}^0$, $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$, to form two of the "good" basis states?

**Student 2:** As long as the basis states are orthonormal, they form a "good" basis. Any two linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ whose inner product is zero forms a pair of "good" orthogonal basis states.

**Student 3:** I disagree with Student 2. There are many possible linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ that are orthogonal that will not form "good" basis states. The linear combination of the initial eigenstates must diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ provides the only pair, neglecting overall phase factors, of orthonormal linear combinations that form a "good" basis set.

Explain why you agree with Student 2 or Student 3.

*** Check your answers to questions 18-21 in EXAMPLE 5. ***

18.

$$\begin{aligned}
\hat{H}^0|\psi_1^0\rangle &= V_0|\psi_1^0\rangle \\
\hat{H}^0|\psi_2^0\rangle &= V_0|\psi_2^0\rangle \\
\hat{H}^0|\psi_3^0\rangle &= 2V_0|\psi_3^0\rangle \\
\hat{H}^0(a|\psi_1^0\rangle + b|\psi_2^0\rangle) &= V_0(a|\psi_1^0\rangle + b|\psi_2^0\rangle) \\
\hat{H}^0(e|\psi_1^0\rangle + f|\psi_3^0\rangle) &= V_0(e|\psi_1^0\rangle + 2f|\psi_3^0\rangle)
\end{aligned}$$

19. Yes. $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ is an eigenstate of $\hat{H}^0$.

e. Yes. $\hat{H}^0$ will still be diagonal if $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ and $c|\psi_1^0\rangle + d|\psi_2^0\rangle$ are used as new basis states instead of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$.

21. No. $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ is not an eigenstate of $\hat{H}^0$.

a. No. $\hat{H}^0$ will no longer be diagonal if $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ is chosen as one of the basis states.

b. No. $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ cannot be used as a basis state to calculate corrections to the energies and energy eigenstates in perturbation theory.

If your answers do not match the checkpoint for questions 18 - 21 in EXAMPLE 5, go back and reconcile any differences you may have.

Now let us determine values of $a, b, c$, and $d$ that correspond to a "good" basis for EXAMPLE 5, for which $\hat{H}^0$ and $\hat{H}'$ given below are represented in the initially chosen basis.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \qquad (\epsilon \ll 1)$$

We will only focus on $\hat{H}'$ in the two-dimensional degenerate subspace of $\hat{H}^0$ for now.

22. Diagonalize $\hat{H}'$ in equation (A.14) in the degenerate subspace of $\hat{H}^0$ and find the eigenstates and eigenvalues of $\hat{H}'$ in that two-dimensional subspace.

Consider the following conversation regarding extending the eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ from a two-dimensional to the three-dimensional Hilbert space.

**Student 1:** When we diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ in equation (A.14), we find two eigenstates of both $\hat{H}'$ and $\hat{H}^0$ in the two-dimensional subspace. How can we use these states to find "good" basis states in the three dimensional Hilbert space?

**Student 2:** In EXAMPLE 5, the eigenstates found by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ are $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. "Good" basis states must be $|\phi_1^0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ c_1 \end{pmatrix}$ and $|\phi_2^0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ c_2 \end{pmatrix}$ when we extend them to the three-dimensional Hilbert space. To determine the values $c_1$ and $c_2$, we must satisfy the orthogonality conditions $\langle\phi_1^0|\phi_3^0\rangle = 0$ and $\langle\phi_2^0|\phi_3^0\rangle = 0$.

**Student 3:** From equation (A.14), $|\phi_3^0\rangle = |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ is already a "good" basis state and any vector orthogonal to $|\phi_3^0\rangle$ must have zero as its third component. Since $\langle\phi_1^0|\phi_3^0\rangle = c_1$ and $\langle\phi_2^0|\phi_3^0\rangle = c_2$, extending the states found from diagonalizing $\hat{H}'$ in the two-dimensional degenerate subspace of $\hat{H}^0$ to find basis states in three dimensions requires adding a zero as the third component to ensure $\langle\phi_1^0|\phi_3^0\rangle = 0$ and $\langle\phi_2^0|\phi_3^0\rangle = 0$. Also, the condition $\langle\phi_1^0|\phi_2^0\rangle = 0$ is satisfied when we extend to three dimensions the states in two dimensions obtained by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

Explain why you agree with Student 2, Student 3, or both.

23. Extend the states you found in the preceding problem (question 22) to the three dimensional space, making use of the preceding conversation, to obtain the two "good" basis states $|\phi_1^0\rangle$ and $|\phi_2^0\rangle$.

24. Express the "good" basis states or eigenstates of $\hat{H}^0$ (obtained by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$) as a linear combination of the initially chosen eigenstates of $\hat{H}^0$, $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$, used in equation (A.14).

25. In the preceding question (question 24), $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ and $c|\psi_1^0\rangle + d|\psi_2^0\rangle$ are "good" orthonormal basis states written in terms of the initially chosen basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. The constants that diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ must be:

$a =$ _____

$b =$ _____

$c =$ _____

$d =$ _____

26. Using your values of $a, b, c$, and $d$ in the preceding question, find the matrix elements of $\hat{H}^0$ in the "good" basis.

$$\hat{H}^0 = \begin{array}{r} \\ a^*\langle\psi_1^0| + b^*\langle\psi_2^0| \\ \\ c^*\langle\psi_1^0| + d^*\langle\psi_2^0| \\ \\ \langle\psi_3^0| \end{array} \begin{array}{c} \begin{array}{ccc} a\ |\psi_1^0\rangle + \ b\ |\psi_2^0\rangle & c|\psi_1^0\rangle + \ d\ |\psi_2^0\rangle & |\psi_3^0\rangle \end{array} \\ \left( \begin{array}{ccc} & & \\ & & \\ & & \\ & & \end{array} \right) \end{array}$$

Summarize your results in one to two sentences.

*** Check your answers to questions 22-26 in EXAMPLE 5. ***

22. Diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$, the eigenvalues of $\hat{H}'$ are $\epsilon V_0$ with corresponding eigenstate $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $-\epsilon V_0$ with corresponding eigenstate $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

**NOTE:** The eigenstates are unique up to a constant multiple (e.g., the eigenstate corresponding to the eigenvalue $-\epsilon V_0$ can be equivalently expressed as $\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$).

23. Using orthogonality with $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, we can extend $\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\}$ to the three dimensional space, so that the other "good" basis states are $\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \right\}$.

24. Therefore, the "good" basis states (in terms of the initially chosen basis states in equation (A.14)) for the entire three-dimensional state space will be $\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$, or equivalently $\left\{ \frac{1}{\sqrt{2}}|\psi_1^0\rangle + \frac{1}{\sqrt{2}}|\psi_2^0\rangle, \frac{1}{\sqrt{2}}|\psi_1^0\rangle - \frac{1}{\sqrt{2}}|\psi_2^0\rangle, |\psi_3^0\rangle \right\}$. These basis states are eigenstates of $\hat{H}^0$ ($\hat{H}^0$ is still diagonal in this basis) as it should be in perturbation theory, but $\hat{H}'$ is also diagonal in the degenerate subspace of $\hat{H}^0$.

25. For the given perturbing Hamiltonian $\hat{H}'$ in equation (A.14), a "good" orthonormal basis that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ is obtained with the constants $a = b = c = \frac{1}{\sqrt{2}}$ and $d = -\frac{1}{\sqrt{2}}$.

**NOTE:** The values of $a, b, c$, and $d$ are unique up to overall phase factors.

26. The entire $\hat{H}^0$ matrix remains diagonal as it must be for an appropriately chosen

"good" basis.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

If your answers do not match the checkpoint for questions 22-26 in EXAMPLE 5, go back and reconcile any differences you may have.

Consider the following conversation regarding whether in the degenerate subspace of $\hat{H}^0$, linear combinations of eigenstates of $\hat{H}^0$ remain eigenstates of $\hat{H}^0$ due to degeneracy.

**Student 1:** Consider EXAMPLE 5. Since any linear combination of the basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ in the degenerate subspace of $\hat{H}^0$ keeps $\hat{H}^0$ diagonal, any linear combination of eigenstates of $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$ will be an eigenstate of $\hat{H}^0$.

**Student 2:** But how can that be? In the context of a one-dimensional infinite square well, a linear combination of the ground state and the first excited state is no longer an energy eigenstate.

**Student 1:** You are correct, a linear combination of the ground state and the first excited state is not an energy eigenstate of the one-dimensional infinite square well. There is no degeneracy in the energy eigenvalue spectrum for the one-dimensional infinite square well. It is the degeneracy that guarantees that any linear combination of eigenstates of $\hat{H}^0$ in the degenerate subspace of $\hat{H}^0$ will be an eigenstate of $\hat{H}^0$.

Explain why you agree or disagree with each student.

**EXAMPLE 6: Interpreting the Matrix Elements of the $\hat{H}'$ Matrix in a Given Representation**

Answer the following questions for this example:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} -3\epsilon & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \qquad (\epsilon \ll 1) \qquad \text{(A.16)}$$

and the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

If we express $\hat{H}^0$ and $\hat{H}'$ in a "good" basis, we have

$$\hat{H}_G^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \hat{H}'_G = V_0 \begin{pmatrix} \epsilon & 0 & \frac{2\epsilon}{\sqrt{5}} \\ 0 & -4\epsilon & \frac{\epsilon}{\sqrt{5}} \\ \frac{2\epsilon}{\sqrt{5}} & \frac{\epsilon}{\sqrt{5}} & 0 \end{pmatrix} \qquad (\epsilon \ll 1) \qquad \text{(A.17)}$$

and the "good" basis states, respectively, are

$$|\phi_1^0\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}, \qquad |\phi_2^0\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\phi_3^0\rangle = |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \text{(A.18)}$$

in which $\hat{H}_G^0$ is the matrix representation of $\hat{H}^0$ expressed in the "good" basis, $\hat{H}'_G$ is the matrix representation of $\hat{H}'$ expressed in a "good" basis, and $\{|\phi_n^0\rangle\}$ are the "good" basis states.

27. Using only the matrix elements in equation (A.17), find the first order corrections to the energies. **No matrix manipulation required!**

28. Using only the matrix elements in equation (A.17), find the first order corrections to the energy eigenstates. **No matrix manipulation required!**

*** Check your answers to questions 27-28 pertaining to EXAMPLE 6. ***

27. $E_1^1 = \epsilon V_0$, $E_2^1 = -4\epsilon V_0$, and $E_3^1 = 0$

28. $|\psi_1^1\rangle = -\frac{2\epsilon}{\sqrt{5}}|\phi_3^0\rangle$, $|\psi_2^1\rangle = -\frac{\epsilon}{\sqrt{5}}|\phi_3^0\rangle$, $|\psi_3^1\rangle = \frac{2\epsilon}{\sqrt{5}}|\phi_1^0\rangle + \frac{\epsilon}{\sqrt{5}}|\phi_2^0\rangle$ (Please note the values of the first order corrections to the energy eigenstates are not unique.)

If your answers to the first order corrections to the energies or energy eigenstates do not match EXAMPLE 6, go back and reconcile any differences.

Consider the following conversation regarding the matrix elements of $\hat{H}'$.

**Student 1:** For the corrections to the energies, we need the diagonal matrix elements of $\hat{H}'$. The matrix elements of $\hat{H}'$ along the diagonal correspond to the first order corrections to the energy.

**Student 2:** But the diagonal elements of $\hat{H}'$ correspond to the first order corrections to the energies only if the $\hat{H}'$ matrix is written in a "good" basis.

**Student 3:** I agree with Student 2. The off-diagonal elements of $\hat{H}'$ must be zero in the degenerate subspace of $\hat{H}^0$ for the basis states to be "good".

**Student 4:** I agree with Student 2 and Student 3. Once we find a "good" basis, the diagonal matrix elements of $\hat{H}'$ can be used to find the first order corrections to the energies. Also, the off-diagonal matrix elements of $\hat{H}'$ are needed when calculating the second or higher order corrections to the energies and any corrections to the energy eigenstates.

Explain why you agree or disagree with each student.

**EXAMPLE 7:** Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$, in which

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 2\epsilon & 0 \\ 2\epsilon & -\epsilon & 3\epsilon \\ 0 & 3\epsilon & \epsilon \end{pmatrix} \qquad (\epsilon \ll 1) \qquad \text{(A.19)}$$

and the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

29. Choose one of the following options to fill in the blank. In the degenerate subspace of $\hat{H}^0$, the matrix representation of $\hat{H}^0$ is _____ and the matrix representation of $\hat{H}'$ is _____, respectively.

(A)
$$V_0 \begin{pmatrix} -\epsilon & 2\epsilon \\ 2\epsilon & -\epsilon \end{pmatrix}, \qquad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

(B)
$$V_0 \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \qquad V_0 \begin{pmatrix} -\epsilon & 3\epsilon \\ 3\epsilon & \epsilon \end{pmatrix}$$

(C)
$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$$

(D)
$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \qquad V_0 \begin{pmatrix} -\epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$$

30. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a "good" basis? Explain.

31. The first order corrections to the energies are

(A) $E_1^1 = -\epsilon V_0, E_2^1 = -\epsilon V_0$, and $E_3^1 = \epsilon V_0$.

(B) $E_1^1 = \epsilon V_0, E_2^1 = \epsilon V_0$, and $E_3^1 = \epsilon V_0$.

(C) $E_1^1 = -\epsilon V_0, E_2^1 = -\epsilon V_0$, and $E_3^1 = 0$.

(D) $E_1^1 = -\epsilon V_0, E_2^1 = 2\epsilon$, and $E_3^1 = 3\epsilon$.

(E) None of the above

***Check your answers to questions 27-28 pertaining to EXAMPLE 7. ***

29. C
30. Yes.
31. A

If your answers to the first order corrections to the energies or energy eigenstates do not match the checkpoint answers for EXAMPLE 7, go back and reconcile any differences.

Consider the following conversation regarding writing the basis states in a different order so that the degenerate eigenvalues of $\hat{H}^0$ along the diagonal are adjacent. With that order, the degenerate subpsace of $\hat{H}^0$ can be identified more easily.

**Student 1:** In equation (A.19), in the degenerate subspace of $\hat{H}^0$, I don't see how the matrix representation of $\hat{H}'$ is $V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$.

**Student 2:** It is a little difficult to recognize the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ because of the order in which the basis states are chosen. However, we are always free to choose the basis states in any order. In this case it may be helpful if we choose to express $\hat{H}^0$ and $\hat{H}'$ with the basis states chosen in a different order than in the order $|\psi_1^0\rangle, |\psi_2^0\rangle$, and $|\psi_3^0\rangle$ selected in equation (A.19). If we choose the basis states in the order $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, and $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ then

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 0 & 2\epsilon \\ 0 & \epsilon & 3\epsilon \\ 2\epsilon & 3\epsilon & -\epsilon \end{pmatrix} \quad (\epsilon \ll 1) \qquad \text{(A.20)}$$

Now we can easily identify the matrix representation of $\hat{H}^0$ and $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

**Student 3:** I disagree with Student 2. Since the first order corrections to the energies depend on the matrix elements of $\hat{H}'$, we cannot choose the basis states in a different order without affecting the first order corrections to each unperturbed energy.

Explain why you agree or disagree with each student.

Consider the following conversation regarding small corrections to the unperturbed energies and eigenstates of the unperturbed Hamiltonian $\hat{H}^0$ due to the perturbation $\hat{H}'$.

**Student 1:** When we use perturbation theory, we are assuming that the perturbation $\hat{H}'$ is small compared to $\hat{H}^0$. Therefore, we use the unperturbed eigenstates of $\hat{H}^0$ as basis states for our calculations of the corrections to the energies and the energy eigenstates.

**Student 2:** Yes, but a "good" basis is still needed to find corrections to the energies and energy eigenstates. We must choose as basis states a set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

Do you agree with Student 1, Student 2, or both? Explain.

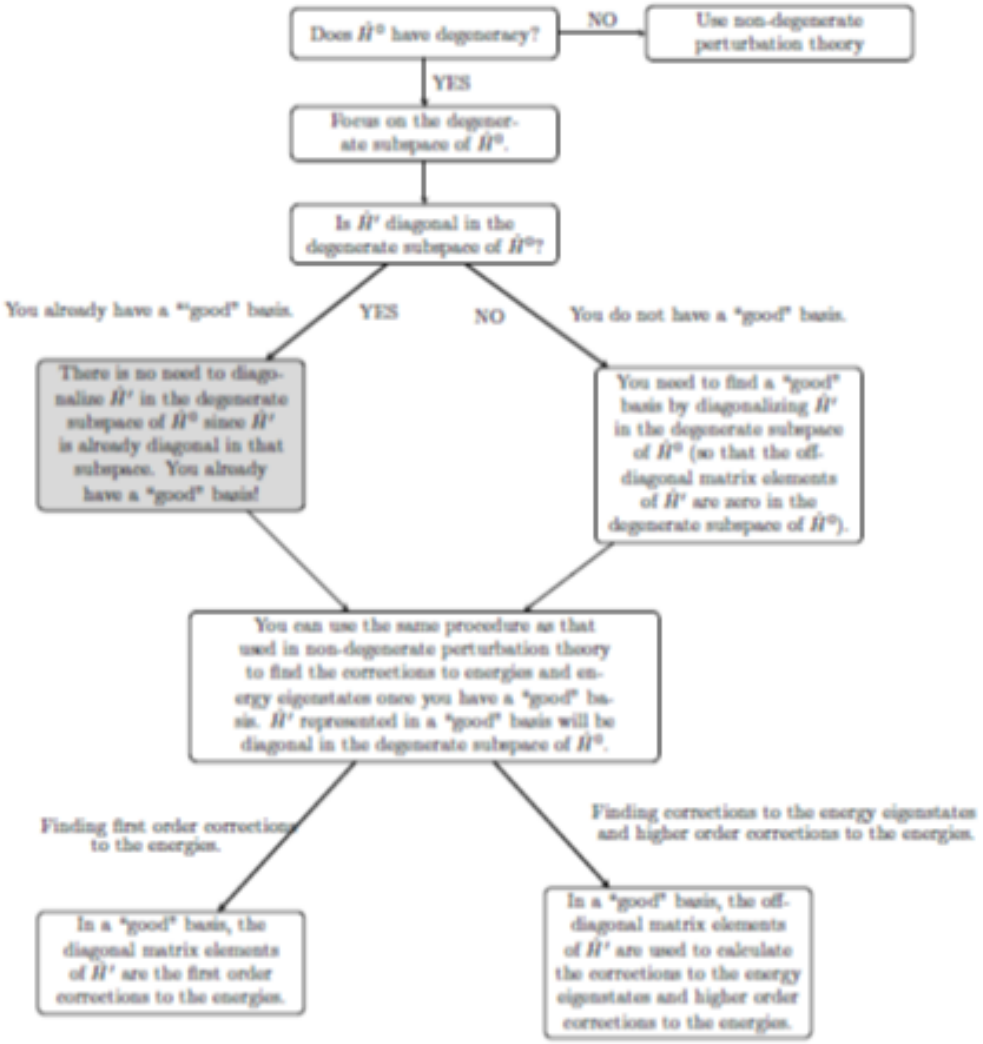
### A.7.7 Checkpoint - Finding a "good" basis for Case 2

For the case in which the unperturbed Hamiltonian $\hat{H}^0$ has degeneracy, we must first ensure that we have a "good" basis before finding the corrections to the energies and energy eigenstates.

- If $\hat{H}'$ **is not diagonal in the degenerate subspace of** $\hat{H}^0$:
  - The initially chosen basis is not "good."
  - We must **DIAGONALIZE** $\hat{H}'$ **in the degenerate subspace of** $\hat{H}^0$ to find a "good" basis.
    - Diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ gives a linear combination of eigenstates of $\hat{H}^0$ that form a "good" basis.
    - Any linear combination of energy eigenstates in the degenerate subspace of $\hat{H}^0$ remains an eigenstate of $\hat{H}^0$.
    - In a "good" basis, $\hat{H}^0$ remains diagonal (i.e., "good" basis states are still eigenstates of $\hat{H}^0$).
  - The diagonal elements of $\hat{H}'$ in a "good" basis are the first order corrections to the energies.
  - The off-diagonal matrix elements of $\hat{H}'$ in a "good" basis are used to determine the first order corrections to the energy eigenstates.

Review the flowchart for the steps in determining corrections to the energies and energy eigenstates **when $\hat{H}'$ is <u>NOT</u> diagonal in the degenerate subspace of $\hat{H}^0$.**

# <u>Finding First Order Corrections to the Energies and Energy Eigenstates</u>



**A.7.7.1 If $\hat{H}^0$ and $\hat{H}'$ do not commute, diagonalizing the entire $\hat{H}'$ matrix makes $\hat{H}^0$ non-diagonal** Consider the following conversation regarding a "good" basis and diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

**Student 1:** In degenerate perturbation theory, to find a "good" basis for a given $\hat{H}^0$ and $\hat{H}'$, we must diagonalize the $\hat{H}'$ matrix.

**Student 2:** We should not diagonalize the entire $\hat{H}'$ matrix, but rather only the part of $\hat{H}'$ that corresponds to the degenerate subspace of $\hat{H}^0$.

**Student 3:** I disagree. If we diagonlize part of the $\hat{H}'$ matrix then we cannot guarantee that it will give us a "good" basis. We must diagonalize the entire $\hat{H}'$ matrix.

**Student 4:** Actually, it is equally valid to diagonalize either the entire $\hat{H}'$ matrix or only the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$. We usually choose to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ simply because it requires less work to diagonalize a matrix with a lower dimension.

Explain why you agree or disagree with each student.

**EXAMPLE 8:** Let's see what happens when we diagonalize the entire $\hat{H}'$ matrix. Consider the example

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 5 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{bmatrix}, \qquad (\epsilon \ll 1). \tag{A.21}$$

Due to the degeneracy in the energy spectrum of $\hat{H}'$, the eigenstates of $\hat{H}'$ are not unique. One possible set of eigenstates of $\hat{H}'$ is

$$|\phi_1^0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, |\phi_2^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\phi_3^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \tag{A.22}$$

in terms of the initially chosen basis states used to write equation (A.21).

If we use the eigenstates of $\hat{H}'$ as the basis states, the $\hat{H}^0$ matrix becomes

$$\hat{H}^0 = \begin{bmatrix} \frac{7}{3} & -\frac{4}{\sqrt{6}} & -\frac{4}{\sqrt{6}} \\ -\frac{4}{\sqrt{6}} & 3 & \frac{5}{2} \\ -\frac{4}{\sqrt{6}} & \frac{5}{2} & 3 \end{bmatrix}. \tag{A.23}$$

32. Is $\hat{H}^0$ in equation (A.23) diagonal in the basis consisting of the eigenstates of $\hat{H}'$?

33. Based upon your answer for whether $\hat{H}^0$ is diagonal in this basis or not, are these basis states, which are eigenstates of $\hat{H}'$, eigenstates of $\hat{H}^0$? Explain.

34. Can this basis be used for finding the corrections to the energies and energy eigenstates in perturbation theory for the Hamiltonian in equation (A.21)? Explain.

With this example in mind, summarize the student conversation on the previous page in one to two sentences and how would you help these students with the issues they are discussing.

*** Check your answers to questions 32-34 in EXAMPLE 8. ***

32. No. $\hat{H}^0$ is not diagonal in the basis consisting of the eigenstates of $\hat{H}'$.

33. No. $\hat{H}^0$ must be diagonal in a basis consisting of the eigenstates of $\hat{H}^0$.

34. No. This is not a "good" basis as $\hat{H}^0$ is not diagonal in a basis consisting of the eigenstates of $\hat{H}'$.

If any of your answers do not match the checkpoint answers for EXAMPLE 8, go back and reconcile any differences you may have with the answers provided.

### A.7.8 Checkpoint

If $\hat{H}^0$ and $\hat{H}'$ do not commute:

- $\hat{H}'$ **must be diagonalized only in the degenerate subspace of** $\hat{H}^0$ in order to ensure that basis states remain eigenstates of $\hat{H}^0$ (i.e., $\hat{H}^0$ is diagonal in that basis).
- Diagonalizing the entire $\hat{H}'$ matrix yields a basis that produces off-diagonal matrix elements in $\hat{H}^0$ when $\hat{H}^0$ and $\hat{H}'$ do not commute, which is not valid for determining the perturbative corrections using perturbation theory (basis states must always be eigenstates of $\hat{H}^0$ since we are finding small corrections to the unperturbed energies).

**A.7.8.1 $\hat{H}^0$ and $\hat{H}'$ do commute** In all the examples up to this point, we have considered systems such that $\hat{H}^0$ and $\hat{H}'$ did not commute. Let's consider whether the same approach is valid for a system in which $\hat{H}^0$ and $\hat{H}'$ do commute.

Consider the following conversation regarding diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ for a system for which $\hat{H}^0$ and $\hat{H}'$ commute.

**Student 1:** Even when $\hat{H} = \hat{H}^0 + \epsilon\hat{H}'$ ($\epsilon \ll 1$) for a system is such that $\hat{H}^0$ and $\hat{H}'$ commute, we can use the same approach to find a "good" basis as when $\hat{H}^0$ and $\hat{H}'$ do not commute. In particular, we can find a "good" basis by only diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.
**Student 2:** I disagree. Since $\hat{H}^0$ and $\hat{H}'$ commute, we must diagonalize the entire $\hat{H}'$ matrix. The "good" basis must consist of a complete set of simultaneous eigenstates of $\hat{H}^0$ and $\hat{H}'$.
**Student 3:** Actually, if $\hat{H}^0$ and $\hat{H}'$ commute, then diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ will diagonalize the entire $\hat{H}'$ matrix. The first order corrections give the exact result.

Explain why you agree or disagree with each student.

### A.7.9 Checkpoint

If $\hat{H}^0$ and $\hat{H}'$ commute, i.e., $[\hat{H}^0, \hat{H}'] = 0$:

- $\hat{H}^0$ and $\hat{H}'$ can be simultaneously diagonalized.
- Diagonalize $\hat{H}'$ **in the degenerate subspace of** $\hat{H}^0$ in order to find corrections to the energies and energy eigenstates.
- Diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ will diagonalize the entire $\hat{H}'$ matrix. The first order corrections (the diagonal matrix elements of $\hat{H}'$) give the exact result.

SUMMARY: Finding First Order Corrections to the Energies and Energy Eigenstates Requires that You Choose a "Good" Basis

The perturbative Hamiltonian $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ will dictate how we proceed to determine the first order corrections to the energies and the energy eigenstates.

CASE 1: $\hat{H}'$ IS DIAGONAL IN THE DEGENERATE SUBSPACE OF $\hat{H}^0$ IN THE INITIAL BASIS.

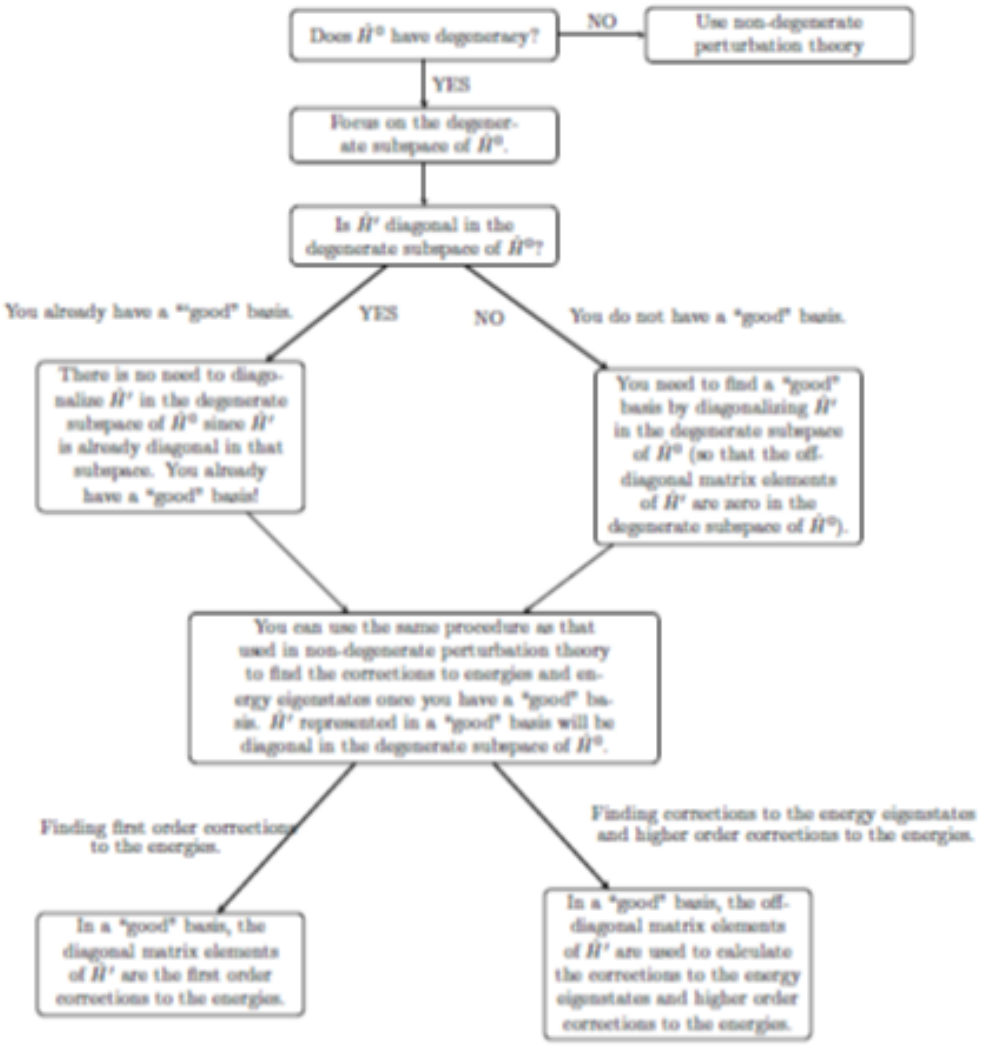
- If $\hat{H}'$ **is diagonal in the degenerate subspace of** $\hat{H}^0$:
  - The initially **chosen eigenstates of** $\hat{H}^0$ **already form a "good" basis** so the corrections to the energies and energy eigenstates can be found simply by **using the matrix elements of** $\hat{H}'$ exactly as in non-degenerate perturbation theory.
    - One can use equations (A.2) and (A.3) with the initial basis states.
    - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ gives the first order correction to the energies.
    - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle$ gives the first order corrections to the energy eigenstates since the numerator will be zero when $E_n^0 = E_m^0$ (if $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$).
      - The terms with $E_n^0 = E_m^0$ in the denominator will not appear in the first order correction to the energy eigenstates $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle$.

CASE 2: $\hat{H}'$ IS NOT DIAGONAL IN THE DEGENERATE SUBSPACE OF $\hat{H}^0$ IN THE INITIAL BASIS.

- In the initially chosen basis, if $\hat{H}'$ **has non-zero off-diagonal matrix elements in the degenerate subspace of** $\hat{H}^0$:
  - The initially **chosen eigenstates of** $\hat{H}^0$ **do not form a "good" basis.**
  - One **CANNOT** use equations (A.2) and (A.3) with the initially chosen basis states (since they do not form a "good" basis).
  - In this case, a "good" basis must be found such that $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$ while $\hat{H}^0$ remains diagonal.
  - To find a "good" basis $\{|\phi_n^0\rangle\}$, **diagonalize** $\hat{H}'$ **in the degenerate subspace of** $\hat{H}^0$.
  - Once a "good" basis is found, the corrections to the energies and energy eigenstates can be found by **inspecting the matrix elements of** $\hat{H}'$ as in non-degenerate perturbation theory.
    - The expression $E_n^1 = \langle\phi_n^0|\hat{H}'|\phi_n^0\rangle$ gives the first order corrections to the energies after finding a "good" basis $\{|\phi_n^0\rangle\}$.
    - The expression $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\phi_m^0|\hat{H}'|\phi_n^0\rangle}{(E_n^0 - E_m^0)}|\phi_m^0\rangle$ gives the first order correction to the energy eigenstates after finding a "good" basis $\{|\phi_n^0\rangle\}$, since the numerator will be zero when $E_n^0 = E_m^0$ (if $\hat{H}'$ is diagonal in the degenerate subspace of $\hat{H}^0$).
      - So the terms with $E_n^0 = E_m^0$ will not appear in the first order corrections to the energy eigenstates $|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle$.

For a given $\hat{H}^0$ and $\hat{H}'$, the following flowchart summarizes the steps required to find the corrections to the energies and energy eigenstates when $\hat{H}^0$ possesses a degeneracy.

## Finding First Order Corrections to the Energies and Energy Eigenstates



### A.7.10 Practice

**EXAMPLE 9:** Now let's apply these ideas to an example (question 35-39): Given

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 1+11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & 2-\epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & 2-4\epsilon \end{bmatrix}, \qquad (\epsilon \ll 1) \tag{A.24}$$

and the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Answer the following questions.

35. Choose the unperturbed Hamiltonian, $\hat{H}^0$, and the perturbing Hamiltonian, $\hat{H}'$ from the choices below.

(A) $\hat{H}^0 = V_0 \begin{pmatrix} 1+11\epsilon & 0 & 0 \\ 0 & 2-\epsilon & 0 \\ 0 & 0 & 2-4\epsilon \end{pmatrix}$ and $\hat{H}' = V_0 \begin{pmatrix} 0 & -8\epsilon & 4\epsilon \\ -8\epsilon & 0 & -2\epsilon \\ 4\epsilon & -2\epsilon & 0 \end{pmatrix}$

(B) $\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$ and $\hat{H}' = V_0 \begin{pmatrix} 11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & -\epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & -4\epsilon \end{pmatrix}$

(C) $\hat{H}^0 = V_0 \begin{pmatrix} 11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & -\epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & -4\epsilon \end{pmatrix}$ and $\hat{H}' = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

(D) $\hat{H}^0 = V_0 \begin{pmatrix} 11\epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & 4\epsilon \end{pmatrix}$ and $\hat{H}' = V_0 \begin{pmatrix} 1 & -8\epsilon & 4\epsilon \\ -8\epsilon & 2 & -2\epsilon \\ 4\epsilon & -2\epsilon & 2 \end{pmatrix}$

36. Choose the unperturbed energies and the normalized eigenstates of $\hat{H}^0$ from the choices below.

(A) The unperturbed energies are $V_0$, $4V_0$, and $11V_0$.

The eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

(B) The unperturbed energies are $\epsilon V_0$, $4\epsilon V_0$, and $11\epsilon V_0$.

The eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

(C) The unperturbed energies are $\epsilon V_0$, and $4\epsilon V_0$.

The eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

(D) The unperturbed energies are $V_0$ and $2V_0$ (twice).

The eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

37. Which one of the following is true about the degeneracy of $\hat{H}^0$?

(A) $\hat{H}^0$ has a two-fold degeneracy with energy eigenvalue of $2V_0$.

(B) $\hat{H}^0$ has a two-fold degeneracy with energy eigenvalues of $-\epsilon V_0$ and $-4\epsilon V_0$.

(C) $\hat{H}^0$ has a two-fold degeneracy with energy eigenvalue of $V_0$.

(D) $\hat{H}^0$ has a two-fold degeneracy with energy eigenvalues of $V_0$ and $2V_0$.

38. Now you will diagonalize part of the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$.

(i) What is the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$?

(A) $V_0 \begin{pmatrix} 11\epsilon & -8\epsilon \\ -8\epsilon & -\epsilon \end{pmatrix}$

(B) $V_0 \begin{pmatrix} -8\epsilon & -\epsilon \\ 4\epsilon & -2\epsilon \end{pmatrix}$

(C) $V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

(D) $V_0 \begin{pmatrix} -\epsilon & -2\epsilon \\ -2\epsilon & -4\epsilon \end{pmatrix}$

(ii) Choose the correct statement below.

(A) In the degenerate subspace of $\hat{H}^0$, the eigenvalues of $\hat{H}'$ are -5 $\epsilon V_0$ and $15\epsilon V_0$, and the normalized eigenstates of $\hat{H}'$ are $\left\{ \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\}$, respectively.

(B) In the degenerate subspace of $\hat{H}^0$, the eigenvalues of $\hat{H}'$ are $-5 - \sqrt{5}\epsilon V_0$ and $\sqrt{5} - 5\epsilon V_0$,
and the normalized eigenstates of $\hat{H}'$ are $\left\{ \frac{1}{4} \begin{pmatrix} -3 - \sqrt{5} \\ 1 \end{pmatrix}, \frac{1}{4} \begin{pmatrix} -3 + \sqrt{5} \\ 1 \end{pmatrix} \right\}$,
respectively.

(C) In the degenerate subspace of $\hat{H}^0$, the eigenvalues of $\hat{H}'$ are 0 and -5$\epsilon V_0$, and the normalized eigenstates of $\hat{H}'$ are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\}$, respectively.

(D) In the degenerate subspace of $\hat{H}^0$, the eigenvalues of $\hat{H}'$ are both 2 $V_0$ and the eigenstates of $\hat{H}'$ are $\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$.

(iii) Choose the true statement (among the following) about extending the eigenstates in the preceding problem to the three-dimensional Hilbert space using the orthogonality of the "good" basis states.

(A) Extending the normalized eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ to the three-dimensional Hilbert space, the "good" states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} \right\}$, respectively.

(B) Extending the normalized eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ to the three-dimensional Hilbert space, the "good" states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -3-\sqrt{5} \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} -3+\sqrt{5} \\ 1 \\ 0 \end{pmatrix} \right\}$, respectively.

(C) Extending the normalized eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ to the three-dimensional Hilbert space, the "good" states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix} \right\}$, respectively.

(D) Extending the normalized eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ to the three-dimensional Hilbert space, the "good" states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} \right\}$, respectively.

39. Now you will determine a "good" basis.

(i) Express the "good" basis states as linear combinations of the initially chosen eigenstates of $H^0$ in equation (A.24).

(A) The "good" states are $\left\{-\frac{2}{\sqrt{5}}|\psi_1^0\rangle + \frac{1}{\sqrt{5}}|\psi_2^0\rangle, \quad \frac{1}{\sqrt{5}}|\psi_1^0\rangle + \frac{2}{\sqrt{5}}|\psi_2^0\rangle, \quad |\psi_3^0\rangle\right\}$.

(B) The "good" states are $\left\{|\psi_1^0\rangle, \quad -\frac{2}{\sqrt{5}}|\psi_2^0\rangle + \frac{1}{\sqrt{5}}|\psi_3^0\rangle, \quad \frac{1}{\sqrt{5}}|\psi_2^0\rangle + \frac{2}{\sqrt{5}}|\psi_3^0\rangle\right\}$.

(C) The "good" states are $\{|\psi_1^0\rangle, \frac{1}{4}(-3-\sqrt{5})|\psi_2^0\rangle + \frac{1}{4}\ |\psi_3^0\rangle,$
$\frac{1}{4}(-3+\sqrt{5})|\psi_2^0\rangle + \frac{1}{4}\ |\psi_3^0\rangle$.

(D) The "good" states are $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$.

(ii) The $\hat{H}'$ matrix in the good basis is:

(A) $\hat{H}'_G = V_0 \begin{pmatrix} 15\epsilon & 0 & 0 \\ 0 & -5\epsilon & 0 \\ 0 & 0 & -4\epsilon \end{pmatrix}$

(B) $\hat{H}'_G = V_0 \begin{pmatrix} 11\epsilon & \frac{20}{\sqrt{5}}\epsilon & 0 \\ \frac{20}{\sqrt{5}}\epsilon & 0 & 0 \\ 0 & 0 & -5\epsilon \end{pmatrix}$

(C) $\hat{H}'_G = V_0 \begin{pmatrix} 0 & -8\epsilon & 4\epsilon \\ -8\epsilon & 0 & -2\epsilon \\ 4\epsilon & -2\epsilon & 0 \end{pmatrix}$

(D) $\hat{H}'_G = V_0 \begin{pmatrix} 1 & -8\epsilon & 4\epsilon \\ -8\epsilon & 2 & 0 \\ 4\epsilon & 0 & 2 \end{pmatrix}$

(iii) Choose the first order corrections to the energies from the choices below.

(A) The first order corrections to the energies are $E_1^1 = 15\epsilon V_0$, $E_2^1 = -5\epsilon V_0$, and $E_3^1 = -4\epsilon V_0$.

(B) The first order corrections to the energies are $E_1^1 = V_0$, $E_2^1 = 2V_0$ and $E_3^1 = 2V_0$.

(C) The first order corrections to the energies are $E_1^1 = 0$, $E_2^1 = -\epsilon V_0$ and $E_3^1 = -4\epsilon V_0$.

(D) The first order corrections to the energies are $E_1^1 = 11\epsilon V_0$, $E_2^1 = 0$ and $E_3^1 = -5\epsilon V_0$.

For a given $\hat{H}^0$ and $\hat{H}'$, when $\hat{H}^0$ has degeneracy, summarize in your own words, the steps necessary to find a "good" basis and the first order corrections to the energies and energy eigenstates.

*** Check your answers to questions 35-39 in EXAMPLE 9. ***

35. B
36. D
37. A
38. i. D
    ii. C
    iii. D
39. i. B
    ii. B
    iii. D

If any of your answers do not match the checkpoint for EXAMPLE 9, go back and reconcile any differences between your predictions and the answers in the checkpoint.

**EXAMPLE 10:** Another example:

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 5 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{bmatrix}, \qquad (\epsilon \ll 1) \tag{A.25}$$

40. Identify the unperturbed Hamiltonian, $\hat{H}^0$, and the perturbation Hamiltonian, $\hat{H}'$.

41. Find the unperturbed energies and the corresponding normalized eigenstates of $\hat{H}^0$ from equation (A.25).

42. How many fold degeneracy is there in the eigenvalue spectrum of $\hat{H}^0$?

43. Diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$:

    (i) Write down $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ in equation (A.25)?

(ii) Calculate the eigenvalues and normalized eigenstates of $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ in the preceding question.

(iii) Extend the states in the preceding question to the three-dimensional Hilbert space by making sure that the basis states found by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ are orthonormal to $|\psi_1^0\rangle$ (the basis states in equation (A.25) corresponding to the non-degenerate eigenvalue of $\hat{H}^0$).

44. Determine "good" basis states

(i) Express the "good" states as a linear combination of the initially chosen eigenstates of $\hat{H}^0$ in equation (A.25).

(ii) Find first order corrections to the energies.

=

*** Check your answers to questions 40-44 in EXAMPLE 10: ***

40.

$$\hat{H}^0 = V_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix}$$

41. The unperturbed energies (eigenvalues of $\hat{H}^0$) are $V_0$ (which is two-fold degenerate) and $5V_0$.The unperturbed energy eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \right.$

$\left. |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

42. $\hat{H}^0$ has a two-fold degeneracy with energy eigenvalue $V_0$.

43. i. $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}$

ii. The eigenvalues of this matrix are $-\epsilon V_0$ and $\epsilon V_0$, and the eigenvectors are $\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\}$ respectively.

iii. Extending to the three-dimensional Hilbert space the "good" states are $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right\}$.

44. i. The "good" basis states in terms of the initially chosen basis states in equation (A.25) are $\left\{ |\psi_1^0\rangle, \quad \frac{1}{\sqrt{2}}(|\psi_2^0\rangle - |\psi_3^0\rangle), \quad \frac{1}{\sqrt{2}}(|\psi_2^0\rangle + |\psi_3^0\rangle) \right\}$

ii. The first order corrections to the energies are $E_1^1 = 0$, $E_2^1 = \epsilon V_0$, and $E_3^1 = -\epsilon V_0$.

If any of your answers to EXAMPLE 10 do not match the checkpoint, go back and reconcile any difference you may have.

**EXAMPLE 11:** Consider the example:

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 4+2\epsilon & 0 & \epsilon \\ 0 & 1-\epsilon & -2\epsilon \\ \epsilon & -2\epsilon & 1-4\epsilon \end{bmatrix}, \qquad (\epsilon \ll 1). \tag{A.26}$$

45. Determine the first order corrections to the energies for $\hat{H}$ given in equation (A.26).

*** Check your answers to questions 45 in EXAMPLE 11. ***

45. $E_1'' = 2\epsilon V_0,\ E_2' = 0,\ E_3' = -5\epsilon V_0$

If any of your answers for EXAMPLE 11 do not match the checkpoint, go back and reconcile any difference you may have with the answers provided.

**EXAMPLE 12:** Consider the unperturbed Hamiltonian

$$\hat{H}^0 = V_0 \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}. \tag{A.27}$$

46. Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis forms a "good" basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use $\epsilon$ as a small parameter.

47. Write an example of a perturbing Hamiltonian $\hat{H}'$ in the same basis as $\hat{H}^0$ such that for that $\hat{H}^0$ and $\hat{H}'$, this basis does NOT form a "good" basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use $\epsilon$ as a small parameter.

*** Check your answers to questions 46-47 in EXAMPLE 12. ***

46. Any $\hat{H}'$ of the form $\hat{H}' = \epsilon V_0 \begin{bmatrix} a & b & 0 \\ b^* & c & d \\ 0 & d^* & e \end{bmatrix}$ in which $a, b, c, d$ and $e$ can be any value such that $a, c$, and $e$ are real and the product with $\epsilon$ remains small.

47. Any $\hat{H}'$ of the form $\hat{H}' = \epsilon V_0 \begin{bmatrix} a & b & f \\ b^* & c & d \\ f^* & d^* & e \end{bmatrix}$ in which $a, b, c, d, e$ and $f$ can be any value such that that $a, c$, and $e$ are real and the product with $\epsilon$ remains small and $f \neq 0$.

If any of your answers do not match the checkpoint for EXAMPLE 12, go back and reconcile any difference you may have with the answers provided.

# APPENDIX B

# FINDING THE SPLITTING IN THE HYDROGEN ATOM ENERGY SPECTRUM DUE TO AN EXTERNAL MAGNETIC FIELD (ZEEMAN EFFECT) TUTORIAL - PART I

Finding the Splitting in the Hydrogen Atom Energy Spectrum Due to an External Magnetic Field (Zeeman Effect)- PART I

## B.1 DEFINITION

For a given unperturbed Hamiltonian $\hat{H}^0$ and perturbation $\hat{H}'$, a **"good"** basis consists of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ ($\hat{H}^0$ remains diagonal everywhere since the basis states are eigenstates of $\hat{H}^0$).

- Once you have a "good" basis for a given $\hat{H}^0$ and $\hat{H}'$, you can use the same expressions that you use in non-degenerate perturbation theory for the perturbative corrections to the energies and energy eigenstates.

## B.2 NOTES FOR THIS TUTORIAL:

* If you are not familiar with the steps to determine a "good" basis for finding corrections to the unperturbed energies when the energy spectrum has degeneracy, please work through the pretest, tutorial and posttest for Basics of Degenerate Perturbation Theory before working on this tutorial.
* A Hermitian operator $\hat{Q}$ must satisfy the property $Q_{ij} = (Q_{ji})^*$. Here $^*$ denotes the complex conjugate.
* For the matrix representation of a Hermitian operator $\hat{Q}$ in a given basis, we will use "$=$" or "is equal to" instead of "$\doteq$" or "is represented by" as in the notation below

$$\hat{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \quad \text{is equivalent to} \quad \hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}.$$

* In this tutorial, "degeneracy" indicates degeneracy in the unperturbed energy eigenvalue spectrum, i.e., the fact that more than one distinct energy eigenstate can have the same energy eigenvalue. For example, if

$$\hat{H}^0|\psi_a\rangle = E_a|\psi_a\rangle \qquad \text{and} \qquad \hat{H}^0|\psi_b\rangle = E_a|\psi_b\rangle,$$

  $|\psi_a\rangle$ and $|\psi_b\rangle$ are degenerate eigenstates of the Hamiltonian $\hat{H}^0$ since they correspond to the same energy $E_a$.
* We will only consider the bound states of the hydrogen atom.
* The unperturbed bound state energy is $E_n$ are given by $E_n = -\frac{13.6\text{eV}}{n^2}$, $n = 1, 2, 3, \ldots$.
* **For any basis we choose, the radial part of the wavefunctions $R_{nl}$ (for given quantum numbers $n$ and $l$) will always be chosen to be the radial parts of a complete set of eigenstates of $\hat{H}^0$. In other words, our focus will be on the choice of the angular part of the wavefunction in order to find a "good" basis for degenerate perturbation theory for the given $\hat{H}^0$ and $\hat{H}'$ for the hydrogen atom.**
* We will restrict our focus to a finite subspace of the infinite dimensional Hilbert space.

  - As an example of a degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$, only the subspace with the principal quantum number $n = 2$ will be considered.
  - The results can be generalized to any quantum number $n$.

* The external magnetic field will be chosen to be a uniform, time independent field along the $\hat{z}$ direction given by $\vec{B} = B_{ext}\hat{z}$.
* We will account for the coupling of the external magnetic field with both the orbital and spin angular momentum.
* We will use the following notations interchangeably to write states in the uncoupled representation (in which basis states are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{L}_Z$, and $\hat{S}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ m_l\ m_s\rangle$
  - $|l,\ m_l\rangle|s,\ m_s\rangle$ (if $n$ is fixed)
  - $|l,\ m_l,\ m_s\rangle$ (if $n$ and $s$ are fixed)
* $\vec{J} = \vec{L} + \vec{S}$
* We will use the following notations interchangeably to write states in the coupled representation (in which basis vectors are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ j\ m_j\rangle$
  - $|l,\ s,\ j,\ m_j\rangle$ (if $n$ is fixed)
  - $|l,\ j,\ m_j\rangle$ (if $n$ and $s$ are fixed)
* In both Part I and Part II of this tutorial, we will consider the case in which $s = \frac{1}{2}$ so this quantum number may be suppressed in writing a state (e.g., $|l\ m_l\ m_s\rangle$ or $|l\ j\ m_j\rangle$).

## B.3 PHYSICAL CONSTANTS

Below is a list of physical constants used in this tutorial.

| | | | |
|---|---|---|---|
| Planck's constant: | $\hbar$ | = | $1.05 \times 10^{-34}$ J s |
| Mass of the electron: | $m$ | = | $9.11 \times 10^{-31}$ kg |
| Magnitude of charge of an electron: | $e$ | = | $1.60 \times 10^{-19}$ C |
| Speed of light: | $c$ | = | $2.99 \times 10^{8}$ m/s |
| Permittivity of space: | $\epsilon_0$ | = | $8.85 \times 10^{-12}$ C$^2$/J m |
| Bohr radius: | $a$ | = | $\frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}$ m |
| Bohr magneton: | $\mu_B$ | = | $\frac{e\hbar}{2m} = 5.79 \times 10^{-5}$ eV/T |
| Fine structure constant: | $\alpha$ | = | $\frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137} = 7.30 \times 10^{-3}$ |

NOTE : The following equations may be helpful.

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$$

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle$$

$$\hat{S}^2|s\ m_s\rangle = \hbar^2 s(s+1)|s\ m_s\rangle \qquad \hat{S}_z|s\ m_s\rangle = \hbar m_s|s\ m_s\rangle$$

$$\hat{S}_\pm|s\ m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1))}|s\ m_s \pm 1\rangle$$

$$\hat{L}^2|l\ m_l\rangle = \hbar^2 l(l+1)|l\ m_l\rangle \qquad \hat{L}_z|l\ m_l\rangle = \hbar m_l|l\ m_l\rangle$$

$$\hat{L}_\pm|l\ m_l\rangle = \hbar\sqrt{l(l+1) - m_l(m_l \pm 1))}|l\ m_l \pm 1\rangle$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$\hat{J}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 j(j+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{J}_z|l,\ s,\ j\ m_j\rangle = \hbar m_j|l,\ s,\ j,\ m_j\rangle$$

$$\hat{S}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 s(s+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{L}^2|l,\ s,\ j\ m_j\rangle = \hbar^2 l(l+1)|l,\ s,\ j,\ m_j\rangle$$

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$$

## B.4 OBJECTIVES:

**Upon completion of this tutorial, you should be able to do the following:**

1. Identify the degeneracy in the unperturbed Hamiltonian $\hat{H}^0$ in each degenerate subspace corresponding to a principal quantum number $n$.
2. In order to find the first order corrections to the unperturbed energies of the hydrogen atom in the presence of an external magnetic field, you should be able to determine:
   - the unperturbed Hamiltonian $\hat{H}^0$ in both the coupled and uncoupled representation (for a given principal quantum number $n$).
   - whether the relativistic correction term $\hat{H}'_r$ is diagonal if the coupled or uncoupled representation is chosen as the basis (for a given principal quantum number $n$).
   - whether the spin-orbit interaction term $\hat{H}'_{SO}$ is diagonal if the coupled or uncoupled representation is chosen as the basis (for a given principal quantum number $n$).
   - whether the Zeeman term $\hat{H}'_Z$ is diagonal if the coupled or uncoupled representation is chosen as the basis.
   - whether a "good" angular part of the basis (angular basis) for a given $\hat{H}^0$ and perturbation $\hat{H}'$ is the uncoupled representation, the coupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or the uncoupled states.

The following questions focus on finding the various quantum numbers for a given principal quantum number $n$.

1. Answer the following questions in the context of the hydrogen atom with Coulomb interaction between the electron and the nucleus (spin quantum number $s = \frac{1}{2}$ for the electron).

   a. For $n = 1$, list the possible values of $l$ and the corresponding possible values of $m_l$.

   b. For $n = 1$, list the possible values of $m_s$ for $s = \frac{1}{2}$.

   c. For $n = 1$, list the possible values of $j$ and the corresponding possible values of $m_j$.

   d. For $n = 2$, list the possible values of $l$ and the corresponding possible values of $m_l$.

   e. For $n = 2$, list the possible values of $m_s$ for $s = \frac{1}{2}$.

   f. For $n = 2$, list the possible values of $j$ and the corresponding possible values of $m_j$.

