IMPROVING THE QUANTUM MECHANICS CONTENT KNOWLEDGE AND PEDAGOGICAL CONTENT KNOWLEDGE OF PHYSICS GRADUATE STUDENTS

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Many physics graduate students face the unique challenge of being both students and teachers concurrently. To succeed in these roles, they must develop both physics content knowledge and pedagogical content knowledge. My research focuses on improving both the content knowledge and pedagogical content knowledge of first year graduate students. To improve their content knowledge, I have focused on improving graduate students' conceptual understanding of quantum mechanics covered in upper-level undergraduate courses since our earlier investigations suggest that many graduate students struggle in developing a conceptual understanding of quantum mechanics. Learning tools, such as the Quantum Interactive Learning Tutorials (QuILTs) that I have developed, have been successful in helping graduate students improve their understanding of Dirac notation and single photon behavior in the context of a Mach-Zehnder Interferometer. In addition, I have been involved in enhancing our semester long course professional development course for teaching assistants (TAs) by including research-based activities. In particular, I have been researching the implications of graduate TAs' reflections on the connections between their grading practices and student learning, i.e., the development of introductory physics students' content knowledge and problem-solving, reasoning, and metacognitive skills. This research involves having graduate students grade sample student solutions to introductory physics problems. Afterward, the graduate TAs discuss with each other the pros and cons of different

grading rubrics on student learning and formulate a joint grading rubric to grade the problem. The graduate TAs are individually asked to reformulate a rubric and grade problems using the rubric several months after the group activity to assess the impact of the intervention on graduate TAs. In addition to the intervention focusing on grading sample student solutions, graduate TAs are also asked to answer a variety of questions to help them reflect upon how introductory physics students learn physics and why grading plays a critical role in improving both their content knowledge and their problem solving, reasoning, and metacognitive skills. The implications of these interventions for the preparation of graduate students is discussed.

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PREFACE

First, I would like to thank my research advisor, Dr. Chandralekha Singh. Her constant assistance and encouragement were invaluable as I embarked on the long journey through graduate school. She has been a wonderful teacher, advisor, mentor, and role model. I am extremely grateful that I have been able to learn from her as I pursue my passion of physics education.

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1.0 INTRODUCTION

The goal of physics education research is to transition students from an initial knowledge state to a desired final knowledge state [1,2]. Graduate students have the unique roles of being both students and teachers simultaneously. Thus, they require assistance to help them transition from an initial knowledge state to a desired state of expertise in both their content knowledge and pedagogical content knowledge. Within this dissertation, I compare graduate students' content knowledge in quantum mechanics with that of upper-level undergraduate students for material covered in a junior-senior level quantum mechanics course before and after they use research-based learning tools and also assess graduate students' pedagogical content knowledge related to grading.

Upper-level undergraduate students and graduate students have various levels of prior preparation and motivation and many do not have well-organized knowledge structure [3] or learn from their mistakes [4]. It is crucial that both upper-level undergraduates and graduate students are provided support to improve their content knowledge and pedagogical content knowledge. If graduate students have a solid foundation in the materials covered in the undergraduate courses, they are more likely to build on them at the graduate level and develop a functional understanding. In addition, graduate students who teach may have unexamined beliefs about how students learn and the types of instructional strategies that are effective for introductory students [5, 6]. In particular, graduate students may teach introductory students in a manner which may have been effective for them while learning introductory physics but which may not necessarily be effective for introductory students who are not majoring in physics [6].

1.1 CONTENT KNOWLEDGE-DEFINITION

We define content knowledge as involving: 1) identifying and generating a concept or principle correctly; 2) using different representations (e.g., words, pictures, mathematical symbols, and graphs) to describe a concept or principle; 3) organizing knowledge of different concepts and principles hierarchically similar to the knowledge organization of domain experts, which facilitates retrieval during problem solving; and 4) developing problem solving, reasoning, and metacognitive skills to solve problems using the concepts and principles learned [1,2]. The development of conceptual knowledge and appropriate skills in physics go hand in hand, and so we include both conceptual knowledge and problem-solving skills in content knowledge.

1.2 CONTENT KNOWLEDGE-CONNECTION TO COGNITIVE SCIENCE

Cognitive research deals with how people learn and solve problems. This type of research can help us understand how people develop expertise in a particular domain. The findings of cognitive research demonstrate how people acquire knowledge and how they organize and retrieve knowledge to solve problems. Cognitive researchers have also developed learning frameworks which provide important guidelines for designing effective instructional strategies for helping people develop content knowledge. The principles of cognitive research can guide the design of effective instructional strategies to help students learn [7].

1.2.1 Memory

According to the information processing view of cognition, human memory has two broad components: 1) long term memory; and 2) short term memory. Long term memory is where prior knowledge is stored and can be used in future problem solving and learning. There does not appear to be a limit to the amount of information that can be stored in long term memory [8]. Short term memory or working memory is where information is processed. While solving problems, the short term memory receives input from sensory buffers (e.g., eyes, hands, ears, etc.) and long term memory [8]. Working memory is limited and has approximately seven "slots" (seven plus or minus two) for storing information for almost all individuals [9,10]. Both components of memory are crucial for learning and developing content knowledge. In order to learn, one must draw upon prior knowledge from long term memory to make connections to the information being processed in working memory.

1.2.2 Cognitive load theory and "Chunking."

Cognitive research also reveals how people organize their knowledge based upon their expertise in a domain and how the retrieval of knowledge is tied to the organization. While solving problems, experts in any field perform better than novices in recalling information in their respective fields of expertise. Chase and Simon compared novice and master chess players' abilities to reproduce game positions from memory (i.e., the chess piece positions on the board of an actual game) and random positions (i.e., the chess piece positions that were randomly placed on the board). They found that masters showed a considerable advantage in reproducing the positions of the chess pieces on the board for actual games [11]. Chase and Simon also used a chess-board reproduction task to examine the nature of the patterns, or chunks, used by the chess masters. The chess masters' task was to reproduce the positions of pieces for a target chessboard (i.e., a chess board with pieces placed on it as would be in an actual game) on a test chessboard. The chess masters glanced at the target board, placed some pieces on the test board, glanced back at the target board, placed some more pieces on the target board, and so on [11]. Each group of chess pieces which were placed on the target board after one glance was considered to be a "chunk." Chunks tended to define meaningful game relations among pieces. These findings demonstrate that experts recognize patterns of elements that repeat in many problems, i.e., chunks. Experts are better at recalling information and generating solutions to problems because they have developed many knowledge chunks which have been organized hierarchically. This type of knowledge structure allows experts to possess a few key ideas which can be remembered easily and flexibly elaborated to solve problems [2]. In contrast, novices' incoherent knowledge structure is fragmented because they have not chunked enough related knowledge. This incoherent knowledge structure inhibits them from being able to recall appropriate knowledge for a particular task and generate solutions [2,12]. It should be noted, however, that there is a spectrum of expertise and each individual falls somewhere in that continuum based upon his/her level of expertise in a given domain.

Due to limited capacity of working memory, Sweller notes that cognitive processing capacity is reduced during problem solving as the problem solver considers the current problem state, the goal state, the relations between the current problem and the goal state, and any subgoals that must be achieved [13]. As the problem solver's cognitive processing capacity becomes limited, there is little room left for the development of a coherent knowledge structure [13]. Sweller suggests that since information is first processed in working memory which has a finite processing capacity, in order for learners to organize their knowledge hierarchically, instructional strategies must be designed to reduce cognitive load while problem solving and learning [13].

1.2.3 Frameworks for learning

Since learners can only hold a limited amount of information in their working memory, this leads to difficulties in developing expertise and building a robust, hierarchical knowledge structure. Cognitive researchers have developed frameworks for learning, which take into account the prior knowledge of the students (information that they already have stored in their long term memory) and build upon it in a manner which can reduce cognitive load. These types of instructional strategies can help learners chunk information and build a hierarchical knowledge structure.

The cognitive apprenticeship model of learning involves three major components: "modeling," "coaching and scaffolding," and "weaning" [14]. In this approach, "modeling" means that the instructor demonstrates and exemplifies the skills that students should learn. "Coaching and scaffolding" refer to providing students suitable practice, guidance, and feedback so that they learn the skills necessary for good performance. To effectively coach and scaffold students, one must know their prior knowledge and implement strategies that can help reduce students' cognitive load. "Weaning" involves gradually fading the support and feedback with a focus on helping students develop self-reliance. As students continue to build a hierarchical knowledge structure and chunk information, the amount of information they can hold in their working memories increases and they can gradually be given more challenging tasks with less support and feedback.

Strategies for coaching and scaffolding students involve frameworks for learning such as Vygotsky's zone of proximal development, Piaget's optimal mismatch, and Bransford and Schwartz's preparation for future learning model that includes elements of innovation and efficiency. The zone of proximal development attributed to Vygotsky is a dynamic zone defined by what a student can accomplish on his/her own at a given time vs. with the help of a guide who is familiar with the student's initial knowledge and targets instruction somewhat above it continuously for effective learning [15]. Piaget's optimal mismatch model suggests that students will benefit if instruction provides a cognitive conflict which makes them realize that there is a mismatch between their prior knowledge and new knowledge being learned [16]. An optimal mismatch occurs when the gap between what is known and what must be learned is neither too great nor too little such that the task is not too cognitively demanding. Then, students are provided appropriate guidance and feedback for the "assimilation and accommodation" of new ideas [16]. Similar to the frameworks put forth by Vygotsky and Piaget, Schwartz et al. recommend a preparation for future learning model, stating that balanced instruction should include opportunities to learn how to rapidly retrieve and accurately apply appropriate knowledge and skills to solve a problem (efficiency) and to adapt knowledge to new situations (innovation) [17]. Students learn most optimally when they follow the "optimal adaptability corridor" in which there are elements of both efficiency and innovation concurrently which helps them be cognitively engaged and prevents them from becoming bored or frustrated [17].

All of the learning frameworks (i.e., cognitive apprenticeship model, and frameworks focusing on the zone of proximal development, optimal mismatch, and preparation for future learning) require that instructors are aware of students' prior knowledge and build on it [18]. In the case of graduate students in physics, instructors must first be aware of the common difficulties they have with topics in upper-level and graduate level courses. Instructors can tailor instruction to reduce cognitive load and help them build an organized knowledge structure (i.e., develop their content knowledge). Instruction must include coaching and scaffolding to help upper-level students and graduate students develop expertise in physics because many of these students are not necessarily building a hierarchical knowledge structure or monitoring their learning [3,4].

1.3 CONTENT KNOWLEDGE-CONNECTION TO PHYSICS EDUCATION RESEARCH

Physics education researchers have used the findings of cognitive research to investigate the initial knowledge states of students, examine the differences between experts and novices, and to develop instructional strategies for helping students become more expert-like.

1.3.1 Expert/Novice differences

Physics education researchers have documented differences between experts' and novices' content knowledge in physics [19-22]. Experts have a hierarchical knowledge structure of physics, with the most fundamental principles at the top of the hierarchy (e.g., Newton's laws, conservation of energy principle, conservation of momentum principle, etc.) and less fundamental principles lower in the hierarchy. Experts also have made many connections between different concepts.