2. How many distinct states $|n\ l\ s\ m_l\ m_s\rangle$ are there in the uncoupled representation for $n = 2$?

3. How many distinct states $|n\ l\ s\ j\ m_j\rangle$ are there in the coupled representation for $n = 2$?

**** Check your answers to questions 1-3: ****

1a. $l = 0; m_l = 0$

1b. $m_s = \frac{1}{2}, -\frac{1}{2}$

1c. $j = \frac{1}{2}; m_j = \frac{1}{2}, -\frac{1}{2}$

1d. $l = 0; m_l = 0$ and $l = 1; m_l = -1, 0, 1$

1e. $m_s = \frac{1}{2}, -\frac{1}{2}$

1f. $j = \frac{1}{2}; m_j = \frac{1}{2}, -\frac{1}{2}$ (appears twice, once for $l = 0$ and once for $l = 1$) and $j = \frac{3}{2}; m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$

2. There are eight distinct states in the uncoupled representation. $|n\ l\ s\ m_l\ m_s\rangle = \{|20\frac{1}{2}0\frac{1}{2}\rangle, |20\frac{1}{2}0-\frac{1}{2}\rangle, |21\frac{1}{2}1\frac{1}{2}\rangle, |21\frac{1}{2}1-\frac{1}{2}\rangle, |21\frac{1}{2}0\frac{1}{2}\rangle, |21\frac{1}{2}0-\frac{1}{2}\rangle, |21\frac{1}{2}-1\frac{1}{2}\rangle, |21\frac{1}{2}-1-\frac{1}{2}\rangle\}$

3. There are eight distinct states in the coupled representation. $|n\ l\ s\ j\ m_j\rangle = \{|21\frac{1}{2}\frac{3}{2}\frac{3}{2}\rangle, |21\frac{1}{2}\frac{3}{2}\frac{1}{2}\rangle, |21\frac{1}{2}\frac{3}{2}-\frac{1}{2}\rangle, |21\frac{1}{2}\frac{3}{2}-\frac{3}{2}\rangle, |21\frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle, |21\frac{1}{2}\frac{1}{2}-\frac{1}{2}\rangle, |20\frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle, |20\frac{1}{2}\frac{1}{2}-\frac{1}{2}\rangle\}$

If any of your answers do not match the checkpoint answers for questions 1-3, go back and reconcile any difference you may have.

## B.5 THE HYDROGEN ATOM PLACED IN AN EXTERNAL MAGNETIC FIELD

The Hamiltonian of the hydrogen atom placed in an external magnetic field is

$$\hat{H} = \hat{H}^0 + \hat{H}'_r + \hat{H}'_{SO} + \hat{H}'_Z = \hat{H}^0 + \hat{H}'_{fs} + \hat{H}'_Z \tag{B.1}$$

in which

- $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$ accounts only for the interaction of the electron with the nucleus via Coulomb attraction
- $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term
- $\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}(\vec{L}\cdot\vec{S})$ is the spin-orbit interaction term

and combining the relativistic and spin-orbit terms

- $\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r$ is the fine structure term
- $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ is the Zeeman term in which $\vec{B}_{ext} = B_{ext}\hat{z}$.

## B.6 UNPERTURBED HAMILTONIAN FOR HYDROGEN ATOM (ONLY ACCOUNTS FOR THE INTERACTION OF THE ELECTRON WITH THE NUCLEUS VIA COULOMB ATTRACTION)

$$\hat{H}^0 = \frac{\hat{p}^2}{2m} + V(r) = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right) \tag{B.2}$$

### B.6.1 Degeneracy of the Unperturbed Hamiltonian $\hat{H}^0$

4. What is one complete set of quantum numbers that describe the eigenstates of $\hat{H}^0$ given by equation (B.2) (include spin degree of freedom)?

5. What is the unperturbed energy corresponding to $\hat{H}^0$ in equation (B.2) in terms of the principal quantum number $n$?

6. Based upon your answers to the two preceding questions, should there be degeneracy in the unperturbed spectrum of hydrogen atom given by equation (B.2)? Explain.

7. What is the degeneracy of an energy level with energy $E_n$ for a given $n$ (including degeneracy due to spin degrees of freedom)?

8. Circle **ALL** the representations below in which $\hat{H}^0$ is a diagonal matrix (fixed $n$).
   a. the coupled representation
   b. the uncoupled representation
   c. any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $n$.
   d. any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $n$.
   e. Neither the coupled nor the uncoupled representation

The entire infinite dimensional unperturbed Hamiltonian $\hat{H}^0$ is diagonal if eigenstates of $\hat{H}^0$ are chosen as basis states. In each degenerate subspace of $\hat{H}^0$ (fixed $n$), the $\hat{H}^0$ matrix is a constant $(-\frac{13.6\text{ eV}}{n^2})$ multiplied by the identity matrix of dimension $2n^2$. For example, the $\hat{H}^0$ matrix in the degenerate subspace for $n = 2$ is shown below when the basis states are eigenstates of $\hat{H}^0$.

$$\hat{H}^0 = \begin{bmatrix} -\frac{13.6\text{eV}}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{13.6\text{eV}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{13.6\text{eV}}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{13.6\text{eV}}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{13.6\text{eV}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{13.6\text{eV}}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{13.6\text{eV}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{13.6\text{eV}}{4} \end{bmatrix} \tag{B.3}$$

$$= -\frac{13.6\text{eV}}{4} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{B.4}$$

9. a. For the $\hat{H}^0$ matrix given above for $n = 2$, can you tell whether the coupled representation or the uncoupled representation is chosen as the basis? Explain why you can or cannot tell.

   b. Can you tell whether the coupled or uncoupled representation was chosen as the basis if you are given the complete infinite dimensional, diagonal matrix for $\hat{H}^0$? Explain your answer.

- In this tutorial, the radial part of the basis states will always chosen to be $R_{nl}(r)$ for the hydrogen atom so the choice of a "good" basis focuses on choosing the angular basis appropriately.

Consider the following conversation regarding whether the unperturbed Hamiltonian $\hat{H}^0$ is diagonal if the coupled or the uncoupled representation is chosen as the angular basis for a given $n$.

**Student 1:** The unperturbed Hamiltonian $\hat{H}^0$ in equation (B.2) is only diagonal when the uncoupled representation is chosen as the basis.

**Student 2:** I disagree that the uncoupled representation is the only basis in which $\hat{H}^0$ is diagonal. $\hat{H}^0$ will also be diagonal when the coupled representation is chosen as the basis.

**Student 3:** I agree with Student 2. Angular basis states in both the coupled and the uncoupled representations are eigenstates of $\hat{H}^0$ since $\hat{H}^0$ is spherically symmetric with unperturbed energy only dependent on $n$. Furthermore, for a fixed $n$, any complete arbitrary orthogonal basis constructed using linear combinations of the coupled or uncoupled states can also be chosen as the angular part of the eigenstates of $\hat{H}^0$ since the unperturbed energy only depends on $n$ as $E_n = -\frac{13.6 \text{ eV}}{n^2}$.

**Student 2:** Yes. And since $\hat{H}^0$ is a diagonal matrix in both the coupled and the uncoupled representations, there is no way to determine whether the basis states were chosen in the coupled or the uncoupled representation in equation (B.3).

**Student 3:** The unperturbed Hamiltonian $\hat{H}^0$ is identical in both the coupled and uncoupled representations. In fact, $\hat{H}^0$ is identical so long as, for a fixed $n$, we choose any complete arbitrary orthonormal basis constructed with linear combinations of states in the coupled or uncoupled representation.

Explain why you agree or disagree with each student.

In one to two sentences, summarize what you have learned about the unperturbed Hamiltonian $\hat{H}^0$ for the hydrogen atom in equation (B.2) (pertaining to whether $\hat{H}^0$ is diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ is chosen as the angular basis).

**** Check your answers to questions 4-9: ****

4. $n, l, m_l, s, m_s$ or $n, l, s, j, m_j$ (If you omitted $s$, that is OK because $s$ is fixed to $s = \frac{1}{2}$ for the electron in the hydrogen atom.)

5. $E_n = -\frac{13.6\text{eV}}{n^2}$

6. Yes, there is degeneracy in the energy spectrum of the hydrogen atom.

7. $2\sum_{l=0}^{n-1}(2l+1) = 2n^2$. (Since for each $n$, there are $(2l+1)$ values of $m_l$ and the factor of 2 corresponds to the spin degeneracy.)

8. $\hat{H}^0$ will be diagonal if the coupled represenation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation or the uncoupled representation with the same principal quantum number $n$ is chosen as the angular basis.

9. (a) and (b). The $\hat{H}^0$ matrix will be a diagonal matrix with the unperturbed energy $E_n$ along the diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation or the uncoupled representation with the same principal quantum number $n$ is chosen as the angular basis. There is no way to distinguish between these bases if we are only given the $\hat{H}^0$ matrix since the basis states are eigenstates of $\hat{H}^0$ in all these cases (so long as we do not take linear superpositions of states with different $n$).

If any of your answers do not match the checkpoint answers for questions 4-9, go back and reconcile any difference you may have.

**Summary: The Unperturbed Hamiltonian of the Hydrogen Atom**

- For a given unperturbed energy $E_n = -\frac{13.6\text{eV}}{n^2}$, there is a $2n^2$-fold degeneracy, i.e., there are $2n^2$ different states with the same energy $E_n$.
  - For $n = 2$, there is an 8-fold degeneracy, so 8 distinctly different states have the same energy $-\frac{13.6\text{ eV}}{4}$.
- For a fixed $n$, the unperturbed Hamiltonian $\hat{H}^0$ is diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ is chosen as the angular basis.

| Unperturbed Hamiltonian | Uncoupled Representation (for a fixed $n$) | Are States in the Uncoupled Representation the Angular Part of an Eigenstate of $\hat{H}^0$? | Coupled Representation (for a fixed $n$) | Are States in the Coupled Representation the Angular Part of an Eigenstate of $\hat{H}^0$? | Is Any Complete Set of Arbitrary Linear Combinations of Orthonormal States (with the same $n$) in the Coupled or Uncoupled Representation the Angular Part of an Eigenstate of $\hat{H}^0$ | Unperturbed Energy |
|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | Yes | Diagonal | Yes | Yes | $E_n = -\frac{13.6\text{eV}}{n^2}$ |

## B.7 PERTURBATION THEORY FOR THE HYDROGEN ATOM IN AN EXTERNAL MAGNETIC FIELD

- For the hydrogen atom placed in an external magnetic field, we will treat the relativistic correction term $\hat{H}'_r$, the spin-orbit coupling term $\hat{H}'_{SO}$, and the Zeeman term $\hat{H}'_Z$ in the Hamiltonian as perturbations on $\hat{H}^0$ to find the corrections to the unperturbed energies (the Bohr energies $E_n = -\frac{13.6\text{eV}}{n^2}$).
- In order to find the corrections to the energies using perturbation theory when the unperturbed Hamiltonian $\hat{H}^0$ possesses degeneracy, we must ensure that the basis states are "**good**" states.
  - **Definition:** For a given $\hat{H}^0$ and $\hat{H}'$, a **"good"** basis consists of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ ($\hat{H}^0$ is diagonal everywhere).
- In order to determine if we have a "good" basis in each case, we can start by determining the matrix elements of the relativistic perturbation $\hat{H}'_r$, the spin-orbit perturbation $\hat{H}'_{SO}$, and the Zeeman perturbation $\hat{H}'_Z$ in the coupled and uncoupled representations and check whether the off-diagonal matrix elements of $\hat{H}'$ are zero in each degenerate subspace of $\hat{H}^0$.
- Given a perturbation $\hat{H}'$, if there are **non-zero off-diagonal matrix elements of $\hat{H}'$ in a degenerate subspace of $\hat{H}^0$** in the coupled and the uncoupled representations, neither is a "good" basis for the given $\hat{H}^0$ and $\hat{H}'$. In that case, we must diagonalize the $\hat{H}'$ matrix (in the initial basis) in each degenerate subspace of the $\hat{H}^0$ matrix explicitly to find a "good" basis.

### B.7.1 Relativistic Correction

Before discussing the relativistic correction perturbation term, let's begin by considering a perturbation $\hat{H}' = \zeta\delta(r)$ that is spherically symmetric (in which $\zeta$ is a constant such that $\hat{H}'$ has the dimensions of energy). Recall that the unperturbed Hamiltonian $\hat{H}^0$ for the hydrogen atom is also spherically symmetric (with energy only depending on $n$) and keep this in mind as you consider the following conversation. Also, note that, in general, energies for spherically symmetric potential energies depend on both quantum numbers $n$ and $l$.

Consider the following conversation regarding whether for the perturbation $\hat{H}' = \zeta\delta(r)$, the coupled representation, the uncoupled representation, or both form a "good" angular basis to find the first order corrections to the unperturbed energies of the hydrogen atom for a fixed $n$.

**Student 1:** When a perturbation $\hat{H}' = \zeta\delta(r)$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$, to find the corrections to the energies, neither the coupled nor the uncoupled representations form a "good" angular basis.

**Student 2:** I agree. Since $\hat{H}'$ only depends on $r$, it means that $n$ and $l$ are the only "good" quantum numbers. Thus neither $\{j, m_j\}$ nor $\{m_l, m_s\}$ is a set of "good" quantum numbers. Neither the coupled nor the uncoupled representation forms a "good" angular basis.

**Student 3:** No, I disagree with both Student 1 and Student 2. Because $\hat{H}'$ is spherically symmetric, its off-diagonal matrix elements will be zero in each degenerate subspace of $\hat{H}^0$ in both the coupled and the uncoupled representations, whichever is chosen as the angular basis for a fixed $n$. $\hat{H}'$ will be diagonal whether we use the uncoupled representation $|m_l, m_s\rangle$ or the coupled representation $|j, m_j\rangle$ as the basis. This implies that the coupled or uncoupled representation each forms a "good" angular basis to find the corrections to the energies.

**Student 4:** I agree with Student 3. The reason the off-diagonal matrix ele-

ments of $\hat{H}'$ are zero in the degenerate subspace of $\hat{H}^0$ is that for each $n$, the matrix elements $\langle\psi'|\hat{H}'|\psi\rangle$ can be written as the product of the radial part and the angular part. If we choose the coupled representation, the angular part is $\langle l,\ j,\ m_j|l',\ j',\ m'_j\rangle = \delta_{l,l'}\delta_{j,j'}\delta_{m_j,m'_j}$. If we choose the uncoupled representation, the angular part is $\langle l,\ m_l,\ m_s|l',\ m'_l,\ m'_s\rangle = \delta_{l,l'}\delta_{m_l,m'_l}\delta_{m_s,m'_s}$. Either way, the Kronecker delta implies that all off-diagonal matrix elements are zero for a fixed $n$. Thus, both the coupled and the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states for the same $n$ and $l$ form a "good" angular basis because $\hat{H}^0$ is diagonal and $\hat{H}' = \zeta\delta(r)$ is diagonal in the degenerate subspace of $\hat{H}^0$.

Explain why you agree or disagree with each student.

10. Is the relativistic correction term $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ diagonal if the coupled representation, the uncoupled representation, or any complete arbitrary orthonormal basis constructed with linear combinations of the coupled or uncoupled states with the same $n$ and $l$ is chosen as the angular basis? Explain. [Hint: $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$, $\hat{H}^0$, and $\hat{H}' = \zeta\delta(r)$ are all spherically symmetric and energies for spherically symmetric potential energies only depend on the quantum numbers $n$ and $l$.]

### B.7.2 Spin-Orbit Interaction

- The spin orbit coupling term in the Hamiltonian, $\hat{H}'_{SO}$, is proportional to $\vec{L} \cdot \vec{S}$. We can write $\vec{L} \cdot \vec{S}$ as $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$ or $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$. The expression that will be most beneficial in determining the matrix elements of $\hat{H}'_{SO}$ will depend on whether the coupled representation or the uncoupled representation is chosen as the basis.

11. If the coupled representation is chosen as the basis, which expression for $\vec{L} \cdot \vec{S}$ is more useful when evaluating the matrix elements of $\vec{L} \cdot \vec{S}$? Explain.

12. If the uncoupled representation is chosen as the basis, which expression for $\vec{L} \cdot \vec{S}$ is more useful when evaluating the matrix elements of $\vec{L} \cdot \vec{S}$? Explain.

- Let's evaluate the matrix elements of $\vec{L} \cdot \vec{S}$ in the coupled and the uncoupled representations in order to determine whether $\vec{L} \cdot \vec{S}$ is diagonal in each basis. This will help us later in determining a "good" angular basis when the perturbation is $\hat{H}'_{SO}$ (which is proportional to $\vec{S} \cdot \vec{L}$).

#### B.7.2.1 Coupled Representation

The spin-orbit coupling term in the Hamiltonian, $\hat{H}'_{SO}$, is proportional to $\vec{L} \cdot \vec{S}$. The expression $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$ is most useful when expressing the matrix elements of $\hat{H}'_{SO}$ in the coupled representation.

13. Evaluate the following matrix elements useful for the perturbation $\hat{H}'_{SO}$, in which the states are written in the coupled representation $|n\ l\ s\ j\ m_j\rangle$.

    a. $\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{1}{2}|\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)|2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{1}{2}\rangle$

    b. $\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{1}{2}|\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)|2\ 1\ \frac{1}{2}\ \frac{3}{2}\ -\frac{1}{2}\rangle$

    c. $\langle 2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{3}{2}|\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)|2\ 1\ \frac{1}{2}\ \frac{3}{2}\ -\frac{1}{2}\rangle$

14. Is $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$ (for a fixed $n$) if the coupled representation is chosen as the basis? [Hint: The answers to the preceding question may be helpful.]

**B.7.2.2 Uncoupled Representation** The spin-orbit coupling term in the Hamiltonian, $\hat{H}'_{SO}$, is proportional to $\vec{L} \cdot \vec{S}$. The expression $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{S}_z\hat{L}_z$ is most useful when expressing the matrix elements of $\hat{H}'_{SO}$ in the uncoupled representation.

15. Evaluate the following expressions. (The states are written in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$).

    a. $\hat{L}_-|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

    b. $\hat{L}_+|2\ 1\ \frac{1}{2}\ -1\ -\frac{1}{2}\rangle$

    c. $\hat{S}_-|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

    d. $\hat{S}_+|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

16. Evaluate the following matrix elements, in which the states are written in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$.

    a. $\langle 2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}|(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+)|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

    b. $\langle 2\ 1\ \frac{1}{2}\ 0\ -\frac{1}{2}|(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+)|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

17. Now let's evaluate the following matrix elements useful for the perturbation $\hat{H}'_{SO}$. We use the fact that $\vec{L} \cdot \vec{S}$ is proportional to $\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$.

    a. $\langle 2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}|\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

    b. $\langle 2\ 1\ \frac{1}{2}\ 0\ -\frac{1}{2}|\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z|2\ 1\ \frac{1}{2}\ -1\ \frac{1}{2}\rangle$

18. Is $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$ (for a fixed $n$) if the uncoupled representation is chosen as the basis? [Hint: The answers to the preceding questions may be helpful.]

Consider the following conversation regarding whether the $\hat{H}'_{SO}$ matrix is a diagonal matrix if, for a fixed $n$, any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states is chosen as the basis.

**Student 1:** Since $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the coupled representation, any linear combination of states in the coupled representation must also be eigenstates of $\hat{H}'_{SO}$. Thus, $\hat{H}'_{SO}$ is diagonal in the coupled representation in each degenerate subspace of $\hat{H}^0$ and also when any arbitrary complete orthonormal basis is constructed with linear combinations of the coupled states.

**Student 2:** I disagree with Student 1. For example, in general, a linear combination of energy eigenstates is NOT an energy eigenstate. For example, if $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenstates of the operator $\hat{H}'_{SO}$ with eigenvalues $E_1$ and $E_2$, respectively, then

$$\begin{aligned} \hat{H}|\psi_1\rangle &= E_1|\psi_1\rangle \\ \hat{H}|\psi_2\rangle &= E_2|\psi_2\rangle. \end{aligned}$$

The linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ gives

$$\hat{H}(|\psi_1\rangle + \psi_2\rangle) \;=\; E_1|\psi_1\rangle + E_2|\psi_2\rangle \;\neq\; E(|\psi_1\rangle + |\psi_2\rangle).$$

Thus $\hat{H}(|\psi_1\rangle + \psi_2\rangle) \neq E(|\psi_1\rangle + \psi_2\rangle)$ unless $E_1 = E_2 = E$.

**Student 3:** I agree with Student 2. If we consider $\hat{H}'_{SO}$, which is proportional to $\frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$, then $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the coupled representation $|n\ l\ s\ j\ m_j\rangle$. However, in general, $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ if linear combinations of states in the coupled representation, even with a fixed $n$, is chosen as the basis. For example, if we consider the states $|\psi_1\rangle = |2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle$ and $|\psi_2\rangle = |2\ 0\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle$

$$\begin{aligned} \tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)|\psi_1\rangle &= \tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)\left|2\ 1\ \tfrac{1}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\right\rangle \\ &= \tfrac{\hbar^2}{2}\left|2\ 1\ \tfrac{1}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\right\rangle \\ \tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)|\psi_2\rangle &= \tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)\left|2\ 0\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\right\rangle \\ &= 0\left|2\ 1\ \tfrac{1}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\right\rangle \end{aligned}$$

But the linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$, both in the $n = 2$ subspace, is not an eigenstate.

$$\begin{aligned}
\tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)(|\psi_1\rangle + |\psi_2\rangle) &= \tfrac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)(\left|2\ 1\ \tfrac{1}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\right\rangle + \left|2\ 0\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\right\rangle) \\
&= \tfrac{1}{2}\left|2\ 1\ \tfrac{1}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\right\rangle \\
&= \tfrac{1}{2}|\psi_1\rangle \\
&\neq \text{Constant}(|\psi_1\rangle + |\psi_2\rangle)
\end{aligned}$$

Explain why you agree or disagree with each student.

Consider the following conversation regarding whether the $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$, for a fixed $n$, when any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states is chosen as the angular basis.

**Student 1:** For a fixed $n$, the spin-orbit interaction term $\hat{H}'_{SO}$ is diagonal if the coupled representation is chosen as the basis. However, $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ if the uncoupled representation or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states is chosen as the basis.

**Student 2:** I disagree. Since $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the coupled representation, then $\hat{H}'_{SO}$ must also be diagonal in each degenerate subspace of $\hat{H}^0$ if any arbitrary complete orthonormal basis constructed with linear combinations of the coupled states is chosen as the basis.

**Student 3:** I disagree with Student 2. For example, the states in the uncoupled representation can be constructed with linear combinations of states in the coupled representation. Therefore, if $\hat{H}'_{SO}$ were to be diagonal in each degenerate subspace of $\hat{H}^0$ when any arbitrary complete orthonormal basis constructed with linear combinations of the coupled states is chosen as the basis, then $\hat{H}'_{SO}$ would also be diagonal if the uncoupled representation were chosen as the basis. However, this is not the case because $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ in the uncoupled representation. But, for a fixed $n$, $\hat{H}'_{SO}$ is diagonal in the coupled representation.

**Student 1:** I agree with Student 3. Also, if a matrix were diagonal if any arbitrary complete orthonormal basis constructed with linear combinations of the **coupled states** is chosen as the angular basis, then that matrix must also be diagonal when any complete orthogonal angular basis is chosen. Therefore, the matrix must also be diagonal if any arbitrary complete orthonormal basis constructed with linear combinations of the **uncoupled states** is chosen as the basis.

Explain why you agree or disagree with each student.

Student 1 and Student 3 are correct in the preceding conversation.

In one to two sentences, summarize what you have learned about the spin-orbit interaction term $\hat{H}'_{SO}$, which is proportional to $\vec{L} \cdot \vec{S}$ for the hydrogen atom (pertaining to whether $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$, for a fixed $n$, is the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ is chosen as the basis).

## SUMMARY: Spin-orbit Interaction ($\hat{H}'_{SO}$ proportional to $\vec{L} \cdot \vec{S}$)

- For a given $n$ (in each degenerate subspace of $\hat{H}^0$), the spin-orbit interaction term in the Hamiltonian, $\hat{H}'_{SO}$, **is diagonal** if the **coupled representation** is chosen as the angular basis.
- For a given $n$ (in each degenerate subspace of $\hat{H}^0$), the spin-orbit interaction term in the Hamiltonian, $\hat{H}'_{SO}$, **is NOT diagonal** if the **uncoupled representation** is chosen as the basis. (You must have found a non-zero off-diagonal matrix element in question 17.)

| Hamiltonian $\hat{H}$ | Uncoupled Representation (for a fixed $n$) | Are States in the Uncoupled Representation the Angular Part of Eigenstates of $\hat{H}$? | Coupled Representation (for a fixed $n$) | Are States in the Coupled Representation the Angular Part of Eigenstates of $\hat{H}$? | Is Any Arbitrary Linear Combination of Orthonormal States (with the same $n$ and $l$) in the Coupled or Uncoupled Representation the Angular Part of an Eigenstate of $\hat{H}$ |
|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | Yes | Diagonal | Yes | Yes |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No |

## ** Check your answers to questions 10-18: **

10. For a given $n$, $\hat{H}'_r$ in each degenerate subspace of $\hat{H}^0$ will be diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same $n$ and $l$ is chosen as the angular basis.

11. If the coupled representation is chosen as the angular basis, $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$ should be used since $|j,\ m_j\rangle$ is an eigenstate of $\hat{J}^2$, $\hat{S}^2$, and $\hat{L}^2$

12. If the uncoupled representation is chosen as the basis, $\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ should be used since $|m_l,\ m_s\rangle$ is an eigenstate of $\hat{L}_z$ and $\hat{S}_z$ and the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$ act on the uncoupled states $|m_l,\ m_s\rangle$.

13a. $\frac{1}{2}\hbar^2$

13b. 0

13c. 0

14. For a fixed $n$, $\hat{H}'_{SO}$ is diagonal if the coupled representation is chosen as the basis. If the basis states are chosen in the coupled representation ($|l,\ j,\ m_j\rangle$) in the order $|\psi_1\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_2\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$ and $|\psi_8\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, the $\hat{H}'_{SO}$ matrix for $n = 2$ is

$$\hat{H}'_{SO} = A\frac{1}{r^3}(\vec{S}\cdot\vec{L}) = \frac{2E_2^2}{3mc^2}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

15a. 0

15b. $\sqrt{2}\hbar|2\ 1\ \frac{1}{2}\ 0\ -\frac{1}{2}\rangle$

15c. $\hbar|2\ 1\ \frac{1}{2}\ -1\ -\frac{1}{2}\rangle$

15d. 0

16a. 0

16b. $\sqrt{2}\hbar^2$

17a. $-\frac{1}{2}\hbar^2$

17b. $\frac{\sqrt{2}}{2}\hbar^2$

18. For a fixed $n$, $\hat{H}'_{SO}$ is not diagonal if the uncoupled representation is chosen as the basis. If the basis states are chosen in the **uncoupled representation** ($|l,\ m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$, the $\hat{H}'_{SO}$ matrix is

$$\hat{H}'_{SO} = A\frac{1}{r^3}(\vec{S}\cdot\vec{L}) = \frac{\alpha^4 mc^2}{96}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

If any of your answers do not match the checkpoint answers to questions 10-18, go back and reconcile any difference you may have.[1]

[1] For a fixed $n$, $\hat{H}'_{SO}$ is also diagonal if an orthonormal basis includes certain **special** linear combinations of states in the coupled representation corresponding to each degenerate subspace of $\hat{H}'_{SO}$. However, $\hat{H}'_{SO}$ is **NOT diagonal** if any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $n$ is chosen as the angular basis. We will not focus on these issues in this tutorial since our goal is to find one "good" basis for perturbation theory.

### B.7.3 Zeeman Effect

If the external magnetic field is chosen to be a uniform, time independent field along the $\hat{z}$ direction given by $\vec{B} = B_{ext}\hat{z}$, the Zeeman term in the Hamiltonian is

$$\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z). \tag{B.5}$$

Consider the following conversation regarding simplifying the hydrogen atom basis states in the coupled or uncoupled representation.

**Student 1:** When we write states in the coupled or uncoupled representation, we must write all the quantum numbers that represent the state $|n\ l\ s\ j\ m_j\rangle$ or $|n\ l\ s\ m_l\ m_s\rangle$.

**Student 2:** If we are dealing with an operator acting on the states that only depends on a subset of all the quantum numbers, we can express the states with only the relevant quantum numbers and suppress the other quantum numbers for convenience. Consider $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$, where the relevant quantum numbers are $m_l$ and $m_s$ if $n$ and $s$ are fixed. We can abbreviate the state in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$ as $|l,\ m_l,\ m_s\rangle$.

**Student 3:** I agree with Student 2. Additionally, if we know we are restricted to a particular set of quantum numbers or can determine the quantum numbers from the context, we can suppress those quantum numbers without loss of generality. For example, if we are considering an electron in the $n = 2$ degenerate subspace of $\hat{H}^0$, the state in the coupled representation $|n\ l\ s\ j\ m_j\rangle = |2\ 1\ \frac{1}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle$ can be written as $|l,\ j,\ m_j\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$ since $s = \frac{1}{2}$.

Explain why you agree or disagree with each student.

19. Evaluate the following matrix elements of $\hat{H}'_Z$ in which the states are written in the uncoupled representation $|l,\ m_l,\ m_s\rangle$.

    a. $\langle 0,\ 0,\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|0,\ 0,\ \frac{1}{2}\rangle$

    b. $\langle 0,\ 0,\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|0,\ 0,\ -\frac{1}{2}\rangle$

    c. $\langle 1,\ 1,\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|1,\ 1,\ \frac{1}{2}\rangle$

    d. $\langle 1,\ 1,\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|1,\ -1,\ -\frac{1}{2}\rangle$

20. Is the $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ matrix a diagonal matrix if the uncoupled representation is chosen as the basis? [Hint: The answers to the preceding question may be helpful.]

**B.7.3.2 Coupled Representation** In the following table, the angular states for $n = 2$ are listed in the coupled representation (left), and each state in the coupled representation is given in terms of a linear combination of states in the uncoupled representation (right) using the Clebsch-Gordon table.

| | Coupled Representation $\lvert l,\ j,\ m_j\rangle$ | Uncoupled Representation $\lvert l,\ m_l\rangle\lvert s,\ m_s\rangle$ |
|---|---|---|
| $\lvert\psi_1\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_2\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_3\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{3}{2}\right\rangle$ | $\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_4\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{3}{2}\right\rangle$ | $\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_5\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{1}{2}\right\rangle$ | $\sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_6\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $-\sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_7\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{1}{2}\right\rangle$ | $\sqrt{\frac{1}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_8\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $-\sqrt{\frac{2}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |

21. Determine the following matrix elements given in the coupled representation ($|l,\ j\ m_j\rangle$). If you need to first express the states in the uncoupled representation ($|l,\ m_l\rangle|s,\ m_s\rangle$) you can use the preceding table.

    a. $\langle\psi_3|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|\psi_3\rangle = \langle 1,\ \frac{3}{2},\ \frac{3}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|1,\ \frac{3}{2},\ \frac{3}{2}\rangle$

    b. $\langle\psi_5|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|\psi_6\rangle = \langle 1,\ \frac{3}{2},\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|1,\ \frac{1}{2},\ \frac{1}{2}\rangle$

    c. $\langle\psi_5|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|\psi_1\rangle = \langle 1,\ \frac{3}{2},\ \frac{1}{2}|\frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)|0,\ \frac{1}{2},\ \frac{1}{2}\rangle$

22. Is the $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ matrix a diagonal matrix if the coupled representation is chosen as the basis? [Hint: The answers to the preceding question may be helpful.]

Consider the following conversation regarding whether the $\hat{H}'_Z$ matrix is a diagonal matrix if any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states is chosen as the basis.

**Student 1:** Since states in the uncoupled representation are eigenstates of $\hat{H}'_Z$, any linear combination of states in the uncoupled representation must also be eigenstates of $\hat{H}'_Z$. Thus, $\hat{H}'_Z$ is diagonal in the uncoupled representation and also when any arbitrary complete orthonormal basis is constructed with a linear combination of a complete set of the uncoupled states.

**Student 2:** I disagree with Student 1. If we consider $\hat{H}'_Z$ which is proportional to $(\hat{L}_z + 2\hat{S}_z)$, then states in the uncoupled representation $|n\ l\ s\ m_l\ m_s\rangle$ are eigenstates of $\hat{H}'_Z$. However, in general, linear combinations of states in the uncoupled representation are NOT eigenstates of $\hat{H}'_Z$. For example, if we consider the states $|\psi_1\rangle = |2\ 0\ \frac{1}{2}\ 0\frac{1}{2}\rangle$ and $|\psi_2\rangle = |2\ 0\ \frac{1}{2}\ 0\ -\frac{1}{2}\rangle$

$$(\hat{L}_z + 2\hat{S}_z)|\psi_1\rangle = (\hat{L}_z + 2\hat{S}_z)\left|2\ 0\tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle = \hbar\left|2\ \ 0\tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle$$

$$(\hat{L}_z + 2\hat{S}_z)|\psi_2\rangle = (\hat{L}_z + 2\hat{S}_z)\left|2\ 0\tfrac{1}{2}\ 0\ -\tfrac{1}{2}\right\rangle = -\hbar\left|2\ 0\tfrac{1}{2}\ 0\ -\tfrac{1}{2}\right\rangle$$

But the linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ is not an eigenstate.

$$\begin{aligned}(\hat{L}_z + 2\hat{S}_z)(|\psi_1\rangle + |\psi_2\rangle) &= (\hat{L}_z + 2\hat{S}_z)\left(\left|2\ 0\tfrac{1}{2}\ 0\tfrac{1}{2}\right\rangle + \left|2\ 0\ \tfrac{1}{2}\ 0\ -\tfrac{1}{2}\right\rangle\right)\\ &= \hbar\left[\left|2\ 0\tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle - \left|2\ 0\tfrac{1}{2}\ 0\ -\tfrac{1}{2}\right\rangle\right]\\ &= \hbar\left[|\psi_1\rangle - |\psi_2\rangle\right]\\ &\neq \text{Constant}(|\psi_1\rangle + |\psi_2\rangle)\end{aligned}$$

Explain why you agree or disagree with each student.

Consider the following conversation regarding whether the $\hat{H}'_Z$ matrix is a diagonal matrix if any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states is chosen as the angular basis.

**Student 1:** The Zeeman term $\hat{H}'_Z$ is diagonal if the uncoupled representation is chosen as the basis. However, $\hat{H}'_Z$ is not diagonal if the coupled representation or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states is chosen as the angular basis.

**Student 2:** I disagree. Since $\hat{H}'_Z$ is diagonal in the uncoupled representation, then $\hat{H}'_Z$ must also be diagonal if any arbitrary complete orthonormal basis constructed with linear combinations of the uncoupled states is chosen as the basis.

**Student 3:** I disagree with Student 2. For example, the states in the coupled representation can be constructed with linear combinations of states in the uncoupled representation. Therefore, if $\hat{H}'_Z$ were to be diagonal when any arbitrary complete orthonormal basis constructed with linear combinations of the uncoupled states is chosen as the basis, then $\hat{H}'_Z$ would also be diagonal if the coupled representation were chosen as the basis. However, this is not the case because $\hat{H}'_Z$ is not diagonal in the coupled representation. But $\hat{H}'_Z$ is diagonal in the uncoupled representation.

**Student 1:** I agree with Student 3. Also, if a matrix is diagonal if any arbitrary complete orthonormal basis constructed with linear combinations of the **coupled states** is chosen as the basis, then that matrix must also be diagonal when any complete orthonormal basis is chosen. Therefore, the matrix must also be diagonal if any arbitrary complete orthonormal angular basis constructed with a linear combination of the **uncoupled states** is chosen as the angular basis.

Explain why you agree or disagree with each student.

In one to two sentences, summarize what you have learned about the Zeeman term $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ for the hydrogen atom (pertaining to whether $\hat{H}'_Z$ is diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ is chosen as the angular basis).

## SUMMARY: Zeeman Effect

- For a given $n$, the Zeeman term in the Hamiltonian, $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$, **is diagonal** if the **uncoupled representation** is chosen as the angular basis.
- For a given $n$, the Zeeman term in the Hamiltonian, $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$, **is NOT diagonal** if the **coupled representation** is chosen as the angular basis. (You must have found some non-zero off-diagonal matrix elements in question 21.)

| Hamiltonian $\hat{H}$ | Uncoupled Representation (for a fixed $n$) | Are States in the Uncoupled Representation the Angular Part of Eigenstates of $\hat{H}$? | Coupled Representation (for a fixed $n$) | Are States in the Coupled Representation the Angular Part of Eigenstates of $\hat{H}$? | Is Any Arbitrary Linear Combination of Orthonormal States (with the same $n$ and $l$) in the Coupled or Uncoupled Representation the Angular Part of an Eigenstate of $\hat{H}$ |
|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | Yes | Diagonal | Yes | Yes |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No |
| $\hat{H}'_Z$ | Diagonal | Yes | Not Diagonal | No | No |

**** Check your answers to questions 19-22: ****

19a. $\mu_B B_{ext}$

19b. 0

19c. $2\mu_B B_{ext}$

19d. 0

20. $\hat{H}'_Z$ is diagonal if the uncoupled representation is chosen as the basis. If the basis states are chosen in the **uncoupled representation** ($|l,\ m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$, the $\hat{H}'_Z$ matrix is

$$\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z) = \mu_B B_{ext} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \end{bmatrix}$$

21a. $2\mu_B B_{ext}$

21b. $-\frac{\sqrt{2}}{3}\mu_B B_{ext}$

21c. 0

22. $\hat{H}'_Z$ is not diagonal if the coupled representation is chosen as the basis. If the basis states are chosen in the coupled representation ($|l,\ j,\ m_j\rangle$) in the order $|\psi_1\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_2\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$ and $|\psi_8\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, the $\hat{H}'_Z$ matrix is

$$\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z) = \mu_B B_{ext} \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

If any of your answers do not match the checkpoint answers to questions 19-22, go back and reconcile any differences you may have.[2]

[2] $\hat{H}'_Z$ is also diagonal if an orthonormal basis includes certain **special** linear combination of states in the uncoupled representation corresponding to each degenerate subspace of $\hat{H}'_Z$. However, $\hat{H}'_Z$ is **NOT diagonal** if any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $n$ is chosen as the basis. We will not focus on these issues in this tutorial since our goal is to find one "good" basis for perturbation theory.

## B.8 CHOOSING A "GOOD" BASIS

To find the first order corrections to the energies of the hydrogen atom in perturbation theory, we must first choose a "good" angular basis for the given $\hat{H}^0$ and $\hat{H}'$. Depending on the nature of the perturbation, the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states can form the "good" angular basis. Recall that the determination of a "good" basis depends on both $\hat{H}^0$ and $\hat{H}'$.

23. In the following questions, a perturbation $\hat{H}'$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For each of the following perturbations, circle **ALL** of the representations that form a "good" angular basis. Assume that for all cases, the principal quantum number is fixed to $n = 2$. ($A$ and $C$ are constants which makes the dimensions of $\hat{H}'$ that of energy in each case.)

    a. $\hat{H}' = C\delta(r)$

        i. Coupled representation

        ii. Uncoupled representation

        iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

        iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

        v. Neither coupled nor uncoupled representation

    b. $\hat{H}' = C\hat{L}_z$

        i. Coupled representation

        ii. Uncoupled representation

        iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

c. $\hat{H}' = C\hat{J}_z$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

d. $\hat{H}' = C(\hat{L}_z + 2\hat{S}_z)$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

e. $\hat{H}' = C(\hat{L}_z + \hat{S}_z)$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

f. $\hat{H}' = C(\vec{L} \cdot \vec{S})$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

g. $\hat{H}' = C\left(\frac{1}{r^n}\right)$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

h. $\hat{H}' = C\hat{p}^2$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

i. $\hat{H}' = C\hat{p}^4$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

j. $\hat{H}' = C(\hat{L}_z + 2\hat{S}_z) + A(\vec{L} \cdot \vec{S})$

i. Coupled representation

ii. Uncoupled representation

iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $l$ (i.e., states with different $l$ values are not mixed),

v. Neither coupled nor uncoupled representation

Consider the following conversation regarding determining a "good" angular basis for the perturbations $\hat{H}' = C(\hat{L}_z + \hat{S}_z)$ and $\hat{H}' = C\hat{J}_z$ acting on the hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$.

**Student 1:** The uncoupled representation forms a "good" basis when the perturbation $\hat{H}' = C(\hat{L}_z + \hat{S}_z)$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$.

**Student 2:** I agree. And the coupled representation forms a "good" basis when the perturbation $\hat{H}' = C\hat{J}_z$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$.

**Student 3:** I agree with both Student 1 and Student 2, but both students are overlooking the fact that $\hat{J}_z = \hat{L}_z + \hat{S}_z$. The perturbation $\hat{H}' = C\hat{J}_z$ is identical to the perturbation $\hat{H}' = C(\hat{L}_z + \hat{S}_z)$. Therefore, both the coupled and uncoupled representations form a "good" basis for the perturbation $\hat{H}' = C(\hat{L}_z + \hat{S}_z) = C\hat{J}_z$.

Explain why you agree or disagree with each student.

Consider the following statement regarding whether any arbitrary orthonormal basis constructed with linear combinations of states in the coupled or uncoupled representation with the same principal quantum number $n$ forms a "good" angular basis if both the coupled and uncoupled representations form a "good" angular basis.

**Student 1:** Since both the uncoupled and coupled representations form a "good" basis when the perturbation is $\hat{H}' = C(\hat{L}_z + \hat{S}_z)$, then any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same $n$ must form a "good" basis. Also, any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same $n$ must form a "good" basis.

Explain why you agree or disagree with the student.

Consider the following conversation regarding whether for the perturbation $\hat{H}' = C(\hat{L}_z + 2\hat{S}_z) + A(\vec{L} \cdot \vec{S})$, the coupled representation, the uncoupled representation, both the coupled and uncoupled representations, or neither the coupled nor uncoupled representation form a "good" angular basis to find the first order corrections to the unperturbed energies of the hydrogen atom.

**Student 1:** When the perturbation $\hat{H}' = C(\hat{L}_z + 2\hat{S}_z) + A(\vec{L} \cdot \vec{S})$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$, to find the corrections to the energies, neither the coupled nor the uncoupled representations form a "good" angular basis.

**Student 2:** I disagree. Both the coupled and the uncoupled representations are "good" angular bases since $C(\hat{L}_z + 2\hat{S}_z)$ is diagonal in the coupled representation and $A(\vec{L} \cdot \vec{S})$ is diagonal in the uncoupled representation.

**Student 3:** I agree with Student 1. Neither the coupled nor uncoupled representation form a "good" angular basis to find the first order corrections to the unperturbed energies of the hydrogen atom due to the perturbation $\hat{H}' = C(\hat{L}_z + 2\hat{S}_z) + A(\vec{L} \cdot \vec{S})$. However, a "good" angular basis will be made up of some special linear combinations of states in the coupled representation that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. These same angular basis states could be expressed as special linear combinations of states in the uncoupled representation.

Explain why you agree or disagree with each student.

**** Check your answers to question 23: ****

23a. i, ii, iii, iv

23b. ii

23c. i, ii

23d. ii

23e. i, ii

23f. i

23g. i, ii, iii, iv

23h. i, ii, iii, iv

23i. i, ii, iii, iv

23j. v

If any of your answers do not match the checkpoint answers to question 23, go back and reconcile any difference you may have.

# APPENDIX C

# FINDING THE SPLITTING IN THE HYDROGEN ATOM ENERGY SPECTRUM DUE TO AN EXTERNAL MAGNETIC FIELD (ZEEMAN EFFECT) TUTORIAL- PART II

Finding the Splitting in the Hydrogen Atom Energy Spectrum Due to an External Magnetic Field (Zeeman Effect)- PART II

The focus in degenerate perturbation theory is on ensuring that $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$. The degeneracy in $\hat{H}^0$ is $2n^2$ fold for each $n$. Our focus is always on a fixed $n$. The radial basis states are always $R_{nl}(r)$, which are solutions to the radial part of the time-independent Schrödinger equation for $\hat{H}^0$. We will learn how to determine a "good" angular basis.

## C.1 DEFINITION

For a given unperturbed Hamiltonian $\hat{H}^0$ and perturbation $\hat{H}'$, a **"good"** basis consists of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ ($\hat{H}^0$ remains diagonal everywhere since the basis states are eigenstates of $\hat{H}^0$).

- Once you have a "good" basis for a given $\hat{H}^0$ and $\hat{H}'$, you can use the same expressions that you use in non-degenerate perturbation theory for perturbative corrections.

## C.2 NOTES FOR THIS TUTORIAL:

* If you are not familiar with the steps to determine a "good" basis for finding corrections to the unperturbed energies when the energy spectrum has degeneracy, please work through the pretest, tutorial and posttest for Basics of Degenerate Perturbation Theory before working on this tutorial.
* A Hermitian operator $\hat{Q}$ has the property $Q_{ij} = (Q_{ji})^*$. Here $^*$ denotes the complex conjugate.
* For the matrix representation of a Hermitian operator $\hat{Q}$ in a given basis, we will use "$=$" or "is equal to" instead of "$\doteq$" or "is represented by" as in the notation below

$$\hat{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \quad \text{is equivalent to} \quad \hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}.$$

* In this tutorial, "degeneracy" indicates degeneracy in the unperturbed energy eigenvalue spectrum, i.e., the fact that more than one distinct energy eigenstate can have the same energy eigenvalue. For example, if

$$\hat{H}^0|\psi_a\rangle = E_a|\psi_a\rangle \qquad \text{and} \qquad \hat{H}^0|\psi_b\rangle = E_a|\psi_b\rangle,$$

  $|\psi_a\rangle$ and $|\psi_b\rangle$ are degenerate eigenstates of the Hamiltonian $\hat{H}^0$ since they correspond to the same energy $E_a$.
* We will only consider the bound states of the hydrogen atom.
* The unperturbed bound state energies $E_n$ are given by $E_n = -\frac{13.6\text{eV}}{n^2}$, $n = 1, 2, 3, \ldots$.
* **For any basis we choose, the radial part of the wavefunctions $R_{nl}$ (for given quantum numbers $n$ and $l$) will always be chosen to be the radial part of a complete set of eigenstates of $\hat{H}^0$. In other words, our focus will be on the choice of the angular part of the wavefunction in order to find a "good" basis for degenerate perturbation theory for the given $\hat{H}^0$ and $\hat{H}'$ for the hydrogen atom.**
* We will restrict our focus to a finite subspace of the infinite dimensional Hilbert space.

  - As an example of a degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$, only the subspace with the principal quantum number $n = 2$ will be considered.
  - The results can be generalized to any quantum number $n$.

* The external magnetic field will be chosen to be a uniform, time independent field along the $\hat{z}$ direction given by $\vec{B} = B_{ext}\hat{z}$.
* We will account for the coupling of the external magnetic field with both the orbital and spin angular momentum.
* We will use the following notations interchangeably to write states in the uncoupled representation (in which basis states are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{L}_Z$, and $\hat{S}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ m_l\ m_s\rangle$
  - $|l,\ m_l\rangle|s,\ m_s\rangle$ (if $n$ is fixed)
  - $|l,\ m_l,\ m_s\rangle$ (if $n$ and $s$ are fixed)
* $\vec{J} = \vec{L} + \vec{S}$
* We will use the following notations interchangeably to write states in the coupled representation (in which basis vectors are eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_Z$) with a given set of quantum numbers (notation for quantum numbers is standard):
  - $|n\ l\ s\ j\ m_j\rangle$
  - $|l,\ s,\ j,\ m_j\rangle$ (if $n$ is fixed)
  - $|l,\ j,\ m_j\rangle$ (if $n$ and $s$ are fixed)
* In both Part I and Part II of this tutorial, we will consider the case in which $s = \frac{1}{2}$ so this quantum number may be suppressed in writing a state (e.g., $|l\ m_l\ m_s\rangle$ or $|l\ j\ m_j\rangle$).

## C.3 PHYSICAL CONSTANTS

Below is a list of physical constants used in this tutorial.

| | | | |
|---|---|---|---|
| Planck's constant: | $\hbar$ | $=$ | $1.05 \times 10^{-34}$ J s |
| Mass of the electron: | $m$ | $=$ | $9.11 \times 10^{-31}$ kg |
| Magnitude of charge of an electron: | $e$ | $=$ | $1.60 \times 10^{-19}$ C |
| Speed of light: | $c$ | $=$ | $2.99 \times 10^{8}$ m/s |
| Permittivity of space: | $\epsilon_0$ | $=$ | $8.85 \times 10^{-12}$ C$^2$/J m |
| Bohr radius: | $a$ | $=$ | $\frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}$ m |
| Bohr magneton: | $\mu_B$ | $=$ | $\frac{e\hbar}{2m} = 5.79 \times 10^{-5}$ eV/T |
| Fine structure constant: | $\alpha$ | $=$ | $\frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137} = 7.30 \times 10^{-3}$ |

NOTE : The following equations may be helpful.

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$$

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle$$

$$\hat{S}^2|s\ m_s\rangle = \hbar^2 s(s+1)|s\ m_s\rangle \qquad \hat{S}_z|s\ m_s\rangle = \hbar m_s|s\ m_s\rangle$$

$$\hat{S}_\pm|s\ m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1))}|s\ m_s \pm 1\rangle$$

$$\hat{L}^2|l\ m_l\rangle = \hbar^2 l(l+1)|l\ m_l\rangle \qquad \hat{L}_z|l\ m_l\rangle = \hbar m_l|l\ m_l\rangle$$

$$\hat{L}_\pm|l\ m_l\rangle = \hbar\sqrt{l(l+1) - m_l(m_l \pm 1))}|l\ m_l \pm 1\rangle$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$\hat{J}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 j(j+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{J}_z|l,\ s,\ j\ m_j\rangle = \hbar m_j|l,\ s,\ j,\ m_j\rangle$$

$$\hat{S}^2|l,\ s,\ j,\ m_j\rangle = \hbar^2 s(s+1)|l,\ s,\ j,\ m_j\rangle \qquad \hat{L}^2|l,\ s,\ j\ m_j\rangle = \hbar^2 l(l+1)|l,\ s,\ j,\ m_j\rangle$$

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$$

## C.4 OBJECTIVES:

**Upon completion of this tutorial, you should be able to do the following for the hydrogen atom:**

1. Identify the unperturbed Hamiltonian $\hat{H}^0$ and the perturbing Hamiltonian $\hat{H}'$.
2. Identify the degeneracy in the unperturbed Hamiltonian $\hat{H}^0$ in each degenerate subspace corresponding to a principal quantum number $n$.
3. Determine a "good" basis for finding the corrections to the unperturbed energies of the hydrogen atom for only the fine structure perturbation $\hat{H}'_{fs}$.
4. Find the first order corrections to energies due to the fine structure perturbation $\hat{H}'_{fs}$.
5. Determine a "good" basis for finding the corrections to the unperturbed energies of the hydrogen atom due to the Zeeman effect (including in intermediate, strong, and weak magnetic field).
6. Find the first order corrections to energies in the intermediate field Zeeman effect.
7. Find the first order corrections to energies in the strong field Zeeman effect.
8. Find the first order corrections to energies in the weak field Zeeman effect.

## C.5 THE HYDROGEN ATOM PLACED IN AN EXTERNAL MAGNETIC FIELD

The Hamiltonian of the hydrogen atom placed in an external magnetic field is

$$\hat{H} = \hat{H}^0 + \hat{H}'_r + \hat{H}'_{SO} + \hat{H}'_Z = \hat{H}^0 + \hat{H}'_{fs} + \hat{H}'_Z \tag{C.1}$$

in which

- $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$ accounts only for the interaction of the electron with the nucleus via Coulomb attraction
- $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term
- $\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}(\vec{L}\cdot\vec{S})$ is the spin-orbit interaction term

and combining the relativistic and spin-orbit terms

- $\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r$ is the fine structure term
- $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ is the Zeeman term, in which $\vec{B}_{ext} = B_{ext}\hat{z}$.

## C.6 PERTURBATION THEORY

- In order to find the first order corrections to the energies due to a perturbation $\hat{H}'$, we must first find a "good" basis for the given $\hat{H}^0$ and $\hat{H}'$.
- A "good" basis is defined as one which satisfies the following two conditions:
  1. The entire unperturbed Hamiltonian $\hat{H}^0$ is diagonal (i.e., basis states are eigenstates of $\hat{H}^0$).
     - We know from Part I of this tutorial that the unperturbed Hamiltonian matrix $\hat{H}^0$ is diagonal if the coupled or uncoupled representation or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ is chosen as the angular basis (as a consequence of the spherical symmetry of $\hat{H}^0$ and the unperturbed energy only depending on $n$ as $E_n = -\frac{13.6\text{ eV}}{n^2}$).

2. The perturbing Hamiltonian $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$.
   - We always choose $R_{nl}$ as the radial part of the basis and focus on the angular basis for determining a "good" basis for a given $\hat{H}^0$ and $\hat{H}'$.
   - We shall consider several types of perturbing Hamiltonian, $\hat{H}'$, and determine whether the coupled representation, the uncoupled representation, some special orthonormal basis constructed with linear combinations of the coupled or the uncoupled states, or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or the uncoupled states with the same principal quantum number $n$ and the same $l$ diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.

- In Part I, we found:
  - $\hat{H}^0$ (spherically symmetric with energy only depending on $n$ as $E_n = -\frac{13.6 \text{ eV}}{n^2}$) is diagonal if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled or the uncoupled representation (with the same $n$) is chosen as the angular basis.
  - $\hat{H}'_r$ (spherically symmetric with energy depending on both $n$ and $l$) is diagonal in each degenerate subspace of $\hat{H}^0$ if the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states with the same $n$ and $l$ in the coupled or the uncoupled representation is chosen as the angular basis.
  - $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ if the coupled representation is chosen as the angular basis.
  - $\hat{H}'_Z$ is diagonal if the uncoupled representation is chosen as the angular basis.

### C.6.1 The Hydrogen Atom in an External Magnetic Field

- In order to find the corrections to the unperturbed energies in the presence of an external magnetic field, we shall consider the following two terms in the Hamiltonian perturbatively:

$$\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z \tag{C.2}$$

  in which $\hat{H}'_{fs}$ is the fine structure correction term and $\hat{H}'_Z$ is the Zeeman term incorporating the effect of the external magnetic field.
- The perturbative corrections due to these terms are small compared to the unperturbed energies due to $\hat{H}^0$, but both terms are important in terms of determining splittings in the energy spectrum so that they should both be considered simultaneously.
- Let's first consider the fine structure. Here is the order in which we shall proceed:

I. Determining a "good" angular basis and corrections to the energies for **ONLY** the fine structure perturbation $\hat{H}'_{fs}$.
   - The fine structure correction $\hat{H}'_{fs}$ is made up of two mechanisms: $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$, in which $\hat{H}'_r$ is the relativistic correction term and $\hat{H}'_{SO}$ is the spin-orbit interaction term (due to the coupling of the orbital and spin angular momenta of the electron).

II. Determining a "good" angular basis and corrections to the energies for **ONLY** the Zeeman perturbation $\hat{H}'_Z$.
   - The Zeeman effect in the hydrogen atom (or any atom) is the splitting of the energy spectrum as a result of placing the atom in an external magnetic field.

III. Determining a "good" angular basis and corrections to the energies for **BOTH** the fine structure and Zeeman perturbations combined: $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

- In this tutorial we will learn about three cases with $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$:
  - **CASE 1: The Intermediate Field Zeeman Effect ($E'_Z \approx E'_{fs}$)**
    - The intermediate field Zeeman effect describes a situation when the corrections to the energies from the fine structure term $E'_{fs}$ and the Zeeman term $E'_Z$ are comparable to one another (We will use the notations $E'_Z \approx E'_{fs}$ to denote the intermediate field Zeeman effect).

- Along with two limiting cases:
  - **CASE 2: The Strong Field Zeeman Effect ($E'_Z \gg E'_{fs}$)**
    - The strong field Zeeman effect describes a situation when the corrections to the energies from the Zeeman term $E'_Z$ are much larger than the corrections to the energies from the fine structure term $E'_{fs}$ (We will use the notation $E'_Z \gg E'_{fs}$ to denote the strong field Zeeman effect).

  - **CASE 3: The Weak Field Zeeman Effect ($E'_{fs} \gg E'_Z$)**
    - The weak field Zeeman effect describes a situation when the corrections to the energies from the fine structure term $E'_{fs}$ are much larger than the corrections to the energies from the Zeeman term $E'_Z$ (We will use the notation $E'_{fs} \gg E'_Z$ to denote the weak field Zeeman effect).

**I. Determining the "GOOD" Angular Basis and Corrections to the Energies for ONLY the Fine Structure Perturbation $\hat{H}'_{fs}$.**

As noted, the fine structure perturbation is comprised of two mechanisms: the relativistic correction $\hat{H}'_r$ and the spin-orbit interaction $\hat{H}'_{SO}$:

$$\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}. \tag{C.3}$$

We shall discuss each separately and then find the first order corrections to the energies of the hydrogen atom due to the combined effect of the relativistic correction and the spin-orbit interaction.

### C.6.2 Finding a "GOOD" Basis for the Relativistic Correction Term as a Perturbation for the Hydrogen Atom

A perturbation $\hat{H}'_r$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ such that the relativistic correction term in the Hamiltonian is

$$\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}. \tag{C.4}$$

1. For the perturbation $\hat{H}'_r$, will a "good" angular basis for finding the corrections to the energies be the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ and the same $l$? Explain.

Consider the following conversation regarding finding a "good" basis for the relativistic term $\hat{H}'_r$ as a perturbation on $\hat{H}^0$ for the hydrogen atom.

**Student 1:** We found that for a fixed $n$ the **spherically symmetric** unperturbed Hamiltonian $\hat{H}^0$ is diagonal in the coupled or the uncoupled representation, as well as in any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation or the uncoupled representation. Since the relativistic correction $\hat{H}'_r$ is also spherically symmetric, $\hat{H}'_r$ will also be diagonal in the coupled or the uncoupled representation, as well as in any arbitrary complete orthonormal basis constructed with linear combinations of basis states with the same $n$ and $l$ in the coupled representation or the uncoupled representation.

**Student 2:** I agree. $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}(\frac{1}{r})$ and $\hat{H}'_r$ is proportional to $\hat{p}^4$. Both terms are spherically symmetric because $[\hat{H}^0, \hat{\vec{L}}] = 0$ and $[\hat{H}'_r, \hat{\vec{L}}] = 0$. However, the eigenvalues of $\hat{H}^0$ only depend on $n$ while the eigenvalues of $\hat{H}'$ depend on both $n$ and $l$. Thus, $\hat{H}'_r$ will also be diagonal in both the coupled and the uncoupled representation, as well as any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation or the uncoupled representation.

**Student 3:** I disagree with both Student 1 and Student 2. The fact that $\hat{H}'_r$ is spherically symmetric is not enough information to determine whether the coupled or uncoupled representation or both will form a "good" angular basis.

**Student 4:** I agree with Student 1 and Student 2. For finding the corrections to the energies due to the perturbation $\hat{H}'_r$, a "good" angular basis can be chosen to be the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ and the same $l$.

Explain why you agree or disagree with each student.

The relativistic correction term $\hat{H}'_r$ is spherically symmetric and its energy eigenvalues depend on the quantum numbers $n$ and $l$, and therefore the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states with a fixed $n$ and $l$ in the coupled or the uncoupled representation will form a "good" basis. For example, using the same reasoning as for the unperturbed Hamiltonian $\hat{H}^0$ and the example when $\hat{H}'$ was proportional to $\delta(r)$ in Part I of this tutorial, for a given $n$ and $l$, $\hat{H}'_r$ will be a diagonal in each degenerate subspace of $\hat{H}^0$ because the angular part of the matrix elements of $\hat{H}'_r$ will involve $\langle l, j, m_j | l', j', m'_j \rangle = \delta_{l,l'}\delta_{j,j'}\delta_{m_j,m'_j}$ if we choose the coupled representation or $\langle l, m_l, m_s | l', m'_l, m'_s \rangle = \delta_{l,l'}\delta_{m_l,m'_l}\delta_{m_s,m'_s}$ if we choose the uncoupled representation. The off-diagonal matrix elements will be zero due to the Kronecker deltas in either case.

**** Check your answers to question 1. ****

1. The coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states with the same $n$ and $l$ in the coupled or the uncoupled representation with the same principal quantum number $n$ and the same $l$ will form a "good" angular basis for finding the corrections to the energies of the hydrogen atom due to the spherically symmetric relativistic correction term $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$.

If your answer to question 1 does not match with the checkpoint, go back and reconcile any differences.

### C.6.3 First Order Corrections to the Energy Spectrum of the Hydrogen Atom Due to the Relativistic Correction Term Using Perturbation Theory

Now that we have determined that the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled or the uncoupled representation will form a "good" angular basis for $\hat{H}'_r$ as the perturbation, we can determine the corrections to the energies.

- Let $\{|\psi_n\rangle\}$ represent a "good" basis set in which the quantum numbers to describe the angular part of the $\{|\psi_n\rangle\}$ have been suppressed (those quantum numbers will depend, e.g., on whether we choose the coupled or uncoupled representation for the angular part).
- If $\{|\psi_n\rangle\}$ forms a "good" basis for $\hat{H}'_r$ as a perturbation on the unperturbed Hamiltonian $\hat{H}^0$, then the first order correction to the energy due to $\hat{H}'_r$ is given by (using the fact that $\hat{p}^2$ is Hermitian, i.e., $(\hat{p}^2)^\dagger = \hat{p}^2$)

$$E'_r = \langle\psi_n|\hat{H}'_r|\psi_n\rangle = \langle\psi_n| - \frac{\hat{p}^4}{8m^3c^2}|\psi_n\rangle = -\frac{1}{8m^3c^2}\langle\hat{p}^2\psi_n|\hat{p}^2\psi_n\rangle. \tag{C.5}$$

Consider the following statement regarding evaluating $\hat{p}^2|\psi_n\rangle$.

**Student 1:** We evaluate $\hat{p}^2|\psi_n\rangle$ by considering the Time-Independent Schrödinger Equation or TISE for the unperturbed Hamiltonian $\hat{H}^0|\psi_n\rangle = E_n|\psi_n\rangle$. Using the TISE $[\frac{\hat{p}^2}{2m} + V(r)]|\psi_n\rangle = E_n|\psi_n\rangle$, rearranging and solving for $\hat{p}^2|\psi_n\rangle$ gives $\hat{p}^2|\psi_n\rangle = 2m[E_n - V(r)]|\psi_n\rangle$ which is helpful in evaluating $E'_r$ in equation (C.5). Using $\langle\hat{p}^2\psi_n|\hat{p}^2\psi_n\rangle = (2m)^2\langle\psi_n|[E_n - V(r)]^2|\psi_n\rangle$, in which $V(r)$ for the hydrogen atom is proportional to $\frac{1}{r}$, we can find the first order corrections to the energies due to $\hat{H}'_r$ in Eq. (C.5).

Do you agree with Student 1's approach? Explain your reasoning.

Student 1's method is helpful in determining $\hat{p}^2|\psi_n\rangle$. The first order correction to the energy due to $\hat{H}'_r$ in the "good" basis $\{|\psi_n\rangle\}$ is given by

$$E'_r = -\frac{1}{8m^3c^2}\langle\hat{p}^2\psi_n|\hat{p}^2\psi_n\rangle = -\frac{1}{8m^3c^2}\langle\psi_n|[2m(E_n - V(r))]^2|\psi_n\rangle \tag{C.6}$$

$$E'_r = -\frac{1}{2mc^2}\langle\psi_n|E_n^2 - 2E_nV(r) + (V(r))^2|\psi_n\rangle. \tag{C.7}$$

For the Coulomb potential energy $V(r) = -\frac{1}{4\pi\epsilon_0}\left(\frac{e^2}{r}\right)$, the first order correction to the energy becomes

$$E'_r = -\frac{1}{2mc^2}\langle\psi_n|\left[E_n^2 + 2E_n\frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right) + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left(\frac{1}{r^2}\right)\right]|\psi_n\rangle. \tag{C.8}$$

It can be shown that using the radial part of the wavefunction $R_{nl}$ (for a given $n$ and $l$) for the unperturbed Hamiltonian $\hat{H}^0$ for the hydrogen atom yields

$$\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2a} \qquad \text{and} \qquad \left\langle\frac{1}{r^2}\right\rangle = \frac{1}{(l+1/2)n^3a^2}$$

with Bohr radius

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2}.$$

The first order correction to the n$^{\text{th}}$ energy state $E_n$ due to the relativistic correction is

$$E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]. \tag{C.9}$$

In one to two sentences, summarize what you have learned about the "good" angular basis states for finding the first order corrections to the energy spectrum of the hydrogen atom due to the relativistic correction $\hat{H}'_r$ (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of a complete set of states with the same principal quantum number $n$ and the same $l$ in the coupled or uncoupled representation form a "good" angular basis or all of them form a "good" angular basis).

## Summary: Finding a "GOOD" Angular Basis for the Relativistic Correction

- The perturbation matrix due to the relativistic correction $\hat{H}'_r$ is a diagonal matrix in the degenerate subspace of $\hat{H}^0$ in both the coupled and the uncoupled representation, or in any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ and the same $l$.
- The coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ and the same $l$ form a "good" basis for finding corrections to the energies.

| Hamiltonian | Uncoupled Representation (for a fixed $n$) | Is the Uncoupled Representation a "Good" Basis? | Coupled Representation (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Is Any Arbitrary Complete Orthonormal Basis Constructed with Linear Combinations of a Complete Set of States with the Same $n$ and $l$ in the Coupled or Uncoupled Representation a "Good" Basis? | Energy |
|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | — | Diagonal | — | — | $E_n = -\frac{13.6\text{eV}}{n^2}$ |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes | $E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$ |

### C.6.4 Finding a "GOOD" Angular Basis for the Spin-orbit Interaction Correction to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory

A perturbation $\hat{H}'_{SO}$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ such that the spin-orbit interaction term in the Hamiltonian is

$$\hat{H}'_{SO} = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S}. \tag{C.10}$$

2. In each degenerate subspace of $\hat{H}^0$, the off-diagonal matrix elements of $\hat{H}'_{SO}$ should be zero in a "good" basis. Does the coupled or the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$ form a "good" angular basis for finding the corrections to the energies? Explain.

Consider the following conversation about finding a "good" angular basis for the hydrogen atom due to the spin-orbit interaction term as the perturbation.

**Student 1:** The spin-orbit interaction term is proportional to $\vec{L} \cdot \vec{S}$. Does the coupled or uncoupled representation, or any arbitrary complete orthonormal basis found with their linear combinations form a "good" angular basis for finding the corrections to the energies?

**Student 2:** Since $\vec{L} \cdot \vec{S} = \hat{L}_x \hat{S}_x + \hat{L}_y \hat{S}_y + \hat{L}_z \hat{S}_z$, the uncoupled representation must be a "good" basis because the basis states in the uncoupled representation are eigenstates of both $\hat{S}_z$ and $\hat{L}_z$.

**Student 3:** I disagree with Student 2. $\vec{L} \cdot \vec{S}$ is diagonal in the coupled representation because $J^2 = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S}) = \hat{L}^2 + \hat{S}^2 + 2\vec{L} \cdot \vec{S}$ which implies $\vec{L} \cdot \vec{S} = \frac{1}{2}(\hat{J}^2 - \hat{S}^2 - \hat{L}^2)$. The basis states in the coupled representation are eigenstates of $\hat{J}^2$, $\hat{S}^2$, and $\hat{L}^2$ and hence eigenstates of $\vec{L} \cdot \vec{S}$.

**Student 4** I agree with Student 3. $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ when the coupled representation is chosen as the basis, but not when the uncoupled representation is chosen as the basis. The coupled representation forms a "good" basis for the given $\hat{H}^0$ and $\hat{H}'_{SO}$.

Do you agree with Student 2 or Student 3? Explain.

(If you need further help with why $\vec{L} \cdot \vec{S}$ is diagonal in the coupled representation, see Part I of this tutorial.)

**** Check your answer to question 2. ****

2. The coupled representation forms a "good" angular basis for finding the corrections to the energies of the hydrogen atom due to the spin-orbit interaction term $\hat{H}'_{SO}$.

If your answer to question 2 does not match with the checkpoint, go back and reconcile any differences.

### C.6.5 First Order Corrections to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory Due to the Spin-orbit Interaction

Student 3 is correct in the preceding conversation in stating that the coupled representation will form a "good" angular basis for finding the correction to the energy due to the spin-orbit interaction as a perturbation. The first order corrections to the energies due to the spin-orbit interaction in this "good" basis are given by

$$E'_{SO} = \langle n\ l\ s\ j\ m_j|\hat{H}'_{SO}|n\ l\ s\ j\ m_j\rangle = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2}\langle n\ l\ s\ j\ m_j|\frac{1}{r^3}\vec{L}\cdot\vec{S}|n\ l\ s\ j\ m_j\rangle$$

$$E'_{SO} = A\langle n\ l\ s\ j\ m_j|\frac{1}{r^3}\vec{L}\cdot\vec{S}|n\ l\ s\ j\ m_j\rangle \tag{C.11}$$

where $A = \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2}$.

Separating the radial ($R_{nl}(r)$) and angular parts of eigenstates $\{|\psi\rangle\}$ of $\hat{H}^0$ in the coupled representation, the angular part is

$$\begin{aligned}\left\langle l\ s\ j\ m_j\left|\vec{L}\cdot\vec{S}\right|l\ s\ j\ m_j\right\rangle &= \left\langle l\ s\ j\ m_j\left|\tfrac{\hat{J}^2-\hat{L}^2-\hat{S}^2}{2}\right|l\ s\ j\ m_j\right\rangle \\ &= \tfrac{\hbar^2}{2}[j(j+1)-l(l+1)-s(s+1)]\end{aligned} \tag{C.12}$$

and the radial part is

$$\left\langle n\ l \left| \frac{1}{r^3} \right| n\ l \right\rangle = \frac{1}{l(l+1)(l+1/2)n^3a^3}. \tag{C.13}$$

Thus, combining equations (C.11), (C.12), and (C.13), the first order correction to the energy due to the spin-orbit interaction is

$$E'_{SO} = \frac{E_n^2}{mc^2}\left[\frac{n(j(j+1)-l(l+1)-3/4)}{l(l+1)(l+1/2)}\right]. \tag{C.14}$$

In one to two sentences, summarize what you have learned about the "good" states for finding the first order corrections to the energy spectrum of the hydrogen atom due to the spin-orbit interaction $\hat{H}'_{SO}$ (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" basis).

**Summary: Finding a "GOOD" Angular Basis for the Spin-orbit Interaction Term $\hat{H}'_{SO}$**

- $\hat{H}'_{SO} = A\frac{1}{r^3}(\vec{L}\cdot\vec{S}) = A\frac{1}{r^3}\left[\frac{1}{2}(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)\right]$ is diagonal in the each degenerate subspace of $\hat{H}^0$ in the coupled representation.
  - The basis states in the coupled representation are eigenstates of $\hat{J}^2$, $\hat{L}^2$ and $\hat{S}^2$ and hence $\hat{H}'_{SO}$ is diagonal in each degenerate subspace of $\hat{H}^0$ if the coupled representation is chosen as the angular basis.
- The coupled representation forms a "good" angular basis for finding the corrections to the energies of the hydrogen atom due to $\hat{H}'_{SO}$.

| Hamiltonian | Uncoupled Representation (for a fixed $n$) | Is the Uncoupled Representation a "Good" Basis? | Coupled Representation (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Is Any Arbitrary Complete Orthonormal Basis Constructed with Linear Combinations of a Complete Set of States with the Same $n$ and $l$ in the Coupled or Uncoupled Representation a "Good" Basis? | Energy |
|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | — | Diagonal | — | — | $E_n = -\frac{13.6\text{eV}}{n^2}$ |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes | $E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$ |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E'_{SO} = \frac{E_n^2}{mc^2}\left[\frac{n(j(j+1)-l(l+1-3/4))}{l(l+1)(l+1/2)}\right]$ |

### C.6.6 Finding a "Good" Angular Basis for the Fine Structure Correction Term to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory

Consider the following conversation regarding finding a "good" angular basis for fine structure term $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ as a perturbation on the unperturbed Hamiltonian $\hat{H}^0$.

**Student 1:** The fine structure term $\hat{H}'_{fs}$ is made up of two mechanisms: $\hat{H}'_{SO}$ and $\hat{H}'_r$. The "good" angular basis is one in which both $\hat{H}'_{SO}$ and $\hat{H}'_r$ are diagonal in each degenerate subspace of $\hat{H}^0$.

**Student 2:** I agree. In the preceding table, the coupled representation is a "good" angular basis for both the relativistic correction term $\hat{H}'_r$ and the spin-orbit interaction term $\hat{H}'_{SO}$, because $\hat{H}'_r$ and $\hat{H}'_{SO}$ are both diagonal in each degenerate subspace of $\hat{H}^0$ in the coupled representation. Therefore, the coupled representation forms a "good" angular basis for finding the corrections to the energies due to the fine structure term $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$.

Explain why you agree or disagree with each student.

### C.6.7 First Order Corrections to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory Due to the Fine Structure

Combining the first order corrections to the energies for the hydrogen atom due to the relativistic correction term in equation (C.9) and spin-orbit interaction term from equation (C.14) gives the first order correction to the energies due to the fine structure correction term in the hydrogen atom.

$$E'_{fs} = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{(j+1/2)} - 3\right] \tag{C.15}$$

3. How many distinct energies does the $n = 2$ state split into? Explain. [Hint: How many possible values of $j$ are there for the $n = 2$ subspace?]

**** Check your answer to question 3. ****

3. For $n = 2$, there are two possible values of $j$, $j = \{\frac{1}{2}, \frac{3}{2}\}$. The energies split into two distinct levels.

| $l$ | $s$ | $j$ | $E'_{fs}$ | Number of States |
|---|---|---|---|---|
| 0 | $\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{5E_2^2}{2mc^2}$ | 2 |
| 1 | $\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{5E_2^2}{2mc^2}$ | 2 |
| 1 | $\frac{1}{2}$ | $\frac{3}{2}$ | $-\frac{E_2^2}{2mc^2}$ | 4 |

If your answers to question 3 do not match with the checkpoint, go back and reconcile any differences.

In one to two sentences, summarize what you have learned about the "good" angular basis states for finding the first order corrections to the energy spectrum of the hydrogen atom due to the fine structure term $\hat{H}'_{fs}$ (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" angular basis).

## Summary: Finding a "GOOD" Angular Basis for the Fine Structure

- For the entire fine structure perturbation $\hat{H}' = \hat{H}'_r + \hat{H}'_{SO}$, the coupled representation forms a "good" angular basis because $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the coupled representation.

| Hamiltonian | Uncoupled Representation (for a fixed $n$) | Is the Uncoupled Representation a "Good" Basis? | Coupled Representation (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Is Any Arbitrary Complete Orthonormal Basis Constructed with Linear Combination of a Complete Set of States with the Same $n$ and $l$ in the Coupled or Uncoupled Representation a "Good" Basis? | Energy |
|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | — | Diagonal | — | — | $E_n = -\frac{13.6\text{eV}}{n^2}$ |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes | $E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$ |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E'_{SO} = \frac{E_n^2}{mc^2}\left[\frac{n(j(j+1)-l(l+1-3/4))}{l(l+1)(l+1/2)}\right]$ |
| $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E'_{fs} = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{(j+1/2)} - 3\right]$ |

# II. Determining a "GOOD" Angular Basis and Corrections to the Energies for ONLY the Zeeman Perturbation $\hat{H}'_Z$.

## Zeeman Effect

### C.6.8 Finding a "GOOD" Angular Basis for the Zeeman term as a Perturbation for the Hydrogen Atom

Note: Treating the Zeeman term as the only perturbation on the unperturbed Hamiltonian is a hypothetical case, one should always consider both the Zeeman term and the fine structure term when an external magnetic field is applied to the hydrogen atom. This hypothetical case is presented here to help when later we consider both the fine structure term and the Zeeman term as perturbations for the hydrogen atom.

- A perturbation $\hat{H}'_Z$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$. The Zeeman perturbation term in the Hamiltonian is

$$\hat{H}'_Z = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}_{ext} = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z) \tag{C.16}$$

  in which $\vec{B}_{ext} = B_{ext}\hat{z}$.

4. In each degenerate subspace of $\hat{H}^0$, the off-diagonal matrix elements of $\hat{H}'_Z$ will be zero in a "good" basis. Is a "good" angular basis for finding the corrections to the energies the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of the coupled or uncoupled states with the same principal quantum number $n$? Explain.

Consider the following conversation regarding choosing a "good" basis when the perturbation is
$\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$.

**Student 1:** When a perturbation $\hat{H}'_Z = \mu_B B_{ext}(\hat{L}_z + 2\hat{S}_z)$ acts on a hydrogen atom, the uncoupled representation is a "good" angular basis for finding the first order corrections to the energies.

**Student 2:** I disagree. We can use either the coupled or the uncoupled representation to find the first order corrections to the energies. Since $\hat{J}_Z = \hat{L}_z + \hat{S}_z$, the perturbation $\hat{H}'_Z = \mu_B B_{ext}(\hat{L}_z + 2\hat{S}_z)$ is not much different from $\hat{J}_Z$ and so the coupled representation is also a "good" angular basis.

**Student 3:** I only agree with Student 1. $\hat{J}_Z$ is diagonal in both the coupled and the uncoupled representation. However, $\hat{H}' = \mu_B B_{ext}(\hat{L}_z + 2\hat{S}_z) = \mu_B B_{ex}(\hat{J}_z + \hat{S}_z)$ is not proportional to $\hat{J}_z$. Therefore, $\hat{H}'_Z = \mu_B B_{ext}(\hat{L}_z + 2\hat{S}_z)$ is only diagonal in the uncoupled representation in which the basis states are eigenstates of $\hat{L}_z$ and $\hat{S}_z$.

Explain why you agree or disagree with each student.

(If you need further help with why $\hat{L}_z + 2\hat{S}_z$ is diagonal in the uncoupled representation and not the coupled representation, refer to the Part I of this tutorial.)

**** Check your answer to question 4. ****

4. The uncoupled representation forms a "good" basis for finding the corrections to the energies of the hydrogen atom due to only the Zeeman term $\hat{H}'_Z$.

If your answer to question 4 does not match with the checkpoint, go back and reconcile any differences.

### C.6.9 First Order Corrections to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory Due to the Zeeman Term

Student 1 and Student 3 are correct in the preceding conversation in stating that the uncoupled representation will form a "good" angular basis for $\hat{H}'_Z$ on $\hat{H}^0$.

5. What are the first order corrections to the energies due to the Zeeman term $\hat{H}'_Z$ using a "good" basis?

6. How many distinct energies does the $n = 2$ state split into when we take into account $\hat{H}'_Z$ as a perturbation on $\hat{H}^0$? Explain. [Hint: How many possible values of $m_l + 2m_s$ are there for $n = 2$?]

**** Check your answer to questions 5-6. ****

5. The first order corrections to the energies due to only the Zeeman term $\hat{H}'_Z$ using a "good" basis (the uncoupled representation) is given by

$$E'_Z = \mu_B B_{ext}(m_l + 2m_s) \tag{C.17}$$

6. 5 distinct energies. For the $n = 2$ subspace, there are three possible values of $m_l$ $(-1, 0, 1)$ for $l = 1$ and one possible values of $m_l$ $(0)$ for $l = 0$. For each value of $l$, there are two possible values of $m_s$ $(\frac{1}{2}, -\frac{1}{2})$.

| $l$ | $m_l$ | $m_s$ | Energy $(E'_Z)$ |
|---|---|---|---|
| 1 | $-1$ | $\frac{1}{2}$ | $0$ |
| | $-1$ | $-\frac{1}{2}$ | $-2\mu_B B_{ext}$ |
| | $0$ | $-\frac{1}{2}$ | $-\mu_B B_{ext}$ |
| | $0$ | $\frac{1}{2}$ | $\mu_B B_{ext}$ |
| | $1$ | $-\frac{1}{2}$ | $0$ |
| | $1$ | $\frac{1}{2}$ | $2\mu_B B_{ext}$ |
| 0 | $0$ | $-\frac{1}{2}$ | $-\mu_B B_{ext}$ |
| | $0$ | $\frac{1}{2}$ | $\mu_B B_{ext}$ |

If your answers to questions 5 and 6 do not match with the checkpoint, go back and reconcile any differences.

In one to two sentences, summarize what you have learned about the "good" states for finding the first order corrections to the energy spectrum of the hydrogen atom due to only the Zeeman term $\hat{H}'_Z$ (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis found with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" basis).

## Summary: Finding a "GOOD" Angular Basis for Various Perturbations on $\hat{H}^0$

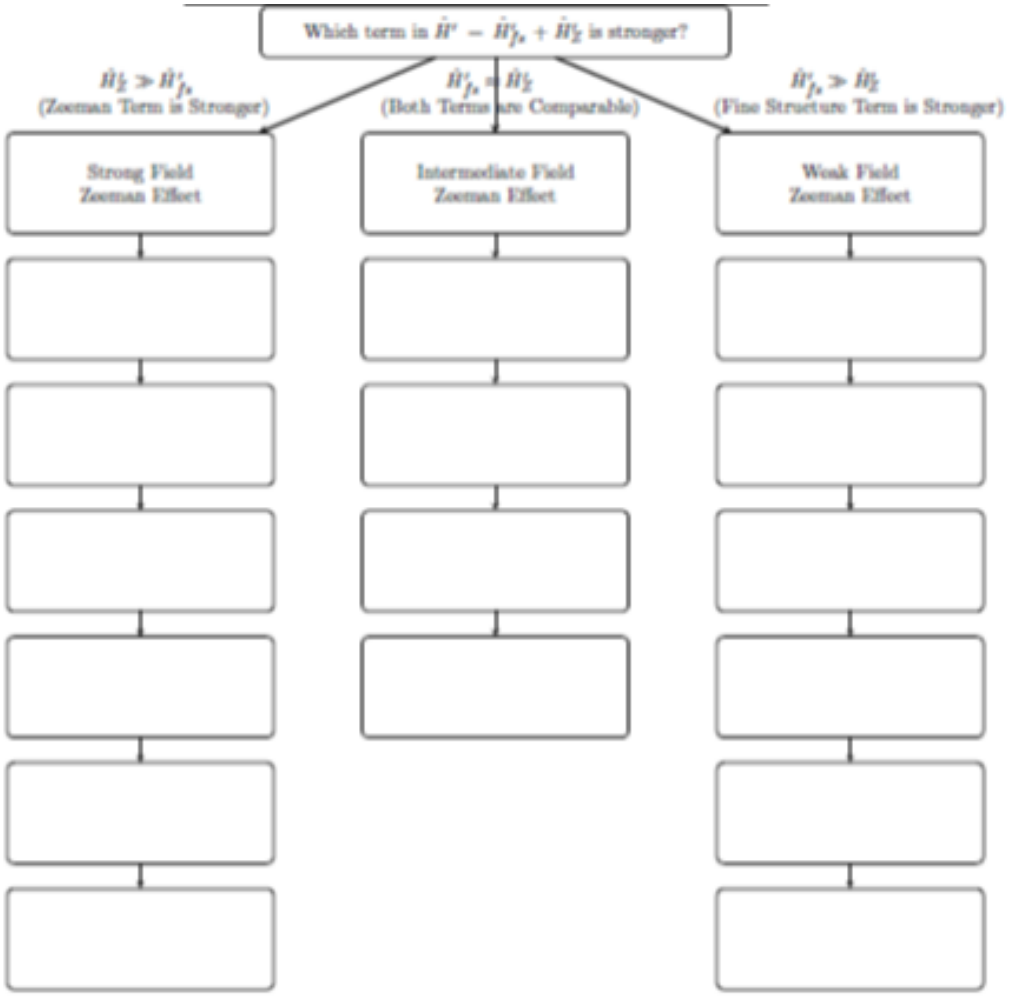
- $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}_0$ in the uncoupled representation.
  - The basis states in the uncoupled representation are eigenstates of $\hat{L}_z$ and $\hat{S}_z$
- The uncoupled representation forms a "good" angular basis for finding the corrections to the energies due to the Zeeman perturbation $\hat{H}'_Z$.

| Hamiltonian | Uncoupled Representation (for a fixed $n$) | Is the Uncoupled Representation a "Good" Basis? | Coupled Representation (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Is Any Arbitrary Complete Orthonormal Basis Constructed with Linear Combinations of a Complete Set of States with the Same $n$ and $l$ in the Coupled or Uncoupled Representation a "Good" Basis? | Energy |
|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | — | Diagonal | — | — | $E_n = -\frac{13.6\text{eV}}{n^2}$ |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes | $E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$ |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E'_{SO} = \frac{E_n^2}{mc^2}\left[\frac{n(j(j+1)-l(l+1-3/4))}{l(l+1)(l+1/2)}\right]$ |
| $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E'_{fs} = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{(j+1/2)} - 3\right]$ |
| $\hat{H}'_Z$ | Diagonal | Yes | Not Diagonal | No | No | $E'_Z = \mu B_{ext}(m_l + 2m_s)$ |

## III. Determining a "GOOD" Angular Basis and Corrections to the Energies due to BOTH the Fine Structure and the Zeeman Perturbations $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_{Z}$.

As we work through the remainder of the tutorial, we will fill in the following flowchart after each section regarding the intermediate, strong, and weak field Zeeman effect.

## Determining a "GOOD" Angular Basis and Corrections to the Energies due to BOTH the Fine Structure and Zeeman Terms



**CASE 1: Intermediate Field Zeeman Effect ($E'_{fs} \approx E'_Z$), when the fine structure term is comparable to the Zeeman term in $\hat{H}'$)**

### C.6.10 Finding a "Good" Angular Basis for the Intermediate Field Zeeman Effect

Consider the following conversation regarding whether the coupled or uncoupled representation forms a "good" angular basis for the intermediate field Zeeman effect (in order to find the first order corrections to the energies).

**Student 1:** In the intermediate field Zeeman effect, we must treat $\hat{H}'_{fs}$ and $\hat{H}'_Z$ on an equal footing. Does the coupled or uncoupled representation form a "good" angular basis?

**Student 2:** Since the coupled representation is a "good" angular basis for the fine structure term and the uncoupled representation is a "good" angular basis for the Zeeman term, both the coupled and uncoupled representation form "good" angular bases and are equally appropriate to find the first order corrections to the energies for $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

**Student 3:** I disagree with Student 2. You cannot consider different bases for different parts of $\hat{H}'$. If we choose the coupled representation, $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ is not diagonal in each degenerate subspace of $\hat{H}^0$ since $\hat{H}'_Z$ is not diagonal in the coupled representation. Similarly, if we choose the uncoupled representation, $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, is not diagonal in each degenerate subspace of $\hat{H}^0$ since $\hat{H}'_{fs}$ is not diagonal in the uncoupled representation. Neither of these representations forms a "good" basis.

Explain why you agree or disagree with Student 2 or Student 3.

Consider the following conversation regarding whether to choose the coupled representation or uncoupled representation as the angular basis for finding the corrections to the energies in the intermediate field Zeeman effect.

**Student 1:** In the intermediate field Zeeman effect, neither the coupled nor uncoupled representation forms a "good" angular basis. How do we determine the "good" angular basis?

**Student 2:** We can express $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ initially in either the coupled or uncoupled representation which will not be a "good" angular basis. Then, a "good" angular basis is found by diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. Thus, the "good" angular basis states will be linear combinations of the originally chosen angular basis states.

Do you agree with Student 2? Explain.

The angular basis states for $n = 2$ are listed below in the coupled representation (left), and each state in the coupled representation is given in terms of a linear combination of states in the uncoupled representation (right) using the Clebsch-Gordon table ($s = 1/2$).

Using the following table, the perturbing Hamiltonian $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in the coupled representation is given on the next page, in which $\gamma = \left(\frac{\alpha}{8}\right)^2$ 13.6 eV, $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$, $\beta = \mu_B B_{ext}$ and the angular basis states are chosen in the order $|\psi_1\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$:

| | Coupled Representation $\lvert l,\ j,\ m_j\rangle$ | Uncoupled Representation $\lvert l,\ m_l\rangle\lvert s,\ m_s\rangle$ |
|---|---|---|
| $\lvert\psi_1\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_2\rangle$ | $\left\lvert 0,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $\lvert 0,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_3\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{3}{2}\right\rangle$ | $\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle$ |
| $\lvert\psi_4\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{3}{2}\right\rangle$ | $\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_5\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ \frac{1}{2}\right\rangle$ | $\sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_6\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ \frac{1}{2}\right\rangle$ | $-\sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 1\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_7\rangle$ | $\left\lvert 1,\ \frac{3}{2},\ -\frac{1}{2}\right\rangle$ | $\sqrt{\frac{1}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |
| $\lvert\psi_8\rangle$ | $\left\lvert 1,\ \frac{1}{2},\ -\frac{1}{2}\right\rangle$ | $-\sqrt{\frac{2}{3}}\lvert 1,\ -1\rangle \left\lvert \frac{1}{2},\ \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\lvert 1,\ 0\rangle \left\lvert \frac{1}{2},\ -\frac{1}{2}\right\rangle$ |

$$\hat{H}' = -\begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$$

Consider the following conversation regarding diagonalizing the $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$ for the intermediate field Zeeman effect.

**Student 1:** In the case of $n = 2$, $\hat{H}^0$ possesses an eight-fold degeneracy, which means that in order to find a "good" angular basis for the correction to the $n = 2$ energy spectrum, we must diagonalize the entire 8 x 8 $\hat{H}'$ matrix in the $n = 2$ degenerate subspace of $\hat{H}^0$.

**Student 2:** While it is true that we must diagonalize the $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$, we are fortunate that the symmetry of the hydrogen atom yields many zero off-diagonal matrix elements. Therefore, $\hat{H}'$ will be block diagonal in the degenerate subspaces of $\hat{H}^0$.

**Student 3:** I agree with Student 2. We must make an effort to diagonalize $\hat{H}'$ only in those block diagonal subspaces with smaller dimensions than the original $8 \times 8$ $\hat{H}'$ matrix in order to diagonalize the entire $\hat{H}'$ matrix in the degenerate subspace of $\hat{H}^0$ to obtain the "good" angular basis set.

**Student 4:** I agree with Student 1, Student 2, and Student 3. When I calculate the $\hat{H}'$ matrix for $n = 2$ in the coupled representation and the angular basis states are chosen in the order $|\psi_1\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, I get the block diagonal matrix $\hat{H}'$ below

$$\hat{H}' = -\begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$$

We will only need to diagonalize the $2 \times 2$ matrices $-\begin{bmatrix} \gamma - \frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma - \frac{1}{3}\beta \end{bmatrix}$ and $-\begin{bmatrix} \gamma + \frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma + \frac{1}{3}\beta \end{bmatrix}$ to obtain the "good" angular basis.

Explain why you agree or disagree with each student.

### C.6.11 First Order Corrections to the Energy Spectrum of the Hydrogen Atom in Perturbation Theory for the Intermediate Field Zeeman Effect

Consider the following conversation regarding whether choosing the coupled representation or the uncoupled representation as the initial angular basis and then carrying out a change of basis by diagonalizing $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ affects the corrections to the energies in the intermediate field Zeeman effect.

**Student 1:** When calculating the first order corrections to the energies in the intermediate field Zeeman effect, we can choose either the coupled or the uncoupled representation as the initial angular basis even if we know it is not a "good" angular basis. Then, a "good" angular basis will be found by diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. After diagonalizing $\hat{H}'$, the new basis is "good" and the first order corrections to the energies are the diagonal matrix elements.

**Student 2:** I disagree. Since the diagonal matrix elements of $\hat{H}'$ will depend on the choice of initial basis, a different choice of the initial basis in which we diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ will change the first order corrections to the energies.

**Student 3:** I disagree with Student 2. After diagonalizing $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$, a "good" basis is obtained and the first order correction to the energy will be the same regardless of which basis, e.g., the coupled or uncoupled representation, you had initially chosen. In a "good" basis, you will end up with the same diagonal matrix elements of $\hat{H}'$ which are the first order corrections to the energies.

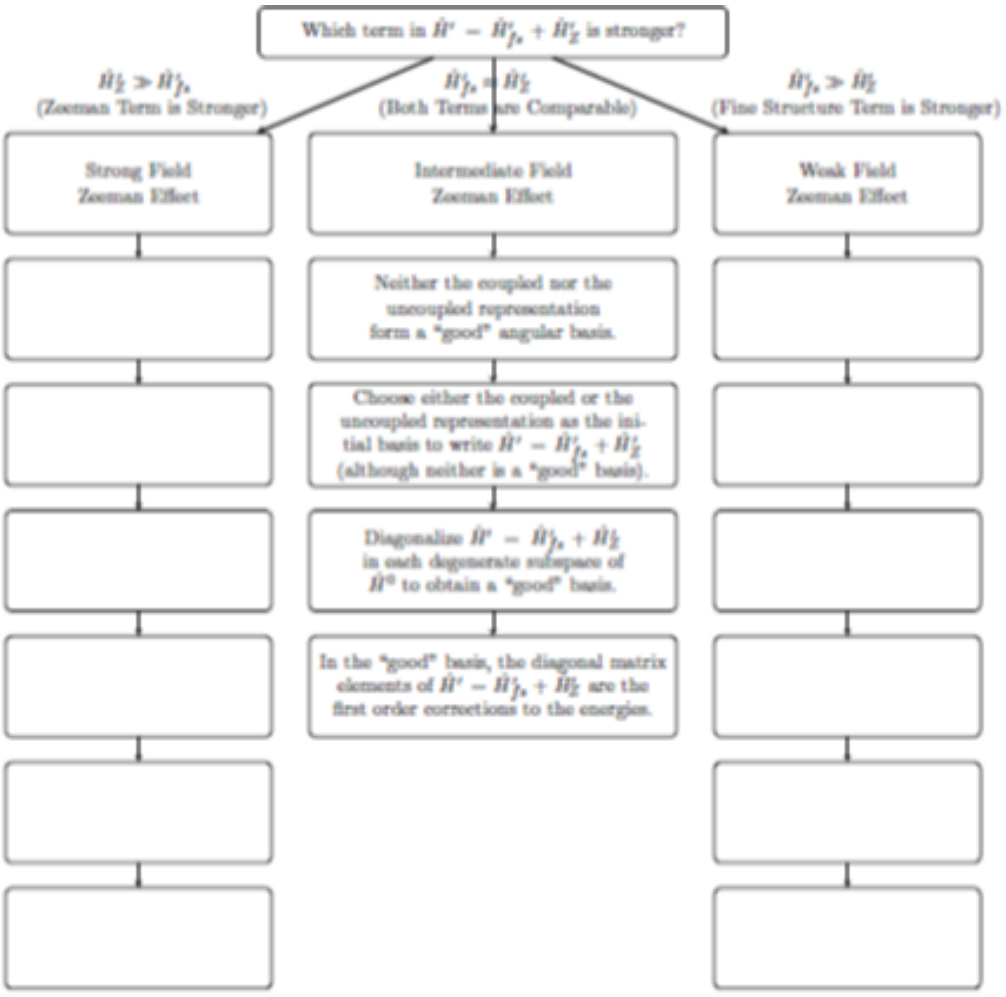
Explain why you agree or disagree with each student.

In one or two sentences, summarize what you have learned about the "good" angular basis states for finding the first order corrections to the energy spectrum of the hydrogen atom due to the intermediate field Zeeman effect (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" angular basis).

Shortly, we shall calculate the first order corrections to the energies due to the intermediate field Zeeman effect. But before we do so, let's first consider the limiting cases when one perturbation is stronger than the other.

Review the following flowchart concerning a "good" angular basis and corrections to the energies for the intermediate field Zeeman effect. Using the intermediate field Zeeman effect as a guide, attempt to fill in the steps required to determine a "good" angular basis and corrections to the energies due to both the fine structure ($\hat{H}'_{fs}$) and Zeeman ($\hat{H}'_Z$) terms for the strong field Zeeman effect ($E_Z \gg E'_{fs}$) and the weak field Zeeman effect ($E'_{fs} \gg E'_Z$). You can add or remove boxes in the flowchart if necessary.

# Determining a "GOOD" Angular Basis and Corrections to the Energies due to BOTH the Fine Structure and Zeeman Term



**Summary: Finding a "GOOD" Angular Basis for the Intermediate Field Zeeman Effect $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$**

- Neither the coupled nor the uncoupled representation forms a "good" angular basis when $E'_Z \approx E'_{fs}$.
- To find a "good" angular basis for the intermediate field Zeeman effect $E'_Z \approx E'_{fs}$:
  - First choose either the coupled or the uncoupled representation as the basis.
  - Diagonalize $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$.
  - The "good" basis will be a special linear combinations of the originally chosen basis set.

### C.6.12 Limiting Cases

Consider the following conversation regarding finding a "good" basis when treating the perturbation in two steps.

**Student 1:** If we have a perturbation that has two terms in which one perturbation is stronger than the other, we can first take into account the correction due to the stronger perturbation and then take into account the weaker perturbation as a second perturbation.

**Student 2:** I agree. In the first step, we must find a "good" basis for $\hat{H}^0$ and $\hat{H}'_{strong}$, so $\hat{H}'_{strong}$ must be diagonal in each degenerate subspace of $\hat{H}^0$. Then in the second step, treat $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ as the unperturbed Hamiltonian and $\hat{H}'_{weak}$ as perturbation on $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$. A "good" basis for step 2 is one in which $\hat{H}'_{weak}$ is diagonal in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$.

**Student 3:** I disagree with Student 2. You cannot find one "good" basis for step 1 and a different "good" basis for step 2.

**Student 4:** I agree with Student 1 and Student 2. It is approprate to use a two step perturbation theory when one part of the perturbation is stronger than another if the error due to this two step process will be negligible. If the basis after step 1 is not a "good" basis for step 2, we would need to diagonalize $\hat{H}'_{weak}$ in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ to find a "good" basis in step 2.

Explain why you agree or disagree with each student.

- Summary of Two-Step Approximation
  - **STEP 1:** First consider only the stronger perturbation $\hat{H}'_{strong}$ as a perturbation on $\hat{H}^0$.
    * Choose a basis in which $\hat{H}^0$ is diagonal and $\hat{H}'_{strong}$ is diagonal in each degenerate subspace of $\hat{H}^0$.
    * Determine the first order corrections to the energies $E'_{strong}$ due to the stronger perturbation $\hat{H}'_{strong}$.
  - **STEP 2:** Consider the weaker perturbation $\hat{H}'_{weak}$ as a perturbation on the new unperturbed Hamiltonian $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$.
    * Treat as the new unperturbed Hamiltonian $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$.
    * Treat $E^0_{strong} = E^0 + E'_{strong}$ as the new unperturbed energies.
    * Determine the degeneracy of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ (i.e., how many distinct states have the same energy $E^0_{strong,i}$).
    * Determine if $\hat{H}'_{weak}$ is diagonal in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$.
      · If $\hat{H}'_{weak}$ is already diagonal in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ then the basis is "good" and the diagonal elements of $\hat{H}'_{weak}$ will give the corrections $E'_{weak}$.
      · If $\hat{H}'_{weak}$ is not diagonal in each degenerate subspace of $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$, diagonalize $\hat{H}'_{weak}$ in each degenerate subspace of $\hat{H}^0_{strong}$ to find a "good" basis.

Consider the following conversation regarding approximating the corrections to the energy when one perturbation is stronger than the other.

**Student 1:** When the hydrogen atom is placed in an external magnetic field, we must consider both the Zeeman term and the fine structure term in the Hamiltonian as perturbations. Therefore, neither the coupled nor the uncoupled representation form a "good" basis. We must diagonalize the entire $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ matrix in the degenerate subspace of $\hat{H}^0$.

**Student 2:** That is true. However, if one term is much stronger than the other, we can approximate the first order corrections to the energy using perturbation theory in two steps. In the first step, consider only the stronger perturbation. Then, as the second step, consider the weaker perturbation. This two-step approximation may simplify the process for finding a "good" basis and provide an alternative to diagonalizing the entire $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ matrix in each degenerate subspace of $\hat{H}^0$.

**Student 3:** I agree with Student 2. We will find that in the limiting case, the first order corrections to the energies obtained using this two-step approximation match with the first order corrections to the energies obtained by diagonalizing the entire $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ matrix in each degenerate subspace of $\hat{H}^0$ as in the intermediate field Zeeman effect when we take the appropriate limit.

Explain why you agree or disagree with each student.

All the students are correct in the preceding conversation. However, we will focus on the limiting cases and use the method described by Student 2 and Student 3.

- When $E'_Z \gg E'_{fs}$ or $E'_{fs} \gg E'_Z$, we can use a two step approximation to find the first order corrections to the energies of the hydrogen atom.
- Two-Step Approximation for the Strong and Weak Field Zeeman Effect
  - **CASE 2: Strong Field Zeeman Effect ($E'_Z \gg E'_{fs}$)**
    - The Zeeman term dominates.
      - **STEP 1:** Treat only $\hat{H}'_Z$ as the perturbation on $\hat{H}^0$.
      - **STEP 2:** Now, treat $\hat{H}'_{fs}$ as the perturbation on the new unperturbed Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ after the first step.
  - **CASE 3: Weak Field Zeeman Effect ($E'_{fs} \gg E'_Z$)**
    - The fine structure term dominates.
      - **STEP 1:** Treat only $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0$.
      - **STEP 2:** Now, treat $\hat{H}'_Z$ as the perturbation on the new unperturbed Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ after the first step.

**CASE 2: Strong Field Zeeman Effect: Perturbation Theory in Two Steps to Find the Corrections to Energy Spectrum**

### C.6.12.1 Finding a "GOOD" Basis for the Strong Field Zeeman Effect in the Hydrogen Atom <u>STEP 1:</u>

For the case $E'_Z \gg E'_{fs}$, in step 1, we treat only $\hat{H}'_Z$ as the perturbation on $\hat{H}^0$.

7. For the case $E'_Z \gg E'_{fs}$, what is a "good" angular basis for step 1 when we only consider $\hat{H}'_Z$ as perturbation? Explain.

8. Write an expression for the first order corrections to the energies due to only the stronger perturbation $\hat{H}'_Z$ acting on the unperturbed Hamiltonian $\hat{H}^0$ (once you have found a "good" basis). Here the first order corrections are the exact results for the energies for the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'_Z$ after STEP 1 since $\hat{H}^0$ and $\hat{H}'_Z$ commute (so $\hat{H}^0$ and $\hat{H}'_Z$ can be diagonalized simultaneously in a "good" basis).

**<u>STEP 2:</u>**

In the strong field when $E'_Z \gg E'_{fs}$, in step 2, the unperturbed Hamiltonian includes the Zeeman term and becomes

$$\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m}B_{ext}(\hat{L}_z + 2\hat{S}_z). \tag{C.18}$$

9. Is the $\hat{H}^0_Z$ matrix a diagonal matrix if the coupled representation or the uncoupled representation is chosen as the basis? Explain your reasoning. Your answer should be consistent with your response to question 7 above.

Now for the $n = 2$ subspace, take a look at the $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ and $\hat{H}'_{fs}$ matrices given below in which $E_2 = -\frac{13.6\text{eV}}{4}$ and the basis vectors are chosen in the **uncoupled representation** ($|l,\ m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $\psi_2\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$. Then answer questions 10-13 for the Strong field Zeeman effect.

$$\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$$

$$\hat{H}_Z^0 = -\frac{13.6\text{eV}}{4}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} + \mu_B B_{ext}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \end{bmatrix}$$

$$= \begin{bmatrix} E_2 + \mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 - \mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 + 2\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 + \mu_B B_{ext} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 - \mu_B B_{ext} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - 2\mu_B B_{ext} \end{bmatrix} \quad \text{(C.19)}$$

$$\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO} = \hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} 15 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{2} & 7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} \quad \text{(C.20)}$$

10. Determine the degeneracy in the energy eigenvalues of the "new" unperturbed Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ after accounting for the stronger perturbation. Then circle the corresponding degenerate subspaces of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ (for the $n = 2$ subspace) in the preceding matrix representation in equation (C.19).

11. Identify the matrix elements of $\hat{H}'_{fs}$ in equation (C.20) that correspond to each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ in equation (C.19) and determine whether $\hat{H}'_{fs}$ is diagonal in any of these subspaces of $\hat{H}_Z^0$.
12. Determine whether the uncoupled representation chosen as the basis in question 9 is a "good" basis for the unperturbed Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ and the perturbation $\hat{H}'_{fs}$. Explain how you made the determination.

**** Check your answers to questions 7-12. ****

7. The uncoupled representation forms a "good" basis when only the Zeeman term $\hat{H}'_Z$ is the perturbation on the unperturbed Hamiltonian $\hat{H}^0$.

8. As we determined in equation (C.17), the first order corrections to the energies due to the Zeeman term $\hat{H}'_Z$ in the uncoupled representation are $E'_Z = \mu_B B_{ext}(m_l + 2m_s)$.

9. $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ is diagonal if the uncoupled representation is chosen as the basis.

10. $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ possesses three two-fold degeneracies (see equation C.19) in the $n = 2$ subspace of $\hat{H}^0$. There are two distinct states that share the new unperturbed energies $E_2 + \mu B_{ext}$, $E_2 - \mu B_{ext}$, and $E_2$.

11. The perturbation $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ treated as the unperturbed Hamiltonian in step 2 of perturbation theory.

12. Yes. The uncoupled representation is a "good" angular basis in this case since $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ is diagonal and $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$.

If your answers to questions 7-12 do not match with the checkpoint answers, go back and reconcile any differences.

For the following conversation, consider the $n = 2$ subspace for which the unperturbed Hamiltonian for the strong field Zeeman effect is $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ after the first step for the strong field Zeeman effect ($E'_Z \gg E'_{fs}$).

**Student 1:** In the limit $E'_Z \gg E'_{fs}$, we can only take the Zeeman term $\hat{H}'_Z$ as the perturbation first when we are using the two-step approximation. Then, after the first step, consider the unperturbed Hamiltonian as $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ with unperturbed energies $E_n^0 = E_n + \mu B_{ext}(m_l + 2m_s)$, and consider the degeneracy left in $E_n^0$ to determine the degenerate subspaces of $\hat{H}_Z^0$. In the second step, treat the fine structure part $\hat{H}'_{fs}$ as the perturbation on $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ .

**Student 2:** What is the degeneracy left in the hydrogen atom energy spectrum when it is placed in a strong external magnetic field after accounting for only the Zeeman term $\hat{H}'_Z$ as the perturbation in the first step?

**Student 3:** In the $n = 2$ subspace, the $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ matrix is the following if the basis states are chosen in the uncoupled representation ($|l,\ m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$,$|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$

$$\hat{H}_Z^0 = \begin{bmatrix} \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \underline{E_2 - \mu_B B_{ext}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 + 2\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \textcircled{E_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \underline{E_2 - \mu_B B_{ext}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \textcircled{E_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - 2\mu_B B_{ext} \end{bmatrix}.$$

$\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ has three separate two-fold degeneracies for the energies $E_2 + \mu_B B_{ext}, E_2 - \mu_B B_{ext}$, and $E_2$ as indicated by the boxed, underlined, and circled matrix elements of $\hat{H}_Z^0$ above.

**Student 4:** I agree with both Student 1 and Student 3. By considering the stronger perturbation $\hat{H}'_Z$ first, some of the degeneracies are broken and the eight-fold degeneracy in the energy spectrum of $\hat{H}^0$ has become three separate two-fold degeneracies plus two nondegenerate levels in the energy spectrum of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the case $E'_Z \gg E'_{fs}$ and treating the perturbation in two steps with the stronger Zeeman term considered as part of the unperturbed Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ to find the corrections due to the weaker perturbation $\hat{H}'_{fs}$.

**Student 1:** Even in a two step process, how can we find a "good" basis easily when both the fine structure term $\hat{H}'_{fs}$ and the Zeeman term $\hat{H}'_Z$ are present? The "good" basis is one in which there are no off-diagonal matrix elements of $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in the degenerate subspace of $\hat{H}^0$. Since $\hat{H}'_{fs}$ is diagonal in the coupled representation and $\hat{H}'_Z$ is diagonal in the uncoupled representation, neither the coupled nor the uncoupled representation could possibly form a "good" basis when we have $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$.

**Student 2:** I agree. In step 1, when we only consider $\hat{H}'_Z$ as the perturbation on $\hat{H}^0$, we choose the uncoupled representation as the "good" basis. Once the uncoupled representation is chosen as the "good" basis, we are guaranteed to have off-diagonal matrix elements in the weaker fine structure perturbation matrix $\hat{H}'_{fs}$. Thus, the "good" basis for step 1 cannot be a "good" basis for step 2.