Furthermore, experts can easily transition from one representation (e.g., a word description) to another representation (e.g., graphical representation). On the other hand, novices' knowledge structures are comprised of facts and formulas that are only loosely connected. Their knowledge structure is not robust. Their learning is often context-dependent, and this causes difficulties when students attempt to translate between different representations.

In terms of their problem-solving, both experts and novices use heuristics to guide their search process by identifying the gap between the problem goal and the state of the solution and taking action to bridge this gap. However, novices approach problems in a haphazard manner, while experts devote time and effort to describe qualitatively the problem situation, identify principles that may be useful in the analysis of the problem, and retrieve effective representations based on their well-organized domain knowledge [1]. In addition, experts devote time to plan a strategy for constructing a solution by devising a useful set of intermediate goals and means to achieve them [1]. Experts also engage more than novices in self-monitoring their progress towards a solution by evaluating former steps and revising their choices [1].

As noted earlier, expertise is a continuous spectrum with different individuals at different points on the "expertise" spectrum. Some upper-level students may fall on the "expert" side of the spectrum in terms of their content knowledge of upper-level topics [3]. However, a significant portion of upper-level undergraduate students (many of whom are future graduate students) have not necessarily built a hierarchical knowledge structure or take the opportunity to learn from their mistakes [3,4]. They may have only a fragmented, loosely connected knowledge structure of advanced topics and also have inadequate problem-solving, reasoning, and metacognitive skills.

1.3.2 Development of instructional strategies for both introductory and advanced students

Physics education researchers have developed various instructional strategies to assist both introductory and advanced students learn physics. These strategies make use of the learning frameworks mentioned earlier to reduce students' cognitive load and assist students in "chunking" information and developing a hierarchically organized knowledge structure. These instructional strategies gradually wean support for students as they learn and require fewer "slots" in their working memory to solve a particular type of problem. This allows them to solve more difficult problems on their own. Research-based active-learning tools such as tutorials, peer-instruction, and group problem-solving are effective scaffolding tools for introductory students [23-25]. They build on students' prior knowledge and explicitly address common difficulties students have in physics. These learning tools give students an opportunity to assimilate and accommodate new ideas while building and organizing their knowledge structure. The guided approach also promotes collaboration and helps students take advantage of each other's strengths and learning styles. Similar strategies, such as tutorials, peer instruction, collaborative learning, and computer simulations have proven to be effective in upper-level courses as well [26-37]. In particular, in quantum mechanics, Quantum Interactive Learning Tutorials (QuILTs) use a guided-inquiry approach to learning in which students predict what should happen in a particular situation and then are provided appropriate feedback. QuILTs often use visualization tools that students can use to check their predictions [26-30]. The peer instruction approach has been used in quantum mechanics and helps advanced students acquire content knowledge because they must answer conceptual questions and also explain their answers to their peers [31]. In addition, upper-level students and graduate students benefit from peer collaboration. Collaboration with a peer often leads to co-construction. Co-construction of knowledge occurs, e.g., when neither student working in a pair was able to answer a question before collaborating with a peer, but after collaborating with a peer, both students were able to answer the question. It was found that on a multiple-choice conceptual survey on topics in quantum mechanics, co-construction occurred in approximately one-fourth of the cases in which both students had selected the incorrect answer before collaboration.

The findings of cognitive science and prior research in physics education are keys in developing graduate students' content knowledge. The instructional strategies based upon learning frameworks in cognitive science are proving to be effective even for graduate students. Thus, in highly abstract and technically difficult subjects, e.g., quantum mechanics, graduate students can benefit from research-based instructional strategies to help them develop hierarchically organized knowledge structure.

1.4 PEDAGOGICAL CONTENT KNOWLEDGE (PCK)-DEFINITION

While having well-developed content knowledge is crucial in teaching a particular subject, pedagogical content knowledge (PCK) is also necessary to effectively address student difficulties and help them learn. Shulman defines PCK as an awareness of student difficulties in a particular subject and the methods of representing and formulating the subject that make it comprehensible to others (e.g., analogies, illustrations, examples, explanations, and demonstrations) [38]. Learners are not blank slates and come into a course with many preconceptions and varying levels of preparation [39]. Thus, teachers need both the knowledge of student difficulties and effective instructional strategies to help them overcome these difficulties.

In addition to developing their content knowledge, graduate students should acquire pedagogical content knowledge since they are often required to teach introductory students. Graduate Teaching Assistants (TAs) often interact more closely with students, have smaller recitation sections, and grade assignments. Thus, TAs play a valuable role in the teaching of introductory students in many universities across the United States. Many graduate students are also future instructors, and thus, they need to both be aware of the difficulties and preconceptions introductory students have as well as the instructional strategies that can help them learn physics.

The process of developing pedagogical content knowledge is similar to the development of content knowledge. To effectively develop instructors' pedagogical content knowledge, leaders of professional development programs must not only be aware of instructors' prior pedagogical content knowledge, but also strategies to help them develop pedagogical content knowledge. The following sections describe prior research on strategies which can help teachers acquire and develop their pedagogical content knowledge and discuss prior work in physics education research regarding TAs' pedagogical content knowledge.

1.5 PEDAGOGICAL CONTENT KNOWLEDGE-CONNECTION TO RESEARCH ON TRAINING TEACHERS

Teachers' decision-making is described in the educational literature as an implicit process, drawing upon tangled and occasionally conflicting conceptions [40-44]. Instructors' interpretations of classroom events are often shaped by their former experiences and beliefs. Teachers activate different beliefs, goals, knowledge, and action plans in response to classroom events, and teachers' reactions to these events are interpreted in light of their former experiences. Experienced teachers' decision making is often automated and the teacher is no longer aware of the reasons that led to the development of the routine actions [45-51]. When instructors work toward an instructional goal, their prior beliefs and experiences may conflict and interfere with the attempt to achieve the goal [51-54]. Professional development programs for teachers aim to help teachers reflect on their goals, actions, and achievements in order for fundamental changes in teacher practice to take place [55-60]. Transformative learning experiences for teachers that develop their PCK create cognitive dissonance between their beliefs and practices, provide time for them to reflect and resolve the cognitive dissonance with peers, and are embedded in practice [60].

1.6 PEDAGOGICAL CONTENT KNOWLEDGE-CONNECTION TO PHYSICS EDUCATION RESEARCH

The principles of professional development discussed above have been effective in the training of physics teachers [57, 59]. These principles can help guide TAs in transforming their perceptions about teaching and learning while taking into account their prior experiences, beliefs, and present teaching situations.

TAs' prior experiences as students affect their views about learning and teaching, and these views are often highly resistant to change [5,6]. For example, TAs often implement instructional strategies that were effective for them (but not necessarily their students) [6]. Furthermore, TAs acknowledge instructional strategies from educational research, but disregard them for their own views of appropriate instruction [6]. They often have internal conflicts between their goals for instruction and their actual practice [5]. TAs' present teaching situations also contribute to their perceptions of teaching and learning. Since limited training and feedback is offered to new TAs, many rely on "on the job" experiences in the classroom to learn how to teach [61]. Professional development for TAs should build upon TAs' prior knowledge (e.g., TAs' past educational experiences, beliefs about teaching and learning, and present teaching experiences) in order to develop their pedagogical content knowledge.

1.7 A STUDY OF THE CONTENT KNOWLEDGE AND PEDAGOGICAL CONTENT KNOWLEDGE OF GRADUATE STUDENTS

The studies in this thesis explore advanced students' content knowledge and pedagogical content knowledge and evaluate effectiveness of strategies designed to develop these types of knowledge. The first three chapters involve determining advanced students' prior content knowledge in quantum mechanics. The first study examined students' content knowledge of quantum mechanics and revealed that advanced students have many common difficulties, e.g., with the wave function and its time development, measurements, the time dependence of expectation values, and formalism and Dirac notation. Many advanced students also have inadequate problem-solving, reasoning, and metacognitive skills. The second study explores how the patterns of difficulties advanced students display when learning quantum mechanics are similar to the patterns of difficulties introductory students display when learning introductory physics. Based on empirical research, a framework is developed that posits that the challenges many students face in developing expertise in quantum mechanics are analogous to the challenges introductory students face in developing expertise in introductory classical mechanics. This framework incorporates both the effects of diversity in upper-level students' prior preparation, goals, and motivation in general (i.e., the facts that even in upper-level courses, students may be inadequately prepared, have unclear goals, and have insufficient motivation to excel) as well as the "paradigm shift" from classical mechanics to quantum mechanics. The third study builds on the results of the first two studies. In this study, a survey was created based upon the common difficulties students have with the formalism and postulates of quantum mechanics. This survey can be used by instructors at the beginning of a course to identify the common difficulties of a particular group of students and build upon these difficulties. The survey can also be administered at the end of a quantum mechanics course to determine the effectiveness of instruction. Chapters 5-7 are studies in which Quantum mechanics Interactive Learning Tutorials (QuILTS) were created to help advanced students develop content knowledge about Dirac notation, single photon interference, and a quantum eraser. In these studies, student difficulties with Dirac notation, single photon interference, and the idea of quantum erasure are investigated. Based upon the difficulties, QuILTs were developed using the principles of learning theory from cognitive science. The results of these studies indicate that students have many common difficulties with Dirac notation, single photon interference, and a quantum eraser and the QuILTs are effective in helping students overcome these difficulties.

The last study discussed in this thesis explores graduate students' pedagogical content knowledge in the context of a grading task. The results of this study indicate that graduate students often have conflicts between their stated goals for grading and their actual grading practice. While many graduate students stated that problem solving should serve as a learning opportunity for both the student and the instructor, they often graded solutions on correctness as opposed to problem solving strategies such as drawing a diagram and explaining steps. The results of this study provides graduate students' prior knowledge about grading. Leaders of professional development can use the results of this study to build on graduate students' prior knowledge and develop their pedagogical content knowledge.

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2.0 A REVIEW OF STUDENT DIFFICULTIES IN UPPER-LEVEL QUANTUM MECHANICS

2.1 INTRODUCTION

2.1.1 Learning in upper-level physics vs. introductory physics

Helping students learn to "think like a physicist" is a major goal of many physics instructors from the introductory to the advanced level [1-9]. In order to become an expert in physics, the development of problem-solving, reasoning, and metacognitive skills must go hand-in-hand with learning content and building a robust knowledge structure [4-6, 10-12]. Expert physicists monitor their own learning and use problem solving as an opportunity for learning, repairing, extending, and organizing their knowledge structure. Much research in physics education has focused on investigating students' reasoning difficulties in learning introductory physics and on the development of research-based curricula and pedagogies that can significantly reduce these difficulties and help students develop a robust knowledge structure [3, 4]. A parallel strand of research in introductory physics has focused on how a typical student in such courses differs from a physics expert and the strategies that may help students become better problem solvers and independent learners [5, 6]. However, relatively few investigations have focused on the nature of expertise of upper-level physics students and strategies that can be effective in such courses to help students learn physics and develop their problem-solving, reasoning, and higher-order thinking skills further [13, 14].