**Student 3:** Actually, once we treat the stronger Zeeman perturbation $\hat{H}'_Z$ in the first step, we lift some of the degeneracy in the energy spectrum of $\hat{H}^0$. There is still degeneracy in the energy spectrum $E^0_n = E_n + \mu_B B_{ext}(m_l + 2m_s)$ after the first step, but now the degeneracy is present in smaller subspaces of $\hat{H}^0$. For example, for the $n = 2$ subspace in step 2, $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ in the uncoupled representation is

$$\hat{H}^0_Z = \begin{bmatrix} \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 - \mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 + 2\mu_B B_{ext} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{E_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 - \mu_B B_{ext} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{E_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - 2\mu_B B_{ext} \end{bmatrix}.$$

In the uncoupled representation, $\hat{H}'_{fs}$ is not diagonal in the entire $n = 2$ subspace, but it is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$. In the $\hat{H}'_{fs}$ matrix below, the elements of the degenerate subspace of $\hat{H}^0_Z$ corresponding to the degenerate energy $E_2 + \mu_B B_{ext}$ are boxed. We see that $\hat{H}'_{fs}$ is diagonal in the $2 \times 2$ subspace corresponding to the degenerate energy $E_2 + \mu_B B_{ext}$.

$$\hat{H}'_{fs} = \frac{(-13.6\text{ eV})\alpha^2}{192}\begin{bmatrix} \boxed{15} & 0 & 0 & 0 & \boxed{0} & 0 & 0 & 0 \\ 0 & 15 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 11 & 4\sqrt{2} & 0 & 0 & 0 \\ \boxed{0} & 0 & 0 & 4\sqrt{2} & \boxed{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 & 4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 4\sqrt{2} & 11 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}.$$

Similarly, $\hat{H}'_{fs}$ is diagonal in the degenerate subspace of $\hat{H}^0_Z$ for the degenerate energies $E_2$ and $E_2 - \mu_B B_{ext}$. Therefore, the uncoupled representation does form a "good" basis in this two step process.

Explain why you agree or disagree with each student.

Consider the following conversation regarding choosing the basis states in a different order to easily determine a "good" basis for the strong field Zeeman effect ($E'_Z \gg E'_{fs}$).

**Student 1:** In the strong field Zeeman effect, for the $n = 2$ subspace, we chose basis states in the uncoupled representation ($|l,\ m_l,\ m_s\rangle$) in the order $|\psi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$,$|\psi_3\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, $|\psi_4\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\psi_5\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$ to write the $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ matrix in equation (C.19) and the $\hat{H}'_{fs}$ matrix in equation (C.20). Can we choose to write the basis states in a different order to make the $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ matrix such that the degenerate eigenvalues along the diagonal are adjacent? Doing so may make it easier to determine if we have a "good" basis.

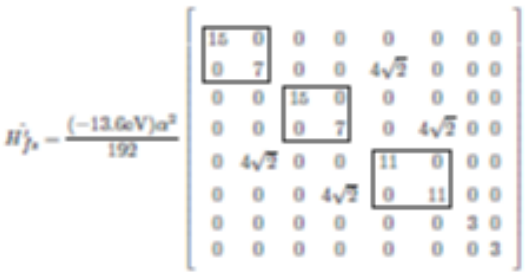
**Student 2:** Yes. Suppose we choose the basis states in the order $|\phi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\phi_2\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\phi_3\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$, $|\phi_4\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\phi_5\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\phi_6\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, $|\phi_7\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, and $|\phi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$, then in the $n = 2$ subspace, the $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ matrix is

$$\hat{H}^0_Z = \begin{bmatrix} \boxed{E_2 + \mu_B B_{ext}} & \boxed{0} & 0 & 0 & 0 & 0 & 0 & 0 \\ \boxed{0} & \boxed{E_2 + \mu_B B_{ext}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{E_2 - \mu_B B_{ext}} & \boxed{0} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{0} & \boxed{E_2 - \mu_B B_{ext}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{E_2} & \boxed{0} & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{0} & \boxed{E_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 + 2\mu_B B_{ext} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - 2\mu_B B_{ext} \end{bmatrix}$$

The degenerate subspaces of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ are boxed. Each degenerate subspace of $\hat{H}^0_Z$ is now diagonal. **Student 3:** I agree with Student 2. In order to determine if the "good" basis for step 1 is also a "good" basis for step 2, we must check that $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$. When basis states are chosen in the order $|\phi_1\rangle = |0,\ 0,\ \frac{1}{2}\rangle$, $|\phi_2\rangle = |1,\ 0,\ \frac{1}{2}\rangle$, $|\phi_3\rangle = |0,\ 0,\ -\frac{1}{2}\rangle$, $|\phi_4\rangle = |1,\ 0,\ -\frac{1}{2}\rangle$, $|\phi_5\rangle = |1,\ 1,\ -\frac{1}{2}\rangle$, $|\phi_6\rangle = |1,\ -1,\ \frac{1}{2}\rangle$, $|\phi_7\rangle = |1,\ 1,\ \frac{1}{2}\rangle$, and $|\phi_8\rangle = |1,\ -1,\ -\frac{1}{2}\rangle$, the $\hat{H}'_{fs}$ matrix is

Now we can more easily see that $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$.

**Student 4:** I disagree with Student 2 and Student 3. We are not permitted to write the basis states in any order we choose. If we change the order of the basis states, we change the first order corrections to the energies. Since the first order corrections to the energies are



the diagonal matrix elements of the perturbation in a "good" basis, writing the basis states in a different order will produce incorrect first order corrections to the energies.

**Student 3:** No! Reordering the basis states just changes the order in which the unperturbed energies and their corrections appear, but corrections to each unperturbed energy will be the same. Remember that we need to reorder both $\hat{H}_Z^0$ and $\hat{H}'_{fs}$ matrices since the basis vectors must be chosen in the same order for all matrices.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the off-diagonal matrix elements of $\hat{H}'$ in each degenerate subspace of $\hat{H}_Z^0$ in the strong field Zeeman effect ($E'_Z \gg E'_{fs}$).

**Student 1:** Since $\hat{H}'_Z$ is diagonal in the uncoupled representation and $\hat{H}'_{fs}$ is diagonal in the coupled representation, we were fortunate that after the first step in our two-step approximation, the off-diagonal matrix elements of $\hat{H}'_{fs}$ were zero in each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ in the uncoupled representation after step 1.

**Student 2:** I agree with Student 1. Considering $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ as the new unperturbed Hamiltonian after the first step, the stronger perturbation $\hat{H}'_Z$ breaks some of the degeneracy in the energy spectrum of $\hat{H}^0$. In the second step in perturbation theory, the non-zero off-diagonal matrix elements of the weaker perturbation $\hat{H}'_{fs}$ are NOT in the degenerate subspaces of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ when we consider the unperturbed Hamiltonian $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ and the uncoupled representation as the basis.

**Student 3:** You are correct. We got lucky! After the first step, if the off-diagonal matrix elements of the weaker perturbation $\hat{H}'_{fs}$ were not zero in the degenerate subspaces of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$, we would need to determine the "good" basis by diagonalizing $\hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z$ in the second step. The uncoupled representation would not have been a "good" basis.

Explain why you agree or disagree with each student.

#### C.6.12.2 Finding Corrections to the Energies for the Strong Field Zeeman Effect

After the first step, the unperturbed Hamiltonian including the Zeeman term is

$$\hat{H}_Z^0 = \hat{H}^0 + \hat{H}'_Z = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m}B_{ext}(L_z + 2S_z) \tag{C.21}$$

and the corresponding unperturbed energies are

$$E_Z^0 = -\frac{13.6\text{eV}}{n^2} + \mu_B B_{ext}(m_l + 2m_s) \tag{C.22}$$

13. After step 2, find one of the first order corrections to the energies due to the weaker perturbation $\hat{H}'_{fs}$ for the hydrogen atom placed in a strong external magnetic field for the $n = 2$ subspace.

**** Check your answers to question 13. ****

13. The first order corrections to the energies due to the fine structure term for the hydrogen atom placed in a strong external magnetic field for the $n = 2$ subspace are the diagonal elements of $\hat{H}'_{fs}$ in equation (**??**).

$$E'_1 = \frac{(-13.6\text{ eV})\alpha^2}{192}(15) \qquad E'_2 = \frac{(-13.6\text{ eV})\alpha^2}{192}(7)$$

$$E'_3 = \frac{(-13.6\text{ eV})\alpha^2}{192}(15) \qquad E'_4 = \frac{(-13.6\text{ eV})\alpha^2}{192}(7)$$

$$E'_5 = \frac{(-13.6\text{ eV})\alpha^2}{192}(11) \qquad E'_6 = \frac{(-13.6\text{ eV})\alpha^2}{192}(11)$$

$$E'_7 = \frac{(-13.6\text{ eV})\alpha^2}{192}(3) \qquad E'_8 = \frac{(-13.6\text{ eV})\alpha^2}{192}(3)$$

If your answers to question 13 do not match with the checkpoint answers, go back and reconcile any differences.

In one to two sentences, summarize what you have learned about the "good" angular basis states for finding the first order corrections to the energy spectrum of the hydrogen atom due to the strong field Zeeman effect (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" angular basis).

**Summary: Finding a "GOOD" Angular Basis for the Strong Field Zeeman Effect ($E'_Z \gg E'_{fs}$)**

- We can use a two step process in perturbation theory to find corrections to the hydrogen atom energy spectrum when $E'_Z \gg E'_{fs}$.

Step 1: Treat the stronger perturbation $\hat{H}'_Z$ as a perturbation on the unperturbed Hamiltonian $\hat{H}^0$.

  - $\hat{H}'_Z$ is diagonal in the uncoupled representation.

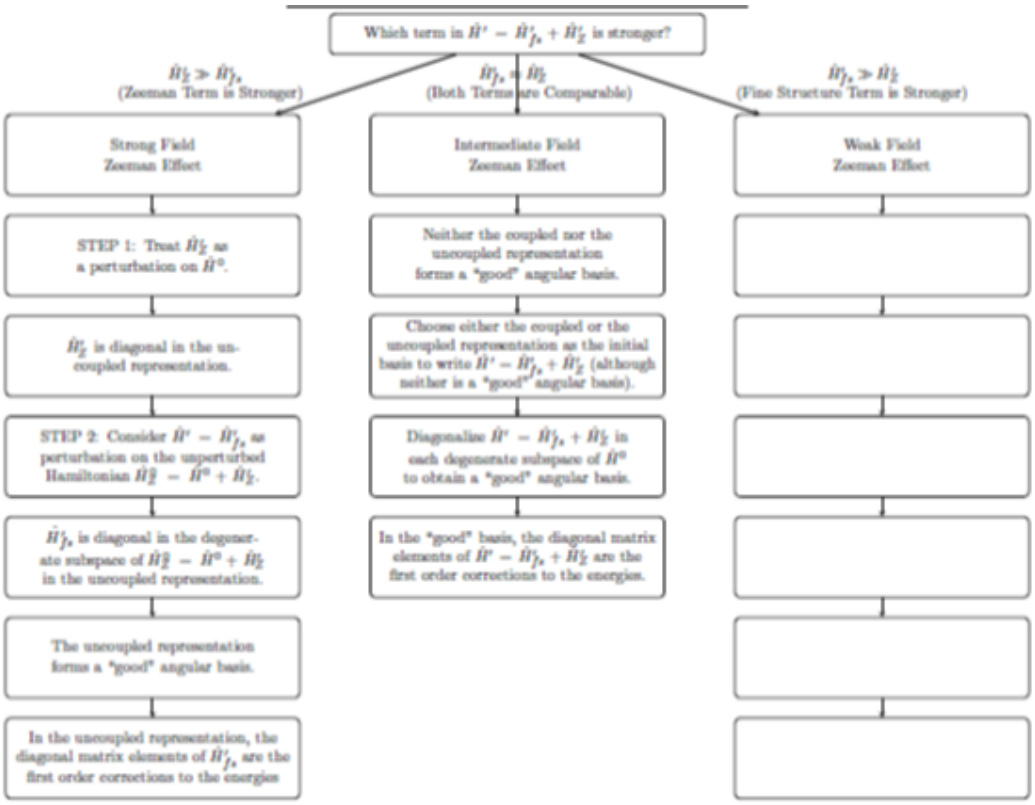
Step 2: Treat the fine structure part of the Hamiltonian, $\hat{H}'_{fs}$, as a perturbation on the new unperturbed Hamiltonian $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$.

  - In the uncoupled representation, $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ (even though $\hat{H}'_{fs}$ has off-diagonal matrix elements in the uncoupled representation, they are not in the degenerate subspaces of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$).

- The uncoupled representation forms a "good" angular basis for finding the corrections to the energies.

Review the following flowchart concerning the "good" basis and how to find the corrections to the energies for the intermediate and strong field Zeeman effect. Using the intermediate and strong field Zeeman effect as a guide, attempt to fill in the steps required to determine a "good" basis and corrections to the energies due to both the fine structure ($\hat{H}'_{fs}$) and Zeeman ($\hat{H}'_Z$) terms for the the weak field Zeeman effect ($E'_{fs} \gg E'_Z$). You may add or remove boxes in the flowchart if necessary.

# Determining a "GOOD" Angular Basis and Corrections to the Energies due to BOTH the Fine Structure and Zeeman Effect




**CASE 3: Weak Field Zeeman Effect: Perturbation Theory in Two Steps to Find the Corrections to the Energy Spectrum**

### C.6.12.3 Finding a "GOOD" Basis for the Weak Field Zeeman Effect ($E'_{fs} \gg E'_Z$) STEP 1:

In step 1, for the case $E'_{fs} \gg E'_Z$, we treat only $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0$.

14. For the case $E'_{fs} \gg E'_Z$, what is the "good" angular basis for step 1 when we ignore $\hat{H}'_Z$? Explain.

15. Write an expression for the first order corrections to the energies due to the stronger perturbation $\hat{H}'_{fs}$.

**STEP 2:**

In the weak field when $\hat{H}'_{fs} \gg \hat{H}'_Z$, in step two, the unperturbed Hamiltonian including the fine structure term becomes

$$\hat{H}^0_{fs} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - \frac{\hat{p}^4}{8m^3c^2} + \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S}. \tag{C.23}$$

16. For $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$, is $\hat{H}^0_{fs}$ diagonal if the angular basis is chosen to be the coupled representation, uncoupled representation, or neither? Explain your reasoning.

Now for the $n = 2$ subspace, take a look at the $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ and $\hat{H}'_Z$ matrices given below in the **coupled representation** ($|l,\ j,\ m_j\rangle$) in which $E_2 = -\frac{13.6\text{eV}}{4}$ and the basis states are chosen in the order $|\Phi_1\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\Phi_2\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\Phi_3\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, $|\Phi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\Phi_5\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\Phi_6\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\Phi_7\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$ and $|\Phi_8\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$. Then, answer questions 16-20 for the weak field Zeeman effect.

$$\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$$

$$\hat{H}^0_{fs} = E_2 \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} + \frac{E_2^2}{mc^2} \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -5 \end{bmatrix}$$

$$^0_{fs} = \begin{bmatrix} E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_2 - \frac{E_2^2}{mc^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_2 - \frac{5E_2^2}{mc^2} \end{bmatrix} \quad \text{(C.24)}$$

$$\hat{H}'_Z = \mu_B B_{ext} \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{3} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \tag{C.25}$$

17. In step 2, determine the degeneracy of the "new" unperturbed Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ after accounting for the stronger perturbation and circle the corresponding degenerate subspaces in $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ for the $n = 2$ subspace in the preceding matrix representation in equation (C.24).

18. Identify the matrix elements of $\hat{H}'_Z$ in equation (C.25) that correspond to each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ in equation (C.24) and determine whether $\hat{H}'_Z$ is diagonal in any of these subspaces of $\hat{H}^0_{fs}$.
19. Determine whether the basis chosen in question 16 is a "good" angular basis for the unperturbed Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ and the perturbation $\hat{H}'_Z$. Explain how you made the determination.

**** Check your answers to questions 14-19. ****

14. The coupled representation forms a "good" basis when only the fine structure term $\hat{H}'_{fs}$ is the perturbation on the unperturbed Hamiltonian $\hat{H}^0$

15. As we determined in equation (C.15), the first order corrections to the energies due to the fine structure term $\hat{H}'_{fs}$ in the coupled representation are $E'_{fs} = \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{j+1/2}\right]$.

16. For a fixed $n$, $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$ if the coupled representation is chosen as the angular basis.

17. $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ possesses two four-fold degeneracies in the $n = 2$ subspace. There are four distinct states that share the new unperturbed energies $E_2 - \frac{5E_2^2}{mc^2}$ and $E_2 - \frac{E_2^2}{mc^2}$.

18. The perturbation $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ treated as the unperturbed Hamiltonian in step 2 of perturbation theory.

19. Yes. The coupled representation is a "good" angular basis. In the second step, the new perturbation term $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ is diagonal in the coupled representation for a fixed $n$ and the perturbation $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$.

If your answers to questions 14-19 do not match with the checkpoint, go back and reconcile any differences.

Consider the following conversation regarding the weak field Zeeman effect ($E'_{fs} \gg E'_Z$) and finding a "good" basis for the two-step process in the weak field Zeeman effect ($E'_{fs} \gg E'_Z$).

**Student 1:** Since $\hat{H}'_Z = \mu_B B_{ext}(\hat{L}_z + 2\hat{S}_z)$, we cannot use the coupled representation as the angular basis. $\hat{H}'_Z$ is not diagonal in the coupled representation. To find the first order corrections to the energies, we must use the uncoupled representation since $\hat{H}'_Z$ is diagonal in the uncoupled representation.

**Student 2:** I don't see how either the coupled or uncoupled representation form a "good" angular basis when we have both $\hat{H}'_{fs}$ and $\hat{H}'_Z$. They simply cannot be diagonalized simultaneously in either basis. We must choose linear combinations of the states in the coupled or uncoupled representation so that the basis diagonalizes the sum of $\hat{H}'_{fs}$ and $\hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$.

**Student 3:** I agree with Student 2 only for the intermediate field Zeeman effect with $E'_{fs} \approx E'_Z$. In the weak field Zeeman effect in which $E'_{fs} \gg E'_Z$, we can use the two step approximation by considering only the stronger perturbation $\hat{H}'_{fs}$ in the first step. In the second step, we consider the "new" unperturbed Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ and the perturbation $\hat{H}'_Z$. If the coupled representation is chosen as the angular basis, then in the $n = 2$ subspace, the $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ matrix is (the basis vectors are chosen the same order as in questions 17-19):

**Student 4:** I agree with Student 3. $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ shown for the $n = 2$ subspace in the following matrix. Therefore, the coupled representation is a "good" basis in the limit $E'_{fs} \gg E'_Z$. When we use a two step process in the limit $\hat{H}'_{fs} \gg \hat{H}'_Z$, some degeneracy is lifted in the first step.

$$\hat{H}'_Z - \mu_B B_{ext} \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2} & 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{3} & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}.$$

Explain why you agree or disagree with each student.

Consider the following conversation regarding the off-diagonal matrix elements of $\hat{H}'_Z$ in the degenerate subspace of $\hat{H}^0_{fs}$ in the weak field Zeeman effect ($E'_{fs} \gg E'_Z$).

**Student 1:** Since $\hat{H}'_Z$ is diagonal in the uncoupled representation and $\hat{H}'_{fs}$ is diagonal in the coupled representation for a fixed $n$, we were fortunate that, after the first step in our approximation, the off-diagonal matrix elements of $\hat{H}'_Z$ are zero in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$.

**Student 2:** I agree with Student 1. The stronger perturbation $\hat{H}'_{fs}$ breaks some of the degeneracy in the energy spectrum of $\hat{H}^0$. When we consider $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ as the new unperturbed Hamiltonian in step 2, the non-zero off-diagonal matrix elements of $\hat{H}'_Z$ are not in the degenerate subspaces of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$.

**Student 3:** You are correct. We got lucky! In step 2, if the off-diagonal matrix elements of the weaker perturbation $\hat{H}'_Z$ were non-zero in any of the degenerate subspaces of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$, we would have needed to determine the "good" basis by diagonalizing $\hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ that is not diagonal already after the first step.

Explain why you agree or disagree with each student.

#### C.6.12.4 Finding Corrections to the Energies for the Weak Field Zeeman Effect

($E'_{fs} \gg E'_Z$) After the first step, the unperturbed Hamiltonian including the fine structure term is

$$\hat{H}^0_{fs} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - \frac{\hat{p}^4}{8m^3c^2} + \left(\frac{e^2}{8\pi\epsilon_0}\right)\frac{1}{m^2c^2r^3}\vec{L}\cdot\vec{S} \tag{C.26}$$

and the corresponding unperturbed energies are

$$E_{njm_j} = -\frac{13.6\text{eV}}{n^2} + \frac{E_n^2}{mc^2}\left[3 - \frac{4n}{j+1/2}\right] \tag{C.27}$$

20. After step 2, find one of the first order corrections to the energies due to the weaker perturbation $\hat{H}'_Z$ for the hydrogen atom placed in a weak external magnetic field for the $n = 2$ subspace.

**** Check your answers to question 20. ****

20. The first order corrections to the energies due to the Zeeman term only for the hydrogen atom placed in a weak external magnetic field for the $n = 2$ subspace are the diagonal elements of $\hat{H}'_Z$

$$\begin{aligned}
E'_1 &= 2\mu_B B_{ext} \\
E'_2 &= \tfrac{2}{3}\mu_B B_{ext} \\
E'_3 &= -\tfrac{2}{3}\mu_B B_{ext} \\
E'_4 &= -2\mu_B B_{ext} \\
E'_5 &= \tfrac{1}{3}\mu_B B_{ext} \\
E'_6 &= -\tfrac{1}{3}\mu_B B_{ext} \\
E'_7 &= \mu_B B_{ext} \\
E'_8 &= -\mu_B B_{ext}
\end{aligned}$$

If your answer to question 20 does not match with the checkpoint, go back and reconcile any differences.

In one to two sentences, summarize what you have learned about the "good" angular basis for finding the first order corrections to the energy spectrum of the hydrogen atom due to the weak field Zeeman effect (pertaining to whether the coupled representation, the uncoupled representation, or any arbitrary complete orthonormal basis constructed with linear combinations of a complete set of states with a fixed principal quantum number $n$ in the coupled or uncoupled representation form a "good" angular basis).

**Summary: Finding a "GOOD" Angular Basis for the Weak Field Zeeman Effect ($E'_{fs} \gg E'_Z$)**

- We can use a two step process for perturbation theory to find the corrections to the hydrogen atom energy spectrum for $E'_{fs} \gg E'_Z$.

Step 1: Treat the stronger perturbation $\hat{H}'_{fs}$ as the entire perturbation on the unperturbed Hamiltonian $\hat{H}^0$.

- $\hat{H}'_{fs}$ is diagonal in the coupled representation for a fixed $n$ (in each degenerate subspace of $\hat{H}^0$).

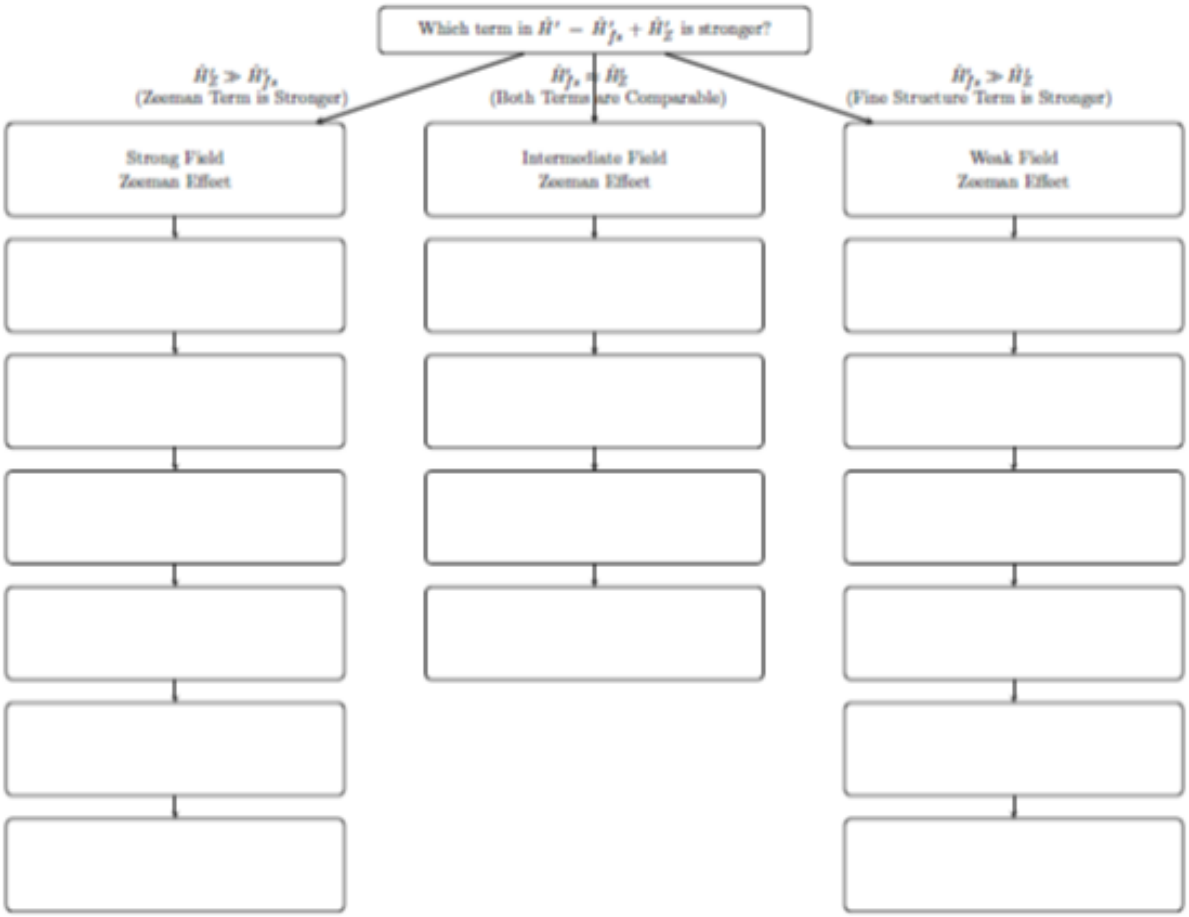
Step 2: Treat the Zeeman part of the Hamiltonian, $\hat{H}'_Z$, as the perturbation on the new unperturbed Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$.

- In the coupled representation, $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ (even though $\hat{H}'_Z$ has off-diagonal matrix elements in the coupled representation, they are not in the degenerate subspaces of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$).
- See equation (C.25) as an example for the $n = 2$ subspace.

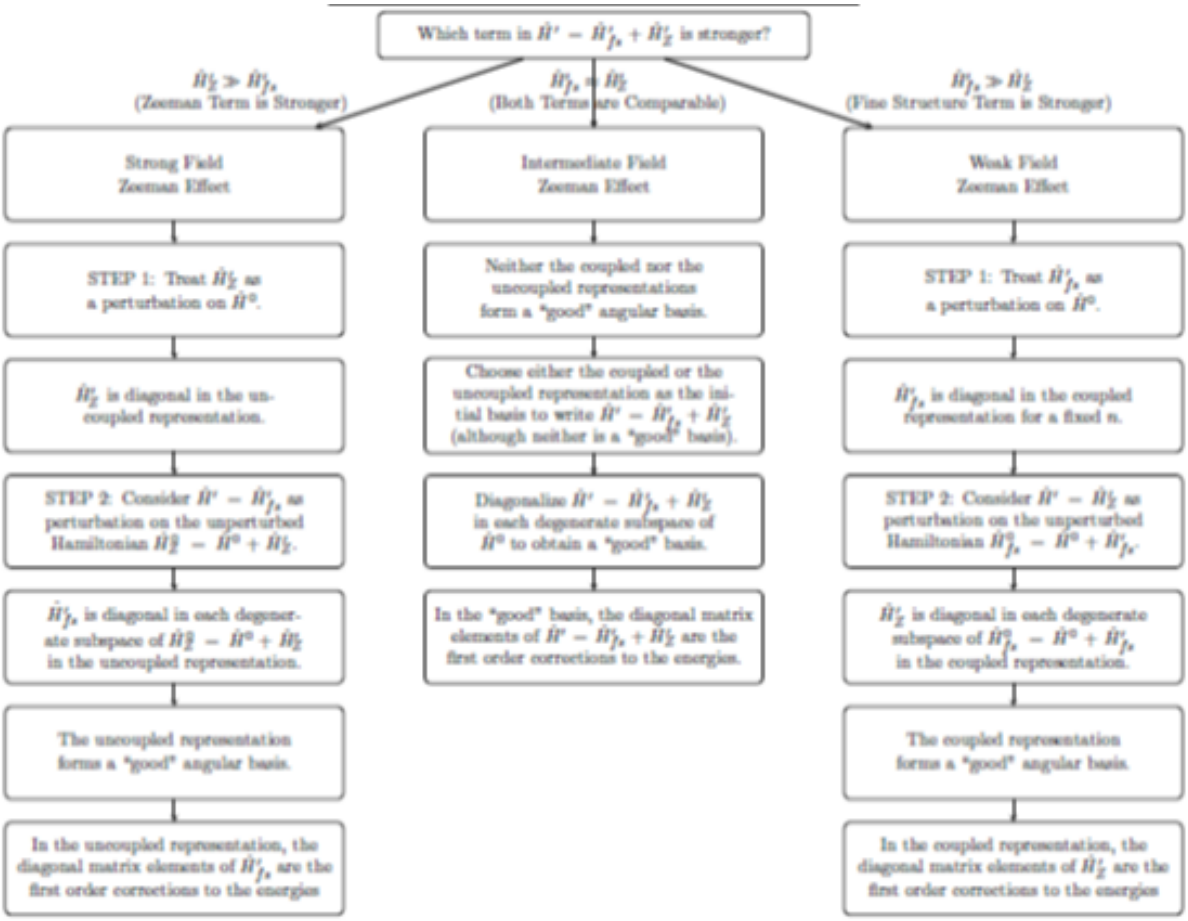
- The coupled representation forms a "good" angular basis for finding the corrections to the energies.

Fill in the following flowchart concerning a "good" angular basis and how to find the corrections to the energies for the intermediate ($E'_{fs} \approx E'_Z$), strong ($E'_Z \gg E'_{fs}$), and weak field Zeeman effect ($E'_{fs} \gg E'_Z$).

# Determining a "GOOD" Angular Basis and Corrections to the Energies Due to BOTH the Fine Structure and Zeeman Effect



# Determining a "GOOD" Angular Basis and Corrections to the Energies Due to BOTH the Fine Structure and Zeeman Effect



Fill in the following table for the Strong Field Zeeman Effect.

# Strong Field Zeeman Effect

| | Hamiltonian | Is the Matrix Diagonal or Non-Diagonal in the Uncoupled Representation? (for a fixed n) | Is the Uncoupled Representation a "Good" Basis? | Is the Matrix Diagonal or Non-Diagonal in the Coupled Representation? (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Energy/ Energy Correction (Using the "Good" Basis) |
|---|---|---|---|---|---|---|
| Step 1 | Unperturbed $\hat{H}^0$ | | | | | |
| | Perturbation $\hat{H}'_Z$ | | | | | |
| Step 2 | Unperturbed $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ | | | | | |
| | Perturbation $\hat{H}'_{fs}$ | | | | | |

Fill in the following table for the Weak Field Zeeman Effect.

# Weak Field Zeeman Effect

| | Hamiltonian | Is the Matrix Diagonal or Non-Diagonal in the Uncoupled Representation? (for a fixed n) | Is the Uncoupled Representation a "Good" Basis? | Is the Matrix Diagonal or Non-Diagonal in the Coupled Representation? (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Energy/ Energy Correction (Using the "Good" Basis) |
|---|---|---|---|---|---|---|
| Step 1 | Unperturbed $\hat{H}^0$ | | | | | |
| | Perturbation $\hat{H}'_{fs}$ | | | | | |
| Step 2 | Unperturbed $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ | | | | | |
| | Perturbation $\hat{H}'_Z$ | | | | | |

**** Check your answers to questions in the preceding tables.****

# Strong Field Zeeman Effect

| | Hamiltonian | Is the Matrix Diagonal or Non-Diagonal in the Uncoupled Representation? (for a fixed n) | Is the Uncoupled Representation a "Good" Basis? | Is the Matrix Diagonal or Non-Diagonal in the Coupled Representation? (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Energy/ Energy Correction (Using the "Good" Basis) |
|---|---|---|---|---|---|---|
| Step 1 | Unperturbed $\hat{H}^0$ | Diagonal | Yes, because $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0$. (actually both $\hat{H}^0$ and $\hat{H}'_Z$ can be diagonalized simultaneously since $[\hat{H}^0, \hat{H}'_Z] = 0$). | Diagonal | No, because $\hat{H}'_Z$ is not diagonal in each degenerate subspace of $\hat{H}^0$. | $E^0 = -\frac{13.6\text{eV}}{n^2}$ |
| | Perturbation $\hat{H}'_Z$ | Diagonal | | Non-Diagonal | | $E'_Z = \mu_B B_{ext}(m_l + 2m_s)$ |
| Step 2 | Unperturbed $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ | Diagonal | Yes, because $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$. | Non-Diagonal | No, because $\hat{H}'_Z$ is not diagonal in each degenerate subspace of $\hat{H}^0$. | $E^0_Z = E^0 + E'_Z$ $= E^0 + \mu_B B_{ext}(m_l + 2m_s)$ |
| | Perturbation $\hat{H}'_{fs}$ | Non-diagonal | | Diagonal | | Use Clebsch-Gordon table to express uncoupled states in the coupled basis to determine $E'_{fs}$ |

# Weak Field Zeeman Effect

| | Hamiltonian | Is the Matrix Diagonal or Non-Diagonal in the Uncoupled Representation? (for a fixed n) | Is the Uncoupled Representation a "Good" Basis? | Is the Matrix Diagonal or Non-Diagonal in the Coupled Representation? (for a fixed $n$) | Is the Coupled Representation a "Good" Basis? | Energy/ Energy Correction (Using the "Good" Basis) |
|---|---|---|---|---|---|---|
| Step 1 | Unperturbed $\hat{H}^0$ | Diagonal | No, because $\hat{H}'_{fs}$ is not diagonal in each degenerate subspace of $\hat{H}^0$. | Diagonal | Yes, because $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$. | $E^0 = -\frac{13.6\text{eV}}{n^2}$ |
| | Perturbation $\hat{H}'_{fs}$ | Non-Diagonal | | Diagonal | | $E'_{fs} = \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{(j+1/2)}\right]$ |
| Step 2 | Unperturbed $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ | Non-Diagonal | No, because $\hat{H}'_{fs}$ is not diagonal in each degenerate subspace of $\hat{H}^0$. | Diagonal | Yes, because $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$. | $E^0_{fs} = E^0 + E'_{fs}$ $= E^0 - \frac{E_n^2}{2mc^2}\left[\frac{4n}{(j+1/2)} - 3\right]$ |
| | Perturbation $\hat{H}'_Z$ | Diagonal | | Non-Diagonal | | Use Clebsch-Gordon table to express coupled states in the uncoupled basis to determine $E'_Z$ |

**Summary: Finding a "GOOD" Basis for the Zeeman Effect in the Hydrogen Atom**

- Intermediate Field Zeeman Effect ($E'_Z \approx E'_{fs}$)
  - Neither the coupled nor the uncoupled representation forms a "good" basis for finding corrections to the energies.
  - One needs to diagonalize $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in each degenerate subspace of $\hat{H}^0$ explicitly to find the "good" basis.
- Strong Field Zeeman Effect ($E'_Z \gg E'_{fs}$)
  - We can carry out perturbation theory in two steps.
  - The uncoupled representation forms a "good" basis for finding corrections to the energies.
- Weak Field Zeeman Effect ($E'_{fs} \gg E'_Z$)
  - We can carry out perturbation theory in two steps.
  - The coupled representation forms a "good" basis for finding corrections to the energies.

| Hamiltonian | Uncoupled Representation (for a fixed $n$) | Is Uncoupled Representation a "Good" Basis? | Coupled Representation (for a fixed $n$) | Is Coupled Representation a "Good" Basis? | Is Any Arbitrary Complete Orthonormal Basis Found with Linear Combinations of a Complete Set of the Coupled or Uncoupled States a "Good" Basis? (with the same $n$ and $l$) | Unperturbed Energy | First Order Correction to the Energy |
|---|---|---|---|---|---|---|---|
| $\hat{H}^0$ | Diagonal | — | Diagonal | — | — | $E_n = -\frac{13.6\text{eV}}{n^2}$ | - |
| $\hat{H}'_r$ | Diagonal | Yes | Diagonal | Yes | Yes | $E_n$ | $E'_r = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$ |
| $\hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E_n$ | $E'_{SO} = \frac{E_n^2}{mc^2}\left[\frac{n(j(j+1)-l(l+1-3/4))}{l(l+1)(l+1/2)}\right]$ |
| $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$ | Not Diagonal | No | Diagonal | Yes | No | $E_n$ | $E'_{fs} = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{(j+1/2)} - 3\right]$ |
| $\hat{H}'_Z$ | Diagonal | Yes | Not Diagonal | No | No | $E_n$ | $E'_Z = \mu B_{ext}(m_l + 2m_s)$ |
| $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$ | Diagonal | Yes | Not Diagonal | No | No | $E_n + \mu B_{ext}(m_l + 2m_s)$ | Diagonal matrix elements of $\hat{H}'_{fs}$ in the uncoupled representation |
| $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ | Not Diagonal | No | Diagonal | Yes | No | $E_n + \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{(j+1/2)}\right]$ | Diagonal matrix elements of $\hat{H}'_Z$ in the coupled representation |

## C.7 FINDING FIRST ORDER ENERGY CORRECTIONS FOR THE INTERMEDIATE FIELD ZEEMAN EFFECT CONTINUED

Reconsider the following perturbing Hamiltonian $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in the coupled representation ($|l,\ j,\ m_j\rangle$) when $E'_{fs} \approx E'_Z$.

$$\hat{H}' = -\begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix} \tag{C.28}$$

in which $\gamma = \left(\frac{\alpha}{8}\right)^2$ 13.6 eV, $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$, $\beta = \mu_B B_{ext}$ and the basis states are chosen in the order of $|\psi_1\rangle = |0,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_2\rangle = |0,\ \frac{1}{2},\ -\frac{1}{2}\rangle$, $|\psi_3\rangle = |1,\ \frac{3}{2},\ \frac{3}{2}\rangle$, $|\psi_4\rangle = |1,\ \frac{3}{2},\ -\frac{3}{2}\rangle$, $|\psi_5\rangle = |1,\ \frac{3}{2},\ \frac{1}{2}\rangle$, $|\psi_6\rangle = |1,\ \frac{1}{2},\ \frac{1}{2}\rangle$, $|\psi_7\rangle = |1,\ \frac{3}{2},\ -\frac{1}{2}\rangle$, and $|\psi_8\rangle = |1,\ \frac{1}{2},\ -\frac{1}{2}\rangle$.

21. Explain in words how to find a "good" basis and corrections to the energies for the intermediate field Zeeman effect ($E'_{fs} \approx E'_Z$).

**OPTIONAL:** The final three questions in this tutorial are optional.

22. Determine the first order corrections to the energies for the intermediate field Zeeman effect ($E'_{fs} \approx E'_Z$) in which the perturbation $\hat{H}' = \hat{H}'_Z + \hat{H}'_{fs}$ in the coupled representation is given in equation (C.28).

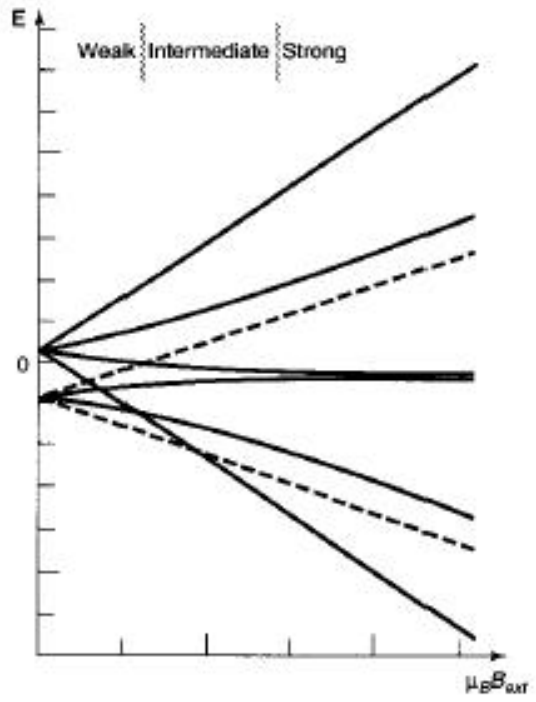
The energy levels for the $n = 2$ states of the hydrogen atom in the intermediate field Zeeman effect are given below.

Table 48: Energy Levels in the Intermediate Field Zeeman Effect ($n = 2$)

$$
\begin{aligned}
\epsilon_1 &= E_2 - 5\gamma + \beta \\
\epsilon_2 &= E_2 - 5\gamma - \beta \\
\epsilon_3 &= E_2 - \gamma + 2\beta \\
\epsilon_4 &= E_2 - \gamma - 2\beta \\
\epsilon_5 &= E_2 - 3\gamma + \beta/2 + \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_6 &= E_2 - 3\gamma + \beta/2 - \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_7 &= E_2 - 3\gamma - \beta/2 + \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_8 &= E_2 - 3\gamma - \beta/2 - \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4}
\end{aligned}
$$

23. Use the appropriate Taylor series expansion to check that the corrections to the energies in the intermediate field Zeeman effect are consistent with the corrections found in the limiting cases of the strong and weak field Zeeman effects earlier.

24. Below is a graph of the splitting of the energy levels of the hydrogen atom for the weak, intermediate, and strong field Zeeman effect for the $n = 2$ subspace. Discuss whether the graph is consistent with what you have learned. Be sure to state whether the number of states is consistent in each regime (weak, strong, and intermediate field Zeeman effect).



[1]

[1]Griffiths, David J. *Introduction to Quantum Mechanics.* 2nd ed. Upper Saddle River, NJ: Pearson Prentice Hall, 2005. pg. 249

**** Check your answers to questions 21-24. ****

21. To find a "good" basis, we must diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. This requires diagonalizing the $2 \times 2$ block diagonals $-\begin{bmatrix} \gamma - \frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma - \frac{1}{3}\beta \end{bmatrix}$ and $-\begin{bmatrix} \gamma + \frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma + \frac{1}{3}\beta \end{bmatrix}$. The "good" basis will be $\{|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle, a|\psi_5\rangle + b|\psi_6\rangle, c|\psi_5\rangle + d|\psi_6\rangle, e|\psi_7\rangle + f|\psi_8\rangle, g|\psi_7\rangle + h|\psi_8\rangle\}$, in which $a, b, c, d, e, f, g$, and $h$ are obtained by diagonalizing the block diagonals.

The corrections to the energies in Table 48 are the diagonal matrix elements of $\hat{H}'$ in the "good" basis.

22.

$$\begin{aligned}
E'_1 &= 5\gamma - \beta \\
E'_2 &= 5\gamma + \beta \\
E'_3 &= \gamma - 2\beta \\
E'_4 &= \gamma + 2\beta \\
E'_5 &= 3\gamma - \beta/2 - \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
E'_6 &= 3\gamma - \beta/2 + \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
E'_7 &= 3\gamma + \beta/2 - \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4} \\
E'_8 &= 3\gamma + \beta/2 + \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4}
\end{aligned}$$

23. In the strong field limit ($\beta \gg \gamma$), $\sqrt{4\gamma^2 \pm \frac{2}{3}\gamma\beta + \frac{1}{4}\beta^2} \approx \frac{1}{2}\beta \pm \frac{2}{3}\gamma$.

$$\begin{aligned}
E'_1 &= E_2 - 5\gamma + \beta \\
E'_2 &= E_2 - 5\gamma - \beta \\
E'_3 &= E_2 - \gamma + 2\beta \\
E'_4 &= E_2 - \gamma - 2\beta \\
E'_5 &= E_2 + \beta - \tfrac{7}{3}\gamma \\
E'_6 &= E_2 - \tfrac{11}{3}\gamma \\
E'_7 &= E_2 - \tfrac{11}{3}\gamma \\
E'_8 &= E_2 - \beta - \tfrac{7}{3}\gamma
\end{aligned}$$

In the weak field limit ($\gamma \gg \beta$), $\sqrt{4\gamma^2 \pm \frac{2}{3}\gamma\beta + \frac{1}{4}\beta^2} \approx 2\gamma \pm \frac{1}{6}\beta$.

$$
\begin{aligned}
E_1' &= E_2 - 5\gamma + \beta \\
E_2' &= E_2 - 5\gamma - \beta \\
E_3' &= E_2 - \gamma + 2\beta \\
E_4' &= E_2 - \gamma - 2\beta \\
E_5' &= E_2 - \gamma + \tfrac{2}{3}\beta \\
E_6' &= E_2 - 5\gamma + \tfrac{1}{3}\beta \\
E_7' &= E_2 - \gamma - \tfrac{2}{3}\beta \\
E_8' &= E_2 - 5\gamma - \tfrac{1}{3}\beta
\end{aligned}
$$

24. In the strong field, we found a two-fold degeneracy remaining in the energy spectrum after the two step approximation. In the weak field, we found no degeneracy remaining in the energy spectrum after the two step approximation. The results are consistent.

If your answers to questions 21-24 do not match with the checkpoint, go back and reconcile any differences.

## APPENDIX D

## SYSTEM OF IDENTICAL PARTICLES QUANTUM INTERACTIVE LEARNING TUTORIAL

### D.1 SYSTEM OF IDENTICAL PARTICLES PRETEST

# Identical Particles Pretest

Notes:

- Do not consider spin of the particles unless explicitly stated in the problem.
- $\hat{\mathbf{H}}_i$ are the single-particle Hamiltonians in the product space.
- $\psi_{n_1}$, $\psi_{n_2}$, etc. are the single-particle stationary state wavefunctions for a non-interacting system.
- For all problems, assume the particles are confined in one spatial dimension.

1. Write the Hamiltonian $\hat{\mathbf{H}}$ for a system of $N$ non-interacting, identical particles in the product space in terms of the Hamiltonian for the $i^{th}$ particle ($i = 1, 2, \ldots, N$).

2. For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction **in the position representation** where **all three particles are in different single-particle states** for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason. **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

   a. The three non-interacting identical particles are fermions.

   b. The three non-interacting identical particles are bosons.

   c. The three non-interacting identical particles are distinguishable.

3. For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction **in the position representation** when two of the particles are in same single-particle state $\psi_{n_1}$ for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason. **Ignore the spin of the particles and only consider the spatial part of the wavefunction (assume $n_1 \neq n_2 \neq n_3$).**

   a. The three non-interacting identical particles are fermions.

   b. The three non-interacting identical particles are bosons.

   c. The three non-interacting identical particles are distinguishable.

4. Consider a system of non-interacting identical particles. For each of the following wavefunctions, identify whether it is a possible wavefunction for a system of identical fermions, identical bosons, both a system of identical fermions and a system of identical bosons, or neither a system of identical fermions or bosons. **Ignore the spin of the particles and only consider the spatial part of the wavefunction**. **Be sure to explain your reasoning**.

   a. $\Psi(x) = \psi_{n_1}(x)\psi_{n_2}(x)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   b. Explain your reasoning.

   c. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   d. Explain your reasoning.

   e. $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   f. Explain your reasoning.

g. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

h. Explain your reasoning.

i. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_2)\psi_{n_1}(x_1)]$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

j. Explain your reasoning.

k. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_1) - \psi_{n_1}(x_2)\psi_{n_2}(x_2)]$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

l. Explain your reasoning.

m. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_2)\psi_{n_1}(x_1)]$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

n. Explain your reasoning.

o. $$\begin{aligned}\Psi(x_1, x_2, x_3) &= \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)]\end{aligned}$$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

p. Explain your reasoning.

q. $$\begin{aligned}\Psi(x_1, x_2, x_3) &= \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)]\end{aligned}$$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

r. Explain your reasoning.

5. For a system of three non-interacting identical particles, there are four distinct single-particle states $\psi_{n_1}(x)$, $\psi_{n_2}(x)$, $\psi_{n_3}(x)$, and $\psi_{n_4}(x)$ available to each single particle. How many different three-particle states can you construct if the particles are

   a. Fermions? (Ignore spin).

   b. Bosons? (Ignore spin).

   c. Distinguishable particles? (Ignore spin).

6. For a system of two non-interacting identical particles in a one-dimensional infinite square well, the total energy of the two particle system is $E_{n_1,n_2} = (n_1^2 + n_2^2)E_1$, in which $E_1$ is the single-particle ground state energy. The total energy of the system is $E = 338E_1$. Assume that all of the possible three-particle states with this total energy $338E_1$ are equally probable.

   Note: The only possible integers $n_1$ and $n_2$ whose squares sum to 338 are given below.

$$\begin{aligned} 338 &= 7^2 + 17^2 \\ &= 13^2 + 13^2 \end{aligned}$$

   a. If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

   b. If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

   c. If the particles are distinguishable and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

7. Suppose a system with eleven single-particle states has 7 particles. The degeneracy of the lowest energy states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited states with energy $E_2$ is $d_2 = 7$. If the total energy of the system is such that 3 particles are in the lowest energy states and 4 particles are in the first-excited states, what is the number of distinct seven-particle states $Q(3, 4)$ corresponding to this particular arrangement $(3, 4)$:

   a. if the particles are indistinguishable fermions? Ignore spin.

   b. if the particles are indistinguishable bosons? Ignore spin.

   c. if the particles are distinguishable? Ignore spin.

   Notes:

   - For the remaining problems, consider the spin of the particles.
   - $|s,\ m_s\rangle$ are eigenstates of $\hat{S}^2$ and $\hat{S}_z$. $|s_i,\ m_{s_i}\rangle$ are eigenstates of $\hat{S}_i^2$ and $\hat{S}_{iz}$ for $i = 1, 2, 3$.
   - We will use the following abbreviated notation for a spin-1/2 particle in the uncoupled representation

$$|\uparrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ 1/2\rangle_1, \qquad \text{and} \qquad |\downarrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ -1/2\rangle_1$$

$$|\uparrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ 1/2\rangle_2, \qquad \text{and} \qquad |\downarrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ -1/2\rangle_2$$

$$|\uparrow\rangle_3 = |s_3,\ m_{s_3}\rangle = |1/2,\ 1/2\rangle_3, \qquad \text{and} \qquad |\downarrow\rangle_3 = |s_3,\ m_{s_3}\rangle = |1/2,\ -1/2\rangle_3$$

   - The following information may be helpful for a system of two particles:

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S}_z = \vec{S}_{1z} + \vec{S}_{2z}$$

- For a system of two spin-1/2 particles $\left(s_1 = \frac{1}{2} \otimes s_2 = \frac{1}{2}\right)$, basis states in the coupled representation $|s,\ m_s\rangle$ are written in terms of the uncoupled representation as follows:

$$\begin{array}{rcccl}
|1,\ 1\rangle & = & |\uparrow\uparrow\rangle & = & |\uparrow\rangle_1|\uparrow\rangle_2 \\
|1,\ -1\rangle & = & |\downarrow\downarrow\rangle & = & |\downarrow\rangle_1|\downarrow\rangle_2 \\
|1,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) \\
|0,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)
\end{array}$$

- In the following table, for spin degrees of freedom for two spin-1 particles ($s_1 = 1 \otimes s_2 = 1$) in the coupled representation the product states, $|s,\ m_s\rangle$, (left) are given in terms of a linear combination of the product states in the uncoupled representation, $|s_1,\ m_{s_1}\rangle_1|s_2,\ m_{s_2}\rangle_2$, (right) using the Clebsch-Gordon table.

| Product states in Coupled Representation $\|s,\ m_s\rangle$ | Written in terms of product states in Uncoupled Representation $\sum_{m_{s_1}+m_{s_2}=m_s} C^{s_1,s_2,s}_{m_{s_1},m_{s_2},m_s}\|s_1,\ m_{s_1}\rangle_1\|s_2,\ m_{s_2}\rangle_2$ |
|---|---|
| $\|2,\ 2\rangle$ | $\|1,\ 1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 + \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|1,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 - \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|2,\ 0\rangle$ | $\frac{1}{\sqrt{6}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 + \sqrt{\frac{2}{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{6}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|1,\ 0\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 1\rangle_2)$ |
| $\|0,\ 0\rangle$ | $\frac{1}{\sqrt{3}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \frac{1}{\sqrt{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{3}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 + \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|1,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|2,\ -2\rangle$ | $\|1,\ -1\rangle_1\|1,\ -1\rangle_2$ |

8. Consider a system of three non-interacting identical spin-1/2 particles. If two of the particles are in the spin up state ($|\uparrow\rangle$) and one of the particles is in the spin down state ($|\downarrow\rangle$), construct a completely symmetric spin state for the three particles. If no such spin state exists, state the reason why.

9. Write one possible spin part of the wavefunction for a system of two non-interacting spin-1/2 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

10. Write one possible spin part of the wavefunction for a system of two non-interacting spin-1/2 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

11. Consider a system with three non-interacting identical spin-1 particles. If the three particles are in different spin states, construct a completely symmetric spin state for the three particles. If no such spin state exists, state the reason why.

12. Write one possible spatial part of the wavefunction for two non-interacting identical spin-1 particles whose spin part of the wavefunction (expressed in terms of the uncoupled representation) is $\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|1\ 1\rangle_1|1\ 0\rangle_2 + |1\ 0\rangle_1|1\ 1\rangle_2]$. If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write not possible and state the reason.

13. Write one possible spatial part of the wavefunction for two non-interacting identical spin-1 particles whose spin part of the wavefunction (expressed in terms of the coupled representation) is $\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|2\ 2\rangle - |1\ 1\rangle]$. If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write not possible and state the reason.

# Identical Particles Posttest

Notes:

- Do not consider spin of the particles unless explicitly stated in the problem.
- $\hat{\mathbf{H}}_i$ are the single-particle Hamiltonians in the product space.
- $\psi_{n_1}$, $\psi_{n_2}$, etc. are the single-particle stationary state wavefunctions for a non-interacting system.
- For all problems, assume the particles are confined in one spatial dimension.

1. Write the Hamiltonian $\hat{\mathbf{H}}$ for a system of $N$ non-interacting, identical particles in the product space in terms of the Hamiltonian for the $i^{th}$ particle ($i = 1, 2, \ldots, N$).

2. For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction **in the position representation** where **all three particles are in different single-particle states** for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason. **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

   a. The three non-interacting identical particles are fermions.

   b. The three non-interacting identical particles are bosons.

   c. The three non-interacting identical particles are distinguishable.

3. For a system of three non-interacting identical particles, write a properly normalized three-particle stationary state wavefunction **in the position representation** when two of the particles are in same single-particle state $\psi_{n_1}$ for the following three cases: indistinguishable fermions, indistinguishable bosons, and identical particles treated as distinguishable. If there is no such possible three-particle stationary state wavefunction for the given system of three particles, state the reason. **Ignore the spin of the particles and only consider the spatial part of the wavefunction**.

   a. The three non-interacting identical particles are fermions.

   b. The three non-interacting identical particles are bosons.

   c. The three non-interacting identical particles are distinguishable.

4. Consider a system of non-interacting identical particles. For each of the following wavefunctions, identify whether it is a possible wavefunction for a system of identical fermions, identical bosons, both a system of identical fermions and a system of identical bosons, or neither a system of identical fermions or bosons. **Ignore the spin of the particles and only consider the spatial part of the wavefunction (assume $n_1 \neq n_2 \neq n_3$). Be sure to explain your reasoning**.

   a. $\Psi(x) = \psi_{n_1}(x)\psi_{n_2}(x)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   b. Explain your reasoning.

   c. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   d. Explain your reasoning.

   e. $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$
      i. Identical fermions
      ii. Identical bosons
      iii. Both identical fermions and identical bosons
      iv. Neither identical fermions nor identical bosons
   f. Explain your reasoning.

g. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

h. Explain your reasoning.

i. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_2)\psi_{n_1}(x_1)]$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

j. Explain your reasoning.

k. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_1) - \psi_{n_1}(x_2)\psi_{n_2}(x_2)]$

   i. Identical fermions

   ii. Identical bosons

   iii. Both identical fermions and identical bosons

   iv. Neither identical fermions nor identical bosons

l. Explain your reasoning.

m. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_2)\psi_{n_1}(x_1)]$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

n. Explain your reasoning.

o. $$\begin{aligned}\Psi(x_1, x_2, x_3) &= \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)]\end{aligned}$$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

p. Explain your reasoning.

q. $$\begin{aligned}\Psi(x_1, x_2, x_3) &= \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)]\end{aligned}$$

i. Identical fermions

ii. Identical bosons

iii. Both identical fermions and identical bosons

iv. Neither identical fermions nor identical bosons

r. Explain your reasoning.

5. For a system of two non-interacting identical particles, there are five distinct single-particle states $\psi_{n_1}(x)$, $\psi_{n_2}(x)$, $\psi_{n_3}(x)$, $\psi_{n_4}(x)$, and $\psi_{n_5}(x)$ available to each single particle. How many different two-particle states can you construct if the particles are

   a. Fermions? (Ignore spin).

   b. Bosons? (Ignore spin).

   c. Distinguishable particles? (Ignore spin).

6. For a system of three non-interacting identical particles in a one-dimensional infinite square well, the total energy of the three particle system is $E_{n_1,n_2,n_3} = (n_1^2 + n_2^2 + n_3^2)E_1$, in which $E_1$ is the single-particle ground state energy. The total energy of the system is $E = 75E_1$. Assume that all of the possible three-particle states with this total energy $75E_1$ are equally probable.

   Note: The only possible integers $n_1$, $n_2$ and $n_3$ whose squares sum to 75 are given below.

$$\begin{aligned} 75 &= 1^2 + 5^2 + 7^2 \\ 75 &= 5^2 + 5^2 + 5^2 \end{aligned}$$

   a. How many distinct three-particle states can you construct if the particles are

      i. Indistinguishable fermions? Explain your reasoning.

      ii. Indistinguishable bosons? Explain your reasoning.

      iii. Identical particles that can be treated as distinguishable? Explain your reasoning.

   b. If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

   c. If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

   d. If the particles are distinguishable and you randomly measure the energy of one particle, what energies might you obtain and with what probabilities?

7. Suppose a system with nine single-particle states has 8 particles. The degeneracy of the lowest energy states with energy $E_1$ is $d_1 = 5$ and the degeneracy of the first-excited states with energy $E_2$ is $d_2 = 4$. If the total energy of the system is such that 3 particles are in the lowest energy states and 5 particles are in the first-excited states, what is the number of distinct eight-particle states $Q(3,5)$ corresponding to this particular arrangement $(3,5)$:

   a. if the particles are indistinguishable fermions? Ignore spin.

   b. if the particles are indistinguishable bosons? Ignore spin.

   c. if the particles are distinguishable? Ignore spin.

   Notes:

   - For the remaining problems, consider the spin of the particles.
   - $|s,\ m_s\rangle$ are eigenstates of $\hat{S}^2$ and $\hat{S}_z$. $|s_i,\ m_{s_i}\rangle$ are eigenstates of $\hat{S}_i^2$ and $\hat{S}_{iz}$ for $i = 1, 2, 3$.
   - We will use the following abbreviated notation for a spin-1/2 particle in the uncoupled representation

$$|\uparrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ 1/2\rangle_1, \qquad \text{and} \qquad |\downarrow\rangle_1 = |s_1,\ m_{s_1}\rangle = |1/2,\ -1/2\rangle_1$$

$$|\uparrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ 1/2\rangle_2, \qquad \text{and} \qquad |\downarrow\rangle_2 = |s_2,\ m_{s_2}\rangle = |1/2,\ -1/2\rangle_2$$

$$|\uparrow\rangle_3 = |s_3,\ m_{s_3}\rangle = |1/2,\ 1/2\rangle_3, \qquad \text{and} \qquad |\downarrow\rangle_3 = |s_3,\ m_{s_3}\rangle = |1/2,\ -1/2\rangle_3$$

   - The following information may be helpful for a system of two particles:

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S_z} = \vec{S}_{1z} + \vec{S}_{2z}$$

- For a system of two spin-1/2 particles $\left(s_1 = \frac{1}{2} \otimes s_2 = \frac{1}{2}\right)$ basis states in the coupled representation $|s,\ m_s\rangle$ are written in terms of the uncoupled representation as follows:

$$\begin{array}{rcccl}
|1,\ 1\rangle & = & |\uparrow\uparrow\rangle & = & |\uparrow\rangle_1|\uparrow\rangle_2 \\
|1,\ -1\rangle & = & |\downarrow\downarrow\rangle & = & |\downarrow\rangle_1|\downarrow\rangle_2 \\
|1,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) \\
|0,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)
\end{array}$$

- In the following table, for spin degrees of freedom for two spin-1 particles ($s_1 = 1 \otimes s_2 = 1$) in the coupled representation the product states, $|s,\ m_s\rangle$, (left) are given in terms of a linear combination of the product states in the uncoupled representation, $|s_1,\ m_{s_1}\rangle_1|s_2,\ m_{s_2}\rangle_2$, (right) using the Clebsch-Gordon table.

| Product states in Coupled Representation $\|s,\ m_s\rangle$ | Written in terms of product states in Uncoupled Representation $\sum_{m_{s_1}+m_{s_2}=m_s} C^{s_1,s_2,s}_{m_{s_1},m_{s_2},m_s}\|s_1,\ m_{s_1}\rangle_1\|s_2,\ m_{s_2}\rangle_2$ |
|---|---|
| $\|2,\ 2\rangle$ | $\|1,\ 1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 + \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|1,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 - \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|2,\ 0\rangle$ | $\frac{1}{\sqrt{6}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 + \sqrt{\frac{2}{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{6}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|1,\ 0\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 1\rangle_2)$ |
| $\|0,\ 0\rangle$ | $\frac{1}{\sqrt{3}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \frac{1}{\sqrt{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{3}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 + \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|1,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|2,\ -2\rangle$ | $\|1,\ -1\rangle_1\|1,\ -1\rangle_2$ |

8. Consider a system with three non-interacting identical spin-1/2 particles. If two of the particles are in the spin up state ($|\uparrow\rangle$) and one of the particles is in the spin down state ($|\downarrow\rangle$), construct a completely symmetric spin state for the three particles. If no such spin state exists, state the reason why.

9. Write one possible spin part of the wavefunction for a system of two non-interacting spin-1/2 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

10. Write one possible spin part of the wavefunction for a system of two non-interacting spin-1/2 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

11. Consider a system of three non-interacting identical spin-1/2 particles. If two of the particles are in the spin up state ($|\uparrow\rangle$) and one of the particles is in the spin down state ($|\downarrow\rangle$), construct a completely antisymmetric spin state for the three particles. If no such spin state exists, state the reason why.

12. Write one possible spatial part of the wavefunction for two non-interacting identical spin-1/2 particles whose spin part of the wavefunction is $\chi(m_{s_1}, m_{s_2}) = |\uparrow\downarrow\rangle$. If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write not possible and state the reason.

13. Write one possible spatial part of the wavefunction for two non-interacting identical spin-1/2 particles whose spin part of the wavefunction is $\chi(m_{s_1}, m_{s_2}) = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle]$. If it is not possible to write a spatial part of the wavefunction with the given spin part of the wavefunction, write not possible and state the reason.

14. Consider a system with three non-interacting identical spin-1 particles. If the three particles are in different spin states, construct a completely antisymmetric spin state for the three particles. If no such spin state exists, state the reason why.

15. Write one possible spin part of the wavefunction for two non-interacting identical spin-1 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

16. Write one possible spin part of the wavefunction for two non-interacting identical spin-1 particles whose spatial part of the wavefunction is $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)]$. If it is not possible to write a spin part of the wavefunction with the given spatial part of the wavefunction, write not possible and state the reason.

## D.3 SYSTEM OF IDENTICAL PARTICLES TUTORIAL

# Identical Particles Tutorial

## D.4 NOTES FOR THIS TUTORIAL:

- We will only consider systems of non-interacting identical particles.
- The word "identical" in this tutorial will refer to one type of particle (all particles with the same properties). For example, all electrons are identical.
- Assume that all systems with more than one particle consist of identical particles. For example, a system of fermions is made up of identical fermions (e.g., electrons) and a system of bosons is made up of identical bosons (e.g., Helium-4 atoms).
- Identical particles (particles of one type with the same properties) are in general indistinguishable (e.g., you cannot distinguish which particle is in which single particle stationary state). Exchanging these indistinguishable particles with each other does not produce a distinctly different many-particle state.
- Assume that particles are restricted to one spatial dimension (spatial coordinate given by $x$) for convenience.
- We will use the notation $\hat{H}_i$ to denote the Hamiltonian in the $M$-dimensional Hilbert space for the $i^{th}$ particle. We will use the boldface notation $\hat{\mathbf{H}}_i$ to denote the Hamiltonian of the $i^{th}$ particle in the $M^N$-dimensional Hilbert space for the $N$ particle system.
- Unless otherwise stated, the single-particle wavefunction, $\psi_n(x)$, in this tutorial refers to the normalized single-particle stationary state wavefunction.
- The $N$-particle wavefunction, $\psi(x_1, x_2, \cdots, x_N) = \psi_{n_1,n_2,\cdots,n_N}(x_1, x_2, \cdots, x_N)$, in this tutorial refers to the many-particle stationary state wavefunction with coordinates $x_1, x_2, \ldots, x_N$ for different particles.

- The wavefunction of a system of two non-interacting identical particles has terms such as $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, where $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for particles in states $n_1$ and $n_2$ and coordinates $x_1$ and $x_2$, respectively.
  - Remark: $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ should be regarded as any single-particle wavefunctions for particles 1 and 2, respectively (i.e., in general, $\psi_{n_1}$ does not refer to the ground state and $\psi_{n_2}$ does not refer to the first-excited state wavefunction).
- Here, for convenience, we will refer to all direct products of single-particle states as "basis states". Please note that for identical fermions, only completely antisymmetric linear combinations of these basis states are allowed, while for bosons only completely symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed.
- The energy of the system of $N$ non-interacting identical particles is given by $E = E_{n_1} + E_{n_2} + \cdots + E_{n_N} = \sum_{i=1}^{N} E_{n_i}$, in which $E_{n_i}$ is the energy corresponding to the single-particle state $\psi_{n_i}$.
- Unless otherwise specified, there is no degeneracy in the energy spectrum of the single-particle states. That is $E_{n_i} \neq E_{n_j}$ for $n_i \neq n_j$, in which $E_{n_i}$ is the energy corresponding to the single-particle state with wavefunction $\psi_{n_i}$ and $E_{n_j}$ is the energy corresponding to the single-particle state $\psi_{n_j}$.
- Unless otherwise specified, assume that the particles are spinless for the purposes of constructing the many-particle wavefunction and ignore the spin part of the wavefunction.
- The product notation, e.g, $\prod_{i=1}^{N} x_i$, will be used to represent the product of $x_i$ for $i = 1, 2, \ldots, N$ (i.e. $\prod_{i=1}^{N} x_i = x_1 x_2 x_3 \cdots x_N$).

## D.5 OBJECTIVES

**Upon completion of this tutorial, you should be able to do the following:**

1. Determine the form of the Hamiltonian for non-interacting identical particles.
2. Determine the basis states in the product space for a system of non-interacting identical particles
3. Determine the form of the wavefunction for a system of non-interacting identical particles if the particles are indistinguishable fermions, indistinguishable bosons, or a hypothetical case in which identical particles can be treated as distinguishable.
4. Construct the wavefunction for the ground state and first-excited state for a specific two-particle system for two non-interacting identical particles (particles of one type with the same properties) if the particles are:
   - Indistinguishable bosons
   - Indistinguishable fermions
   - Hypothetical case: Identical particles which can be treated as distinguishable
5. Determining the Number of Distinct Many-Particle States
   a. CASE 1: The total energy of the many-particle system is not fixed, but a fixed number of single-particle states are available to the system:
      i. Calculate the number of distinct many-particle states if you have two particles, three particles, or $N$ particles ($N \gg 1$) in the following cases:
         - Particles are indistinguishable bosons
         - Particles are indistinguishable fermions
         - Hypothetical case: Identical particles which can be treated as distinguishable
      ii. Compare the results for the cases of indistinguishable bosons and indistinguishable fermions to the results for the hypothetical case when identical particles can be treated as distinguishable.
   b. CASE II: The total energy of the many-particle system is fixed:
      i. Calculate the number of distinct many-particle states if you have two particles or three particles in the following cases:
         - Particles are indistinguishable bosons

- Particles are indistinguishable fermions
- Hypothetical case: Identical particles which can be treated as distinguishable

ii. Compare the results for the cases of indistinguishable bosons and indistinguishable fermions to the results for the hypothetical case when identical particles can be treated as distinguishable.

iii. For a system of two non-interacting identical particles, determine the probability of obtaining a particular value of the energy of a particle when the single-particle energy is measured at random and the total energy is fixed for a specified many-particle system if the particles are:

- Indistinguishable bosons
- Indistinguishable fermions
- Hypothetical case: Identical particles which can be treated as distinguishable

iv. Compare the results for the cases of indistinguishable bosons and indistinguishable fermions to the results for the hypothetical case when identical particles can be treated as distinguishable.

c. CASE III: The single-particle states have degeneracy and the total energy of the many-particle system is fixed by fixing the number of particles in each group of degenerate single-particle states with a given energy.

i. Calculate the number of distinct many-particle states in the following cases:

- Particles are indistinguishable bosons
- Particles are indistinguishable fermions
- Hypothetical case: Identical particles which can be treated as distinguishable.

6. Determine the wavefunction including spin for a system of non-interacting identical particles if the particles are indistinguishable fermions or bosons.
7. Construct the wavefunction for the ground state and first-excited state for specific many-particle system for many non-interacting identical particles if the particles are:
   - Indistinguishable bosons
   - Indistinguishable fermions.

8. Determine the form of the wavefunction for a system of non-interacting identical particles in the limiting case when identical particles can be treated as distinguishable.

## D.6 BASICS FOR A SYSTEM OF $N$ NON-INTERACTING PARTICLES

### D.6.1 Hamiltonian for a System of Non-interacting Particles

- Before we determine the form of the stationary state wavefunction for a system of $N$ non-interacting identical particles, let's determine the form of the Hamiltonian for a system of non-interacting particles in terms of the single-particle Hamiltonian.
- We will use the notation $\hat{H}_i$ to denote the Hamiltonian in the $M$-dimensional Hilbert space for the $i^{th}$ particle. We will use the boldface notation $\hat{\mathbf{H}}_i$ to denote the Hamiltonian of the $i^{th}$ particle in the $M^N$-dimensional Hilbert space for the many-particle system.
- The following question and conversations will guide you as you think about the Hamiltonian for a system of $N$ non-interacting identical particles in which each particle is in a $M$-dimensional space.

1. For a system of $N$ **non-interacting** particles, write the Hamiltonian of the system in the product space $\hat{\mathbf{H}}$, in terms of $\hat{\mathbf{H}}_i$, the Hamiltonian for the $i^{th}$ particle ($i = 1, 2, \ldots, N$) in the product space.

Consider the following conversation regarding constructing the Hamiltonian for a system of $N$ **non-interacting** identical particles in which each particle is in a $M$-dimensional space.

**Student 1:** The Hamiltonian for the non-interacting $N$-particle system in the $M^N$-dimensional product space is $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 \otimes \hat{\mathbf{H}}_2 \otimes \hat{\mathbf{H}}_3 \otimes \cdots \otimes \hat{\mathbf{H}}_N$, in which $\hat{\mathbf{H}}_i = \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{i-1} \otimes \hat{H}_i \otimes \hat{I}_{i+1} \cdots \otimes \hat{I}_N$ is the Hamiltonian of the $i^{th}$ particle in the $M^N$-dimensional space. The single-particle Hamiltonian, $\hat{H}_i$, and the identity operator, $\hat{I}_i$, are for the $i^{th}$ particle in the $M$-dimensional space.

**Student 2:** I disagree with Student 1. The Hamiltonian $\hat{\mathbf{H}}$ for non-interacting particles in the $M^N$-dimensional product space is $\hat{\mathbf{H}} = \hat{H}_1 \otimes \hat{H}_2 \otimes \hat{H}_3 \otimes \cdots \otimes \hat{H}_N$.

**Student 3:** I disagree with Student 1 and Student 2. If we know the single-particle Hamiltonian $\hat{H}_i$ for the $i^{th}$ particle in the system in the $M$-dimensional space, then the Hamiltonian for a system of $N$ non-interacting identical particles in the $M^N$-dimensional product space has the form $\hat{\mathbf{H}} = \hat{H}_1 + \hat{H}_2 + \cdots + \hat{H}_N$.

**Student 4:** I disagree with Student 1, Student 2, and Student 3. Since the Hamiltonian for the system must be in the $M^N$-dimensional product space, $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \cdots + \hat{\mathbf{H}}_N$. The single-particle Hamiltonian for the $i^{th}$ particle in the $M^N$-dimensional product space is $\hat{\mathbf{H}}_i = \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \hat{I}_{i-1} \otimes \hat{H}_i \otimes \hat{I}_{i+1} \otimes \cdots \otimes \hat{I}_N$, where the boldface notation $\hat{\mathbf{H}}_i$ is for the $M^N$-dimensional product space. The sum of the $M$-dimensional single-particle Hamiltonians $\hat{H}_1 + \hat{H}_2 + \cdots + \hat{H}_N$ is only $M$-dimensional and is not in the $M^N$-dimensional product space.

Explain why you agree or disagree with each student.

Consider the following conversation regarding constructing the Hamiltonian for a system of $N$ **non-interacting** identical particles in which each particle is in a $M$-dimensional space.

**Student 1:** If we know the single-particle Hamiltonian $\hat{\mathbf{H}}_i$ for the $i^{th}$ particle in the system in the $M^N$-dimensional space, then the Hamiltonian for a system of $N$ non-interacting identical particles has the form $\hat{\mathbf{H}} = (\hat{H}_1 \otimes \hat{I}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N) + (\hat{I}_1 \otimes \hat{H}_2 \otimes \hat{I}_3 \otimes \cdots \otimes \hat{I}_N) + \cdots + (\hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{N-2} \otimes \hat{H}_{N-1} \otimes \hat{I}_N) + (\hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{N-1} \otimes \hat{H}_N)$, with the single-particle Hamiltonian, $\hat{H}_i$, and the identity operator, $\hat{I}_i$, for the $i^{th}$ particle in the $M$-dimensional space.

**Student 2:** I agree with Student 1. Since the particles are non-interacting, the Hamiltonian $\hat{\mathbf{H}}_i$ for the $i^{th}$ particle is not entangled with the Hamiltonian $\hat{\mathbf{H}}_j$ for the $j^{th}$ particle. A short hand notation for the sum is $\hat{\mathbf{H}} = \sum_{i=1}^{N} \hat{\mathbf{H}}_i = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 + \cdots + \hat{\mathbf{H}}_N$.

Explain why you agree or disagree with each student.

**** CHECKPOINT: Check your answer to question 1. ****

1. $\hat{\mathbf{H}} = \sum_{i=1}^{N} \hat{\mathbf{H}}_i = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 + \cdots + \hat{\mathbf{H}}_N$

If your answer does not match the checkpoint, go back and reconcile any difference you may have with the checkpoint answer.

Consider the following conversation regarding two non-interacting identical particles in a one-dimensional infinite square well.

**Student 1:** In an infinite square well, we are only permitted to have one-particle in the well. If the system has two non-interacting identical particles, we MUST have two infinite square wells in order to place each particle.

**Student 2:** I disagree. We can have two non-interacting identical particles in the same infinite square well. If the particles are non-interacting and confined to a well of width $a$, the Hamiltonian for each particle in the product space will be $\hat{\mathbf{H}}_i = \frac{\hat{p}_i^2}{2m} + V(x_i)$, in which

$$V(x_i) = \begin{cases} 0 & \text{if} \quad 0 \leq x_i \leq a \\ \infty & \text{otherwise} \end{cases} \qquad (i = 1, 2).$$

The Hamiltonian for the system of two non-interacting identical particles in the same well in the product space is $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2$, where $\hat{\mathbf{H}}_1$ and $\hat{\mathbf{H}}_2$ are the single-particle Hamiltonians in the product space and $\hat{H}_1$ and $\hat{H}_2$ are the single-particle Hamiltonians in the subspaces for the individual particles.

Explain why you agree or disagree with each student.

**Summary of the Hamiltonian for a System of $N$ Non-interacting Particles.**

- The Hamiltonian $\hat{\mathbf{H}}$ for a system of $N$ non-interacting particles in the product space is the sum of the Hamiltonians for each particle in the product space, $\hat{\mathbf{H}} = \sum_{i=1}^{N} \hat{\mathbf{H}}_i = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \hat{\mathbf{H}}_3 + \cdots + \hat{\mathbf{H}}_N$ with $\hat{\mathbf{H}}_i = \hat{I}_1 \otimes \hat{I}_2 \otimes \cdots \otimes \hat{I}_{i-1} \otimes \hat{H}_i \otimes \hat{I}_{i+1} \otimes \cdots \otimes \hat{I}_N$.

### D.6.2 Determining Whether the Basis States in the Product Space for a System of $N$ Non-Interacting Identical Particles Should be Written in Terms of the Sum or Product of the Single-Particle Stationary State Wavefunctions

- Now that we know the form of the Hamiltonian $\hat{\mathbf{H}}$ for a system of $N$ non-interacting identical particles in terms of the single-particle Hamiltonian $\hat{\mathbf{H}}_i$ in the product space, let's think about the form of the stationary state wavefunction for this system.
- The form of the stationary state wavefunction for a system of non-interacting identical particles will depend on the type of particle. We will consider three cases:
  - Indistinguishable fermions
  - Indistinguishable bosons
  - Hypothetical case: Identical particles which can be treated as distinguishable.
- Here, for convenience, we will refer to all direct products of single-particle states as "basis states". Please note that for identical fermions, only completely antisymmetric linear combinations of these basis states are allowed, while for bosons only completely symmetric linear combinations are allowed. For distinguishable particles, all basis states are allowed..
  - Let's consider the appropriate basis states, e.g., whether the wavefunction for a system of $N$ non-interacting identical particles can be written in terms of the sum or the product of the single-particle wavefunctions of individual particles.

2. Explain why you agree or disagree with the following student. If you disagree, write a correct statement.

   **Student 1:** The wavefunction $\psi_{n_1}(x_1)$ describes a particle in a single-particle state denoted by quantum number $n_1$ specifying a single-particle energy and coordinate $x_1$.

3. Write the right-hand side without operators if possible in the following questions for a system of two non-interacting identical particles, whose single-particle wavefunctions satisfy the Time Independent Schrödinger Equation (TISE), $\hat{H}_i\psi_{n_j}(x_i) = E_{n_j}\psi_{n_j}(x_i)$ for the $i^{th}$ particle with coordinate $x_i$ in the single-particle state given by $n_j$. Assume $n_1 \neq n_2$. If it is not possible to write the right-hand side without operators and without encountering difficulties or inconsistencies, explain why.

   a. $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$ _____

   b. $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$ _____

   c. $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)] =$ _____

   d. $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] =$ _____

   e. $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] =$ _____

   f. $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) =$ _____

   g. $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)] =$ _____

   h. $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)] =$ _____

4. Circle all of the following wavefunctions "$\Psi$" (taken from question 3) that are "possible" two-particle stationary state wavefunctions. Ignore normalization. (Hint: The wavefunction $\Psi$ should satisfy $\hat{\mathbf{H}}\Psi = E\Psi$ in which $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ is the Hamiltonian in the product space and $E = E_1 + E_2$ is the energy, respectively, of the two-particle system.)
   a. $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$
   b. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$
   c. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)$
   d. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)$

Consider the following conversation regarding whether the basis states for constructing the two-particle stationary state wavefunction for a system of two non-interacting identical particles can be written in terms of the sum of the single-particle wavefunctions.

**Student 1:** The basis states that can be used to construct a two-particle stationary state wavefunction for a system of two non-interacting identical particles can be written in terms of the sum of the single-particle wavefunctions, $\Psi(x_1, x_2) = \psi_{n_1}(x_1) + \psi_{n_2}(x_2)$.

**Student 2:** I disagree. The sum of the single-particle states $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$ is not in the Hilbert space of the two-particle system. When the two-particle Hamiltonian $\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ acts on the state $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$, there are inconsistencies. Consider terms of the type $\hat{\mathbf{H}}_\mathbf{1}\psi_{n_2}(x_2)$ when $\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$ acts on $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$.

**Student 1:** Isn't $\hat{\mathbf{H}}_1\psi_{n_2}(x_2) = 0$?

**Student 2:** No. The single-particle Hamiltonian $\hat{H}_1$ only acts on the wavefunction corresponding to particle one. The wavefunction $\psi_{n_2}(x_2)$ can be written as $1 \cdot \psi_{n_2}(x_2)$. The wavefunction corresponding to particle one is "1", which is not normalizable.

**Student 3:** I agree with Student 2. The sum of the single-particle states $\psi_{n_1}(x_1) + \psi_{n_2}(x_2)$ cannot be a basis state for a two-particle system.

Explain why you agree or disagree with the students.

Consider the following conversation regarding whether the basis states for constructing the many-particle stationary state wavefunction for a system of two non-interacting identical particles can be written in terms of the product of the single-particle wavefunctions.

**Student 1:** The basis states used to construct a two-particle stationary state wavefunction for a system of two non-interacting identical particles can be written in terms of the product of the single-particle wavefunctions, such as $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$.

**Student 2:** I agree with Student 1. Also, if we consider terms of the type $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ in the wavefunction for a system of two non-interacting identical particles, then it satisfies the TISE, as follows:

$$\begin{aligned}
\hat{\mathbf{H}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (\hat{H}_1 \otimes \hat{I}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) + (\hat{I}_1 \otimes \hat{H}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= \hat{H}_1\psi_{n_1}(x_1)\hat{I}_2\psi_{n_2}(x_2) + \hat{I}_1\psi_{n_1}(x_1)\hat{H}_2\psi_{n_2}(x_2) \\
&= \hat{H}_1\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \hat{H}_2\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= [\hat{H}_1\psi_{n_1}(x_1)]\psi_{n_2}(x_2) + \psi_{n_1}(x_1)[\hat{H}_2\psi_{n_2}(x_2)] \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_1)E_{n_2}\psi_{n_2}(x_2) \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (E_{n_1} + E_{n_2})\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= E\psi_{n_1}(x_1)\psi_{n_2}(x_2) \qquad \text{in which } E = E_{n_1} + E_{n_2}.
\end{aligned}$$

Explain why you agree or disagree with each student.

Consider the following conversation regarding whether the basis states consisting of the product of the single-particle stationary state wavefunctions span the product space of the many-particle system.

**Student 1:** The products of the single-particle stationary state wavefunctions are solutions to the TISE and therefore, they must be basis states for the system of $N$ non-interacting identical particles.

**Student 2:** I agree. A complete set of energy eigenstates $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ will span the product space and will form a suitable basis.

**Student 3:** I agree with both Student 1 and Student 2. Since the products of the single-particle stationary state wavefunctions form a complete set of energy eigenstates for the many-particle system, they must span the product space for the many-particle system.

Explain why you agree or disagree with each student.

Summarize in your own words whether the sums or products of the single-particle wavefunctions can form a suitable basis for $N$ non-interacting identical particles in the product space.

- The following conversation and questions will help you learn about the notation for the stationary state wavefunction for a system of $N$ non-interacting identical particles

Consider the following conversation regarding whether the single-particle wavefunctions in the basis states should have the same or different coordinates to properly specify a three-particle wavefunction for a system of three non-interacting identical particles.

**Student 1:** We must assign a different coordinate to each identical particle. The wavefunction will have basis states such as $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$.

**Student 2:** No. I disagree with Student 1. When the particles are indistinguishable, we can't possibly distinguish their individual coordinates. So the wavefunction will have basis states such as $\psi_{n_1}(x)\psi_{n_2}(x)\psi_{n_3}(x)$.

Explain why you agree or disagree with each student.

5. After each statement, explain why you agree or disagree with the following students. If you disagree, write a correct statement.

   a. **Student 1:** $\psi_{n_1}(x)\psi_{n_2}(x)$ is a basis state that can be used to construct the two-particle stationary state wavefunction for a system of two non-interacting particles. Particle 1 is in a single-particle state denoted by $n_1$ and particle 2 is in a single-particle state denoted by $n_2$.

   b. **Student 2:** $\psi_{n_1}(x_2)\psi_{n_2}(x_1)$ is a basis state that can be used to construct the two-particle stationary state wavefunction for a system of two non-interacting particles. Particle 1 with coordinate $x_2$ is in a single-particle state denoted by $n_1$ and particle 2 with coordinate $x_1$ is in a single-particle state denoted by $n_2$.

   c. **Student 3:** $\psi_{n_2}(x_2)\psi_{n_1}(x_1)$ is a basis state that can be used to construct the two-particle stationary state wavefunction for a system of two non-interacting particles. Particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$ and particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_2$.

   d. **Student 4:** $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ is a basis state that can be used to construct the three-particle stationary state wavefunction for a system of three non-interacting particles. Particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$, particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_2$, and particle 3 with coordinate $x_3$ is in a single-particle state denoted by $n_3$.

6. In your own words, describe what the symbols $x_1$, $x_2$, and $x_3$ in the basis state $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)$ mean to you. (Labels representing the single-particle states are $n_1$, $n_2$ and $n_1$, respectively, with two of the labels being the same.)

Consider the following conversation regarding whether a different ordering of the single-particle wavefunctions in the basis states yields a different basis state for a system of non-interacting identical particles.

**Student 1:** For a system of two non-interacting identical particles, the terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ and $\psi_{n_2}(x_2)\psi_{n_1}(x_1)$ represent two different basis states.

**Student 2:** No. I disagree with Student 1. When writing the basis states, different orderings of the single-particle wavefunctions does not produce a different basis state. Both terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ and $\psi_{n_2}(x_2)\psi_{n_1}(x_1)$ represent the same basis state in which particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$, and particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_2$.

Explain why you agree or disagree with each student.

**** CHECKPOINT: Check your answers to questions 2-6. ****

2. Student 1 is correct.

3a. There is an inconsistency in the term $\hat{\mathbf{H}}_1[\psi_{n_2}(x_2)]$. The single-particle Hamiltonian $\hat{H}_1$ can only act on the wavefunction in the part of the Hilbert space corresponding to particle 1 but this term has a wavefunction "1" corresponding to particle 1 which is not possible (in other words, $\hat{H}_1$ acts on "1" for the wavefunction which is not a possible wavefunction since it is not normalizable)

3b. There is an inconsistency in the term $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1)]$. The single-particle Hamiltonian $\hat{H}_2$ can only act on the wavefunction in the part of the Hilbert space corresponding to particle 2 but this term has a wavefunction "1" corresponding to particle 2 which is not possible (in other words, $\hat{H}_1$ acts on "1" for the wavefunction which is not a possible wavefunction since it is not normalizable)

$\hat{\mathbf{H}}_2[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)]$ is undefined as the term $\hat{\mathbf{H}}_2\psi_{n_1}(x_1) = (\hat{I}_1 \otimes \hat{H}_2)\psi_{n_1}(x_1) = [\hat{I}_1\psi_{n_1}(x_1)][\hat{H}_2 1]$ and 1 is not a normalizable wavefunction for particle 2.

3c. $(\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)[\psi_{n_1}(x_1) + \psi_{n_2}(x_2)]$ is undefined by reasoning as in a and b.

3d. $\hat{\mathbf{H}}_1[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = E_{n_1}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]$

3e. $\hat{\mathbf{H}}_2[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = E_{n_2}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]$

3f.

$$
\begin{aligned}
\hat{\mathbf{H}}\psi_{n_1}(x_1)\psi_{n_2}(x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (\hat{H}_1 \otimes \hat{I}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) + (\hat{I}_1 \otimes \hat{H}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= \hat{H}_1\psi_{n_1}(x_1)\hat{I}_2\psi_{n_2}(x_2) + \hat{I}_1\psi_{n_1}(x_1)\hat{H}_2\psi_{n_2}(x_2) \\
&= [\hat{H}_1\psi_{n_1}(x_1)]\psi_{n_2}(x_2) + \psi_{n_1}(x_1)[\hat{H}_2\psi_{n_2}(x_2)] \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_1)E_{n_2}\psi_{n_2}(x_2) \\
&= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2) + E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= (E_{n_1} + E_{n_2})\psi_{n_1}(x_1)\psi_{n_2}(x_2) \\
&= E\psi_{n_1}(x_1)\psi_{n_2}(x_2)
\end{aligned}
$$

3g.

$$\begin{aligned}(\hat{\mathbf{H}}_1+\hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2)+\psi_{n_2}(x_1)\psi_{n_1}(x_2)] &= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad +E_{n_2}\psi_{n_2}(x_1)\psi_{n_1}(x_2)\\ &\quad +E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad +E_{n_1}\psi_{n_2}(x_1)\psi_{n_1}(x_2)\\ &= (E_{n_1}+E_{n_2})[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad +\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\\ &= E[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad +\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\end{aligned}$$

3h.

$$\begin{aligned}(\hat{\mathbf{H}}_1+\hat{\mathbf{H}}_2)[\psi_{n_1}(x_1)\psi_{n_2}(x_2)-\psi_{n_2}(x_1)\psi_{n_1}(x_2)] &= E_{n_1}\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad -E_{n_2}\psi_{n_2}(x_1)\psi_{n_1}(x_2)\\ &\quad +E_{n_2}\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad -E_{n_1}\psi_{n_2}(x_1)\psi_{n_1}(x_2)\\ &= (E_{n_1}+E_{n_2})[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad -\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\\ &= E[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\\ &\quad -\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\end{aligned}$$

4. b, c, and d. The wavefunctions in the preceding question f, g, and h, which are products of the single-particle wavefunctions, all satisfy the TISE for $\hat{\mathbf{H}}_1+\hat{\mathbf{H}}_2$ and are possible many-particle stationary state wavefunctions.

5a. Student 1 is incorrect. The coordinates for each particle must be unique in the basis states (e.g., particle 1 has coordinate $x_1$ and particle 2 has coordinate $x_2$).

5b. Student 2 is incorrect. $\Psi(x_1,x_2)=\psi_{n_1}(x_2)\psi_{n_2}(x_1)$ is a basis state that can be used to construct the two-particle stationary state wavefunction for a system of two non-interacting particles. Particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_2$ and particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_1$.

5c. Student 3 is correct.

5d. Student 4 is correct.

56. For the system of three non-interacting particles, particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$, particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_2$, and particle 3 with coordinate $x_3$ is in a single-particle state denoted by $n_1$.

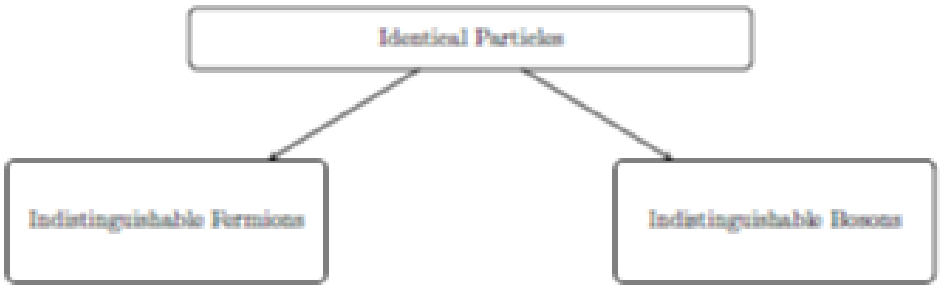
If your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

**Summary of the Basis States for a System of $N$ Non-Interacting Particles.**

- The basis states used to construct the many-particle stationary state wavefunction for a system of $N$ non-interacting identical particles are written in terms of products of the single-particle wavefunctions (NOT the sum of the single-particle wavefunctions) with different coordinates $x_i$ for each particle.

### D.6.3 Stationary State Wavefunction for a System of $N$ Identical Particles which are Indistinguishable

- Now that we know that the products of the single-particles wavefunctions form appropriate basis states for the product space, let's focus on how to use these basis states to construct the many-particle stationary state wavefunction (i.e., the form of the many-particle stationary state wavefunction for identical particles which reflects indistinguishability).
- A system of identical particles which are indistinguishable can consist of either a system of identical fermions or identical bosons.



Consider the following conversation regarding identical particles which are indistinguisble.

**Student 1:** If we have two identical fermions, we can paint one fermion red and the other fermion green. Then, all we need to do is to keep track of the color to keep track of each fermion.

**Student 2:** In general, in quantum mechanics, if two particles in a system are identical fermions, we couldn't paint one red and the other green. Quantum particles are truly indistinguishable. There is no measurement we can perform that could distinguish one identical fermion from the other. For example, there is no measurement that can distinguish which fermion was in which single-particle state and had which coordinate. The wavefunction must reflect the fact that we cannot attach identifiers to each identical fermion.

**Student 3:** Yes. Similarly, if both particles are identical bosons, we couldn't paint one red and the other green either. In general, when the single-particle wavefunctions for the two identical bosons overlap, there is no measurement we can perform that could distinguish one boson from the other, for example, which boson had which coordinate and was in which single-particle state.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the spin of identical particles regardless of whether the particles are fundamental particles (indivisible or composite).

**Student 1:** When we have a system of identical particles, all particles have the same intrinsic properties such as mass, charge, and spin.

**Student 2:** I agree. Also, the property of spin differentiates a boson from a fermion. The spin of a boson must be an integer. For example, Helium-4 is a boson since it has integer spin. The spin of a fermion must be a half-integer. For example, an electron, proton, and neutron are fermions with spin 1/2.

Explain why you agree or disagree with the students.

Consider the following conversation regarding whether the coordinates of each particle should be the same or different in the wavefunction for a system of non-interacting identical particles which are indistinguishable.

**Student 1:** For a system of three identical particles, the wavefunction will have terms such as

$\psi_{n_1}(x)\psi_{n_2}(x)\psi_{n_3}(x)$ in which $\psi_{n_1}(x), \psi_{n_2}(x)$, and $\psi_{n_3}(x)$ are the single-particle wavefunctions with the same coordinate for all three particles since the particles are indistinguishable.

**Student 2:** I disagree. Even though the particles are indistinguishable, we must still assign a different coordinate to each particle in a given state. The wavefunction will have terms such as $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$.

**Student 3:** No. I agree with Student 1 and disagree with Student 2. When the particles are indistinguishable, we can't possibly distinguish their individual coordinates. So the wavefunction will have terms such as $\psi_{n_1}(x)\psi_{n_2}(x)\psi_{n_3}(x)$.

Explain why you agree or disagree with each student.

Student 2 is correct in the preceding conversation.

- The coordinates do not account for the indistinguishability of the particles, rather the indistinguishability is reflected in the way the many-particle wavefunction is written (either as a completely symmetric or antisymmetric wavefunction).
- The wavefunction for indistinguishable fermions has different properties than the wavefunction for indistinguishable bosons.
- Before considering the wavefunction for indistinguishable fermions or indistinguishable bosons, let's review how to determine whether a many-particle wavefunction is completely symmetric versus antisymmetric with respect to the exchange of any two particles.

**Symmetric Wavefunction:** A **symmetric wavefunction** of two-particles $\Psi(x_1, x_2)$ produces the same wavefunction (with the same sign) when the two particles are exchanged. Therefore,

$$\Psi(x_2, x_1) = \Psi(x_1, x_2).$$

A completely **symmetric wavefunction** for $N$ particles $\Psi(x_1, x_2, x_3 \ldots, x_i, \ldots, x_j, \ldots, x_N)$ produces the same wavefunction (with the same sign) when any two particles labeled by $x_i$ and $x_j$ are exchanged:

$$\Psi(x_1, x_2, x_3 \ldots, x_j, \ldots, x_i, \ldots, x_N) = \Psi(x_1, x_2, x_3 \ldots, x_i, \ldots, x_j, \ldots, x_N).$$

The following permutations of coordinates of the particles underlined are all examples of the consequences of exchanging particles for a completely symmetric wavefunction (i.e., the many-particle wavefunction is unchanged)

i. One permutation

$$\Psi(\underline{x_1}, \underline{x_2}, x_3, \ldots, x_N) = \Psi(\underline{x_2}, \underline{x_1}, x_3, \ldots, x_N) \quad \text{(Permuting } x_1 \text{ and } x_2\text{)}$$

ii. Two total permutations

$$\begin{aligned} \Psi(x_1, x_2, x_3, x_3, x_4, \ldots, x_N) &= \Psi(\underline{x_2}, \underline{x_1}, x_3, x_4, \ldots, x_N) \quad \text{(First permutation: Permuting } x_1 \text{ and } x_2\text{)} \\ &= \Psi(x_2, \underline{x_3}, \underline{x_1}, x_4, \ldots, x_N) \quad \text{(Second permutation: Permuting } x_1 \text{ and } x_3\text{)} \end{aligned}$$

iii. Three total permuations

$$\begin{aligned} \Psi(x_1, x_2, x_3, x_4, \ldots, x_N) &= \Psi(\underline{x_2}, \underline{x_1}, x_3, x_4, \ldots, x_N) \quad \text{(First permutation: Permuting } x_1 \text{ and } x_2\text{)} \\ &= \Psi(x_2, \underline{x_3}, \underline{x_1}, x_4, \ldots, x_N) \quad \text{(Second permutation: Permuting } x_1 \text{ and } x_3\text{)} \\ &= \Psi(\underline{x_3}, \underline{x_2}, x_1, x_4, \ldots, x_N) \quad \text{(Third permutation: Permuting } x_2 \text{ and } x_3\text{)} \end{aligned}$$

Continuing in this manner, you can perform any number of permutations to show that the many-particle is unchanged for each exchange of particles.

- The wavefunction for indistinguishable bosons must be a completely symmetric wavefunction with respect to exchange of any two particles.

**Antisymmetric Wavefunction:** An **antisymmetric wavefunction** of two-particles $\Psi(x_1, x_2)$ produces a wavefunction that is related to the original wavefunction as follows when the two particles are exchanged:

$$\Psi(x_2, x_1) = -\Psi(x_1, x_2).$$

A completely **antisymmetric wavefunction** of $N$ particles $\Psi(x_1, x_2, x_3, \ldots, x_N)$ produces a wavefunction that is related to the original wavefunction as follows when two particles are exchanged. The following permutations of the coordinates are all examples of the consequences of exchanging particles for a completely antisymmetric wavefunction

i. One permutation

$$\Psi(\underline{x_1}, \underline{x_2}, x_3, \ldots, x_N) = -\Psi(\underline{x_2}, \underline{x_1}, x_3, \ldots, x_N) \quad \text{(Permuting } x_1 \text{ and } x_2\text{)}$$

ii. Two total permutations

$$\begin{aligned}
\Psi(x_1, x_2, x_3, x_4, \ldots, x_N) &= -\Psi(\underline{x_2}, \underline{x_1}, x_3, x_4, \ldots, x_N) && \text{(First Permutation: Permuting } x_1 \text{ and } x_2\text{)} \\
&= -[-\Psi(x_2, \underline{x_3}, \underline{x_1}, x_4, \ldots, x_N)] && \text{(Second Permutation: Permuting } x_1 \text{ and } x_3\text{)} \\
&= \Psi(x_2, x_3, x_1, x_4, \ldots, x_N) && \text{(Simplifying } -1 \times -1 \text{ for two permutations)}
\end{aligned}$$

iii. Three total permutations

$$\begin{aligned}
\Psi(x_1, x_2, x_3, x_4, \ldots, x_N) &= -\Psi(\underline{x_2}, \underline{x_1}, x_3, x_4, \ldots, x_N) && \text{(First Permutation:} \\
&&& \text{Permuting } x_1 \text{ and } x_2) \\
&= -[-\Psi(x_2, \underline{x_3}, \underline{x_1}, x_4, \ldots, x_N)] && \text{(Second Permutation:} \\
&&& \text{Permuting } x_1 \text{ and } x_3) \\
&= \Psi(x_2, x_3, x_1, x_4, \ldots, x_N) && \text{(Simplifying } -1 \times -1 \\
&&& \text{for two permutations)} \\
&= -\Psi(\underline{x_3}, \underline{x_2}, x_1, x_4, \ldots, x_N) && \text{(Third Permuation:}
\end{aligned}$$

Permuting $x_2$ and $x_3$)

Continuing in this manner, you can perform any number of permutations to show that the many-particle wavefunction develops a plus or minus sign for each exchange of particles depending upon whether the number of exchanges was even or odd, respectively.

- The wavefunction for indistinguishable fermions must be a completely antisymmetric wavefunction with respect to the exchange of any two particles.

Consider the following conversation regarding the only two ways of constructing a wavefunction for identical particles which are indistinguishable (either completely symmetric or completely antisymmetric with respect to exchange of any two particles).

**Student 1:** Since there is no measurement we can perform to distinguish different identical particles in a system consisting of $N$ identical particles, the wavefunction must reflect this symmetry.

**Student 2:** I agree with Student 1. There are two possible ways to construct the wavefunction for a system of $N$ non-interacting indistinguishable particles from the single-particle wavefunctions for that system. The wavefunction could be either completely symmetric or completely antisymmetric with respect to exchange of two particles because it is $|\psi|^2$ that determines the measurable properties and the overall sign of the many-particle wavefunction is not important.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the eigenvalues of the "permutation operator."

**Student 1:** Let's consider the permutation operator $\hat{P}_{ij}$ acting on a many-particle stationary state wavefunction for a system of identical particles. The permutation operator $\hat{P}_{ij}$ acting on the many-particle stationary state wavefunction exchanges particle $i$ and particle $j$ in the many-particle stationary state wavefunction.

**Student 2:** I agree. If the permutation operator $\hat{P}_{ij}$ is applied twice, the original wavefunction is obtained. That is,

$$\hat{P}_{ij}^2 \Psi(x_1, x_2, \ldots, x_i, \ldots, x_j, \ldots, x_N) = \Psi(x_1, x_2, \ldots, x_i, \ldots, x_j, \ldots, x_N).$$

Therefore, $\hat{P}_{ij}^2 = \hat{I}$, in which $\hat{I}$ is the identity operator. Thus, the eigenvalues of the permutation operator $\hat{P}_{ij}$ are $\pm 1$. The eigenvalue 1 corresponds to the completely symmetric bosonic wavefunction and the eigenvalue $-1$ corresponds to the completely antisymmetric fermionic wavefunction.

Explain why you agree or disagree with the students.

#### D.6.3.1 Stationary State Wavefunction for a System of $N$ Indistinguishable Fermions

- Now let's consider the case in which the identical particles are indistinguishable fermions.
- We will begin with a system of two fermions and then consider a system of three fermions and finally consider a system of $N$ fermions.

7. Consider a system of two non-interacting identical fermions in which $\psi_{n_1}(x)$ and $\psi_{n_2}(x)$ are the single-particle wavefunctions for the system and $n_1 \neq n_2$. Choose all of the following normalized wavefunctions that are appropriate for a system of two non-interacting fermions considering that indistinguishable fermions must have a completely antisymmetric wavefunction.
   a. $\psi_{n_1}(x_1)\psi_{n_2}(x_1)$ (same coordinate)
   b. $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$
   c. $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$
   d. $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$
   e. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ (same state label $n_1$)

Consider the following conversation regarding the wavefunction for a system of two non-interacting indistinguishable fermions.

**Student 1:** For a system of two non-interacting indistinguishable fermions, the wavefunction describing the system is $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, in which $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for the two-particles.

**Student 2:** I disagree. If the system consists of two fermions, there is no way to distinguish which fermion is in the state labeled by $n_1$ and which is in the state labeled by $n_2$. The wavefunction must reflect this symmetry.

**Student 3:** I agree with Student 2. The wavefunction describing a system of non-interacting indistinguishable fermions must be completely antisymmetric. Therefore, the normalized wavefunction for a system of two non-interacting fermions must be $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.[1]

Explain why you agree or disagree with each student.

Consider the following conversation regarding whether the Pauli exclusion principle and identical fermions having a completely antisymmetric wavefunction are consistent with each other.

**Student 1:** The fact that a wavefunction for a system of fermions must be completely antisymmetric is consistent with the Pauli exclusion principle.

**Student 2:** I thought the Pauli exclusion principle states that no two fermions can be in the same single-particle state. How is that consistent with the wavefunction being completely antisymmetric?

**Student 1:** Let's suppose we have two fermions in the same single-particle state. Then $n_1 = n_2$ and the wavefunction would be

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_1}(x_1)] = 0.$$

Thus $\Psi(x_1, x_2) = 0$ is not a possible wavefunction.

**Student 3:** The same is true for a system of more than two indistinguishable fermions. Since a system of fermions has a completely antisymmetric wavefunction, no two fermions can be in the same single-particle state. If you try to put two or more fermions in the same state, the wavefunction will be zero for the $N$-fermion system.

Explain why you agree or disagree with Student 1 and Student 3.

[1] The wavefunction for a system of indistinguishable fermions must always be completely antisymmetric. This must also be true when the system includes interactions between the indistinguishable fermions so that the stationary state wavefunction cannot be expressed as $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.

Consider the following conversation regarding whether different orderings of the single-particle stationary state wavefunctions yield different many-particle wavefunctions.

**Student 1:** The basis states for a system of non-interacting identical fermions with only two available single-particle states $n_1$ and $n_2$ are $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, $\psi_{n_2}(x_2)\psi_{n_1}(x_1)$, $\psi_{n_2}(x_1)\psi_{n_1}(x_2)$, and $\psi_{n_1}(x_2)\psi_{n_2}(x_1)$. The normalized many-particle stationary state wavefunction for a system of two indistinguishable fermions is $\frac{1}{\sqrt{4}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_2)\psi_{n_1}(x_1) - \psi_{n_2}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.

**Student 2:** I disagree with Student 1. The terms $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ and $\psi_{n_2}(x_2)\psi_{n_1}(x_1)$ are two ways to write the same basis state. Changing the order of the single-particle wavefunctions does not give a different basis state.

**Student 3:** I agree with Student 2. The expression $\frac{1}{\sqrt{4}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)$
$+ \psi_{n_2}(x_2)\psi_{n_1}(x_1) - \psi_{n_2}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)] = \frac{1}{\sqrt{4}}[2\psi_{n_1}(x_1)\psi_{n_2}(x_2)$
$- 2\psi_{n_2}(x_1)\psi_{n_1}(x_2)] = \psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)$, which is not a properly normalized wavefunction. The normalization factor should be $\frac{1}{\sqrt{2}}$.

Explain why you agree or disagree with Student 1 and Student 3.

8. Is the completely antisymmetric wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ a stationary state wavefunction for the two-fermion system? Explain.

Consider the following conversation regarding whether, after antisymmetrizing the wavefunction for a system of two non-interacting fermions, the state remains a stationary state wavefunction of the many-particle system with $n_1 \neq n_2$.

**Student 1:** When we completely antisymmetrize the wavefunction for two fermions, the wavefunction is $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$. However, since this is a linear superposition of two basis states, it is not a stationary state wavefunction for the two-particle system.

**Student 2:** I disagree with Student 1's claim that $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ is not a stationary state wavefunction for the two-particle system. If we completely antisymmetrize the wavefunction for a system of two non-interacting fermions, then this completely antisymmetric wavefunction
$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ constructed from products of single-particle wavefunctions is a stationary state wavefunction for the two-particle system. That is,

$$\begin{aligned}
\hat{\mathbf{H}}\Psi(x_1, x_2) &= \hat{\mathbf{H}}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= E_1\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&\quad + E_2\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= E\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= E\Psi(x_1, x_2).
\end{aligned}$$

This is true because each basis state in the product space satisfies the TISE with the same energy $E = E_1 + E_2$

Explain why you agree or disagree with each student.

Use the following questions to check your answer to the preceding question about the conversation.

9. Consider a system of two non-interacting identical fermions. As we learned, the Hamiltonian for a system of two non-interacting identical particles is given by $\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2$. Using the TISE, determine whether the completely antisymmetric wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ is a stationary state wavefunction for the two fermion system.

$\hat{\mathbf{H}}\Psi(x_1, x_2) = \hat{\mathbf{H}}\{\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\} =$

10. What is the energy for a system of two non-interacting identical fermions in which one fermion is in a single-particle state labeled by $n_1$ with energy $E_{n_1}$ and the other fermion is in a single-particle state labeled by $n_2$ with energy $E_{n_2}$?

- Now, let's construct the completely antisymmetric wavefunction for a system of more than one non-interacting, indistinguishable fermion.
- We will begin with a system of two indistinguishable fermions followed by a system of three indistinguishable fermions.

11. Starting with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, construct the completely antisymmetric wavefunction for a system of two non-interacting, indistinguishable fermions by permuting the coordinates (hold $n_1$ and $n_2$ fixed) and combining the terms with different permutations to make the wavefunction completely antisymmetric.

12. Starting with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, construct the completely antisymmetric wavefunction for a system of two non-interacting, indistinguishable fermions by permuting the labels $n_1$ and $n_2$ for the states (hold $x_1$ and $x_2$ fixed) and combining the terms with different permutations to make the wavefunction completely antisymmetric.

13. Compare your answers to questions 11 and 12 and state the reasoning for what you found.

Consider the following conversation regarding constructing a completely antisymmetric wavefunction for a system of two indistinguishable fermions starting with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$.