Learning physics is challenging even at the introductory level because it requires drawing meaningful inferences and unpacking and applying the few fundamental physics principles, which are in compact mathematical forms, to diverse situations [3, 4]. Learning upper-level physics is also challenging because one must continue to build on all of the prior knowledge acquired at the introductory and intermediate levels. In addition, the mathematical sophistication required is generally significantly higher for upper-level physics. In order to develop a functional understanding, students must focus on the physics concepts while solving problems and be able to go back and forth between the mathematics and the physics, regardless of whether they are converting a physical situation to a mathematical representation or contemplating the physical significance of the result of a complex mathematical procedure during problem solving. However, little is actually known about how expertise in physics develops as a student makes a transition from introductory to intermediate to advanced physics courses and whether the cognitive and metacognitive skills [15] of advanced students are significantly superior to those of physics majors in the introductory and intermediate level courses. In particular, there is a lack of research on whether the development of these skills from the introductory level to the point at which the students take up scientific careers is a continuous process of development or whether there are some discontinuous boosts in this process, for example, when students become involved in undergraduate or graduate research or when they independently start teaching and/or researching. There are also little research data on what fraction of students who have gone through the entire traditional physics curriculum including the upper-level courses have developed sufficient cognitive and metacognitive skills to excel professionally in the future, e.g., in graduate school or a future career. Investigations in which students in advanced physics courses are asked to perform tasks related to simple introductory physics content cannot properly assess their learning and self-monitoring skills [15]. Advanced students may possess a large amount of compiled knowledge about introductory physics due to repetition of the basic content in various courses and may not need to do much self-monitoring while solving introductory problems. Therefore, the task of evaluating upper-level students' learning and self-monitoring skills should involve physics topics at the periphery of their own understanding.

2.1.2 Effect of the "Paradigm Shift" on Student Difficulties in Quantum Mechanics

Among upper-level courses, quantum mechanics can be especially challenging for students because the paradigms of classical mechanics and quantum mechanics are very different [16, 17]. For example, unlike classical physics, in which position and momentum are deterministic variables, in quantum mechanics they are operators that act on a wave function (or a state) which lies in an abstract Hilbert space. In addition, according to the Copenhagen interpretation, which is most commonly taught in quantum mechanics courses, an electron in a hydrogen atom does not, in general, have a definite distance from the nucleus; it is the act of measurement that collapses the wave function and makes it localized at a certain distance. If the wave function is known right before the measurement, quantum theory only provides the probability of measuring the distance in a narrow range.

The significantly different paradigms of classical mechanics and quantum mechanics suggest that even students with a good knowledge of classical mechanics will start as novices and gradually build their knowledge structure about quantum mechanics. The "percolation model" of expertise can be particularly helpful in knowledge-rich domains such as physics [10]. In this model of expertise, a person's long term memory contains different "nodes" which represent different knowledge pieces within a particular knowledge domain. Experts generally have their knowledge hierarchically organized in pyramid-shaped schema in which the top nodes are more foundational than nodes at a lower level and nodes are connected to other nodes through links that signify the relation between those concepts. As a student develops expertise in a domain, links are formed which connect different knowledge nodes. If a student continues her effort to organize, repair, and extend her knowledge structure, she will reach a percolation threshold when all knowledge nodes become connected to each other by at least one link in an appropriate manner. At this point, the student will become at least a nominal expert. The student can continue on her path to expertise with further strengthening of the nodes and building additional appropriate links. Redundancy in appropriate links between different nodes is useful because it provides alternative pathways during problem solving when other pathways cannot be accessed, e.g., due to memory decay. As a student starts to build a knowledge structure about quantum mechanics, her knowledge nodes will not be appropriately connected to other nodes farther away, and her reasoning about quantum mechanics will only be locally consistent and lack global consistency [18, 19]. In fact, a person who begins a pursuit of expertise in any knowledge-rich domain must go through a phase in which her knowledge is in small disconnected pieces which are only locally consistent but lack global consistency, leading to reasoning difficulties. Therefore, introductory students learning classical mechanics and advanced students learning quantum mechanics are likely to show similar patterns of reasoning difficulties as they move up along the expertise spectrum in each of these sub-domains of physics.

2.1.3 Overview of Student Difficulties in Quantum Mechanics

Students taking upper-level quantum mechanics often develop survival strategies for performing reasonably well in their course work. For example, they become proficient at solving algorithmic problems such as the time-independent Schrödinger equation with a complicated potential energy and boundary conditions. However, research suggests that they often struggle to make sense of the material and build a robust knowledge structure. They have difficulty mastering concepts and applying the formalism to answer qualitative questions, e.g., questions related to the properties of wave functions, possible wave functions for a given system, the time-development of a wave function, measurement of physical observables within the Copenhagen interpretation, and the meaning of expectation values as an ensemble average of a large number of measurements on identically prepared systems [7, 20-24].

Here, we review research on student reasoning difficulties and on their problem-solving and metacognitive skills in learning upper-level quantum mechanics. Difficulties in learning quantum mechanics can result from its novel paradigm, the abstractness of the subject matter, and mathematical sophistication. Also, the diversity in students' prior preparation for upper-level courses such as quantum mechanics has increased significantly [25] and makes it difficult for instructors to target instruction at the appropriate level. Moreover, in order to transfer previous learning, e.g., knowledge of linear algebra, waves, or probability concepts learned in other contexts, students must first learn the basic structure of quantum mechanics and then contemplate how the previously learned knowledge applies to this novel framework [26]. Research suggests that students in upper-level quantum mechanics have common difficulties independent of their background, teaching style, textbook, and institution that are analogous to the patterns of difficulties observed in introductory physics courses, and many students in these courses have not acquired a functional understanding of the fundamental concepts [7, 24]. The nature of conceptual difficulties in learning quantum mechanics is analogous in nature to conceptual difficulties found via research in introductory physics courses.