**Student 1:** If we start with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, we can construct a completely antisymmetric wavefunction by **interchanging the two single-particle wavefunction labels**, multiplying the new permutation by -1 and then summing over all the permutations, which in this case is just two permutations. If we permute $\underline{n_1}$ and $\underline{n_2}$ in $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, the new term is $-\psi_{n_2}(x_1)\psi_{n_1}(x_2)$. After normalization, the completely antisymmetric wavefunction for a system of two identical fermions is $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$.

**Student 2:** If we start with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, we can construct a completely antisymmetric wavefunction by **interchanging the coordinates**, multiplying the new permutation by -1 and then summing over all the permutations, which in this case is just two permutations. If we permute $\underline{x_1}$ and $\underline{x_2}$ in $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, the new term is $-\psi_{n_1}(x_2)\psi_{n_2}(x_1)$. The sum of the terms after normalization for the completely antisymmetric wavefunction for a system of two identical fermions is $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$.

**Student 3:** I agree with both Student 1 and Student 2. Both students constructed the same completely antisymmetric wavefunction. The single-particle wavefunctions are not operators, so we can switch the order of single-particle wavefunctions, i.e., $\psi_{n_1}(x_2)\psi_{n_2}(x_1) = \psi_{n_2}(x_1)\psi_{n_1}(x_2)$. The completely antisymmetric wavefunction can be generated by interchanging either the coordinates or the labels for the states.

Explain why you agree or disagree with the students.

Consider the following conversation regarding constructing a completely antisymmetric wavefunction for a system of indistinguishable fermions by switching both the coordinates and the labels for the states.

**Student 1:** If we interchange **both** the labels for the states and the coordinates, the resulting wavefunction is a completely antisymmetric wavefunction for the system of identical fermions.

**Student 2:** I disagree with Student 1. Let's consider a system of two indistinguishable fermions. If we start with the basis state $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ and interchange two single-particle wavefunction labels and multiply the new permutation by -1, the new term is $-\psi_{n_2}(x_1)\psi_{n_1}(x_2)$. Now if we interchange the coordinates of the two-particles and multiply the new permutation by -1, the new term is $\psi_{n_2}(x_2)\psi_{n_1}(x_1) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$. By switching both the coordinates and the labels, we recovered the original expression and did not generate a new term. The original expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ that we got back by exchanging both the labels for the states and the coordinates is not antisymmetric and therefore it cannot be the wavefunction for a system of two indistinguishable fermions.

**Student 3:** I agree with Student 2. For a system of indistinguishable fermions, we cannot generate a completely antisymmetric wavefunction by switching **both** the coordinates and the labels for the states. We should only permute one of them to generate a completely antisymmetric wavefunction.

Explain why you agree or disagree with each student.

14. Starting with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, construct the completely antisymmetric wavefunction for the system of three indistinguishable fermions. Hint: Switch either the coordinates or the states (but not both) two at a time and remember to make the wavefunction completely antisymmetric by multiplying the new permutation by -1 each time you interchange two particles. Two interchanges will produce -1 $\times$ -1 =1 times the new permutation. Then sum all of the permutations and normalize the completely antisymmetric wavefunction.

Consider the following conversation regarding the number of terms and the normalization factor for a completely antisymmetric wavefunction for a system of indistinguishable fermions.

**Student 1:** When constructing the completely antisymmetric wavefunction for a system of three indistinguishable fermions, how do I know that I have found all the possible permutations?

**Student 2:** In general, for a system of $N$ indistinguishable fermions, there are $N!$ permutations of the labels. For example, there are $N!$ permutations of the coordinates $x_1, x_2, \ldots, x_N$ or $N!$ permutations of the labels for the single-particle states $\psi_{n_1}, \psi_{n_2}, \ldots, \psi_{n_N}$. The normalization factor is $\frac{1}{\sqrt{N!}}$.

**Student 3:** I agree with Student 2. For a system of three indistinguishable fermions, the completely antisymmetric wavefunction will have $3! = 6$ terms and the normalization factor will be $\frac{1}{\sqrt{6}}$.

Explain why you agree or disagree with Student 2 and Student 3.

Consider the following conversation regarding a method for constructing completely antisymmetric wavefunctions for indistinguishable fermions.

**Student 1:** To find the completely antisymmetric wavefunction for a system of three indistinguishable fermions, we start with the expression $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ and then find all possible permutations of either the coordinates $(x_1, x_2, x_3)$ or the state indices $(n_1, n_2, n_3)$. Each time we interchange two labels, we multiply the new permuted term by -1. Once we find all the permutations, we add them and normalize the completely antisymmetric wavefunction obtained.

**Student 2:** Although I agree with Student 1's method for more than two-particles, it can be easy to make a mistake with the sign of each term or omit a term altogether. A more systematic approach to help eliminate these sign mistakes is to use the "Slater determinant". For three-particles, the Slater determinant is

$$A\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_2}(x_1) & \psi_{n_3}(x_1) \\ \psi_{n_1}(x_2) & \psi_{n_2}(x_2) & \psi_{n_3}(x_2) \\ \psi_{n_1}(x_3) & \psi_{n_2}(x_3) & \psi_{n_3}(x_3) \end{vmatrix} = \begin{array}{l} A[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ -\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) + \psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) \\ +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)] \end{array}$$

in which $A$ is the normalization constant which needs to be found separately. Here, $A = \frac{1}{\sqrt{N!}} = \frac{1}{\sqrt{6}}$ for a system of three fermions since each single-particle state is itself normalized. The Slater determinant can equivalently be expressed as

$$A\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) & \psi_{n_1}(x_3) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) & \psi_{n_2}(x_3) \\ \psi_{n_3}(x_1) & \psi_{n_3}(x_2) & \psi_{n_3}(x_3) \end{vmatrix} = \begin{array}{l} A[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2) \\ -\psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2) - \psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)]. \end{array}$$

**Student 3:** I agree with Student 2. The wavefunction is the same using either form of the Slater determinant since the rows and columns are transposed. Also, the Slater determinant works for a system of any number of fermions although even this method can become tedious when applied to more than three fermions.

Explain why you agree or disagree with the students.

15. Using the Slater determinant, determine the stationary state wavefunction of a system of two fermions and check your answer to question 7.

Consider the following conversation regarding the Slater determinant and the Pauli exclusion principle for a system of two identical fermions.

**Student 1:** The Slater determinant yields a many-particle wavefunction which is consistent with the Pauli exclusion principle. For example, for a system of two fermions, if we put both fermions in the same single-particle state, then

$$\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) \\ \psi_{n_1}(x_1) & \psi_{n_1}(x_2) \end{vmatrix} = \psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_1}(x_1) = 0$$

which is not a possible wavefunction since zero represents the absence of a wavefunction.

**Student 2:** I agree with Student 1. We can extend the Slater determinant method to find the many-particle wavefunction for a system with more than two particles. Consistent with Pauli's exclusion principle, having two particles in the same single-particle state produces two columns or rows with the same entries so the Slater determinant of the many-particle wavefunction is zero, which is not a possible wavefunction.

Explain why you agree or disagree with the students.

****CHECKPOINT: Check your answers to questions 7-14. ****

7. d

8. Yes, the completely antisymmetric wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ is a stationary state wavefunction for the two fermion system as it satisfies the TISE, $\hat{H}\Psi(x_1, x_2) = E\Psi(x_1, x_2)$

9.

$$\begin{aligned}
\hat{\mathbf{H}}\Psi(x_1,x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= \hat{\mathbf{H}}_1\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} - \hat{\mathbf{H}}_1\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&\quad +\hat{\mathbf{H}}_2\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} - \hat{\mathbf{H}}_2\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= E_{n_1}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} - E_{n_2}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&\quad +E_{n_2}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} - E_{n_1}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= E_{n_1}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&\quad +E_{n_2}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&= (E_{n_1} + E_{n_2})\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= E\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]\right\} \\
&\qquad \text{in which } E = E_{n_1} + E_{n_2} \\
&= E\Psi(x_1,x_2)
\end{aligned}$$

10. $E = E_{n_1} + E_{n_2}$

11. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$

12. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$

13. The completely antisymmetric wavefunction for the system of two fermions is the same if we permute either the coordinates or the labels for the states (but NOT both simultaneously).

14.

| Permutation | Switch | New Permutation |
|---|---|---|
| $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ | $n_1 \leftrightarrow n_2$ | $-\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3)$ |
| $-\psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3)$ | $n_1 \leftrightarrow n_3$ | $\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)$ |
| $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$ | $n_2 \leftrightarrow n_3$ | $-\psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3)$ |
| $-\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3)$ | $n_1 \leftrightarrow n_3$ | $\psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3)$ |
| $\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)$ | $n_1 \leftrightarrow n_2$ | $-\psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)$ |

Adding the different permutations, we get the completely antisymmetric wavefunction

$$\begin{aligned}\Psi(x_1,x_2,x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_3}(x_3) \\ &\quad +\psi_{n_3}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) - \psi_{n_1}(x_1)\psi_{n_3}(x_2)\psi_{n_2}(x_3) \\ &\quad +\psi_{n_2}(x_1)\psi_{n_3}(x_2)\psi_{n_1}(x_3) - \psi_{n_3}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)]\end{aligned}$$

15. $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

**Summary for the Properties of the Wavefunction for Fermions**

- The wavefunction for a system of indistinguishable fermions is completely antisymmetric with respect to exchange of any two particles.

#### D.6.3.2 Stationary State Wavefunction for a System of $N$ Indistinguishable Bosons

- Now let's consider the case in which the particles are indistinguishable bosons.

16. Consider a system of two non-interacting, indistinguishable bosons in which $\psi_{n_1}(x)$ and $\psi_{n_2}(x)$ are the single-particle wavefunctions for the system ($n_1 \neq n_2$). Choose all of the following wavefunctions that are appropriate for a system of two non-interacting indistinguishable bosons considering that bosons must have a completely symmetric wavefunction.

    a. $\psi_{n_1}(x_1)\psi_{n_2}(x_1)$

    b. $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$

    c. $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$

    d. $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$

    e. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ (same label $n_1$ for the states)

    Consider the following conversation regarding the wavefunction for a system of two non-interacting indistinguishable bosons.

    **Student 1:** For a system of two non-interacting, indistinguishable bosons, if the bosons are in the same single-particle state, say $\psi_{n_1}$, the wavefunction describing the two-particle system is $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$.

    **Student 2:** I disagree. If the system consists of two indistinguishable bosons, the bosons cannot be in the same single-particle state. So, $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is not a possible wavefunction for a system of two non-interacting, indistinguishable bosons. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is the wavefunction for distinguishable particles only.

    Explain why you agree or disagree with each student.

Consider the following conversation regarding two indistinguishable bosons in the same single-particle state.

**Student 1:** If we have a system consisting of two indistinguishable bosons, then the Pauli exclusion principle tells us that the bosons must be in different single-particle states.

**Student 2:** I disagree with Student 1. The Pauli exclusion principle applies only to fermions. Since the wavefunction for a system of indistinguishable bosons is symmetric with respect to exchange of two particles, the wavefunction is not zero when the indistinguishable bosons are in the same single-particle state.

**Student 3:** I agree with Student 2. The antisymmetrized wavefunction for two indistinguishable fermions in the same single-particle state is zero, which is not a possible wavefunction consistent with the Pauli's exclusion principle. However, for two indistinguishable bosons, if both bosons are in state $n_1$, then the normalized two-particle wavefunction would be $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding two indistinguishable bosons having the same two-particle stationary state wavefunction as a system of identical particles that can be treated as distinguishable.

**Student 1:** For two indistinguishable bosons, if both bosons are in state $n_1$, then the normalized two-particle wavefunction is $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$.

**Student 2:** I disagree with Student 1. The wavefunction $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is not a possible stationary state wavefunction for a system of bosons. The wavefunction for a system of indistinguishable bosons must be completely symmetric and we must have a sum of terms in the wavefunction for it to be completely symmetric. The wavefunction $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is only possible for a system of identical particles that can be treated as distinguishable.

**Student 3:** I agree with Student 1 and disagree with Student 2. A completely symmetric wavefunction does not necessarily have to be written in terms of a sum. The wavefunction $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is completely symmetric with respect to exchange of the two particles. If all of the indistinguishable bosons are in the same single-particle state, then the many-particle wavefunction for a system of indistinguishable bosons is the same as the wavefunction for a system of identical particles that can be treated as distinguishable.

Explain why you agree or disagree with each student.

17. Check whether the wavefunction $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ satisfies the TISE and is symmetric with respect to exhange of the two particles.

Consider the following conversation regarding the wavefunction for a system of two non-interacting indistinguishable bosons when $n_1 \neq n_2$.

**Student 1:** For a system of two non-interacting indistinguishable bosons, if the two bosons are in different single-particle states, the wavefunction describing the two-particle system is $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, in which $\psi_{n_1}(x_1)$ and $\psi_{n_2}(x_2)$ are the single-particle wavefunctions for the two-particles.

**Student 2:** I disagree. If the system consists of two bosons, there is no way to distinguish which boson is in the single-particle state denoted by $n_1$ and which is in the single-particle state denoted by $n_2$. The wavefunction must reflect this symmetry.

**Student 3:** The wavefunction describing a system of non-interacting indistinguishable bosons must be completely symmetric.[2] Therefore, the two-particle wavefunction for a system of two non-interacting, indistinguishable bosons, where the bosons are in different single-particle states, must be $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$.

Explain why you agree or disagree with each student.

[2]The wavefunction for a system of indistinguishable bosons must always be completely symmetric. This must also be true when the system includes interactions between the indistinguishable bosons so that the stationary state wavefunction cannot be expressed as $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$.

18. Does the two-particle wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)+\psi_{n_2}(x_1)\psi_{n_1}(x_2)]$ satisfy the TISE for a two-particle system? Explain.

19. What is the energy for a system of two non-interacting identical bosons in which one boson is in a single-particle state labeled by $n_1$ and the other boson is in a single-particle state labeled by $n_2$?

20. For a system of two non-interacting, indistinguishable bosons, how many terms will be present in the two-particle wavefunction for the system if the bosons are in different single-particle states?

21. For a system of two non-interacting, indistinguishable bosons, how many terms will be present in the two-particle wavefunction for the system if the bosons are in the same single-particle state?

22. For a system of three non-interacting, indistinguishable bosons, how many terms will be present in the three-particle wavefunction for the system if two of the three bosons are in the same single-particle stationary state?

Consider the following conversation regarding the normalization factor for a system of indistinguishable bosons.

**Student 1:** For a system of $N$ non-interacting, indistinguishable bosons, the normalization factor must be $\frac{1}{\sqrt{N!}}$.

**Student 2:** I agree with Student 1. To ensure we have a symmetric wavefunction, the many-particle wavefunction will be the sum of all the permutations of the product of the single-particle wavefunctions. Since there are $N!$ ways to permute the $N$ single-particle wavefunctions, the normalization factor will be $\frac{1}{\sqrt{N!}}$.

**Student 3:** I disagree with both Student 1 and Student 2. The normalization factor will be $\frac{1}{\sqrt{N!}}$ only if all the bosons are in different single-particle states. If we have all of the bosons in one single-particle state, $\prod_{i=1}^{N} \psi_n(x_i)$ is a valid many-particle state, e.g., $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ is an appropriately symmetrized wavefunction and the overall normalization factor for $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ is 1 since all three particles are in the same single-particle state given by the label $n_1$. We must be careful not to over count the number of unique permutations of the $N$ single-particle states.

Explain why you agree or disagree with each student.

23. Construct the completely symmetric normalized three-particle wavefunction for the system of three non-interacting, indistinguishable bosons in the following cases:

    a. All the bosons are in different states.

    b. Two of the bosons are in the same state $\psi_{n_1}$.

    c. All the bosons are in the same state $\psi_{n_1}$.

****CHECKPOINT: Check your answers to questions 16-23. ****

16. c and e

17. Yes, the wavefunction $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ is symmetric with respect to exchange of the two particles and satisfies the TISE.

$$\hat{\mathbf{H}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = (E_{n_1} + E_{n_2})[\psi_{n_1}(x_1)\psi_{n_2}(x_2)] = E[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]$$

18. Yes, the completely symmetric wavefunction $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)+\psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ is a stationary state wavefunction for the two boson system as it satisfies the TISE, $\hat{H}\Psi(x_1, x_2) = E\Psi(x_1, x_2)$.

$$\begin{aligned}
\hat{\mathbf{H}}\Psi(x_1, x_2) &= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= \hat{\mathbf{H}}_1\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} + \hat{\mathbf{H}}_1\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&\quad +\hat{\mathbf{H}}_2\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} + \hat{\mathbf{H}}_2\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= E_{n_1}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} + E_{n_2}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&\quad +E_{n_2}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)]\right\} + E_{n_1}\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= (E_{n_1} + E_{n_2})\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= E\left\{\tfrac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]\right\} \\
&= E\Psi(x_1, x_2)
\end{aligned}$$

19 $E = E_{n_1} + E_{n_2}$

20. There must be two terms to satisfy the symmetrization requirement for bosons. $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$

21. One. For example, if both bosons are in the single-particle state $\psi_{n_1}$, the many-particle stationary state wavefunction is $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$

22. There must be three terms to satisfy the symmetrization requirement for bosons. For example, if two of the three bosons are in the single-particle state $\psi_{n_1}$, the many-particle stationary state wavefunction is $\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) +$

$\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)]$

23a.

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2) \\ &\quad +\psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1) \\ &\quad +\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2) + \psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)]\end{aligned}$$

23b. $\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)]$

c. $\Psi(x_1, x_2, x_3) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

**Summary of Properties of the Wavefunction for Bosons**

- The wavefunction for a system of indistinguishable bosons is completely symmetric with respect to exchange of any two particles.

#### D.6.3.3 Hypothetical Case: Stationary State Wavefunction for a System of $N$ Non-Interacting Identical Particles if They Could Be Treated as Distinguishable

- Let's contrast the cases of indistinguishable fermions and indistinguishable bosons with a hypothetical case in which the identical particles could be treated as distinguishable.
- We compare the resulting many-particle stationary state wavefunctions to what was obtained for indistinguishable fermions and indistinguishable bosons to learn why care must be taken to ensure that the many-particle wavefunction reflects the indistinguishability of the particles.
- If identical particles (particles of one type with the same properties) could be treated as **distinguishable**, we can assign a distinct label (e.g., red, blue, etc.) to distinguish each particle from the other particles in the system even though the particles have the same properties.

Consider the following conversation regarding the symmetrization requirements of the wavefunction for a system of two non-interacting identical particles if they could be treated as **distinguishable**.

**Student 1:** For a system of two non-interacting identical particles which can be treated as distinguishable, we must still symmetrize the wavefunction.

**Student 2:** I disagree with Student 1. Since the particles can be treated as distinguishable, we can determine which particle is in which single-particle state. There is no requirement to symmetrize the wavefunction.

Explain why you agree or disagree with the students.

24. Consider a system of two non-interacting, identical particles which can be treated as distinguishable, in which $\psi_{n_1}$ and $\psi_{n_2}$ are the single-particle wavefunctions for the system ($n_1 \neq n_2$). Choose all of the following wavefunctions that are appropriate two-particle stationary state wavefunctions for a system of two non-interacting, identical particles which can be treated as distinguishable.

    a. $\psi_{n_1}(x_1)\psi_{n_2}(x_1)$ (same label $x_1$)

    b. $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$

    c. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ (same label $n_1$)

    d. $\psi_{n_1}(x)\psi_{n_1}(x)$ (same label $x$)

    Consider the following conversation regarding the appropriate wavefunctions for a system of two non-interacting identical particles that can be treated as **distinguishable**.

    **Student 1:** For a system of two non-interacting identical particles which can be treated as distinguishable, the wavefunction describing the system can be $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ in which $n_1 \neq n_2$. $\psi_{n_1}(x_1)$ means that particle 1 with coordinate $x_1$ is in a single-particle energy state denoted by $n_1$. Similarly, $\psi_{n_2}(x_2)$ means that particle 2 with coordinate $x_2$ is in a single-particle energy state denoted by $n_2$.

    **Student 2:** I agree with Student 1. Additionally, $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ is also a valid wavefunction for two identical particles which can be treated as distinguishable as there is nothing prohibiting both particles from occupying the same single-particle state with label $n_1$.

    **Student 3:** Only for the case when both particles are in the same single-particle state $\psi_{n_1}$ is the two-particle wavefunction $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ the same as for the case of identical bosons.

    Explain why you agree or disagree with the students.

Consider the following conversation regarding constructing a wavefunction for a system of $N$ non-interacting identical particles which can be treated as distinguishable from the corresponding single-particle wavefunctions $\psi_{n_i}$, $i = 1, 2, \ldots, \infty$.

**Student 1:** For a system of $N$ non-interacting identical particles which can be treated as distinguishable, a stationary state wavefunction describing the system must be a product of the single-particle wavefunctions, i.e.,

$$\Psi(x_1, x_2, \ldots, x_N) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)\cdots\psi_{n_N}(x_N),$$

in which the $n_i$ need not be different. **Student 2:** How can the stationary state wavefunction describing the system be the product of the single-particle wavefunctions $\Psi(x_1, x_2, \ldots, x_N) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)\cdots\psi_{n_N}(x_N)$ when the Hamiltonian for a system of the $N$ non-interacting identical particles which can be treated as distinguishable is the sum of the Hamiltonian of each particle $\hat{\mathbf{H}} = \sum_{i=1}^{N} \hat{\mathbf{H}}_i$?

**Student 3:** Let's consider the stationary state wavefunction to be the product of the single-particle wavefunctions $\Psi(x_1, x_2, \ldots, x_N) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)\cdots\psi_{n_N}(x_N)$. From the TISE, $\hat{\mathbf{H}}\Psi = E\Psi$, where $\hat{\mathbf{H}}$ is the Hamiltonian, $\Psi$ is a stationary state wavefunction, and $E$ is the energy of the many-particle system. Thus,

$$\hat{\mathbf{H}}\Psi(x_1, x_2, \ldots, x_N) = \sum_{i=1}^{N} \hat{\mathbf{H}}_i \Psi(x_1, x_2, \ldots, x_N)$$
$$= \sum_{i=1}^{N} \hat{\mathbf{H}}_i \left( \prod_{j=1}^{N} \psi_{n_j}(x_j) \right)$$
$$= (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2 + \ldots + \hat{\mathbf{H}}_N)(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$= \hat{\mathbf{H}}_1(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N)) + \hat{\mathbf{H}}_2(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$+ \ldots + \hat{\mathbf{H}}_N(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$= E_{n_1}(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N)) + E_{n_2}(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$+ \ldots + E_{n_N}(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$= (E_{n_1} + E_{n_2} + \ldots + E_{n_N})(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_N}(x_N))$$
$$= (E_{n_1} + E_{n_2} + \ldots + E_{n_N}) \left( \prod_{i=1}^{N} \psi_{n_i}(x_i) \right)$$
$$= \left( \sum_{i=1}^{N} E_{n_i} \right) \left( \prod_{j=1}^{N} \psi_{n_j}(x_j) \right)$$

$$= E\left(\prod_i = 1^N \psi_{n_j}(x_j)\right)$$
$$= E\Psi(x_1, x_2, \ldots, x_N)$$

which is the constant $E$ times the same wavefunction and so $\prod_{i=1}^{N} \psi_{n_i}(x_i)$ is a many-particle stationary state wavefunction. Therefore, stationary state wavefunctions for a system of $N$ non-interacting particles which can be treated as distinguishable are products of the single-particle wavefunctions.

Explain why you agree or disagree with Student 1 and Student 3 .

25. Write the wavefunction for a system of two **non-interacting**, identical particles which can be treated as distinguishable in which particle 1 is in the single-particle state labeled by $n_1$ and particle 2 is in a single-particle state labeled by $n_2$ with $n_1 \neq n_2$. Do not forget to use appropriate coordinates for each particle.

26. Is the wavefunction in question 25 a stationary state wavefunction for a system of two non-interacting identical particles which can be treated as distinguishable? Explain.

27. What is the energy for a system of two **non-interacting** identical particles which can be treated as distinguishable in which particle 1 is in the single-particle state labeled by $n_1$ and particle 2 is in a single-particle state labeled by $n_2$?

28. Compare your answer for question 27 to the energy for a system of two indistinguishable particles (questions 10 and 19 for fermions and bosons, respectively) where one particle is in a single-particle state labeled by $n_1$ and the other particle is in a single-particle state labeled by $n_2$.

29. For a system of $N$ **non-interacting** identical particles which can be treated as distinguishable, write the stationary state wavefunction for the $N$-particle system, in which $\psi_{n_i}$ is the single-particle wavefunction for the $i^{th}$ particle. Do not forget to use appropriate coordinates for each particle.

30. Write the stationary state wavefunctions for a system of two non-interacting indistinguishable fermions and a system of two indistinguishable bosons (for the distinct single-particle states $\psi_{n_1}$ and $\psi_{n_2}$) and compare to the stationary state wavefunction for a system of two non-interacting identical particles which can be treated as distinguishable in question 25.

**** Checkpoint: Check your answer to questions 24-30. ****

24. b and c

25. $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$

26. Yes. $\hat{\mathbf{H}}\Psi = (\hat{\mathbf{H}}_1 + \hat{\mathbf{H}}_2)\psi_{n_1}(x_1)\psi_{n_2}(x_2) = (E_{n_1} + E_{n_2})\psi_{n_1}(x_1)\psi_{n_2}(x_2) = E\Psi(x_1, x_2)$

27. $E = E_{n_1} + E_{n_2}$

28. The energy of a system of two identical particles which are indistinguishable fermions or bosons is the same as the energy for a system of two identical particles which can be treated as distinguishable, for which $E = E_{n_1} + E_{n_2}$ for all three cases.

29. $\Psi(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N} \psi_{n_i}(x_i) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\cdots\psi_{n_N}(x_N)$.

30. The stationary state wavefunctions for two non-interacting identical particles occupying the two distinct single-particle states $\psi_{n_1}$ and $\psi_{n_2}$ are given in the following chart

| System | Stationary State Wavefunction |
|---|---|
| Distinguishable Particles | $\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$ or $\Psi(x_1, x_2) = \psi_{n_2}(x_1)\psi_{n_1}(x_2)$ |
| Indistinguishable Fermions | $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$ |
| Indistinguishable Bosons | $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)]$ |

The wavefunction for a system of indistinguishable particles must reflect symmetrization requirements.

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

**Summary of the Properties of the Wavefunction for Distinguishable Particles**

- There is no symmetrization requirement for the many-particle stationary state wavefunction for a system of identical particles which can be treated as distinguishable.
- The wavefunction for a system of non-interacting identical particles which can be treated as distinguishable is the product of the single-particle wavefunctions:
  - $\Psi(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N} \psi_{n_i}(x_i)$.

In two to three sentences, summarize the properties of the wavefunction for identical particles (particles of the same type with the same properties). Be sure to describe the properties of indistinguishable fermions, indistinguishable bosons, and identical particles if they could be treated as distinguishable.

Fill in the table below with the properties of an $N$-particle system consisting of identical particles.

| **IDENTICAL PARTICLES**<br>How would you explain to someone why in an $N$-particle quantum system consisting of identical particles, the particles must be treated as indistinguishable? | |
|---|---|
| **Type of Particle** | **Properties** |
| INDISTINGUISHABLE FERMIONS | What is the constraint on the spin of a fermion? |
| | Give an example of a physical system consisting of identical fermions in which the fermions must be treated as indistinguishable. |
| | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)? |
| INDISTINGUISHABLE BOSONS | What is the constraint on the spin of a boson? |
| | Give an example of a physical system consisting of identical bosons in which the bosons must be treated as indistinguishable. |
| | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)? |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)? |

Construct the wavefunction for the following systems of three non-interacting particles with correct normalization. Use thelabels $n_1$, $n_2$, and $n_3$ to represent the single-particle stationary state wavefunctions of the system when necessary. If no suchwavefunction is permissible, mark the box with an X.

| | All 3 particles in the same single-particle state labeled by $n_1$. | 2 particles in the same single-particle state labeled by $n_1$<br>1 particle in a different single-particle state labeled by $n_2$. | All 3 particles in different single-particle states labeled by $n_1$, $n_2$, and $n_3$. |
|---|---|---|---|
| INDISTINGUISHABLE FERMIONS | | | |
| INDISTINGUISHABLE BOSONS | | | |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | | | |

## ** Check your answers in the preceding tables.**

**IDENTICAL PARTICLES**

How would you explain to someone why in an $N$-particle quantum system consisting of identical particles, the particles must be treated as indistinguishable?

**Nature is found to behave in this manner. A system of identical particles consists of $N$ particles in which all the particles are of the same type with the same properties and the particles must be treated as indistinguishable.**

| **Type of Particle** | **Properties** |
|---|---|
| INDISTINGUISHABLE FERMIONS | What is the constraint on the spin of a fermion?<br><br>**The $N$ fermions must all be the same half-integer spin particle.** |
| | Give an example of a physical system consisting of identical fermions in which the fermions must be treated as indistinguishable.<br><br>**Electrons in a metal.** |
| | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)?<br><br>**Completely antisymmetric** |
| INDISTINGUISHABLE BOSONS | What is the constraint on the spin of a boson?<br><br>**The $N$ bosons must all be the same integer spin particle.** |
| | Give an example of a physical system consisting of identical bosons in which the bosons must be treated as indistinguishable.<br><br>**He-4 atoms for which there is overlap of the single-particle wavefunctions (i.e., the average separation between atoms is less than the de Broglie wavelength).** |
| | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)?<br><br>**Completely symmetric** |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | What is the symmetrization requirement of the $N$-particle wavefunction (i.e. Completely symmetric, Completely antisymmetric, or No requirement)?<br><br>**No Requirement** |

| | All 3 Particles in the same single-particle state labeled by $n_1$. | 2 particles in the same single-particle state labeled by $n_1$ 1 particle in a different single-particle state labeled by $n_2$. | All 3 particles in different single-particle states labeled by $n_1$, $n_2$, and $n_3$. |
|---|---|---|---|
| INDISTINGUISHABLE FERMIONS | X | X | $\frac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2)$ $-\psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1)$ $+\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2) - \psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)]$ |
| INDISTINGUISHABLE BOSONS | $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ | $\frac{1}{\sqrt{3}}[\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)$ $+\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)$ $+\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)]$ | $\frac{1}{\sqrt{6}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2)$ $\psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3) + \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1)$ $+\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2) + \psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)]$ |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$ | $\psi_{n_1}(x_1)\psi_{n_1}(x_2)\psi_{n_2}(x_3)$[3] | $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$[4] |

[3] There are two other possibilities: $\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_1}(x_3)$ and $\psi_{n_2}(x_1)\psi_{n_1}(x_2)\psi_{n_1}(x_3)$

[4] There are five other possibilities: $\psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2)$, $\psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3)$, $\psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1)$, $\psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2)$, and $\psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)$

## Summary of the Properties of the Wavefunction for Non-Interacting Identical Particles

- Indistinguishable Fermions
  - The basis states used to construct the many-particle stationary state wavefunction for a system of indistinguishable fermions are written in terms of the products of single-particle wavefunctions.
  - The coordinate corresponding to each particle is different in the many-particle stationary state wavefunction.
  - The many-particle wavefunction describing a system of indistinguishable fermions must be completely antisymmetric with respect to exchange of any two particles.
- Indistinguishable Bosons
  - The basis states used to construct the many-particle stationary state wavefunction for a system of $N$ indistinguishable bosons are written in terms of the products of single-particle wavefunctions.
  - The coordinate corresponding to each particle is different in the many-particle stationary state wavefunction.
  - The many-particle wavefunction describing a system of indistinguishable bosons must be completely symmetric with respect to exchange of any two particles.
- Hypothetical Case: Identical Particles if they could be treated as Distinguishable
  - The basis states for the many-particle stationary state wavefunction for a system of identical particles which can be treated as distinguishable can be written in terms of the product of the single-particle wavefunctions.
  - The coordinate corresponding to each particle is different in the many-particle stationary state wavefunction.
  - There is no symmetrization requirement for the many-particle wavefunction for a system of identical particles which can be treated as distinguishable.

## D.7 EXAMPLES OF FINDING MANY-PARTICLE STATIONARY STATE WAVEFUNCTIONS AND ENERGIES

### D.7.1 One-Dimensional Infinite Square Well (Ignoring spin)

**Recall:** The single-particle wavefunctions for the infinite square well are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \qquad 0 < x < a \qquad n = 1, 2, 3, \ldots$$

and the single-particle energies are given by

$$E_n = n^2 \left(\frac{\pi^2\hbar^2}{2ma^2}\right) = n^2 E_1.$$

31. Suppose we have two non-interacting particles, both of mass $m$, in a one-dimensional infinite square well of width $a$ (the well is between $x = 0$ and $x = a$). Find the ground state and first-excited state energies of the many-particle system for the following cases:

    a. Indistinguishable fermions. (Ignore spin)

    b. Indistinguishable bosons. (Ignore spin)

    c. Hypothetical case: Identical particles which can be treated as distinguishable. (Ignore spin)

32. Construct the ground state and first-excited state wavefunctions for two non-interacting particles in that infinite square well for the following cases:

a. Indistinguishable fermions. (Ignore spin)

b. Indistinguishable bosons. (Ignore spin)

c. Hypothetical case: Identical particles which can be treated as distinguishable. (Ignore spin)

Consider the following conversation regarding finding the ground state energy of the many-particle system in a one-dimensional infinite square well of width $a$ (ignore spin).
**Student 1:** For a system of two non-interacting identical particles, the energy is $E_{n_1,n_2} = E_{n_1} + E_{n_2} = \left(\frac{n_1^2\pi^2\hbar^2}{2ma^2}\right) + \left(\frac{n_2^2\pi^2\hbar^2}{2ma^2}\right) = (n_1^2 + n_2^2)\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = (n_1^2 + n_2^2)\,E_1$.
**Student 2:** I agree with Student 1. The ground state energy for a system of two identical particles corresponds to the case in which both particles are in the single-particle state labeled by $n_1 = n_2 = 1$. Thus, the ground state energy of the two-particle system is $E_{1,1} = (1^2 + 1^2)\,E_1 = 2E_1$
**Student 3:** I agree with Student 2 only for the cases in which the two particles are indistinguishable bosons or particles which can be treated as distinguishable. In both cases, the particles are permitted to occupy the same lowest single-particle state labeled by $n_1 = n_2 = 1$. However, two indistinguishable fermions cannot occupy the same single-particle state. The ground state energy for a system of two indistinguishable fermions is $E_{1,2} = E_{2,1} = (1^2 + 2^2)\,E_1 = 5E_1$.

Explain why you agree or disagree with the students.

Consider the following conversation regarding finding the first-excited state energy of the many-particle system in a one-dimensional infinite square well of width $a$ (ignore spin).

**Student 1:** For a system of two non-interacting identical particles, the first-excited state energy is $E_{1,2} = (1^2 + 2^2)\, E_1 = 5E_1$.

**Student 2:** I agree with Student 1 only for the cases in which the identical particles are indistinguishable bosons or identical particles which can be treated as distinguishable. The ground state for a system of two indistinguishable fermions corresponds to the case in which one fermion is in the single-particle state labeled by $n_1 = 1$ and the other fermion is in the single-particle state labeled by $n_2 = 2$. The first-excited state energy for a system of two identical fermions corresponds to the case in which one fermion is in the single-particle state labeled by $n_1 = 1$ and the other fermion is in the single-particle state labeled by $n_2 = 3$. Thus, the first-excited state energy for a system of two fermions is $E_{1,3} = (1^2 + 3^2)\, E_1 = 10E_1$.

Explain why you agree or disagree with each student.

Consider the following conversation about finding the ground state wavefunction of the many-particle system involving a one-dimensional infinite square well of width $a$ (ignore spin).

**Student 1:** For a system of two non-interacting identical particles, the ground state wavefunction is $\Psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$.

**Student 2:** I agree with Student 1 only for the cases in which the identical particles are indistinguishable bosons or particles which can be treated as distinguishable since in both cases the particles are permitted to be in the same single-particle state. However, two indistinguishable fermions must be in different single-particle states and the ground state wavefunction for a system of two indistinguishable fermions must be completely antisymmetric.

**Student 3:** I agree with Student 2. The ground state wavefunction for a system of two indistinguishable fermions is $\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)]$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding finding the first-excited state wavefunction of the many-particle system in a one-dimensional infinite square well of width $a$ (ignore spin).

**Student 1:** For a system of two non-interacting identical particles, the first-excited state wavefunction is $\Psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$.

**Student 2:** I agree with Student 1 only if the particles can be treated as distinguishable.

**Student 3:** I agree with Student 2. Also, the first-excited state wavefunction for a system of two indistinguishable bosons ignoring spin is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)] .$$

**Student 2:** I agree with Student 3. Furthermore, the first-excited state wavefunction for a system of two indistinguishable fermions ignoring spin is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_1(x_1)\psi_3(x_2) - \psi_3(x_1)\psi_1(x_2)] .$$

Explain why you agree or disagree with each student.

****CHECKPOINT: Check your answers to questions 31-32. ****

31a. Ground state: $E = E_1 + E_2 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2} = 5E_1$

First excited state:$E = E_1 + E_3 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{9\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{ma^2} = 10E_1$

31b. Ground state: $E = E_1 + E_1 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{\pi^2\hbar^2}{2ma^2} = \frac{\pi^2\hbar^2}{ma^2} = 2E_1$

First excited state:$E = E_1 + E_2 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2} = 5E_1$

31c. Ground state: $E = E_1 + E_1 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{\pi^2\hbar^2}{2ma^2} = \frac{\pi^2\hbar^2}{ma^2} = 2E_1$

First excited state:$E = E_1 + E_2 = \frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2} = 5E_1$

32a. Ground state:

$$\begin{aligned}\Psi(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right] \\ &= \tfrac{1}{\sqrt{2}}\left[\tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{2\pi}{a}x_2\right) - \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_2\right)\sin\left(\tfrac{2\pi}{a}x_1\right)\right]\end{aligned}$$

First excited:

$$\begin{aligned}\Psi(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_3(x_2) - \psi_1(x_2)\psi_3(x_1)\right] \\ &= \tfrac{1}{\sqrt{2}}\left[\tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{3\pi}{a}x_2\right) - \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_2\right)\sin\left(\tfrac{3\pi}{a}x_1\right)\right]\end{aligned}$$

32b. Ground state:

$$\begin{aligned}\Psi(x_1,x_2) &= \psi_1(x_1)\psi_1(x_2) \\ &= \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{\pi}{a}x_2\right)\end{aligned}$$

First excited:

$$\begin{aligned}\Psi(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\right] \\ &= \tfrac{1}{\sqrt{2}}\left[\tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{2\pi}{a}x_2\right) + \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_2\right)\sin\left(\tfrac{2\pi}{a}x_1\right)\right]\end{aligned}$$

32c. Ground state:

$$\begin{aligned}\Psi(x_1,x_2) &= \psi_1(x_1)\psi_1(x_2) \\ &= \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{\pi}{a}x_2\right)\end{aligned}$$

First excited:

$$\begin{aligned}\Psi(x_1,x_2) &= \psi_1(x_1)\psi_2(x_2)\\ &= \tfrac{2}{a}\sin\left(\tfrac{\pi}{a}x_1\right)\sin\left(\tfrac{2\pi}{a}x_2\right)\end{aligned}$$

or

$$\begin{aligned}\Psi(x_1,x_2) &= \psi_2(x_1)\psi_1(x_2)\\ &= \tfrac{2}{a}\sin\left(\tfrac{2\pi}{a}x_1\right)\sin\left(\tfrac{\pi}{a}x_2\right)\end{aligned}$$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

## D.8 COUNTING THE NUMBER OF DISTINCT MANY-PARTICLE STATES

- Now that we know how to construct stationary state wavefunctions from the single-particle wavefunctions for indistinguishable fermions, indistinguishable bosons, and identical particles if they could be treated as distinguishable, let's determine the number of distinct many-particle states for the three different cases, beginning with indistinguishable fermions.
- We will only consider systems in which there is no degeneracy in the single-particle wavefunctions (i.e., $E_{n_i} \neq E_{n_j}$ in which $E_{n_i}$ is the energy corresponding to the single-particle state $\psi_{n_i}$ and $E_{n_j}$ is the energy corresponding to the single-particle state $\psi_{n_j}$)
- Recall: The number of ways to arrange $K$ identical objects among $N$ available slots is $\binom{N}{K} = \frac{N!}{K!(N-K)!}$

## CASE I: A Fixed Number of Single Particle States are Available to the System (but the Total Energy of the Many-Particle System is NOT Fixed).

### D.8.1 Determining the Number of Distinct Many-Particle States for INDISTINGUISHABLE FERMIONS (no constraints on the total energy of the many-particle system)

33. Suppose you have two indistinguishable fermions and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct two-particle states can you construct (neglecting spin)? Think about how you could use the diagram below to answer this question by placing the fermions into the single-particle states.

_____ $\psi_{n_1}$

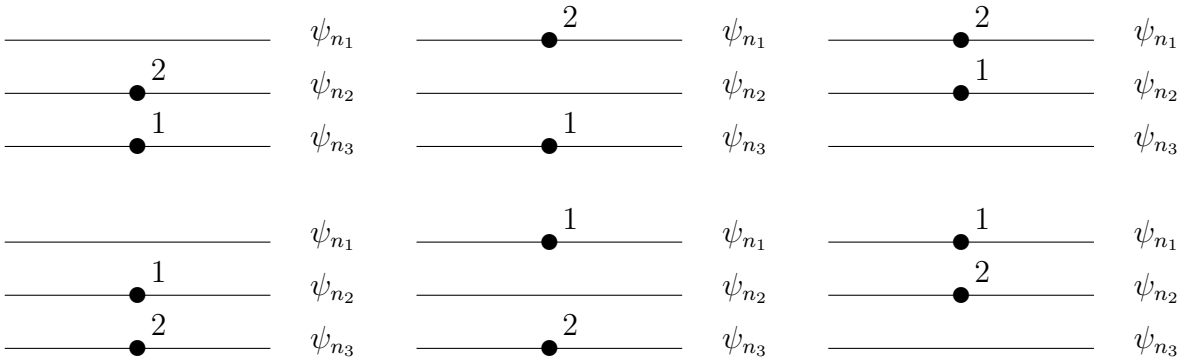
_____ $\psi_{n_2}$

_____ $\psi_{n_3}$

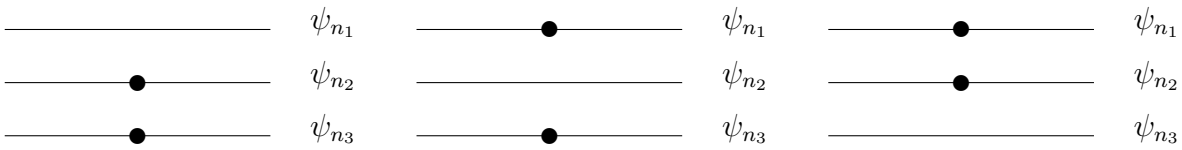
Consider the following conversation regarding the number of distinct two-particle states for a system of two indistinguishable fermions and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$.

**Student 1:** For a system of two fermions and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$, there are three available single-particle states for the first fermion. That leaves two single-particle states for the second fermion since the second fermion cannot occupy the same single-particle state as the first fermion. The number of two-particle states is $3 \times 2 = 6$.

**Student 2:** I agree with Student 1. Here is the diagrammatic representation for the 6 distinct two-particle states:




**Student 3:** I disagree with Student 1 and Student 2. You are overcouting the number of distinct two-particle states. Since the fermions are indistinguishable, we cannot distinguish which fermion is in which single-particle state. We can only tell that one fermion is in single-particle state $\psi_{n_2}$ and another fermion in single-particle state $\psi_{n_3}$. But there is no way to tell which fermion is in which single-particle state. This indistinguishability is reflected in the antisymmetrized wavefunction. There are 3 distinct two-particle states. Here is the diagrammatic representation for the 3 distinct two-particle states:



Explain why you agree or disagree with each student.

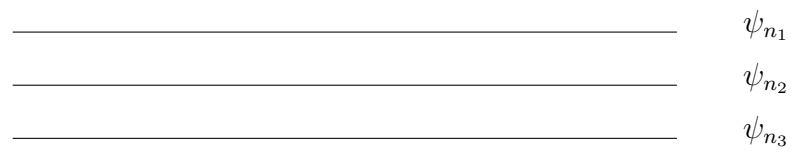
Consider the following conversation regarding the number of distinct two-particle states that you can construct for a system of two indistinguishable fermions and three distinct single-particle states.

**Student 1:** The Pauli exclusion principle forbids two fermions from occupying the same single-particle state. Each single-particle state can either have one or zero fermions.

**Student 2:** I agree. There are three distinct single-particle states available to the fermions and we must choose any two for the fermions to occupy. The number of distinct two-particle states for a system of two indistinguishable fermions and three distinct single-particle states is $\binom{3}{2}=\frac{3!}{2!(3-2)!}=3$.

Explain why you agree or disagree with the students.

34. Suppose you have three indistinguishable fermions and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct three-particle states can you construct (neglecting spin)? If you would like, you can think about how you could use the diagram below to answer this question by placing the fermions into the corresponding states.




Consider the following conversation regarding the number of distinct three-particle states for a system of three indistinguishable fermions.

**Student 1:** For a system of three indistinguishable fermions and three available single-particle states, there is only one distinct three-particle state. There must be one fermion is each single-particle state.

**Student 2:** I agree. There are three distinct single-particle states available to the fermions and we must choose three single-particle states for the fermions to occupy. The number of distinct three-particle states for a system of three indistinguishable fermions and three distinct single-particle states is $\binom{3}{3}=\frac{3!}{3!(3-3)!}=1$.

Explain why you agree or disagree with the students.

35. Suppose you have $N$ indistinguishable fermions ($N \gg 1$) and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct $N$-particle states can you construct (neglecting spin)?

Consider the following conversation regarding the number of distinct three-particle states for a system of $N$ ($N \gg 1$) indistinguishable fermions.

**Student 1:** For a system of $N$ fermions ($N \gg 1$) and three distinct single-particle states, there is no possible way to place the fermions into the three distinct single-particle states such that no two particles are in the same single-particle state. Therefore, this situation is impossible.

**Student 2:** I agree. We need at least as many distinct single-particle states available in a situation as the number of fermions in order for such a many-particle system to be possible.

Explain why you agree or disagree with the students.

36. Suppose you have $N$ fermions ($N \gg 1$) and $M$ distinct single-particle states ($M \gg 1$). How many distinct $N$-particle states can you construct (neglecting spin)?

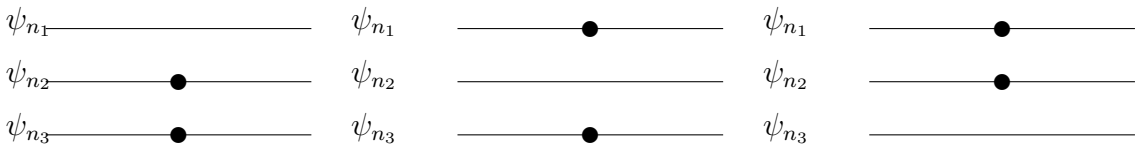
In two to three sentences, describe in words how to determine the number of distinct $N$-particle states for $N$ indistinguishable fermions and $M$ distinct single-particle states when there are no constraints on the total energy of the many-particle system.

Let's connect the number of distinct single-particle states with the number of possible many-particle stationary state wavefunctions for fermions.

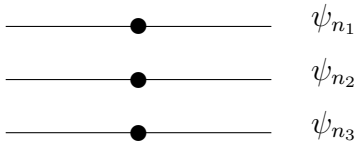
37. Write all the possible two-particle stationary state wavefunctions you found for two indistinguishable fermions in three distinct single-particle states $\psi_{n_1}, \psi_{n_2}$, and $\psi_{n_3}$ in question 33.

****CHECKPOINT: Check your answers to questions 33-37. ****

33. $\binom{3}{2}=3$




34. $\binom{3}{3}=1$




35. 0. There cannot be more fermions than available single-particle states since that would mean there would be more than one fermion in at least one single-particle state, which is not permitted.

36. The number of distinct $N$-particle states for a system of $N$ fermions with $M$ available single-particle states is $\begin{cases} \binom{M}{N} & M \geq N \\ 0 & M < N \end{cases}$

37.

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$$

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_3}(x_2) - \psi_{n_3}(x_2)\psi_{n_1}(x_1)]$$

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_3}(x_2) - \psi_{n_3}(x_2)\psi_{n_2}(x_1)]$$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

**Summary for Determining the Number of Distinct Many-Particle States of INDISTINGUISHABLE FERMIONS for a Fixed Number of Single-Particle States (no constraints on the total energy of the many-particle system)**

- The number of distinct $N$-particle states for a system of $N$ indistinguishable fermions with $M$ available single-particle states when $N \leq M$ is $\binom{M}{N}$.
- The number of distinct $N$-particle states for a system of $N$ indistinguishable fermions with $M$ available single-particle states when $N > M$ is 0.

### D.8.2 Determining the Number of Distinct Many-Particle States for INDISTINGUISHABLE BOSONS (no constraints on the total energy of the many-particle system)

38. Suppose you have two indistinguishable bosons and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct two-particle states can you construct (neglecting spin)? Think about how you could use the diagram below to answer this question by placing the bosons into the corresponding single-particle states.

_____ $\psi_{n_1}$

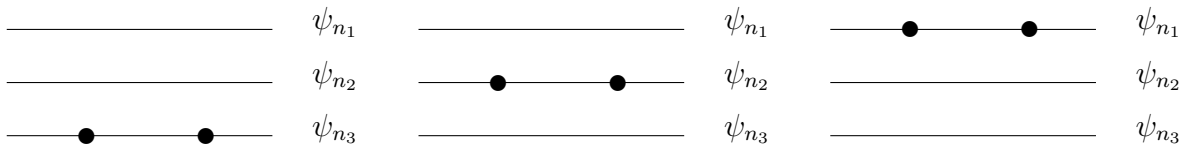
_____ $\psi_{n_2}$

_____ $\psi_{n_3}$

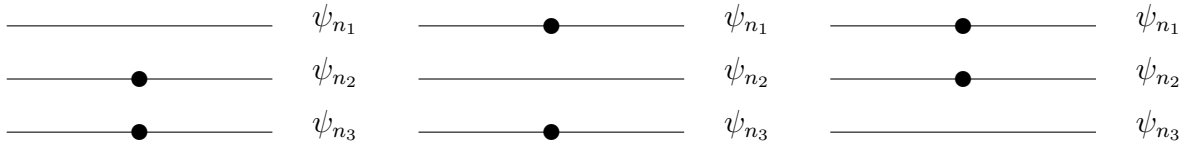
Consider the following conversation regarding the number of distinct two-particle states for a system of two indistinguishable bosons and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$ available.

**Student 1:** For a system of two bosons and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$, there are three available states for the first boson and three available states for the second boson. The number of two-particle states is $3 \times 3 = 9$.

**Student 2:** I disagree with Student 1. You are overcounting since you are not taking into account the fact that bosons are indistinguishable. If the bosons are in the same single-particle state, there are three possibilities as follows:




But, if the bosons are in different single-particle states, there are three possibilities since bosons are indistinguishable and swapping the two bosons in the two single-particle states in each of the following situations does not produce a new two-particle state:




There are 6 distinct two-particle states for a system of two bosons and three distinct single-particle states.

Explain why you agree or disagree with each student.

Consider the following conversation about a method for determining the number of distinct ways two indistinguishable bosons can be arranged in the three distinct single-particle states.

**Student 1:** For a system of two bosons, there can be more than one boson in a given single-particle state. We can treat the single-particle states as bins to be filled with bosons and dividers to separate the different single-particle states or bins. For example, if the system had two bosons in the first single-particle state then the first bin would have two bosons. For a system with three single-particle states available, we would need two dividers between the three single-particle states. In the case of three single-particle states and two bosons, we must find the number of possible arrangements of the two bosons and two dividers.

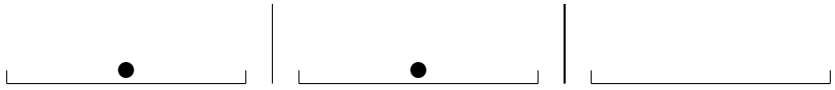
**Student 2:** I agree with Student 1. Furthermore, since the two dividers cannot be distinguished from one another and the bosons cannot be distinguished from one another, we can permute the indistinguishable dividers with the indistinguishable bosons to find all possible ways to permute two bosons in the three single-particle states as follows:

Two Bosons in the First State

Two Bosons in the Second State

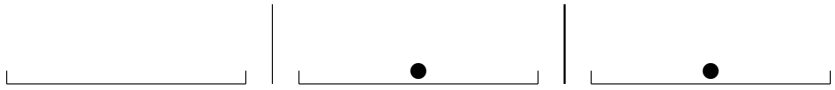
Two Bosons in the Third State

One Boson in the First State and One Boson in the Second State



One Boson in the First State and One Boson in the Third State

One Boson in the Second State and One Boson in the Third State

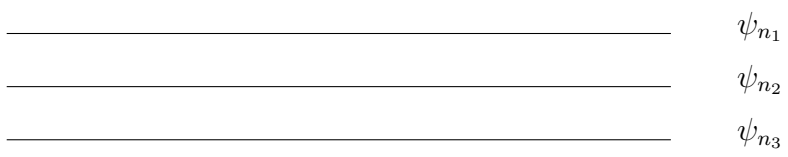


**Student 3:** I agree with both Student 1 and Student 2. The number of distinct many-particle states comes from the number of ways the two bosons and two dividers can be permuted. We have a total of four objects (two bosons and two dividers) and we can find the number of ways to permute the two bosons or equivalently the number of ways to permute the two dividers among the four objects. The number of distinct two-particle states is $\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$.

**Student 2:** Yes! Since the dividers are indistinguishable, permuting them with each other does not give us a new two-particle state. Similarly, since the bosons are indistinguishable, permuting them with each other does not give us a new two-particle state.

Explain why you agree or disagree with the students.

39. Suppose you have three indistinguishable bosons and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct three-particle states can you construct (neglecting spin)? If you would like, you can think about how you could use the diagram below to answer this question by placing the bosons into the corresponding states.




Consider the following conversation regarding determining the number of distinct ways three indistinguishable bosons can be arranged in the three distinct single-particle states.

**Student 1:** Using the bin and divider method, we have three bosons and three bins or single-particle states constructed with two dividers. There are five total objects, three bosons and two dividers, and we must calculate the number of distinct permutations remembering that the bosons are indistinguishable and the dividers are indistinguishable.