Several investigations have strived to improve the teaching and learning of quantum mechanics at the introductory or intermediate level [27-43]. For example, some investigations have focused on students' conceptions about modern physics early in college or at the pre-college level [33-37]. Zollman et al. [27] have proposed that quantum concepts be introduced much earlier in physics course sequences and have designed tutorials and visualization tools [44] which illustrate concepts that can be used at a variety of levels. Redish et al. [29, 30] have conducted investigations of student difficulties and developed research-based material to teach quantum mechanics concepts to a wide range of science and engineering students. Robinett et al. [45] designed a "visualization" test related to quantum physics concepts that can be administered to students in introductory quantum physics. Other visualization tools have also been developed to help students learn quantum mechanics better [46-51].

While there is overlap between the content in introductory, intermediate, and upper-level quantum mechanics courses, here we focus only on student difficulties in upper-level (junior/senior level) quantum mechanics. We first describe theoretical frameworks that inform why investigations of student difficulties in learning quantum mechanics are important. Then, we summarize the methodologies used in the investigations that explore the difficulties. We then present a summary of common student difficulties in learning upper-level quantum mechanics found via research. We conclude with a brief summary of research-based learning approaches that take into account the research on student difficulties and strive to help students develop a good knowledge structure of quantum mechanics.

2.2 THEORETICAL FRAMEWORKS THAT INFORM THE INVESTIGATIONS ON STUDENT DIFFICULTIES

Research on student reasoning difficulties in learning upper-level quantum mechanics and on students' problem-solving and metacognitive skills in these courses is inspired by cognitive theories that point to the importance of knowing student difficulties in order to help them develop a functional understanding of relevant concepts. For example, Hammer proposed a "resource" model that suggests that students' prior knowledge, including their learning difficulties, should be used as a resource to help students learn better [55]. Similarly, the Piagetian model of learning emphasizes an "optimal mismatch" between what the student knows and is able to do and the instructional design [56, 57]. In particular, this model focuses on the importance of knowing students' skill levels and reasoning difficulties and using this knowledge to design instruction to help them assimilate and accommodate new ideas and build a good knowledge structure. Similarly, Bransford and Schwartz's framework, "preparation for future learning" (PFL), suggests that to help students be able to transfer their knowledge from one context to another, instructional design should include elements of both innovation and efficiency [58]. While there are multiple interpretations of their model, efficiency and innovation can be considered two orthogonal dimensions in instructional design. If instruction only focuses on efficiently transferring information, cognitive engagement will be diminished and learning will not be effective. On the other hand, if the instruction is solely focused on innovation, students will struggle to connect what they are learning with their prior knowledge and learning and transfer will be inhibited. Incorporating the efficiency and innovation elements into an instructional design based upon this framework and being in the “optimal adaptability corridor” demands that instruction build on students’ existing skills and take into account their reasoning difficulties.

With this knowledge for a given student population, an instructor can determine what is innovative and what is efficient. Vygotsky developed a theory which introduces the notion of the “zone of proximal development” (ZPD). The ZPD refers to the zone defined by the difference between what a student can do on his/her own and what a student can do with the help of an instructor who is familiar with his/her prior knowledge and skills [59]. Scaffolding is at the heart of this model and can be used to stretch students’ learning beyond their current knowledge by carefully crafted instruction. Even within this model of learning, knowing the ZPD requires knowledge of student reasoning difficulties and the current level of expertise in their problem-solving, reasoning, and self-monitoring skills. These cognitive theories (i.e., “resource” model, “optimal mismatch” model, PFL model, and Vygotsky’s model focusing on ZPD) all point to the fact that one must determine the initial knowledge states of the students in order to design effective instruction commensurate with students’ current knowledge and skills. Thus, the investigation of student difficulties, which is reviewed in the following sections, can help in the development of curricula and pedagogies to reduce the difficulties and improve learning of quantum mechanics.

2.3 SUMMARY OF METHODOLOGY

The research studies on learning difficulties in upper-level quantum mechanics summarized in this report use both quantitative and qualitative methodologies. In fact, almost all of the investigations that we draw upon use a mixed methodology involving both quantitative and qualitative data. The complete details of the methodologies can be found in the respective references. However, generally, for the quantitative part of the studies, students in various upper-level undergraduate quantum mechanics courses (after traditional instruction) or in various graduate core quantum mechanics courses (before instruction) were given written surveys with free-response and/or multiple-choice questions on topics that are covered in a typical undergraduate quantum mechanics course. Some of these studies were conducted at several universities simultaneously (with the total number of students varying from close to a hundred to more than two hundred depending upon the investigation) while others were conducted at typical state universities where the student population in the upper-level quantum mechanics courses is likely to be representative of students in similar courses at other typical state universities.

In most studies (which used a mixed research methodology), a subset of students (a smaller number of students than in the quantitative classroom investigations involving written tasks) were interviewed to investigate difficulties with quantum mechanics concepts in more depth and to unravel the underlying cognitive mechanisms. For these qualitative studies, upper-level undergraduate students in various quantum mechanics courses and physics graduate students who were taking or had taken core graduate level quantum mechanics were interviewed individually outside of the class using semi-structured, think-aloud interviews [60] and were asked to solve similar problems to those that were administered in written tests. As noted, the rationale was to understand the cognitive mechanism for students' written responses in-depth. In these semi-structured interviews, students were asked to verbalize their thought processes while they worked on the problems. They were not disturbed while they answered the questions except when asked to "keep talking" if they became quiet for a long time. After the students had answered the questions to the best of their ability, they were asked for clarifications of points they had not made clear earlier. In some interviews, students were also asked about their problem solving and learning strategies and what difficulties they faced in learning quantum mechanics. These interviews were semi-structured in the sense that the interviewers had a list of issues that they definitely wanted to discuss. These issues were not brought up initially because the researchers wanted to give students an opportunity to articulate their thought processes and formulate their own responses. However, some of the later probing questions were from the list of issues that researchers had planned to discuss ahead of time (and interviewers asked students at the end of the interview if students did not bring the issue up themselves). Other probing questions were designed on-the-spot by the interviewer to get a better comprehension of a particular student's reasoning and thought process. We note that in some investigations, the individual interview protocol was somewhat different and can be found by consulting the individual references.