**Student 2:** I agree. We can find the number of ways to permute the three bosons among the five total objects or equivalently the number of ways to permute the two dividers among the five total objects. When we calculate the number of ways to place the two dividers between the three bins, we get $\binom{5}{2} = \frac{5!}{2!(5-2)!} = \frac{5!}{2!3!} = 10$. If instead, we calculate the number of ways to place the three bosons among the two dividers, we get $\binom{5}{3} = \frac{5!}{3!(5-3)!} = \frac{5!}{3!2!} = 10$. Either way it is the same!

Explain why you agree or disagree with the students.

40. Suppose you have $N$ bosons ($N \gg 1$) and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct $N$-particle states can you construct (neglecting spin)?

Consider the following conversation regarding determining the number of distinct ways $N$ indistinguishable bosons can be arranged in the three distinct single-particle states.

**Student 1:** Using the bin and divider method, there are $N + 2$ total objects to be permuted out of which the $N$ bosons are indistinguishable from each other and the two dividers are indistinguishable from each other. We must calculate the number of distinct arrangements.

**Student 2:** I agree. When we calculate the number of ways to place the two dividers among the $N$ bosons, we get

$$\binom{N+2}{2} = \frac{(N+2)!}{2![(N+2)-2)]!} = \frac{(N+2)!}{2!N!} = \frac{(N+2)(N+1)}{2}$$

. If instead, we calculate the number of ways to place the $N$ bosons among the two dividers, we get

$$\binom{N+2}{M} = \frac{(N+2)!}{N![(N+2)-N)]!} = \frac{(N+2)!}{N!2!} = \frac{(N+2)(N+1)}{2}$$

.

Explain why you agree or disagree with each student.

41. Suppose you have $N$ bosons ($N \gg 1$) and $M$ distinct single-particle states ($M \gg 1$). How many distinct $N$-particle states can you construct (neglecting spin)?

Consider the following conversation regarding determining the number of distinct ways $N$ indistinguishable bosons can be arranged in the $M$ distinct single-particle states.

**Student 1:** Using the bin and divider method, there are $N + M - 1$ total objects that must be permuted, out of which $N$ bosons are indistinguishable from each other and the $M - 1$ dividers are indistinguishable from each other. We must calculate the number of distinct arrangements.

**Student 2:** I agree. When we choose the number of ways to place the $M - 1$ indistinguishable dividers among the $N$ bosons, we get

$$\binom{N+M-1}{M-1} = \frac{(N+M-1)!}{(M-1)![(N+M-1)-(M-1))]!} = \frac{(N+M-1)!}{(M-1)!N!}$$

. If instead we choose the number of ways to place the $N$ bosons among $M-1$ dividers, we get

$$\binom{N+M-1}{N} = \frac{(N+M-1)!}{N![(N+M-1)-N)]!} = \frac{(N+M-1)!}{N!(M-1)!}$$

. Either way it is the same!

Explain why you agree or disagree with the students.

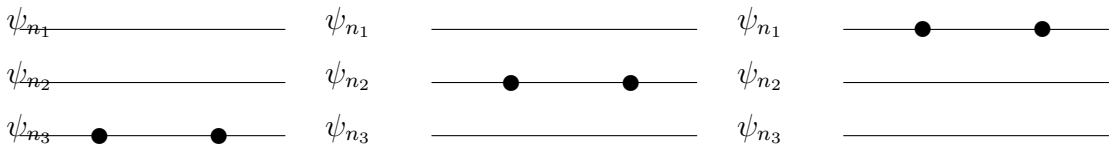
In two to three sentences, describe how to determine the number of distinct $N$-particle states for $N$ indistinguishable bosons and $M$ distinct one-particle states.

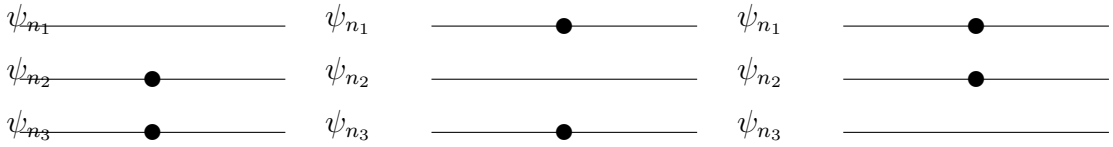
Let's connect the number of distinct many-particle states with the number of possible many-particle stationary state wavefunctions for bosons.

42. Write the two-particle stationary state wavefunctions for the two indistinguishable bosons in three distinct single-particle states $\psi_{n_1}, \psi_{n_2}$, and $\psi_{n_3}$ in question 38.

****CHECKPOINT: Check your answers to questions 38-42. ****

38. $\binom{4}{2} = 6$




39. $\binom{5}{2} = 10$

40. $\binom{N+2}{N} = \frac{(N+2)(N+1)}{2}$

41. $\binom{N+M-1}{N} = \binom{N+M-1}{M-1} = \frac{(N+M-1)!}{N!(M-1)!}$

42.

$$\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$$

$$\Psi(x_1, x_2) = \psi_{n_2}(x_1)\psi_{n_2}(x_2)$$

$$\Psi(x_1, x_2) = \psi_{n_3}(x_1)\psi_{n_3}(x_2)$$

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$$

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_3}(x_2) + \psi_{n_1}(x_2)\psi_{n_3}(x_1)]$$

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_2}(x_1)\psi_{n_3}(x_2) + \psi_{n_2}(x_2)\psi_{n_3}(x_1)]$$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

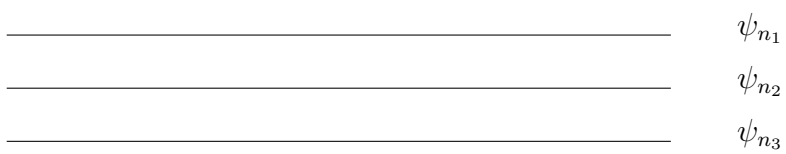
**Summary for Determining the Number of Distinct Many-Particle States of INDISTINGUISHABLE BOSONS for a Fixed Number of Single-Particle States (no constraints on the total energy of the many-particle system)**

- The number of distinct $N$-particle states for a system of $N$ indistinguishable bosons with $M$ available single-particle states is
$\binom{N+M-1}{N} = \binom{N+M-1}{M-1} = \frac{(N+M-1)!}{N!(M-1)!}$

### D.8.3 Hypothetical Case: Determining the Number of Distinct Many-Particle States for IDENTICAL PARTICLES IF THEY COULD BE TREATED AS DISTINGUISHABLE (no constraints on the total energy of the many-particle system)

- Now that we know how to determine the number of distinct many-particle states for indistinguishable fermions and indistinguishable bosons, let's consider a contrasting case in which the particles can be treated as distinguishable.
- Next, compare the resulting number of many-particle states to what was obtained for indistinguishable fermions and indistinguishable bosons to learn why care must be taken to ensure that the many-particle wavefunction reflects the indistinguishability of the particles.

43. Suppose you have two identical particles which can be treated as distinguishable and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct two-particle states can you construct (neglecting spin)? Think about how you could use the diagram below to answer this question by placing the distinguishable particle into the single-particle states.

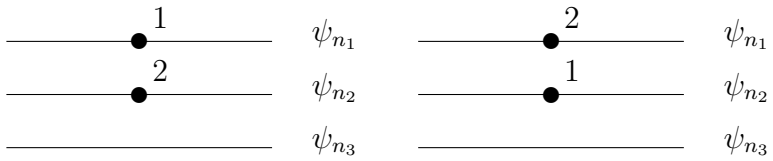


Consider the following conversation regarding the number of distinct two-particle states for a system of two identical particles which can be treated as distinguishable and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$.

**Student 1:** The first particle can be placed in one of the three states so there are three possibilities. The same is true about the second particle since there is no restriction on how many particles can be placed in a given single-particle state. Thus, the total number of distinct two-particle states for the system of two identical particles which can be treated as distinguishable with three available single-particle states is $3 \times 3 = 9$.

**Student 2:** I disagree with Student 1. You are double counting when the particles occupy the same two single-particle states. For example, you are counting the states $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ and $\psi_{n_1}(x_2)\psi_{n_2}(x_1)$ as two distinctly different states. However, there must be only one distinctly different state $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ in which one particle is in the state labeled by $\psi_{n_1}$ and the other particle is in the state labeled by $\psi_{n_2}$.

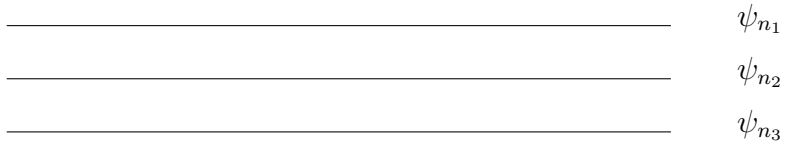
**Student 3:** I agree with Student 1. There are three two-particle states when the particles are in the same single-particle state and six two-particle states when the particles are in different single-particle states. Since the particles can be treated as distinguishable, we know which particles is in which state. $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ is the stationary state wavefunction corresponding to particle 1 in the single particle state $\psi_{n_1}$ and particle 2 in the single particle state $\psi_{n_2}$. Also, particle 1 in state $\psi_{n_1}$ and particle 2 in state $\psi_{n_1}$ is different than particle 2 in state $\psi_{n_1}$ and particle 1 in state $\psi_{n_1}$. These are two possible stationary state wavefunctions and must be determined as two distinct two-particle states as illustrated in the diagram below.




Explain why you agree or disagree with each student.

Student 1 and Student 3 are correct in the previous conversation. Let's extend the rationale to three identical particles which can be treated as distinguishable.

44. Suppose you have three identical particles which can be treated as distinguishable and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct three-particle states can you construct (neglecting spin)? If you would like, think about how you could use the diagram below to answer this question by placing the distinguishable particles into the single-particle states.



Consider the following conversation regarding the number of distinct three-particle states for a system of three identical particles which can be treated as distinguishable and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$.

**Student 1:** The first particle can be placed in one of the three states so there are three possibilities. The same is true for the second particle and the third particle since there is no restriction on how many particles we can place in a given single-particle state. The total number of distinct three-particle states for the system of three identical particles which can be treated as distinguishable with three available single-particle states is $3 \times 3 \times 3 = 27$.

**Student 2:** I agree with Student 1. The total number of distinct three-particle states for the system of three identical particles which can be treated as distinguishable with three available single-particle states is

$$[\text{Three single-particle states}]^{(\text{Three Particles})} = 3^3 = 27.$$

**Student 3:** I agree with both Student 1 and Student 2. And in general, the total number of distinct states for a system of identical particles which can be treated as distinguishable is

$$[\text{Number of Single-Particle States}]^{(\text{Number of Particles})}.$$

Explain why you agree or disagree with the students.

45. Suppose you have $N$ identical particles which can be treated as distinguishable ($N \gg 1$) and three distinct single-particle states $\psi_{n_1}$, $\psi_{n_2}$, and $\psi_{n_3}$. How many distinct $N$-particle states can you construct (neglecting spin)?

46. Suppose you have $N$ identical particles which can be treated as distinguishable ($N \gg 1$) and $M$ distinct single-particle states ($M \gg 1$). How many distinct $N$-particle states can you construct?

In two to three sentences, summarize how to determine the number of distinct $N$-particle states for $N$ identical particles which can be treated as distinguishable and $M$ distinct single-particle states.

Rank the number of distinct $N$-particle states for identical particles if they are indistinguishable fermions, indistinguishable bosons, or identical particles that can be treated as distinguishable for $N$ identical particles ($N \gg 1$) and $M$ distinct single-particle states ($M \gg 1$).

Let's connect the number of distinct single-particle states with the number of possible stationary state wavefunctions for identical particles which can be treated as distinguishable.

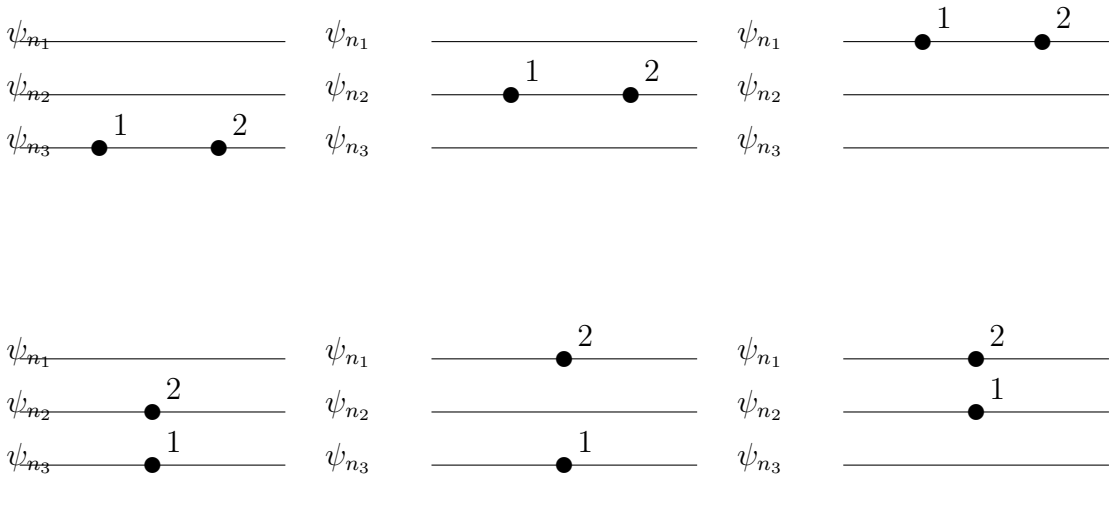
47. Write all of the possible two-particle stationary state wavefunctions you found for two identical particles which can be treated as distinguishable in three distinct single-particle states given by the wavefunctions $\psi_{n_1}, \psi_{n_2}$, and $\psi_{n_3}$ in question 43 for the following situations:

    - Both particles are in the same single-particle state: (Hint: There are three possible two-particle stationary state wavefunctions).

    - Two particles are in different single-particle states: (Hint: There are six possible two-particle stationary state wavefunctions).

****CHECKPOINT: Check your answers to questions 43-47. ****

43. $3 \times 3 = 3^2 = 9$




44. $3 \times 3 \times 3 = 3^3 = 27$

45. $3^N$

46. $M^N$

47.

Two particles in the same state:

$$\Psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_1}(x_2)$$
$$\Psi(x_1, x_2) = \psi_{n_2}(x_1)\psi_{n_2}(x_2)$$
$$\Psi(x_1, x_2) = \psi_{n_3}(x_1)\psi_{n_3}(x_2)$$

| | | | |
|---|---|---|---|
| Two particles in different states: | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$ |
| | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_1}(x_1)\psi_{n_3}(x_2)$ |
| | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_2}(x_1)\psi_{n_1}(x_2)$ |
| | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_2}(x_1)\psi_{n_3}(x_2)$ |
| | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_3}(x_1)\psi_{n_1}(x_2)$ |
| | $\Psi(x_1, x_2)$ | $=$ | $\psi_{n_3}(x_1)\psi_{n_2}(x_2)$ |

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

**Summary for Determining the Number of Distinct Many-Particle States of IDENTICAL PARTICLES IF THEY COULD BE TREATED AS DISTINGUISHABLE for a Fixed Number of Single-Particle States (no constraints on the total energy of the many-particle system)**

- The number of distinct $N$-particle states for a system of $N$ identical particles if they could be treated as distinguishable with $M$ available single-particle states is $M^N$.

To summarize what you have learned about determining the number of distinct many-particle states for a fixed number of single-particle states (total energy of the many-particle system is not fixed), fill in the following table with how many disinct many-particle states you can construct for the given situation.

| Identical Particles | |
|---|---|
| INDISTINGUISHABLE FERMIONS | 5 particles and 7 distinct single-particle states |
| | 5 particles and 3 distinct single-particle states |
| INDISTINGUISHABLE BOSONS | 5 particles and 7 distinct single-particle states |
| | 5 particles and 3 distinct single-particle states |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | 5 particles and 7 distinct single-particle states |
| | 5 particles and 3 distinct single-particle states |

In two to three sentences, summarize how to determine the number of distinct $N$-particle states for $N$ identical particles and $M$ distinct single-particle states. Be sure to describe the cases of indistinguishable fermions, indistinguishable bosons, and the hypothetical case of identical particles which can be treated as distinguishable.

Review your answers to the questions in the preceding table for the given system of identical particles for a fixed number of single-particle states (no constraints on the total energy of the many-particle system).

| Identical Particles | |
|---|---|
| INDISTINGUISHABLE FERMIONS | 5 particles and 7 distinct single-particle states<br><br>$\binom{7}{5} = 21$ |
| | 5 particles and 3 distinct single-particle states<br><br>None, there are more particles than available states. |
| INDISTINGUISHABLE BOSONS | 5 particles and 7 distinct single-particle states<br><br>$\binom{11}{5}=\binom{11}{6}=462$ |
| | 5 particles and 3 distinct single-particle states<br><br>$\binom{7}{5}=\binom{7}{2}=21$ |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | 5 particles and 7 distinct single-particle states<br><br>$7^5 = 16,807$ |
| | 5 particles and 3 distinct single-particle states<br><br>$3^5 = 243$ |

**Summary of CASE I: Determining the Number of Distinct Many-Particle States for a Fixed Number of Single-Particle States (no constraints on the total energy of the many-particle system)**

- Indistinguishable Fermions
  - The number of distinct $N$-particle states for a system of $N$ indistinguishable fermions with $M$ available single-particle states when $N \leq M$ is $\binom{M}{N}$.
  - The number of distinct $N$-particle states for a system of $N$ indistinguishable fermions with $M$ available single-particle states when $N > M$ is 0 (such a state is NOT possible).
- Indistinguishable Bosons
  - The number of distinct $N$-particle states for a system of $N$ indistinguishable bosons with $M$ available single-particle states is

$$\binom{N+M-1}{N} = \binom{N+M-1}{M-1} = \frac{(N+M-1)!}{N!(M-1)!}$$

- Identical Particles which are Distinguishable
  - The number of distinct $N$-particle states for a system of $N$ identical particles which can be treated as distinguishable with $M$ available single-particle states is $M^N$.

## CASE II: Determining the Number of Distinct Many-Particle States when the Total Energy of the Many-Particle System is Fixed (Ignore spin).

- Let's consider three non-interacting identical particles of mass $m$ in a one-dimensional infinite square well of width "$a$".
- Recall that the total energy of the many-particle system can be written in terms of the single-particle energy as

$$E = E_{n_1} + E_{n_2} + E_{n_3} = (n_1^2 + n_2^2 + n_3^2)\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = (n_1^2 + n_2^2 + n_3^2)E_1.$$

  Here $n_1, n_2, n_3$ are positive integers that label the single-particle states in which the three particles can be placed.
- Suppose the total energy is $E = 243\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 243E_1$
- Note: The only possible integers $n_1, n_2$, and $n_3$ whose squares sum to 243 are given below.

$$\begin{aligned} 243 &= 1^2 + 11^2 + 11^2 \\ 243 &= 3^2 + 3^2 + 15^2 \\ 243 &= 5^2 + 7^2 + 13^2 \\ 243 &= 9^2 + 9^2 + 9^2 \end{aligned}$$

48. List all of the combinations of three positive integers $(n_1, n_2, n_3)$ whose squares sum to 243. For example, two combinations would be $(1, 11, 11)$ and $(11, 1, 11)$.

### D.8.4 Determining the Number of Distinct Many-Particle States for Three INDISTINGUISHABLE FERMIONS in a One-Dimensional Infinite Square Well with a Fixed Total Energy for the Many-Particle System

49. Suppose you have three indistinguishable fermions and the total energy of the three-particle system is $E = 243\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 243E_1$. How many distinct three-particle states can you construct? [Hint: Consider the combinations in question 48 that are possible for indistinguishable fermions and the antisymmetric requirement for the wavefunction.]

50. Write all of the possible three-particle stationary state wavefunctions for the system of three indistinguishable fermions in the one-dimensional infinite square well with total energy $E = 243E_1$. (The Slater determinant may be helpful.)

Consider the following conversation regarding the number of distinct three-particle states you can construct for a system of three indistinguishable fermions with a total energy of $E = 243E_1$.

**Student 1:** For a system of three indistinguishable fermions with a total energy of $E = 243E_1$, there is only one three-particle state. There is one fermion in the single-particle state $\psi_5$, one fermion in the state $\psi_7$, and one fermion in the state $\psi_{13}$.

**Student 2:** I disagree with Student 1. There are four disinct three-particle states for the three fermions: $\psi_1(x_1)\psi_{11}(x_2)\psi_{11}(x_3)$, $\psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3)$, $\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3)$, and $\psi_9(x_1)\psi_9(x_2)\psi_9(x_3)$.

**Student 3:** I agree with Student 1. There cannot be more than one fermion in each single-particle state. The combination $(9, 9, 9)$ is a system with three fermions in the state $\psi_9$. The combinations $(3, 3, 15)$, $(3, 15, 3)$, and $(15, 3, 3)$ have two fermions in the state $\psi_3$ and the combinations $(1, 11, 11)$, $(11, 1, 11)$, and $(11, 11, 1)$ have two fermions in the state $\psi_{11}$. None of these are possible for fermions.

**Student 1:** I agree with Student 3. A system of indistinguishable fermions must satisfy the antisymmetrization requirement, so there is only one distinct three-particle state, corresponding to the combinations $(5, 7, 13), (5, 13, 7), (7, 5, 13), (7, 13, 5)$, $(13, 5, 7)$, and $(13, 7, 5)$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the number of three-particle states you can construct for a system of three indistinguishable fermions with total energy of $E = (5^2 + 7^2 + 13^2)\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 243E_1$.

**Student 1:** How can there only be one distinct three-particle state for a system of three indistinguishable fermions corresponding to the six combinations $(5, 7, 13)$, $(5, 13, 7), (7, 5, 13), (7, 13, 5), (13, 5, 7)$, and $(13, 7, 5)$?

**Student 2:** Since the fermions are indistinguishable, we cannot say which fermion is in which single-particle state. All we can say is that one fermion is in the single-particle state $\psi_5$, one fermion is in the single-particle state $\psi_7$, and one fermion is in the single-particle state $\psi_{13}$. The stationary state wavefuntion for the three indistinguishable fermions must be completely antisymmetric. The six combinations $(5, 7, 13), (5, 13, 7), (7, 5, 13), (7, 13, 5), (13, 5, 7)$, and $(13, 7, 5)$ correspond to the labels for the products of the single-particle states to be summed to obtain the three-particle stationary state wavefunction.

**Student 3:** I agree with Student 2. To find the three-particle stationary state wavefunction for a system of three indistinguishable fermions, we must ensure that the wavefunction is completely antisymmetric and normailized. The normalization factor is $\frac{1}{\sqrt{3!}}$. We can use the Slater determinant to ensure that we include all the terms with the correct sign and obtain

$$\frac{1}{\sqrt{6}}\begin{vmatrix} \psi_5(x_1) & \psi_7(x_1) & \psi_{13}(x_1) \\ \psi_5(x_2) & \psi_7(x_2) & \psi_{13}(x_2) \\ \psi_5(x_3) & \psi_7(x_3) & \psi_{13}(x_3) \end{vmatrix} = \begin{array}{l} \frac{1}{\sqrt{6}}[\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3) - \psi_5(x_1)\psi_{13}(x_2)\psi_7(x_3) \\ \quad -\psi_7(x_1)\psi_5(x_2)\psi_{13}(x_3) + \psi_7(x_1)\psi_{13}(x_2)\psi_5(x_3) \\ \quad +\psi_{13}(x_1)\psi_5(x_2)\psi_7(x_3) - \psi_{13}(x_1)\psi_7(x_2)\psi_5(x_3)]. \end{array}$$

Explain why you agree or disagree with Student 2 and Student 3.

****CHECKPOINT: Check your answers to questions 48-50. ****

48.

$$(9, 9, 9)$$

$$(3, 3, 15), (3, 15, 3), (15, 3, 3)$$

$$(1, 11, 11), (11, 1, 11), (11, 11, 1)$$

$$(5, 7, 13), (5, 13, 7), (7, 5, 13), (7, 13, 5), (13, 5, 7), (13, 7, 5)$$

49. 1. Two or more fermions in the same single-particle state are not possible. Identical fermions must satisfy the antisymmetrization requirement.

50.

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{6}}[\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3) - \psi_5(x_1)\psi_{13}(x_2)\psi_7(x_3) \\ &\quad -\psi_7(x_1)\psi_5(x_2)\psi_{13}(x_3) + \psi_7(x_1)\psi_{13}(x_2)\psi_5(x_3) \\ &\quad +\psi_{13}(x_1)\psi_5(x_2)\psi_7(x_3) - \psi_{13}(x_1)\psi_7(x_2)\psi_5(x_3)]\end{aligned}$$

If your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.

### D.8.5 Determining the Number of Distinct Many-Particle States for Three INDISTINGUISHABLE BOSONS in a One-Dimensional Infinite Square Well with a Fixed Total Energy for the Many-Particle System (Ignore Spin)

51. Suppose you have three indistinguishable bosons and the total energy of the three-particle system is $E = 243E_1$. How many distinct three-particle states can you construct? [Hint: Consider the combinations in question 48 that are possible for indistinguishable bosons.]

52. Write all of the possible three-particle stationary state wavefunctions for the system of three indistinguishable bosons in the one-dimensional infinite square well with total energy $E = 243E_1$.

Consider the following conversation regarding the number of three-particle states you can construct for a system of three indistinguishable bosons with total energy $E = 243E_1$.

**Student 1:** For a system of three indistinguishable bosons with a total energy of $E = 243E_1$, there is only one three-particle state. There is one boson in the state $\psi_5$, one boson in the state $\psi_7$, and one boson in the state $\psi_{13}$.

**Student 2:** I disagree with Student 1. It is possible for bosons to occupy the same single-particle state. Since the bosons are indistinguishable, there are four disinct three-particle states for the three bosons with the total energy $E$.

**Student 3:** I agree with Student 2. All three bosons could be in the state $\psi_9$. There could also be two bosons in state $\psi_3$ and one boson in state $\psi_{15}$, two bosons in state $\psi_{11}$ and one boson in state $\psi_1$, or one boson in each of the states $\psi_5$, $\psi_7$, and $\psi_{13}$.

Explain why you agree or disagree with each student.

****CHECKPOINT: Check your answers to questions 51-52. ****

51. 4.

52.

$$\Psi(x_1, x_2, x_3) = \psi_9(x_1)\psi_9(x_2)\psi_9(x_3)$$

$$\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3) + \psi_3(x_1)\psi_{15}(x_2)\psi_3(x_3) + \psi_{15}(x_1)\psi_3(x_2)\psi_3(x_3)]$$

$$\Psi(x_1, x_2, x_3) = \frac{1}{\sqrt{3}}[\psi_1(x_1)\psi_{11}(x_2)\psi_{11}(x_3) + \psi_{11}(x_1)\psi_1(x_2)\psi_{11}(x_3) + \psi_{11}(x_1)\psi_{11}(x_2)\psi_1(x_3)]$$

$$\begin{aligned}\Psi(x_1, x_2, x_3) &= \tfrac{1}{\sqrt{6}}[\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3) + \psi_5(x_1)\psi_{13}(x_2)\psi_7(x_3) \\ &+\psi_7(x_1)\psi_5(x_2)\psi_{13}(x_3) + \psi_7(x_1)\psi_{13}(x_2)\psi_5(x_3) \\ &+\psi_{13}(x_1)\psi_5(x_2)\psi_7(x_3) + \psi_{13}(x_1)\psi_7(x_2)\psi_5(x_3)]\end{aligned}$$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.[5]

[5]Note, the four states can be regarded as a basis for the three-particle system and any linear superposition of the four states listed in question 52 would also be a three-particle stationary state wavefunction for the system of three indistinguishable bosons due to the degeneracy in the energy spectrum. However, in this tutorial we will not focus on the linear superpostion of these states.

### D.8.6 Hypothetical Case: Determining the Number of Distinct Many-Particle States for Three IDENTICAL PARTICLES IF THEY COULD BE TREATED AS DISTINGUISHABLE in a One-Dimensional Infinite Square Well with a Fixed Total Energy for the Many-Particle System (Ignore spin)

53. Suppose you have three identical particles which can be treated as distinguishable and the total energy of the three-particle system $E = 243E_1$. How many distinct three-particle states can you construct if the total energy of the many-particle system is fixed? [Hint: Consider the combinations in question 48 that are possible for identical particles which can be treated as distinguishable.]

54. Write four possible three-particle stationary state wavefunctions for a system of three identical particles which can be treated as distinguishable in the one-dimensional infinite square well with total energy $E = 243E_1$.

Consider the following conversation regarding the number of three-particle states you can construct with a total energy $E = 243E_1$ for a system of three identical particles which can be treated as distinguishable.

**Student 1:** For a system of three identical particles which can be treated as distinguishable with a total energy $E = 243E_1$, there are four distinct three-particle states with wavefunctions: $\psi_1(x_1)\psi_{11}(x_2)\psi_{11}(x_3)$, $\psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3)$, $\psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3)$, and $\psi_9(x_1)\psi_9(x_2)\psi_9(x_3)$.

**Student 2:** I disagree with Student 1. Since the particles can be treated as distinguishable, we can tell which particle is in which single-particle state. For example, there are three distinct many-particle states corresponding to the particles in the single-particle states $\psi_3$, $\psi_3$, and $\psi_{15}$: $\psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3)$, $\psi_3(x_1)\psi_{15}(x_2)\psi_3(x_3)$, and $\psi_{15}(x_1)\psi_3(x_2)\psi_3(x_3)$. Similarly, there are three distinct states corresponding to the particles in the single-particle states $\psi_1$,$\psi_{11}$, and $\psi_{11}$.

**Student 3:** I agree with Student 2. There is one distinct many-particle state corresponding to all three particles in the single-particle state $\psi_9$ and six distinct many-particle states corresponding to the particles in the single-particle states $\psi_5$, $\psi_7$, and $\psi_{13}$ because the particles can be treated as distinguishable.

**Student 2:** I agree with Student 3. There are 13 distinct many-particle states for the system of three identical particles which can be treated as distinguishable with energy $E = 243E_1$.

Explain why you agree or disagree with each student.

****CHECKPOINT: Check your answers to questions 53-54. ****

53. 13. There are 13 combinations that are distinct for identical particles which can be treated as distinguishable.

54.

$$\Psi(x_1, x_2, x_3) = \psi_9(x_1)\psi_9(x_2)\psi_9(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_3(x_1)\psi_3(x_2)\psi_{15}(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_3(x_1)\psi_{15}(x_2)\psi_3(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_{15}(x_1)\psi_3(x_2)\psi_3(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_1(x_1)\psi_{11}(x_2)\psi_{11}(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_{11}(x_1)\psi_1(x_2)\psi_{11}(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_{11}(x_1)\psi_{11}(x_2)\psi_1(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_5(x_1)\psi_7(x_2)\psi_{13}(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_5(x_1)\psi_{13}(x_2)\psi_7(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_7(x_1)\psi_5(x_2)\psi_{13}(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_7(x_1)\psi_{13}(x_2)\psi_5(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_{13}(x_1)\psi_5(x_2)\psi_7(x_3)$$

$$\Psi(x_1, x_2, x_3) = \psi_{13}(x_1)\psi_7(x_2)\psi_5(x_3)$$

If your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answers.[6] In two or three sentences, compare the hypothetical case if particles could be treated as distinguishable to the case of indistin-

[6]Note, the thirteen states can be regarded as a basis for the three-particle system and any linear superposition of the thirteen states listed in question 54 is a three-particle stationary state wavefunction for the system of three distinguishable particles due to the degeneracy in the energy spectrum. However, in this tutorial we will not focus on linear superpostions of these states.

guishable fermions and bosons.

**Summary of CASE II: Determining the Number of Distinct Many-Particle States for a Many-Particle System with Fixed Energy (Ignore spin)**

To summarize what you have learned about determining the number of distinct many-particle states for a many-particle system with fixed energy, answer the following questions in the table below for a system of two particles in a one-dimensional infinite square well with fixed total energy $E = 200\left(\frac{\pi^2\hbar^2}{2ma^2}\right) = 200E_1$.

a. What are the possible combinations (i.e., what are the possible combinations of $(n_1, n_2)$ that yield a total energy of $200E_1$ for the two-particle system)?

b. How many disinct two-particle states can you construct?

Note: The only possible integers $n_1$ and $n_2$ whose squares sum to 200 are given below

$$\begin{aligned} 200 &= 10^2 + 10^2 \\ 200 &= 2^2 + 14^2 \end{aligned}$$

| Identical Particles | |
|---|---|
| INDISTINGUISHABLE FERMIONS | (a) Possible combinations $(n_1, n_2)$ |
| | (b) How many distinct two-particle states? |
| INDISTINGUISHABLE BOSONS | (a) Possible combinations $(n_1, n_2)$ |
| | (b) How many distinct two-particle states? |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | (a) Possible combinations $(n_1, n_2)$ |
| | (b) How many distinct two-particle states? |

**Summary of CASE II: Determining the Number of Distinct Many-Particle States for a Many-Particle System with Fixed Energy (Ignore Spin)**

Check your answers to the questions in the preceding table.

| Identical Particles | |
|---|---|
| INDISTINGUISHABLE FERMIONS | (a) Possible combinations $(n_1, n_2)$<br>$(2, 14), (14, 2)$ |
| | (b) How many distinct two-particle states?<br>1 |
| INDISTINGUISHABLE BOSONS | (a) Possible combinations $(n_1, n_2)$<br>$(2, 14), (14, 2), (10, 10)$ |
| | (b) How many distinct two-particle states?<br>2 |
| HYPOTHETICAL CASE: DISTINGUISHABLE PARTICLES | (a) Possible combinations $(n_1, n_2)$<br>$(2, 14), (14, 2), (10, 10)$ |
| | (b) How many distinct two-particle states?<br>3 |

55. Suppose that for a system of two non-interacting identical particles in a one-dimensional infinite square well, the total energy of the two-particle system is $E_{n_1,n_2} = (n_1^2 + n_2^2)E_1$, in which $E_1$ is the ground state energy for the single-particle system. The total energy of the two-particle system is $E = 50E_1$. Assume all of the possible combinations are equally probable.[7]

Note: The only possible integers $n_1$ and $n_2$ whose squares sum to 50 are given below.

$$\begin{aligned} 50 &= 1^2 + 7^2 \\ &= 5^2 + 5^2 \end{aligned}$$

a. If the particles are indistinguishable fermions and you randomly measure the energy of one particle, what single-particle energies might you obtain and with what probability? Explain.

b. If the particles are indistinguishable bosons and you randomly measure the energy of one particle, what single-particle energies might you obtain and with what probability? Explain.

c. Hypothetical case: If the particles could be treated as distinguishable and you randomly measure the energy of one particle, what single-particle energies might you obtain and with what probability? Explain.

Briefly describe how the probability of the possible values of energy differs in the case of indistinguishable fermions, indistinguishable bosons, and the hypothetical case in which particles can be treated as distinguishable.

[7] Due to the degeneracy of the two-particle system, any linear combination of degenerate two-particle stationary states is a two-particle stationary state with the same energy. However, in this tutorial we will not focus on linear superpostions of these states.

Consider the following conversation regarding the possible outcomes if you measure the energy of a single particle and the corresponding probability if the particles are indistinguishable fermions.

**Student 1:** For a system of two indistinguishable fermions in which the total energy of the two-particle system is $E = 50E_1$, there are two possible combinations: $(1, 7)$ and $(7, 1)$. The two combinations contribute to the completely antisymmetric wavefunction in which one fermion is in the state $\psi_1$ and one fermion is in the state $\psi_7$.

**Student 2:** I agree with Student 1. Additionally, the fermions could have the combination $(5, 5)$ in which both fermions are in the single-particle state $\psi_5$. Therefore, if you randomly measure the energy you could obtain the energies $E_1$, $49E_1$, or $25E_1$ with equal probability $1/3$.

**Student 1:** I disagree with Student 2. The fermions cannot be in the same single-particle state $\psi_5$. One fermion must be in the single-particle state $\psi_1$ and one fermion must be in the single-particle state $\psi_7$. If you randomly measure the energy, you could obtain the energy $E_1$ or $49E_1$ with equal probability of $1/2$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the possible outcomes if you measure the energy of a single particle and the corresponding probability if the particles are indistinguishable bosons.

**Student 1:** For a system of two indistinguishable bosons in which the total energy of the two-particle system is $E = 50E_1$, there are three possible combinations: $(1, 7)$, $(7, 1)$, and $(5, 5)$. The combinations $(1, 7)$ and $(7, 1)$ correspond to the completely symmetric state $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_7(x_2) + \psi_7(x_1)\psi_1(x_2)]$. The combination $(5, 5)$ corresponds to two bosons in the same state $\psi_5$.

**Student 2:** I agree with Student 1. It is equally probable that the bosons are in the same state $\psi_5$ or one boson is in the state $\psi_1$ and the other boson is in the state $\psi_7$. If you randomly measure the energy you could obtain the energies $E_1$, $49E_1$, or $25E_1$.

**Student 3:** I agree with Student 2. Since the three combinations are equally likely, the probability that the system has the combination $(1, 7)$, $(7, 1)$, or $(5, 5)$ is $1/3$. For the combination $(1, 7)$, the probability of obtaining $1^2E_1$ is $1/2$. Similarly, the probability of obtaining $E_1$ for the combination $(7, 1)$ is $1/2$. Therefore, the probability of obtaining $E_1$ is $(1/3) \times (1/2) + (1/3) \times (1/2) = 1/3$. By the same reasoning, the probability of obtaining $49E_1$ is $(2/3) \times (1/2) = 1/3$. The probability of the system with the combination $(5, 5)$ is $1/3$ and for bosons with the combination $(5, 5)$, the probability of being in state $\psi_5$ is 1. Thus, the probability of obtaining $25E_1$ is $(1/3) \times 1 = 1/3$.

**Student 1:** I agree with Student 2, but disagree with Student 3. The probability of the bosonic system having the combination $(5, 5)$ is $1/2$ and the probability of having the combinations $(1, 7)$ and $(7, 1)$, which correspond to one two-particle state $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_7(x_2) + \psi_7(x_1)\psi_1(x_2)]$ is $1/2$. The probability of obtaining $E_1$ is $(1/2) \times (1/2) = 1/4$, the probability of obtaining $49E_1$ is $(1/2) \times (1/2) = 1/4$, and the probability of obtaining $25E_1$ is $(1/2) \times 1 = 1/2$.

Explain why you agree or disagree with each student.

**Hypothetical Case: Treating the identical particles as distinguishable.**

Consider the following conversation regarding the possible outcomes if you measure the energy of a single particle and the corresponding probability if identical particles could be treated as distinguishable.

**Student 1:** For a system of two identical particles if they could be treated as distinguishable, there are three possible combinations $(1, 7)$, $(7, 1)$ and $(5, 5)$ if the total energy of the two-particle system is $E = 50E_1$. Each combination is equally probable with probability $1/3$.

**Student 2:** I agree with Student 1. If identical particles which can be treated as distinguishable are in the combination $(1, 7)$ and you measure the energy, you could obtain the energy $E_1$ with probability $(1/3) \times (1/2) = 1/6$ and the energy $49E_1$ with probability $(1/3) \times (1/2) = 1/6$.

**Student 3:** I agree with Student 1 and Student 2. If identical particles which can be treated as distinguishable are in the combination $(7, 1)$ and you measure the energy, you could obtain the energy $E_1$ with probability $(1/3) \times (1/2) = 1/6$ and the energy $49E_1$ with probability $(1/3) \times (1/2) = 1/6$.

**Student 1:** I agree with Student 2 and Student 3. If identical particles which can be treated as distinguishable are in the combination $(5, 5)$ and you measure the energy you would obtain the energy, $25E_1$ with probability $(1/3) \times 1 = 1/3$.

**Student 2:** To sum up, if you randomly measure the energy, you could obtain the energy $E_1$ with probability $(1/3) \times (1/2) + (1/3) \times (1/2) = 1/3$, the energy $49E_1$ with probability $(1/3) \times (1/2) + (1/3) \times (1/2) = 1/3$, and the energy $25E_1$ with probability $(1/3) \times 1 = 1/3$.

Explain why you agree or disagree with each student.

****CHECKPOINT: Check your answers to question 55. ****

a. $E_1$ with probability $\frac{1}{2}$ or $49E_1$ with probability $\frac{1}{2}$

b. $E_1$ with probability $\frac{1}{4}$, $49E_1$ with probability $\frac{1}{4}$ or $25E_1$ with probability $\frac{1}{2}$

c. $E_1$ with probability $\frac{1}{3}$, $49E_1$ with probability $\frac{1}{3}$ or $25E_1$ with probability $\frac{1}{3}$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

## D.9 DETERMINING THE NUMBER OF DISTINCT MANY-PARTICLE STATES WHEN THE TOTAL ENERGY OF THE MANY-PARTICLE SYSTEM IS FIXED AND THE SINGLE-PARTICLE STATES HAVE DEGENERACY

- Here, we will consider a system of identical particles in which there is degeneracy in the single-particle energy spectrum and there are constraints on the number of particles in different single-particle states with a certain energy. We will focus on the spatial part of the wavefunction and ignore the spin degrees of freedom.
- We will consider a group of degenerate states together and the arrangement $(N_1, N_2, N_3, \ldots, N_n, \ldots)$ is such that for all of the single-particle states with energy $E_i$, the total number of particles is $N_i$. We will use the notation $Q(N_1, N_2, N_3, \ldots, N_n, \ldots)$ to represent the number of distinct many-particle states for a given arrangement $(N_1, N_2, N_3, \ldots, N_n, \ldots)$.
- If there are no particles with energy greater than $E_m$, then for the arrangement $(N_1, N_2, N_3, \ldots, N_n, \ldots)$, we only list the number of particles $(N_m)$ up to and including the highest occupied energy level $E_m$.
  - For example, $(3, 4)$ denotes that there are three particles in the single-particle states with the lowest energy $E_1$, four particles in the single-particle states with the first-excited state energy $E_2$, and zero particles in the single-particle states with higher energy.
- We will use the symbol $d_i$ to represent the degeneracy corresponding to the energy $E_i$.
  - For example, if $d_i = 5$ then there are five degenerate single-particle states with energy $E_i$.
- We will ignore the spin degrees of freedom and only consider the spatial part of the wavefunction.

56. Suppose a system with ten single-particle states has 4 particles. The degeneracy of the lowest single-particle stationary states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$. If the energy of the system is such that 2 particles occupy the lowest single-particle stationary states and 2 particles occupy the first-excited single-particle states, what is the number of distinct four-particle states $Q(2, 2)$ corresponding to this particular arrangement $(2, 2)$:

a. if the particles are indistinguishable fermions? Ignore spin.

b. if the particles are indistinguishable bosons? Ignore spin.

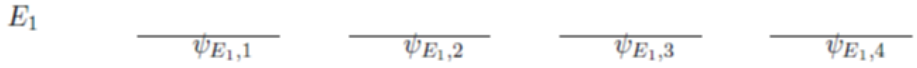
c. (Hypothetical case) if the identical particles can be treated as distinguishable? Ignore spin.

Consider the following conversation regarding the number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of identical particles in which the degeneracy of the lowest energy single-particle states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$.

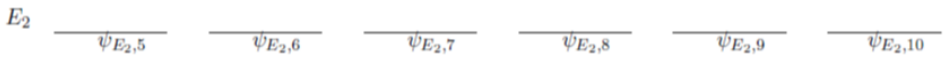
**Student 1:** In the given example, since the lowest energy single-particle states with energy $E_1$ have degeneracy $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$, there are a total of 10 available single-particle states. We must determine all the permutations of the four particles among the 10 single-particle states.

**Student 2:** I agree with Student 1 only in the case in which there is no constraint on the total energy of the system. However, in this example, the permutations of the four particles must be consistent with the fixed total energy of the system. Therefore, only two particles with energy $E_1$ and two particles with energy $E_2$ are permitted.

**Student 3:** I agree with Student 2. To determine the number of ways to arrange the two identical particles in the single-particle states with energy $E_1$, we find the number of ways to arrange the two identical particles when there are four single-particle state available. We can use the following diagram to arrange the two identical particles in the four single-particle states with energy $E_1$:



**Student 2:** I agree with Student 3. Similarly to determine the number of ways to arrange the two identical particles in the first-excited single-particle states with energy $E_2$, we find the number of ways to arrange the two identical particles when there are six single-particle states available. We can use the following diagram to arrange the two identical particles in the six single-particle states with energy $E_2$:



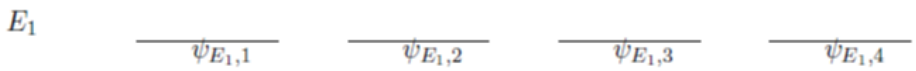

Then combine the number of ways to arrange the particles in the lowest energy single-particle states with the number of ways to arrange the particles in the first-excited single-particle states to find the total number of distinct four-particle states.

Explain why you agree or disagree with each student.

Consider the following three conversations regarding the number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of indistinguishable fermions in which the degeneracy of the lowest energy single-particle states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$. Two students consider the number of ways two indistinguishable fermions can be arranged in the lowest energy single-particle states.

Consider the following conversation in which three students consider the number of ways two indistinguishable fermions can be arranged in the lowest energy single-particle states.

**Student 1:** For the lowest energy single-particle states with energy $E_1$, which have degeneracy $d_1 = 4$, we must find the number of ways to arrange the two indistinguishable fermions among the four degenerate single-particle states with energy $E_1$.

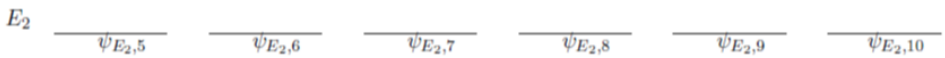



**Student 2:** I agree with Student 1. There are four states in which to arrange the two fermions. Since there can only be one or zero fermions in each degenerate state, there are $\binom{4}{2} = 6$ ways to arrange the two fermions among the lowest energy single-particle states with energy $E_1$.

Explain why you agree or disagree with each student.

Consider the following conversation in which two students consider the number of ways in which two indistinguishable fermions can be arranged in the first-excited single-particle states.

**Student 1:** For the first-excited single-particle states with energy $E_2$ which have degeneracy $d_2 = 6$, we must find the number of ways to arrange the two indistinguishable fermions among the six degenerate single-particle states with energy $E_2$.




**Student 2:** I agree with Student 1. There are six states in which to arrange the two fermions. Since there can only be one or zero fermions in each degenerate state, there are $\binom{6}{2} = 15$ ways to arrange the two fermions among the first-excited single-particle states with energy $E_2$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the total number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of indistinguishable fermions.

**Student 1:** Since there are 6 ways to arrange the two indistinguishable fermions among the four degenerate single-particle states with energy $E_1$ and 15 ways to arrange the two indistinguishable fermions among the six degenerate single-particle states with energy $E_2$, there are a total of $6 + 15 = 21$ distinct four-particle states corresponding to the arrangment of two fermions in the lowest energy states and two fermions in the first-excited states.

**Student 2:** I disagree with Student 1. The total number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement of two fermions in the lowest energy states and two fermions in the first-excited states is the product of the number of ways to arrange the indistinguishable fermions in the four degenerate states with energy $E_1$ and the six degenerate states with energy $E_2$, not the sum. The number of distinct four-particle states corresponding to the arrangement of two fermions in the lowest energy states and two fermions in the first-excited states of the system is $6 \times 15 = 90$.

Do you agree with Student 1 or Student 2? Explain your reasoning.

Consider the following conversation regarding the number of distinct $N$-particle states $Q(N_1, N_2, N_3, \ldots, N_n, \ldots)$ for a system of indistinguishable fermions in which $N_n$ particles are in the $n^{th}$ single-particle states with energy $E_n$, which have degeneracy $d_n$.

**Student 1:** For each set of degenerate single-particle states, we must find the number of ways to arrange the $N_n$ fermions among the $d_n$ degenerate states. Since each state can contain at most one fermion, the number of ways to choose the $N_n$ occupied states is $\binom{d_n}{N_n}$ in which $N_n \leq d_n$.

**Student 2:** I agree with Student 1. The total number of distinct $N$-particle states is the product of the number of ways to arrange the fermions into each single-particle state and is given by

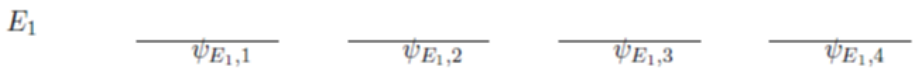
$$\prod_n \frac{d_n!}{N_n!(d_n - N_n)!} = \binom{d_1}{N_1}\binom{d_2}{N_2}\binom{d_3}{N_3}\cdots .$$

Explain why you agree or disagree with the students.

Consider the following two conversations regarding the number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of indistinguishable bosons in which the degeneracy of the lowest energy single-particle states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$. Three students consider the number of ways two indistinguishable bosons can be arranged in the lowest energy single-particle states.

Consider the following conversation in which three students consider the number of ways in which two indistinguishable bosons can be arranged among the lowest energy single-particle states.

**Student 1:** For the lowest energy single-particle states with energy $E_1$ which have degeneracy $d_1 = 4$, we must find the number of ways to arrange the two indistinguishable bosons among the four degenerate single-particle states with energy $E_1$.




**Student 2:** I agree with Student 1. Using the bin and divider method, there are two indistinguishable bosons and three indistinguishable dividers between the four degenerate states. There are five total objects that must be permuted.

**Student 3:** I agree with both Student 1 and Student 2. When we calculate the number of ways to permute the three indistinguishable dividers with the two bosons, we get $\binom{5}{3} = 10$. There are 10 ways to arrange the two indistinguishable bosons in the lowest energy single-particle states with energy $E_1$.

Explain why you agree or disagree with the students.

Consider the following conversation in which three students consider the number of ways two indistinguishable bosons can be arranged among the first-excited single-particle states and the total number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of indistinguishable bosons.

**Student 1:** For the first-excited single-particle states with energy $E_2$ which have degeneracy $d_2 = 6$, we must find the number of ways to arrange the two indistinguishable bosons among the six degenerate single-particle states with energy $E_2$.


**Student 2:** I agree with Student 1. Using the bin and divider method, there are two indistinguishable bosons and five indistinguishable dividers between the six degenerate states. There are seven total objects to be permuted, two indistinguishable bosons and five indistinguishable dividers. When we calculate the number of ways to permute the five indistinguishable dividers with the two bosons, we get $\binom{7}{2} = 21$.

**Student 3:** I agree with both Student 1 and Student 2. There are 10 ways to arrange the two indistinguishable bosons among the lowest stationary states with energy $E_1$ and 21 ways to arrange the two indistinguishable bosons among the first-excited single-particle states with energy $E_2$. The total number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ is $10 \cdot 21 = 210$.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the number of distinct $N$-particle states $Q(N_1, N_2, N_3, \ldots, N_n, \ldots)$ for a system of indistinguishable bosons in which $N_n$ particles are in the $n^{th}$ single-particle states with energy $E_n$, which has degeneracy $d_n$.

**Student 1:** For each set of degenerate single-particle states, we must find the number of ways to arrange the $N_n$ bosons among the $d_n$ degenerate states. Using the bin and divider method, there are $N_n$ indistinguishable bosons and $d_n - 1$ indistinguishable dividers between the $d_n$ degenerate states. There are $N_n + d_n - 1$ total objects that must be permuted. When we calculate the number of ways to permute the $d_n - 1$ indistinguishable dividers with the $N_n$ bosons, we get $\binom{N_n+d_n-1}{d_n-1} = \binom{N_n+d_n-1}{N_n}$.

**Student 2:** I agree with Student 1. The total number of distinct $N$-particle states is the product of the ways to arrange the bosons into each group of degenerate single-particle states and is given by

$$\prod_{n=1}^{\infty} \frac{(N_n + d_n - 1)!}{N_n!(d_n - 1)!} = \binom{N_1 + d_1 - 1}{d_1 - 1}\binom{N_2 + d_2 - 1}{d_2 - 1}\binom{N_3 + d_3 - 1}{d_3 - 1} \cdots .$$

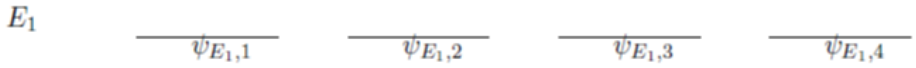
Explain why you agree or disagree with the students.

**Hypothetical Case: Treating the identical particles as distinguishable.**

Consider the following two conversations regarding the number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of identical particles which can be treated as distinguishable, in which the degeneracy of the lowest energy single-particle states with energy $E_1$ is $d_1 = 4$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 6$. Three students consider the number of ways two identical particles can be arranged in the lowest energy single-particle states if they can be treated as distinguishable.

In the following conversation three students consider the number of ways two distinguishable particles can be arranged among the lowest energy single-particle states.

**Student 1:** For the lowest energy single-particle states with energy $E_1$ which has degeneracy $d_1 = 4$, we must find the number of ways to arrange the two distinguishable particles among the four degenerate single-particle states with energy $E_1$.




**Student 2:** I agree with Student 1. Since the particles can be treated as distinguishable, we need to take into account which particles we are choosing, i.e., there are $\binom{4}{2} = 6$ different two particle combinations to arrange in the lowest energy single-particle states with energy $E_1$. Within the 4-fold degenerate lowest energy single-particle states, there are four degenerate single-particle states available to the first particle and four degenerate single-particle states for the second particle. There are $4^2$ ways to arrange the two particles.

**Student 3:** I agree with both Student 1 and Student 2. There is a total of $6 \cdot 16 = 96$ ways to arrange two of the four identical particles which can be treated as distinguishable in the lowest energy single-particle states.

Explain why you agree or disagree with the students.

Consider the following conversation in which three students consider the number of ways two distinguishable particles can be arranged among the first-excited single-particle states and the total number of distinct four-particle states $Q(2,2)$ corresponding to the arrangement $(2,2)$ for a system of distinguishable particles.

**Student 1:** For the set of degenerate first-excited single-particle states with energy $E_2$ which has degeneracy $d_2 = 6$, we must find the number of ways to arrange the two distinguishable particles among the six degenerate single-particle states with energy $E_2$.


**Student 2:** I agree with Student 1. If the **particles can be treated as distinguishable**, we need to take into account which particles we are choosing. Since we chose two particles for the lowest energy single-particle states, there are two identical particles remaining for the first-excited single-particle states. There is only $\binom{4-2}{2} = \binom{2}{2} = 1$ two particle combination to arrange among the first-excited single-particle states with energy $E_2$. Within the 6-fold degenerate first-excited single-particle states, there are six degenerate single-particle states available to the first particle and six degenerate single-particle states for the second particle. There are $6^2 = 36$ ways to arrange the two particles.

**Student 3:** I agree with both Student 1 and Student 2. There are 96 ways to arrange two particles among the lowest energy single particle stationary states first and 36 ways to arrange the remaining two particles among the first-excited single-particle states. The number of distinct four-particle states corresponding to the arrangement $(2,2)$ for a system of identical particles which can be treated as distinguishable is $96 \cdot 36 = 3456$.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the number of distinct $N$-particle states $Q(N_1, N_2, N_3, \ldots, N_n, \ldots)$ for a system of $N$ identical particles which can be treated as distinguishable in which $N_n$ particles are in the $d_n$-fold degenerate single-particle states with energy $E_n$.

**Student 1:** To determine the number of distinct $N$-particle states for a system of $N$ **identical particles which can be treated as distinguishable** in which $N_n$ particles are in the $d_n$-fold degenerate single-particle states with energy $E_n$, we can first choose which of the $N$ particles are in the set of degenerate states with energy $E_n$ and then multiply by the number of ways to arrange the particles among the single-particle states.

**Student 2:** I agree with Student 1. If there are $N_1$ particles in the $d_1$-fold degenerate lowest stationary state, then there are $\binom{N}{N_1}$ ways to choose the $N_1$ particles in the lowest stationary state and there are $d_1^{N_1}$ ways to arrange the $N_1$ particles among the $d_1$ degenerate lowest single-particle states.

**Student 3:** I agree with Student 2. If there are $N_2$ particles in the $d_2$-fold degenerate first-excited single-particle states, then there are $N - N_1$ particles from which to choose the $N_2$ particles in the first-excited single-particle states. Then, there are $d_2$ states available to the $N_2$ particles so there are $d_2^{N_2}$ ways to arrange the particles in the first-excited single-particle states.

**Student 1:** I agree with both Student 2 and Student 3. We can continue this way and the total number of distinct $N$-particle states for a system of $N$ identical particles which can be treated as distinguishable is

$$\left[\binom{N}{N_1} d_1^{N_1}\right] \cdot \left[\binom{N-N_1}{N_2} d_2^{N_2}\right] \cdot \left[\binom{N-N_1-N_2}{N_3} d_3^{N_3}\right] \cdots$$

$$= \left[\frac{N!}{N_1!(N-N_1)!} d_1^{N_1}\right] \cdot \left[\frac{(N-N_1)!}{N_2!(N-N_1-N_2)!} d_2^{N_2}\right] \cdot \left[\frac{(N-N_1-N_2)!}{N_3!(N-N_1-N_2-N_3)!} d_3^{N_3}\right] \cdots$$

$$= N! \frac{d_1^{N_1} d_2^{N_2} d_3^{N_3} \cdots}{N_1! N_2! N_3! \cdots}$$

$$= N! \prod_n \frac{d_n^{N_n}}{N_n!}$$

Explain why you agree or disagree with each student.

## Summary for Determining the Number of Distinct Many-Particle States when the Total Energy of the Many-Particle System is Fixed and the Single-Particle States have Degeneracy

To summarize what you have learned about determining the number of distinct many-particle states for a many-particle system with fixed energy and in which the single-particle states have degeneracy, answer the following question.

57. Suppose a system with six single-particle states has 6 particles. The degeneracy of the lowest single-particle states with energy $E_1$ is $d_1 = 3$ and the degeneracy of the first-excited single-particle states with energy $E_2$ is $d_2 = 3$. If the system has the arrangement $(2, 4)$ such that 2 particles are in the lowest single-particle states and 4 particles are in the first-excited single-particle states, what is the number of distinct six-particle states $Q(2, 4)$ corresponding to this particular arrangement $(2, 4)$:

    a. if the particles are indistinguishable fermions? Ignore spin.

    b. if the particles are indistinguishable bosons? Ignore spin.

    c. (Hypothetical case) if the identical particles can be treated as distinguishable? Ignore spin.

Compare the number of distinct four-particle states $Q(2, 4)$ for the cases in which the 6 particles are indistinguishable fermions, indistinguishable bosons, and the hypothetical case in which particles can be treated as distinguishable particles.

****CHECKPOINT: Check your answers to questions 56-57. ****

56a. $\binom{4}{2} \cdot \binom{6}{2} = 6 \times 15 = 90$

or equivalently $\prod_n \frac{d_n!}{N_n!(d_n - N_n)!} = \left(\frac{4!}{2!(4-2)!}\right)\left(\frac{6!}{2!(6-2)!}\right) = 90$

56b. $\binom{2+4-1}{2} \cdot \binom{2+6-1}{2} = \binom{5}{2} \cdot \binom{7}{2} = 10 \times 21 = 210$

or equivalently $\prod_n \frac{(N_n + d_n - 1)!}{N_n!(d_n - 1)!} = \left(\frac{(2+4-1)!}{2!(4-1)!}\right)\left(\frac{(2+6-1)!}{2!(6-1)!}\right) = 210$

56c. $\left[\binom{4}{2} \cdot 4^2\right]\left[\binom{4-2}{2} \cdot 6^2\right] = 96 \times 36 = 3456$

or equivalently $N! \prod_n \frac{{d_n}^{N_n}}{N_n!} = 4!\left(\frac{4^2}{2!}\right)\left(\frac{6^2}{2!}\right) = 3456$

57a. 0. There cannot be four fermions in the second single-particle state with energy $E_2$ since it has degeneracy $d_2 = 3$. There must at least as many available states as the number of fermions.

57b. $\binom{2+3-1}{2} \cdot \binom{4+3-1}{4} = \binom{4}{2} \cdot \binom{6}{4} = 6 \times 15 = 90$

or equivalently $\prod_n \frac{(N_n + d_n - 1)!}{N_n!(d_n - 1)!} = \left(\frac{(2+3-1)!}{2!(3-1)!}\right)\left(\frac{(4+3-1)!}{4!(3-1)!}\right) = 90$

57c. $\left[\binom{6}{2} \cdot 3^2\right]\left[\binom{6-2}{4} \cdot 3^4\right] = [15 \cdot 9][1 \cdot 81] = 10,935$

or equivalently $N! \prod_n \frac{{d_n}^{N_n}}{N_n!} = 6!\left(\frac{3^2}{2!}\right)\left(\frac{3^4}{4!}\right) = 10,935$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

## D.10 STATIONARY STATE WAVEFUNCTION FOR A SYSTEM OF $N$ NON-INTERACTING PARTICLES (INCLUDING SPIN)

- When considering the spin part of the wavefunction for a single-particle, we will use the notation $|s_i,\ m_{s_i}\rangle$ (in which $s_i$ and $m_{s_i}$ are the quantum numbers corresponding to the total spin and z-component of the spin for the $i^{th}$ particle, respectively).
  - The states $|s_1,\ m_{s_1}\rangle$ are eigenstates of $\hat{S}_1^2$ and $\hat{S}_{1z}$ and the states $|s_2,\ m_{s_2}\rangle$ are eigenstates of $\hat{S}_2^2$ and $\hat{S}_{2z}$.
- When considering the spin part of the wavefunction for the two particles in the **uncoupled representation** in the product space, we will use the notation $|s_1,\ m_{s_1}\rangle_1|s_2,\ m_{s_2}\rangle_2$ for the basis states.
- Unless otherwise specified, we will consider only systems of spin-1/2 particles confined in one spatial dimension.
- Even though the spatial and spin parts of the wavefunction can be entangled in many situations, we will only consider separable many-particle wavefunctions in one-dimension that can be written as the product of the spatial part of the wavefunction $\psi(x_1, x_2, x_3, \ldots)$ and the spin part of the wavefunction $\chi(m_{s_1}, m_{s_2}, m_{s_3}, \ldots)$

$$\Psi(x_1, x_2, x_3, \ldots, m_{s_1}, m_{s_2}, m_{s_3}, \ldots) \ = \ \psi(x_1, x_2, x_3, \ldots)\chi(m_{s_1}, m_{s_2}, m_{s_3}, \ldots)$$

**Recall:** The eigenstates of the $z$-component of spin for a spin-1/2 system $|s_i\ m_{s_i}\rangle_i$ can be $\left\{\left|\frac{1}{2},\ \frac{1}{2}\right\rangle_i, \left|\frac{1}{2},\ -\frac{1}{2}\right\rangle_i\right\}$ (since for $s_i = \frac{1}{2}$, $m_{s_i} = \frac{1}{2}$ or $-\frac{1}{2}$). For a system of two spin-1/2 particles, e.g. electrons, we will use the following notation for the spin state of each particle since it can have spin "up" or spin "down":

$$\text{Spin "Up"} \quad |\uparrow\rangle_i \ = \ \left|\frac{1}{2},\ \frac{1}{2}\right\rangle_i \quad \text{Spin "Down"} \quad |\downarrow\rangle_i \ = \ \left|\frac{1}{2},-\frac{1}{2}\right\rangle_i$$

- When considering the spin part of the wavefunction for the two spin-1/2 particles ($s_1 = 1/2 \otimes s_2 = 1/2$) in the **uncoupled representation** in the product space, we will use the notation $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, $|\downarrow\rangle_1|\uparrow\rangle_2$, and $|\downarrow\rangle_1|\downarrow\rangle_2$ for the basis states.

- We will also use the notation in the **coupled representation** $|s,\ m_s\rangle$ in which the quantum numbers $s$ and $m_s$ correspond to the total spin angular momentum and the $z$ component of the total spin angular momentum including both spins, respectively (we will use the notation that a state in the coupled representation will not have a subscript whereas states in the uncoupled representation will have a subscript indicating the particle associated with each spin state).
  - The states $|s,\ m_s\rangle$ in the coupled representation are eigenstates of $\hat{S}^2$ and $\hat{S}_z$ where $\vec{S} = \vec{S}_1 + \vec{S}_2$.
- For a system of two spin-1/2 particles ($s_1 = 1/2 \otimes s_2 = 1/2$), the total spin quantum number $s = s_1 + s_2 = 1/2 + 1/2 = 1$ or $s = |s_1 - s_2| = |1/2 - 1/2| = 0$.
  - If the total spin quantum number is $s = 1$ then the corresponding $m_s = -1, 0, 1$ and the states in the coupled representation are given by $|s, m_s\rangle = \{|1,\ 1\rangle, |1,\ 0\rangle, |1,\ -1\rangle\}$. If $s = 0$, then the corresponding $m_s = 0$ and the state in the coupled representation is given by $|s, m_s\rangle = |0,\ 0\rangle$.
- We will use the following abbreviated notation for a complete set of normalized states for a system of two spin-1/2 particles in the coupled representation $|s,\ m_s\rangle$ written in terms of the uncoupled representation.

$$\boxed{\begin{array}{lcccl} |1,\ 1\rangle & = & |\uparrow\uparrow\rangle & = & |\uparrow\rangle_1|\uparrow\rangle_2 \\ |1,\ -1\rangle & = & |\downarrow\downarrow\rangle & = & |\downarrow\rangle_1|\downarrow\rangle_2 \\ |1,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right) \\ |0,\ 0\rangle & = & \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) & = & \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right) \end{array}}$$

- If you are not familiar with the formalism of addition of angular momentum (including how to write a complete set of basis states in the coupled and uncoupled representations or how to write various operators in the coupled and uncoupled representations), please work through the pretest, warm-up, tutorial and posttest for the Addition of Angular Momentum Tutorial (since it would help you in writing the spin part of the many-particle state in a particular representation).

58. For the spin part of the wavefunction (spin state) of a two-particle system ($s_1 = 1/2 \otimes s_2 = 1/2$) given below in the uncoupled representation, identify whether the spin state is symmetric, antisymmetric, or neither symmetric nor antisymmetric with respect to exchange of the two particles. Labels 1 and 2 denote particles 1 and 2, respectively. Explain your reasoning.

a. $|\uparrow\rangle_1|\uparrow\rangle_2$

b. $|\downarrow\rangle_1|\downarrow\rangle_2$

c. $C_1|\uparrow\rangle_1|\uparrow\rangle_2 + C_2|\downarrow\rangle_1|\downarrow\rangle_2$ (with $C_1 \neq C_2$ and $|C_1|^2 + |C_2|^2 = 1$)

d. $|\uparrow\rangle_1|\uparrow\rangle_2 - |\downarrow\rangle_1|\downarrow\rangle_2$

e. $|\uparrow\rangle_1|\downarrow\rangle_2$

f. $|\downarrow\rangle_1|\uparrow\rangle_2$

g. $C_1|\uparrow\rangle_1|\downarrow\rangle_2 + C_2|\downarrow\rangle_1|\uparrow\rangle_2$ (with $C_1 \neq \pm C_2$ and $|C_1|^2 + |C_2|^2 = 1$)

h. $C_1|\uparrow\rangle_1|\uparrow\rangle_2 + C_2|\downarrow\rangle_1|\downarrow\rangle_2 + \frac{C_3}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2)$ (with $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$)

59. Based on your answer to 58, in the uncoupled representation ($s_1 = 1/2 \otimes s_2 = 1/2$), are the spin states $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\downarrow\rangle_1|\downarrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, $|\downarrow\rangle_1|\uparrow\rangle_2$, $|\uparrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2$ and $|\uparrow\rangle_1|\uparrow\rangle_2 - |\downarrow\rangle_1|\downarrow\rangle_2$ an appropriate spin part of the wavefunction for a system of two indistinguishable spin-1/2 particles for writing a completely symmetric/antisymmetric wavefunction? Explain your reasoning.

60. For the spin part of the wavefunction (spin state) for ($s_1 = 1/2 \otimes s_2 = 1/2$) of a two-particle system given below in the coupled representation and expressed in terms of the uncoupled representation, identify whether the spin state is symmetric, antisymmetric, or neither symmetric nor antisymmetric with respect to exchange of the two particles. Explain your reasoning.

    a. $|1,\ 1\rangle = |\uparrow\uparrow\rangle$

    b. $|1,\ -1\rangle = |\downarrow\downarrow\rangle$

    c. $|1,\ 0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

    d. $|0,\ 0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

    e. $C_1|1,\ 0\rangle + C_2|0,\ 0\rangle = \frac{C_1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) + \frac{C_2}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ (with $C_1 \neq 0$, $C_2 \neq 0$, and $|C_1|^2 + |C_2|^2 = 1$)

    f. $C_1|1,\ 1\rangle + C_2|1,\ -1\rangle + C_3|1,\ 0\rangle = C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + \frac{C_3}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$ (with $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$)

61. Based on your answer to question 60, in the coupled representation, are the spin states $|1,\ 1\rangle$, $|1,\ -1\rangle$, $|1,\ 0\rangle$, $|0,\ 0\rangle$, and $\frac{1}{\sqrt{3}}[|1,\ 1\rangle + |1,\ -1\rangle + |0,\ 0\rangle]$ an appropriate spin part of the wavefunction for a system of two indistinguishable spin-1/2 particles for writing a completely symmetric/antisymmetric wavefunction? Explain your reasoning.

Consider the following conversation regarding whether a spin state in the coupled representation is symmetric or antisymmetric for a system of two spin-1/2 particles ($s_1 = 1/2 \otimes s_2 = 1/2$).

**Student 1:** The spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2\rangle - |\downarrow\rangle_1|\uparrow\rangle_2)$ is symmetric since exchanging the particles results in the same spin state.

**Student 2:** I disagree with Student 1. The spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ $= \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2\rangle - |\downarrow\rangle_1|\uparrow\rangle_2)$ is antisymmetric. If we exchange the particles, we get $\frac{1}{\sqrt{2}}(|\uparrow\rangle_2|\downarrow\rangle_1\rangle - |\downarrow\rangle_2|\uparrow\rangle_1) = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle) = -\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

**Student 3:** I agree with Student 2. The antisymmetric spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is referred to as the "singlet" state since it corresponds to the total spin quantum number $s = 0$ for a system of two spin-1/2 particles for which the only possibility for $m_s$ is $m_s = 0$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding whether a spin state in the coupled representation for a system of two spin-1/2 particles ($s_1 = 1/2 \otimes s_2 = 1/2$) is symmetric or antisymmetric.

**Student 1:** The spin state $|\uparrow\uparrow\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$ is symmetric since exchanging the two particles results in the same spin state $|\uparrow\uparrow\rangle = |\uparrow\rangle_2 |\uparrow\rangle_1$. Similarly, the spin state $|\downarrow\downarrow\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2$ is symmetric.

**Student 2:** I agree with Student 1. The spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$
$= \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 |\downarrow\rangle_2\rangle + |\downarrow\rangle_1 |\uparrow\rangle_2)$ is also symmetric since exchanging the two particles results in the same spin state.

**Student 3:** The spin states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, and $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ are all symmetric and referred to as the "triplet" states since they correspond to the total spin quantum number $s = 1$ for a system of two spin-1/2 particles with $m_s = +1, -1, 0$, respectively.

Explain why you agree or disagree with the students.

Consider the following conversation regarding choosing states for a system of two spin-1/2 particles with regard to symmetrization requirements.

**Student 1:** In the uncoupled representation, the two-particle spin states $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\downarrow\rangle_1|\downarrow\rangle_2$, $|\uparrow\rangle_1|\downarrow\rangle_2$, and $|\downarrow\rangle_1|\uparrow\rangle_2$ are all appropriate choices for spin part of the wavefunction to satisfy the symmetrization requirement.

**Student 2:** I disagree with Student 1. In order to satisfy the symmetrization requirement of the wavefunction, we must choose spin states which are either symmetric or antisymmetric. In the uncoupled representation, the two-particle spin states $|\uparrow\rangle_1|\downarrow\rangle_2$ and $|\downarrow\rangle_1|\uparrow\rangle_2$ are neither symmetric nor antisymmetric. For example, exchanging particles 1 and 2 transforms the state $|\uparrow\rangle_1|\downarrow\rangle_2$ to $|\uparrow\rangle_2|\downarrow\rangle_1 = |\downarrow\rangle_1|\uparrow\rangle_2$ but $|\uparrow\rangle_1|\downarrow\rangle_2 \neq \pm|\downarrow\rangle_1|\uparrow\rangle_2$ so $|\uparrow\rangle_1|\downarrow\rangle_2$ is neither symmetric nor antisymmetric. The same is true for the spin state $|\downarrow\rangle_1\uparrow\rangle_2$.

**Student 3:** I agree with Student 2. The two-particle spin states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, and $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ in the coupled representation expressed in terms of states in the uncoupled representation, are symmetric. The two-particle spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is antisymmetric. Therefore, the two-particle spin states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$,
$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, and $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ are all appropriate choices for spin part of the two-particle wavefunction with suitable spatial wavefunction to satisfy the symmetrization requirement.

Explain why you agree or disagree with each student.

62. Write four possible two-particle wavefunctions including spin for a system of two non-interacting indistinguishable fermions in single-particle states labeled by $n_1$ and $n_2$.

Consider the following conversation regarding constructing a completely antisymmetric wavefunction for a system of indistinguishable non-interacting fermions.

**Student 1:** For a system of two fermions, the two-particle wavefunction, which is made up of the product of the spatial part and spin part of the wavefunction, must be antisymmetric.

**Student 2:** I disagree with Student 1. We must only ensure that the spatial part of the two-particle wavefunction is antisymmetric. The spatial part of the two-particle stationary state wavefunction must be $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$. The spin part of the two-particle wavefunction can be either the antisymmetric singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ or one of the three symmetric triplet states $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\}$.

**Student 3:** I agree with Student 2 in that the spatial part of the two-particle wavefunction must be antisymmetric. However, we must also choose the antisymmetric singlet state as the spin part of the two-particle wavefunction.

**Student 4:** I disagree with both Student 2 and Student 3. The overall two-particle wavefunction must be antisymmetric. If the spatial part of the two-particle wavefunction is symmetric $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$, the spin part of the two-particle wavefunction must be the antisymmetric singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

**Student 1:** I agree with Student 4. Additionally, the spatial part of the two-particle wavefunction could be antisymmetric $\frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$ which would imply that the spin part of the two-particle wavefunction can be one of the symmetric triplet states $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\}$. In either case, the product of one symmetric and one antisymmetric wavefunction produces an overall antisymmetric two-particle wavefunction.

**Student 4:** I agree with Student 1. However, remember that a linear combination of the triplet states such as $C_1|\uparrow\uparrow\rangle + C_2|\downarrow\downarrow\rangle + \frac{C_3}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ is a completely symmetric spin state. This state is normalized if we choose $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

Explain why you agree or disagree with each student.

63. Fill in all the possibilities in the table below based on what you learned about the symmetric/antisymmetric characteristic (with respect to exchange of two particles) of the many-particle wavefunction for a system of identical particles.

| Type of Particle | Spatial Part of the Many-Particle Wavefunction (Symmetric/Antisymmetric) | Spin part of the Many-Particle Wavefunction (Symmetric/Antisymmetric) | Complete Many-Particle Wavefunction (Symmetric/Antisymmetric) |
|---|---|---|---|
| Indistinguishable Fermions | | | |
| | | | |
| Indistinguishable Bosons | | | |
| | | | |

****CHECKPOINT: Check your answers to questions 58-63. ****

58a. Symmetric

58b. Symmetric

58c. Symmetric

58d. Symmetric

58e. Neither symmetric nor antisymmetric

58f. Neither symmetric nor antisymmetric

58g. Neither symmetric nor antisymmetric

58h. Symmetric

59. The spin states $|\uparrow\rangle_1|\downarrow\rangle_2$ and $|\downarrow\rangle_1|\uparrow\rangle_2$ are neither symmetric nor antisymmetric. It is not possible to combine either of these two spin states individually with the spatial part of the wavefunction to produce a wavefunction that is either completely symmetric or completely antisymmetric.

The spin states $|\uparrow\rangle_1|\uparrow\rangle_2$, $|\downarrow\rangle_1|\downarrow\rangle_2$, and $|\uparrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2$ are symmetric and the spin state $|\uparrow\rangle_1|\uparrow\rangle_2 - |\downarrow\rangle_1|\downarrow\rangle_2$ is antisymmetric and could be combined with the spatial part of the wavefunction to produce a wavefunction that is either completely symmetric or completely antisymmetric.

60a. Symmetric

60b. Symmetric

60c. Symmetric

60d. Antisymmetric

60e. Neither symmetric nor antisymmetric

60f. Symmetric

61. The spin states $C_1|1,\ 0\rangle + C_2|0,\ 0\rangle$ is neither symmetric nor antisymmetric. It is not possible to combine this spin states individually with the spatial part of the wavefunction to produce a wavefunction that is either completely symmetric or completely antisymmetric.

The spin states $|1,\ 1\rangle$, $|1,\ -1\rangle$, $|1,\ 0\rangle$, and $C_1|1,\ 1\rangle + C_2|1,\ -1\rangle + C_3|1,\ 0\rangle$ in the coupled representation are symmetric. The spin state $|0,\ 0\rangle$ is antisymmetric. Therefore it is possible to combine these spin states with the spatial part of the wavefunction to produce a wavefunction that is either completely symmetric or completely antisymmetric.

62. The following are examples of a two-particle wavefunction including spin for a system of two non-interacting indistinguishable fermions in single-particle states labeled by $n_1$ and $n_2$

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= [\tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}][|\uparrow\uparrow\rangle] \\
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= [\tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}][|\downarrow\downarrow\rangle] \\
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= [\tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\} \\
&\quad ][\tfrac{1}{\sqrt{2}}\{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\}] \\
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= [\tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}] \\
&\quad [\tfrac{1}{\sqrt{2}}\{|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\}]
\end{aligned}$$

$$\begin{aligned}
\Psi(x_1, x_2, m_{s_1}, m_{s_2}) &= [\tfrac{1}{\sqrt{2}}\{\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\}] \\
&\quad [\tfrac{1}{\sqrt{2}}\{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\}]
\end{aligned}$$

63.

| Type of Particle | Spatial Part of the Wavefunction (Symmetric/ Antisymmetric) | Spin part of the Wavefunction (Symmetric/ Antisymmetric) | Complete Wavefunction (Symmetric/ Antisymmetric) |
|---|---|---|---|
| Indistinguishable Fermions | Symmetric | Antisymmetric | Antisymmetric |
| | Antisymmetric | Symmetric | |
| Indistinguishable Bosons | Symmetric | Symmetric | Symmetric |
| | Antisymmetric | Antisymmetric | |

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

64. Consider a system with three identical non-interacting spin-1/2 particles. If two of the particles are in the spin up state and one of the particles is in the spin down state, construct a completely symmetric spin state for the three particle system. If no such spin state exists, state the reason why. (Hint: Start with the basis state $|\uparrow\rangle_1|\uparrow\rangle_2|\downarrow\rangle_3$.)

65. Consider a system with three identical non-interacting spin-1/2 particles. If two of the particles are in the spin up state and one of the particles is in the spin down state, construct a completely antisymmetric spin state for the three particle system. If no such spin state exists, state the reason why. (Hint: Start with the basis state $|\uparrow\rangle_1|\uparrow\rangle_2|\downarrow\rangle_3$.)

64. $\frac{1}{\sqrt{3}}[|\uparrow\rangle_1|\uparrow\rangle_2|\downarrow\rangle_3 + |\uparrow\rangle_1|\downarrow\rangle_2|\uparrow\rangle_3 + |\downarrow\rangle_1|\uparrow\rangle_2|\uparrow\rangle_3]$

65. It is not possible to construct a completely antisymmetric spin state for a system with two particles in the same spin state.

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

## D.11 EXAMPLES OF FINDING THE MANY-PARTICLE STATIONARY STATE WAVEFUNCTIONS AND ENERGIES (INCLUDING SPIN)

In this section and the next, we shall focus on determining the many-particle stationary state wavefunction for a system of non-interacting particles placed in a one-dimensional harmonic oscillator potential well. Previously, we considered the many-particle stationary state wavefunction for a system of non-interacting particles placed in an infinite square well potential. Take a moment to think about the form of the many-particle stationary state wavefunction for a system of identical fermions or bosons in these two systems and whether the different potential energy terms affect the form of the many-particle stationary state wavefunction.

### D.11.1 One-Dimensional Harmonic Oscillator - Two Spin-1/2 Fermions

Two identical non-interacting spin-1/2 fermions are placed in a one-dimensional harmonic oscillator potential energy well with Hamiltonian $\hat{H}_i = \frac{\hat{p}_i^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_i{}^2$. The single-particle energies are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \qquad n = 0, 1, 2, \ldots$$

For the following questions, you can denote the spatial state of the $i^{th}$ particle in the $n_i{}^{th}$ single-particle state of the oscillator by $\psi_{n_i}(x_i)$.

66. Find the two-particle ground state and first-excited state energies of the two-particle system if the particles are

    a. Indistinguishable fermions with spin-1/2 in a total spin $s = 0$ state.

    b. Indistinguishable fermions with spin-1/2 in a total spin $s = 1$ state.

67. Construct the spatial part of the two-particle ground state and first-excited state for two non-interacting particles in the one-dimensional harmonic oscillator potential energy well if the particles are

a. Indistinguishable fermions with spin-1/2 in a total spin $s = 0$ state.

b. Indistinguishable fermions with spin-1/2 in a total spin $s = 1$ state.

Consider the following conversation regarding the two-particle ground state and ground state energy for two indistinguishable fermions with spin-1/2 in a total spin $s = 0$ state placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** For the two-particle ground state for a system of two indistinguishable fermions with spin-1/2 in a total spin $S = 0$ state, both fermions are in the single-particle spatial state $\psi_0$, so $n_1 = n_2 = 0$. The many-particle ground state energy is $E_{00} = E_0 + E_0 = \hbar\omega$.

**Student 2:** I disagree with Student 1. The two fermions cannot both be in the same single-particle spatial state $\psi_0$. For the two-particle ground state, one fermion is in the lowest single-particle spatial state $\psi_0$ and the other fermion is in the first-excited single-particle spatial state $\psi_1$, so $n_1 = 0$ and $n_2 = 1$ or $n_1 = 1$ and $n_2 = 0$. The two-particle ground state energy is $E_{10} = E_1 + E_0 = 2\hbar\omega$.

**Student 3:** I agree with Student 1 and disagree with Student 2. For a system of indistinguishable fermions, the overall two-particle state must be antisymmetric. Since the fermions are in the total spin $s = 0$ antisymmetric singlet state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, the spatial part of the many-particle state must be symmetric. Two fermions in the same single-particle spatial state $\psi_0$ correspond to the symmetric spatial state $\psi_0(x_1)\psi_0(x_2)$

**Student 1:** I agree with Student 3. The overall two-particle ground state including both spatial and spin parts is $\Psi_{00} = [\psi_0(x_1)\psi_0(x_2)][\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)]$. In the total spin $s = 0$ state, the two fermions can be in the same single-particle spatial state $\psi_0$ since the fermions are in different spin states with the two-particle spin-state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ being antisymmetric.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the two-particle first-excited state and first-excited state energy for two indistinguishable fermions with spin-1/2 in a total spin $s = 0$ state placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** For a system of indistinguishable fermions, the overall two-particle state must be antisymmetric. Since the fermions are in the total spin $s = 0$ antisymmetric singlet state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, the spatial part of the two-particle state must be symmetric.

**Student 2:** In the two-particle first-excited spatial state for a system of two indistinguishable fermions with spin-1/2 in a total spin $s = 0$ state, one fermion is in the lowest single-particle spatial state $\psi_0$ and the other fermion is in the first-excited single-particle spatial state $\psi_1$, so $n_1 = 1$ and $n_2 = 0$ or $n_1 = 0$ and $n_2 = 1$. The two-particle first-excited state energy is $E_{10} = E_1 + E_0 = 2\hbar\omega$.

**Student 3:** I agree with Student 1 and Student 2. The spatial part of the two-particle first-excited state is symmetric and given by $\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2))$. The overall two-particle first-excited state including both spatial and spin parts is $\Psi_{01} = [\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2))][\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)]$.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the two-particle ground state and ground state energy for two indistinguishable fermions with spin-1/2 in a total spin $s = 1$ state placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** For the two-particle ground state for a system of two indistinguishable fermions with spin-1/2 in a total spin $S = 1$ state, both fermions are in the single-particle spatial state $\psi_0$, so $n_1 = n_2 = 0$. The two-particle ground state energy is $E_{00} = \hbar\omega$.

**Student 2:** I disagree. For a system of indistinguishable fermions, the overall two-particle state including both spatial and spin parts must be antisymmetric. Since the fermions are in a total spin $s = 1$ symmetric triplet state, the spatial part of the two-particle state must be antisymmetric. The two fermions cannot be in the same single-particle spatial state $\psi_0$ because that is a symmetric state.

**Student 3:** I agree with Student 2. The two-particle ground state must include the antisymmetric spatial state in which one fermion is in the single-particle state $\psi_0$ and the other fermion is in the single-particle spatial state $\psi_1$, so $n_1 = 1$ and $n_2 = 0$ or $n_1 = 0$ and $n_2 = 1$.

**Student 2:** Right! The antisymmetric spatial part of the two-particle ground state is $\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2))$. One possible two-particle ground state including both spatial and spin parts is $\Psi_{00} = [\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2))][|\uparrow\uparrow\rangle]$. The two-particle ground state energy is $E_{10} = 2\hbar\omega$.

**Student 3:** I agree with Student 2. Additionally, if the spatial part of two-particle ground state is $\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2))$, then the spin part of the wavefunction could be $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, or $C_1|\uparrow\rangle + C_2|\downarrow\rangle + \frac{C_3}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ in which $|C_1|^2 + |C_2|^2 + |C_3|^2 = 1$.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the two-particle first-excited state and first-excited state energy for two indistinguishable fermions with spin-1/2 in a total spin $s = 1$ state placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** The two-particle first-excited state energy for two spin-1/2 fermions in a total spin $s = 1$ state is $E_{11} = 3\hbar\omega$, in which both fermions are in the same single-particle spatial state $\psi_1$.

**Student 2:** I disagree. In the total spin $s = 1$ state, both fermions are in the same spin state and therefore cannot be in the same single-particle spatial state $\psi_1$.

**Student 3:** I disagree with Student 1's reasoning. Since the fermions are in a total spin $s = 1$ symmetric triplet state, the spatial part of the two-particle state must be antisymmetric so that the overall two-particle state is antisymmetric. The two fermions cannot be in the same spatial state $\psi_1$ because this would mean that both the spatial part and spin part of the wavefunction are symmetric, which is not allowed. I disagree with Student 2's reasoning, as it does not hold for the triplet state $|\chi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 + |\uparrow\rangle_2|\downarrow\rangle_1)$.

**Student 4:** In the two-particle first-excited state for a system of two indistinguishable fermions with spin-1/2 in a total spin $s = 1$ state, one fermion is in the single-particle spatial state $\psi_0$ and the other fermion is in the single-particle spatial state $\psi_2$, so $n_1 = 2$ and $n_2 = 0$ or $n_1 = 0$ and $n_2 = 2$. The spatial part of the two-particle first-excited state is antisymmetric and given by $\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_0(x_2))$. Neglecting various superpositions, one of the three possible two-particle first-excited state including both spatial and spin parts is $\Psi_{01} = [\frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_0(x_2))][\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)]$. The two-particle first-excited state energy is $E_{20} = 3\hbar\omega$.

Explain why you agree or disagree with each student.

****CHECKPOINT: Check your answers to questions 66-67. ****

66a. Ground state: $E_{00} = \hbar\omega$

First-excited state: $E_{01} = 2\hbar\omega$

66b. Ground state: $E_{01} = 2\hbar\omega$

First-excited state: $E_{02} = 3\hbar\omega$

67a. Ground state: $\Psi_{00} = \psi_0(x_1)\psi_0(x_2)$

First-excited state: $\Psi_{01} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2))$

67b. Ground state: $\Psi_{01} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2))$

First-excited state: $\Psi_{02} = \frac{1}{\sqrt{2}}(\psi_0(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_0(x_2))$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

### D.11.2 One-Dimensional Harmonic Oscillator - Two Spin-1 Bosons

Two identical non-interacting spin-1 bosons ($s_1 = 1 \otimes s_2 = 1$) are placed in a one-dimensional harmonic oscillator potential energy well with Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$. The single-particle energies are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \qquad n = 0, 1, 2, \ldots$$

- For a spin-1 boson, $|s_i, m_{s_i}\rangle = \{|1,\ -1\rangle, |1,\ 0\rangle, |1,\ 1\rangle\}$ for each particle.
- When considering the spin part of the wavefunction for the two spin-1 particles ($s_1 = 1 \otimes s_2 = 1$) in the uncoupled representation in the product space, we will use the notation $|1,1\rangle_1|1,\ 1\rangle_2$, $|1,1\rangle_1|1,\ 0\rangle_2$, $|1,1\rangle_1|1,\ -1\rangle_2$, $|1,0\rangle_1|1,\ 1\rangle_2$, $|1,0\rangle_1|1,\ 0\rangle_2$, $|1,0\rangle_1|1,\ -1\rangle_2$, $|1,-1\rangle_1|1,\ 1\rangle_2$, $|1,-1\rangle_1|1,\ 0\rangle_2$, and $|1,-1\rangle_1|1,\ -1\rangle_2$ for the basis states.
- In the following table, for two identical non-interacting spin-1 bosons ($s_1 = 1 \otimes s_2 = 1$), the product states for spin degrees of freedom in the coupled representation $|s,\ m_s\rangle$ (left) are given in terms of a linear combination of product states in the uncoupled representation $|s_1,\ m_{s_1}\rangle_1|s_2,\ m_{s_2}\rangle_2$ (right) using the Clebsch-Gordon table.

| Product states in Coupled Representation<br><br>$\|s,\ m_s\rangle$ | Written in terms of product states in Uncoupled Representation<br><br>$\sum_{m_{s_1}+m_{s_2}=m_s} C^{s_1,s_2,s}_{m_{s_1},m_{s_2},m_s}\|s_1,\ m_{s_1}\rangle_1\|s_2,\ m_{s_2}\rangle_2$ |
|---|---|
| $\|2,\ 2\rangle$ | $\|1,\ 1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 + \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|1,\ 1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ 0\rangle_2 - \|1,\ 0\rangle_1\|1,\ 1\rangle_2)$ |
| $\|2,\ 0\rangle$ | $\frac{1}{\sqrt{6}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 + \sqrt{\frac{2}{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{6}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|1,\ 0\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 1\rangle_2)$ |
| $\|0,\ 0\rangle$ | $\frac{1}{\sqrt{3}}\|1,\ 1\rangle_1\|1,\ -1\rangle_2 - \frac{1}{\sqrt{3}}\|1,\ 0\rangle_1\|1,\ 0\rangle_2 + \frac{1}{\sqrt{3}}\|1,\ -1\rangle_1\|1,\ 1\rangle_2$ |
| $\|2,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 + \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|1,\ -1\rangle$ | $\frac{1}{\sqrt{2}}(\|1,\ 0\rangle_1\|1,\ -1\rangle_2 - \|1,\ -1\rangle_1\|1,\ 0\rangle_2)$ |
| $\|2,\ -2\rangle$ | $\|1,\ -1\rangle_1\|1,\ -1\rangle_2$ |

68. Find the two-particle ground state and first-excited state energies of the two-particle system if the particles are indistinguishable bosons with spin 1.

69. Construct at least two possible overall two-particle ground state wavefunctions (including both spatial and spin parts) for two non-interacting particles in the one-dimensional harmonic oscillator potential energy well if the particles are indistinguishable bosons with spin 1.

70. Construct at least two possible overall two-particle first-excited state wavefunctions (including both spatial and spin parts) for two non-interacting particles in the one-dimensional harmonic oscillator potential energy well if the particles are indistinguishable bosons with spin 1.

Consider the following conversation regarding the two-particle ground state and ground state energy for two non-interacting indistinguishable bosons with spin 1 ($s_1 = 1 \otimes s_2 = 1$) placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** The two-particle ground state for a system of two indistinguishable bosons with spin 1 ($s_1 = 1 \otimes s_2 = 1$) must be symmetric. There are two possibilities for the two-particle ground state: both the spatial part and the spin part are symmetric or both the spatial part and spin part are antisymmetric.

**Student 2:** While that is generally the case, the two-particle ground state must be a state with the lowest energy. The lowest energy occurs when both bosons are in the same single-particle spatial state $\psi_0$. Therefore, the spatial part of the two-particle ground state is the symmetric state $\psi_0(x_1)\psi_0(x_2)$. The two-particle ground state energy is $E_{00} = \hbar\omega$.

**Student 3:** I agree with Student 2. Since the spatial part of the two-particle ground state is symmetric, the spin part of the two-particle ground state must also be symmetric. Six possible symmetric combinations for the spin part of the many-particle state for two indistinguishable spin-1 bosons ($s_1 = 1, s_2 = 1$) in coupled representation are $|2,\ 2\rangle$, $|2,\ 1\rangle$, $|2,\ 0\rangle$, $|0,\ 0\rangle$, $|2,\ -1\rangle$, and $|2,\ -2\rangle$ in the preceding table. One possible overall two-particle ground state including both spatial and spin parts is $\Psi_{00} = [\psi_0(x_1)\psi_0(x_2)][|2,\ 2\rangle]$.

**Student 2:** I agree with Student 3. We can also construct a completely symmetric spin state by taking a linear combination of these symmetric states. $C_1|2,\ 2\rangle + C_2|2,\ 1\rangle + C_3|2,\ 0\rangle + C_4|0,\ 0\rangle + C_5|2,\ -1\rangle + C_6|2,\ -2\rangle$ where $|C_1|^2 + |C_2|^2 + |C_3|^2 + |C_4|^2 + |C_5|^2 + |C_6|^2 = 1$ will yeild a normalized state.

Explain why you agree or disagree with each student.

Consider the following conversation regarding the two-particle first-excited state and first-excited state energy for two non-interacting indistinguishable spin-1 bosons ($s_1 = 1 \otimes s_2 = 1$) placed in a one-dimensional harmonic oscillator potential energy well.

**Student 1:** If the two-particle first-excited state energy is $E_{01} = 2\hbar\omega$, one boson is in the single-particle spatial state $\psi_0$ and the other boson is in the single-particle spatial state $\psi_1$. The spatial part of the two-particle first-excited state MUST be $\frac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2) + \psi_1(x_1)\psi_0(x_2)]$ since the overall wavefunction should be symmetric. Therefore, the spin part of the two-particle first-excited state must be a symmetric spin state.

**Student 2:** The spatial part of the two-particle first-excited state can also be $\frac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2)]$ in which case the spin part of the two-particle first-excited state must be an antisymmetric spin state.

Explain why you agree or disagree with each student.

In the preceding conversation, Student 1 is correct that both the spatial and spin part of the two-particle stationary state wavefunction can be symmetric to produce an overall symmetric first-excited state wavefunction for the two bosons. However, it is also possible that both the spatial and spin parts of the two-particle stationary state wavefunction can be antisymmetric resulting in an overall symmetric first-excited state wavefunction for the two bosons as stated by Student 2.

****CHECKPOINT: Check your answers to questions 68-69. ****

68. Ground state: $E_{00} = \hbar\omega$

First-excited state: $E_{01} = 2\hbar\omega$

69. We will use the following notation, $|s,_i \ m_{s_i}\rangle_i$ represents the spin state of particle $i$.

Ground State:

$$\begin{aligned}
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][|1,\ 1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2 + |1,\ 0\rangle_1|1,\ 1\rangle_2)] \\
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{6}}|1,\ 1\rangle_1|1,\ -1\rangle_2 + \sqrt{\tfrac{2}{3}}|1,\ 0\rangle_1|1,\ 0\rangle_2 \\
&\quad + \tfrac{1}{\sqrt{6}}|1,\ -1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{3}}|1,\ 1\rangle_1|1,\ -1\rangle_2 - \tfrac{1}{\sqrt{3}}|1,\ 0\rangle_1|1,\ 0\rangle_2 \\
&\quad + \tfrac{1}{\sqrt{3}}|1,\ -1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 0\rangle_1|1,\ -1\rangle_2 + |1,\ -1\rangle_1|1,\ 0\rangle_2)] \\
\Psi_{00} &= \psi_0(x_1)\psi_0(x_2)][|1,\ -1\rangle_1|1,\ -1\rangle_2]
\end{aligned}$$

70. We will use the following notation, $|s,\ m_s\rangle_i$ represents the spin state of particle $i$.

First-excited state:

$$
\begin{aligned}
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][|1,\ 1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2+|1,\ 0\rangle_1|1,\ 1\rangle_2)] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{6}}|1,\ 1\rangle_1|1,\ -1\rangle_2 \\
&\quad +\sqrt{\tfrac{2}{3}}|1,\ 0\rangle_1|1,\ 0\rangle_2+\tfrac{1}{\sqrt{6}}|1,\ -1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{3}}|1,\ 1\rangle_1|1,\ -1\rangle_2 \\
&\quad -\tfrac{1}{\sqrt{3}}|1,\ 0\rangle_1|1,\ 0\rangle_2+\tfrac{1}{\sqrt{3}}|1,\ -1\rangle_1|1,\ 1\rangle_2] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 0\rangle_1|1,\ -1\rangle_2+ \\
&\quad |1,\ -1\rangle_1|1,\ 0\rangle_2)] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)+\psi_1(x_1)\psi_0(x_2)][|1,\ -1\rangle_1|1,\ -1\rangle_2] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)-\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ 0\rangle_2 \\
&\quad -|1,\ 0\rangle_1|1,\ 1\rangle_2)] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)-\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 1\rangle_1|1,\ -1\rangle_2 \\
&\quad -|1,\ -1\rangle_1|1,\ 1\rangle_2)] \\
\Psi_{01} &= \tfrac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2)-\psi_1(x_1)\psi_0(x_2)][\tfrac{1}{\sqrt{2}}(|1,\ 0\rangle_1|1,\ -1\rangle_2 \\
&\quad -|1,\ -1\rangle_1|1,\ 0\rangle_2)]
\end{aligned}
$$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

71. Consider a system with three identical non-interacting spin-1 particles. If the three particles are in different spin states, construct a completely symmetric spin state for the three particles starting with the basis state $|1,\ 1\rangle_1|1,\ 0\rangle_2|1,\ -1\rangle_3$. If no such spin state exists, state the reason why.

72. Consider a system with three identical non-interacting spin-1 particles. If the three particles are in different spin states, construct a completely antisymmetric spin state for the three particles starting with the basis state $|1,\ 1\rangle_1|1,\ 0\rangle_2|1,\ -1\rangle_3$. If no such spin state exists, state the reason why.

****CHECKPOINT: Check your answers to questions 71-72. ****

71. $\frac{1}{\sqrt{6}}[|1,\ 1\rangle_1|1,\ 0\rangle_2|1,\ -1\rangle_3 + |1,\ 1\rangle_1|1,\ 0\rangle_3|1,\ -1\rangle_2 + |1,\ 1\rangle_2|1,\ 0\rangle_3|1,\ -1\rangle_1 + |1,\ 1\rangle_2|1,\ 0\rangle_1|1,\ -1\rangle_3 + |1,\ 1\rangle_3|1,\ 0\rangle_1|1,\ -1\rangle_2 + |1,\ 1\rangle_3|1,\ 0\rangle_2|1,\ -1\rangle_1]$

72. $\frac{1}{\sqrt{6}}[|1,\ 1\rangle_1|1,\ 0\rangle_2|1,\ -1\rangle_3 - |1,\ 1\rangle_1|1,\ 0\rangle_3|1,\ -1\rangle_2 + |1,\ 1\rangle_2|1,\ 0\rangle_3|1,\ -1\rangle_1 - |1,\ 1\rangle_2|1,\ 0\rangle_1|1,\ -1\rangle_3 + |1,\ 1\rangle_3|1,\ 0\rangle_1|1,\ -1\rangle_2 - |1,\ 1\rangle_3|1,\ 0\rangle_2|1,\ -1\rangle_1]$

If any of your answers do not match the checkpoint, go back and reconcile any differences you may have with the checkpoint answer.

**OPTIONAL: This final optional section of this tutorial deals with examples of limiting cases when identical paticles can be treated as distinguishable.**

## D.12 LIMITING CASE: WHEN IDENTICAL PARTICLES CAN BE TREATED AS DISTINGUISHABLE

- So far we considered the distinguishable particle case as a hypothetical case for contrast with the cases of identical fermions and identical bosons. Now we will learn about some limiting cases in which identical microscopic particles can be treated as distinguishable.
- In limiting situations in which identical particles (particles of one type with the same properties) can be treated as distinguishable, you can distinguish which particle is in which single-particle stationary state. Exchanging distinguishable particles in different single-particle states with each other produces a distinctly different many-particle state.

Consider the following conversation regarding identical particles which can be treated as distinguishable versus indistinguishable.

**Student 1:** In general, in quantum mechanics, if two particles in a system are identical, we couldn't paint one red and the other green. Quantum particles are truly indistinguishable. There is no measurement we can perform that could distinguish one identical particle from the other. For example, there is no measurement that can distinguish which fermion was in which single-particle state and had which coordinate.

**Student 2:** I agree with Student 1. Identical particles are indistinguishable. However, under certain circumstances, for example, when the overlap of the single-particle wavefunctions is negligible, we can treat the particles as distinguishable.

Explain why you agree or disagree with the students.

Consider the following conversation regarding when identical particles (particles of the same type with the same properties) can be treated as distinguishable.

**Student 1:** In nature, aren't all identical microscopic particles with the same properties, e.g., electrons, indistinguishable? How can we consider the identical particles as distinguishable?

**Student 2:** That is a good question! In certain limits, microscopic identical particles can be treated as distinguishable. For example, when the overlap of the single-particle wavefunctions of the identical fermions or identical bosons is negligible, we can treat them as distinguishable particles. As an example, if we are considering electrons in two metal blocks with a macroscopic separation between them, then there is negligible overlap in their single-particle wavefunctions and the electrons in the two metal blocks can be treated as distinguishable from those in the other block.

**Student 3:** I agree with Student 2. Also, in the classical limit, for a system of electrons at "high" temperature, the de Broglie wavelength of the electron in a material becomes small compared to the average separation between the particles. The overlap of the single-particle wavefunctions for the electrons becomes negligible and the electrons can be treated as distinguishable.

Explain why you agree or disagree with Student 2 and Student 3.

73. Consider a system of two non-interacting, identical particles in the limiting case in which they can be treated as distinguishable. $\psi_{n_1}(x)$ and $\psi_{n_2}(x)$ are the single-particle wavefunctions for the system ($n_1 \neq n_2$). Choose all of the following wavefunctions that are appropriate two-particle stationary state wavefunctions for a system of two non-interacting, identical particles if they can be treated as distinguishable.

a. $\psi_{n_1}(x_1)\psi_{n_2}(x_1)$ (same label $x_1$)

b. $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$

c. $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$ (same label $n_1$)

d. $\psi_{n_1}(x)\psi_{n_1}(x)$

Consider the following conversation regarding appropriate wavefunctions for a system of two non-interacting identical particles in the limiting case in which they can be treated as distinguishable.

**Student 1:** For a system of two non-interacting identical particles which can be treated as distinguishable, the wavefunction describing the system can be $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$. Here $\psi_{n_1}(x_1)$ means that particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$. Similarly, $\psi_{n_2}(x_2)$ means that particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_2$.

**Student 2:** I agree with Student 1. In this limiting case, we can treat the identical particles independently and we can just multiply their single-particle wavefunctions. There is no need to symmetrize or antisymmetrize the many-particle stationary state wavefunction.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the appropriate wavefunction for a system of two non-interacting identical fermions which can be treated as distinguishable.

**Student 1:** For a system of two non-interacting identical fermions which can be treated as distinguishable, it is possible for the wavefunction describing the system to be $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$. Here $\psi_{n_1}(x_1)$ means that particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$. Similarly, $\psi_{n_1}(x_2)$ means that particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_1$.

**Student 2:** I disagree with Student 1. Two fermions can never be in the same single-particle state even in limiting cases for which fermions can be treated as distinguishable.

**Student 3:** I agree with Student 2. In limiting cases where fermions can be treated as distinguishable, the average occupancy of each single-particle state is less than 1. In this case, we can treat the fermions independently and we can just multiply their single-particle wavefunctions in which all the single-particle states have different indices. There is no need to antisymmetrize the many-particle stationary state wavefunction.

Explain why you agree or disagree with the students.

Consider the following conversation regarding the appropriate wavefunction for a system of two non-interacting identical bosons which can be treated as distinguishable.

**Student 1:** For a system of two non-interacting identical bosons which can be treated as distinguishable, the wavefunction describing the system can be $\psi_{n_1}(x_1)\psi_{n_1}(x_2)$. $\psi_{n_1}(x_1)$ means that particle 1 with coordinate $x_1$ is in a single-particle state denoted by $n_1$. Similarly, $\psi_{n_1}(x_2)$ means that particle 2 with coordinate $x_2$ is in a single-particle state denoted by $n_1$.

**Student 2:** I agree with Student 1. There is nothing that prohibits two bosons from occupying the same single-particle state. In the limiting case in which identical bosons can be treated as distinguishable, the stationary state wavefunction is the product of the single-particle stationary state wavefunctions.

**Student 3:** While I agree with Student 2 that nothing forbids two identical bosons from occupying the same single-particle state, in the limit in which identical bosons can be treated as distinguishable, the average number of bosons in any given single-particle state is less than 1.

**Student 4:** I agree with Student 3. In this limiting case, we can just multiply their single-particle wavefunctions in which all the single-particle states have different indices. There is no need to symmetrize the many-particle stationary state wavefunction.

Explain why you agree or disagree with each students.

Consider the following conversation regarding a physical system in which two non-interacting identical bosons can be treated as distinguishable.

**Student 1:** If we consider two He-4 atoms separated by a distance greater than the de Broglie wavelength such that there is negligible overlap in their single-particle wavefunctions, we can treat the He-4 atoms as distinguishable and treat each atom independently.

**Student 2:** I agree. For example, if we treat each He-4 atom as a separate system and each is in its OWN ground state, the two-particle stationary state wavefunction would be the product of the single-particle ground state wavefunctions for each He-4 atom.

**Student 3:** I disagree with Student 2. If both He-4 atoms are in their ground states, then the He-4 atoms are in the same single-particle state $\psi_1$. The two-particle stationary state wavefunction would be $\Psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$.

**Student 2:** I disagree with Student 3. Even though the He-4 atoms are both in their respective ground states, the He-4 atoms are not in the SAME single-particle state because they are separated spatially by a macroscopic distance. They are essentially two different systems. There is no overlap in these ground state wavefunctions for the two He-4 atoms.

**Student 1:** I agree with Student 2. Perhaps using identifiers for the two ground states would help. For example, the two-particle stationary state wavefunction would be $\Psi(x_1, x_2) = \psi_1(x_1)\psi_1'(x_2)$ in which $\psi_1(x_1)$ is the ground state of the first He-4 atom and $\psi_1'(x_2)$ is the ground sate of the second He-4 atom.

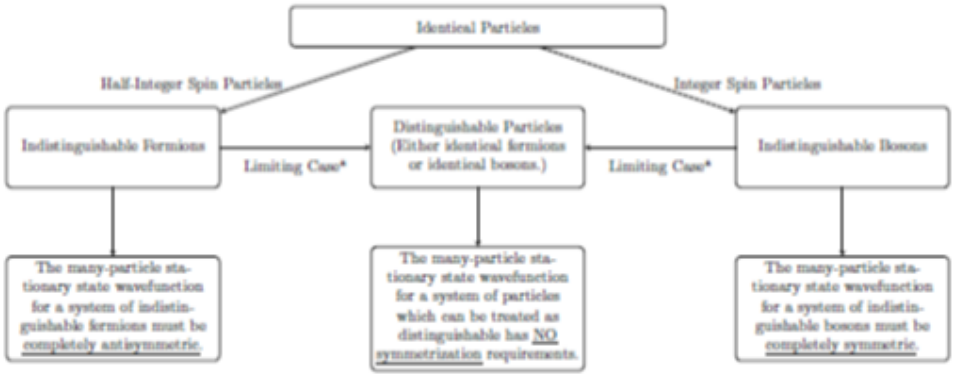
Explain why you agree or disagree with each students.

****CHECKPOINT: Check your answer to question 73. ****

73. b

If your answer does not match the checkpoint, go back and reconcile any difference you may have with the checkpoint answer.

Review the following flowchart which summarizes the properties of non-interacting identical particles




* In certain circumstances, e.g., when the overlap of the wavefunctions of the identical particles is negligible, we can treat them as distinguishable. In this limiting case, the average occupancy of each single-particle state is less than 1 and Pauli's exclusion principle is not violated.