2.4 STUDENT REASONING DIFFICULTIES IN UPPER-LEVEL QUANTUM MECHANICS

Learning content and development of skills go hand in hand. This section focuses on student reasoning difficulties with different topics in upper-level quantum mechanics and the next section focuses on evidence that students in these courses often have inadequate problem-solving, reasoning, and metacognitive skills.

Similar to research in introductory physics learning, research in learning quantum mechanics suggests that student reasoning difficulties are often context dependent. In other words, a student reasoning difficulty related to a particular topic may manifest itself in one context but not in another context. This is expected because students are developing expertise and their knowledge structure is not robust. They may recognize the relevance of a particular principle or concept in one context but not in another. Moreover, even students who have a good knowledge structure of mathematics may have conceptual difficulties, especially in a traditional course that focuses mostly on algorithmic problems rather than on sense making.

Furthermore, student responses are sensitive to the wording of a question, particularly for multiple-choice questions which include an explicit mention of a particular difficulty. For example, students were asked if "$\hat{H}\Psi = E\Psi$" is true for all possible wave functions for a system (where $\hat{H}$ and Ψ are the Hamiltonian and wave function, respectively). About one out of ten students incorrectly claimed that it is not true because, instead, the Hamiltonian acting on a generic state corresponds to energy measurement and implies that "$\hat{H}\Psi = E_n\phi_n$" [23]. On the other hand, when students are explicitly asked to evaluate the correctness of the statement that "$\hat{H}\Psi = E_n\phi_n$ is true because the Hamiltonian operator acting on a generic state corresponds to the measurement of energy which collapses the state to an energy eigenstate ϕ_n and the corresponding energy eigenvalue E_n is measured," more than one-third of students incorrectly agree with this statement [61]. The difference between the percentages of students in these contexts is mainly due to the fact that in one case, students may generate the incorrect expression "$\hat{H}\Psi = E_n\phi_n$" themselves, whereas in the other case they are evaluating the correctness of a statement that explicitly involves

"$\hat{H}\Psi = E_n\phi_n$." This type of context dependence of student responses should be kept in mind in the research studies discussed below. In particular, even if only $5 - 10\%$ of the students show a certain type of difficulty in a particular context, it is likely that a higher percentage will display the same difficulty in a different context.

We also note that in several studies, very similar problems were chosen to probe student reasoning difficulties in upper-level quantum mechanics. In some cases, the contexts of the problems in two different investigations were very similar except that one study asked students to solve a problem in an open-ended format while the other study asked them to solve the same problem in a multiple-choice format. If there are several contexts in which reasoning difficulties related to a particular topic were investigated, we only present a few examples to illustrate the main issues involved. The original references should be consulted for further details.

2.4.1 Difficulties in reconciling quantum concepts with classical concepts

Quantum mechanics is abstract and its paradigm is very different from the classical paradigm. A good grasp of the principles of quantum mechanics requires building a knowledge structure consistent with the quantum postulates. However, students often have difficulty reconciling classical concepts with quantum concepts. For example, the fact that measurements are probabilistic and position and momentum do not have the usual meaning in quantum mechanics is very difficult for students. While there are many examples that fall in this broad category of student difficulties in reconciling quantum concepts with classical concepts, here we give a few examples.

Incorrect belief that a particle loses energy in quantum tunneling: Students have difficulty with the concept of quantum tunneling. Research has shown that students often transfer classical reasoning when thinking about quantum tunneling [62, 63]. Many students state that a particle “loses energy” when it tunnels through a rectangular potential barrier. This reasoning is incorrect because the particle does not lose energy when tunneling through the barrier, although the wave function of the particle inside the potential barrier is described by exponential decay. In interview situations, common responses regarding tunneling involve statements such as: “the particle collides and loses energy in the barriers" and “it requires energy to go through the barrier” [62, 63]. These types of responses indicate that many students incorrectly apply classical concepts to quantum mechanical situations.

Difficulties distinguishing between a quantum harmonic oscillator vs. a classical harmonic oscillator: In one investigation, students had difficulty with the fact that for a simple quantum harmonic oscillator in the ground state, the probability of finding the particle is maximum at the center of the well. For a classical harmonic oscillator, e.g., a simple pendulum, the particle is more likely to be found close to the classical turning points [65, 64]. Discussions with individual students suggest that this difficulty often has its origin in their experiences with how much time a particle spends near the turning points in a classical system.

Incorrect belief that quantities with labels “x,” “y,” and “z” are orthogonal to each other: One common difficulty upper-level students in quantum mechanics courses have is assuming that an object with a label “x” is orthogonal to or cannot influence an object with a label “y” [66-68]. This is evident from responses such as: “The magnetic field is in the z-direction so the electron is not influenced if it is initially in an eigenstate of $\hat{S}_x$” or “Eigenstates of $\hat{S}_x$ are orthogonal to eigenstates of $\hat{S}_y$.” In introductory physics, x, y and z are indeed conventional labels for orthogonal components of a vector. Unless students are given an opportunity to understand the structure of quantum mechanics and that the eigenstates of spin components are vectors in Hilbert space and not the physical space in which the magnetic field is a vector, such difficulties will persist. Students must learn that although an electron in an external magnetic field pointing in the z-direction is in a real, physical, three-dimensional space of the laboratory, making predictions about the measurement performed in the laboratory using quantum mechanics requires mapping the problem to an abstract Hilbert space in which the state of the system lies and where all the observables of the real physical space get mapped onto operators acting on states.

Difficulties with photon polarization states: In an investigation involving photon polarization states, some interviewed students claimed that the polarization states of a photon cannot be used as basis vectors for a two-state system due to the fact that a photon can have an infinite number of polarization states [69-71]. They argued that since a polarizer can have any orientation and the orientation of the polarizer determines the polarization state of a photon after it passes through the polarizer, it did not make sense to think about the polarization states of a photon as a two-state system. These students were often so fixated on their experiences with polarizers from introductory physics courses (which can be rotated to make their polarization axis along any direction perpendicular to the direction of propagation) that they had difficulty thinking about the polarization states of a photon as vectors in a two-dimensional space. It is interesting to note that most students who had difficulty accepting that the polarization states of a photon can be used as basis states for a two-state system had no difficulty accepting that spin states of a spin-1/2 particle can be used as basis states for a two-state system despite the fact that these two systems are isomorphic from an expert perspective. Interviews suggest that this difference in their perception was often due to how a spin-1/2 system and polarization were first introduced and the kinds of mental models students had built about each system. Generally, students are introduced to polarization in an introductory course and to spin-1/2 systems in a quantum mechanics course.

Discussions suggest that some students were so used to thinking about a beam of light passing through a polarizer according to their own mental model that they had difficulty thinking about the polarization states of a photon as vectors in a two-dimensional Hilbert space. Many instructors introduce polarization basis vectors in classical electricity and magnetism, but many students do not remember these concepts. Since students had learned about the spin-1/2 system only in quantum mechanics, thinking of the spin states of a spin-1/2 particle as vectors in a two-dimensional space often did not create a similar conflict.

Difficulties with the wave-particle duality: The double-slit experiment reveals that the wave function of a single electron can be non-zero through both slits. In particular, if electrons are sent one at a time through two slits, under appropriate conditions, one observes an interference pattern after a large number of electrons have arrived on a distant phosphor screen. This experiment is very difficult to reconcile with classical ideas. While the wave function of a single electron is non-zero through both slits, when the electron arrives at a detecting screen, a flash is seen in one location due to the collapse of the wave function. The wave-particle duality of a single electron, which is evident at different times in the same experiment, is very difficult for students to rationalize [17, 20, 31]. Students may have used vocabulary such as "particle" to describe a localized entity in their classical mechanics courses. Consequently, they may find it very difficult to think of the electron as a wave in part of the experiment (when it is going through the two slits) and as a particle in another part of the experiment (when it lands on the detecting screen and the wave function collapses).

2.4.2 Difficulties with the wave function

Any smooth, normalized function that satisfies the boundary conditions for a system is a possible wave function. However, students struggle to determine possible wave functions, especially if they are not explicitly written as a linear superposition of stationary states. The following difficulties have been found via research [24, 28, 64, 74]:

Incorrect belief that "$\hat{H}\Psi = E\Psi$" holds for any possible wave function Ψ: In a multi-university study [24], many students claimed that the Time-Independent Schrödinger Equation (TISE) $\hat{H}\Psi = E\Psi$ is true for all possible wave functions, even when Ψ is not an energy eigenstate (stationary state). In general, $\Psi = \sum_{n=1}^{\infty} C_n \phi_n$, where ϕ_n are the stationary states and $C_n = \langle \phi_n | \Psi \rangle$. Therefore, $\hat{H}\Psi = \sum_{n=1}^{\infty} C_n E_n \phi_n \neq E\Psi$. More than one-third of the students incorrectly stated that the expression "$\hat{H}\Psi = E\Psi$" is unconditionally correct, with statements such as the following being typical: "Agree. This is what 80 years of experiment has proven. If future experiments prove this statement wrong, then I'll update my opinion on this subject." Students with such responses misunderstood what the instructor taught, perhaps due to an overemphasis on the TISE in the course. This incorrect notion that all possible wave functions should satisfy the TISE makes it challenging for students to determine possible wave functions for a given system. In individual interviews, students were explicitly asked whether "$\hat{H}\Psi = E\Psi$" is true for a linear superposition of the ground and first excited state wave functions, ϕ_1 and ϕ_2, respectively, for a one-dimensional infinite square well. Many students incorrectly claimed that "$\hat{H}\Psi = E\Psi$" is indeed true for this wave function. When these students were asked to explicitly show that this equation is true in this given context, most of them verbally argued without writing that since the TISE works for each ϕ_1 and ϕ_2 individually, it implies that it should be satisfied by their linear superposition. In fact, even when students were told that the TISE is not satisfied for this linear superposition, many had difficulty believing it until they explicitly wrote these equations on paper (mostly after additional encouragement to do so) and noted that since E_1 and E_2 are not equal, $\hat{H}\Psi \neq E\Psi$ in this case.

Difficulties with mathematical representations of non-stationary state wave functions: Students have difficulties in determining non-stationary possible wave functions for a given quantum system. For example, in a multi-university study in Ref. [24], student interviewees were given three wave functions and asked if they were possible wave functions for an electron in a one-dimensional infinite square well between $x = 0$ and $x = a$ and to explain their reasoning. Students had to note that the first wave function $Ae^{-((x-a)/a)^2}$ is not possible because it does not satisfy the boundary conditions (does not go to zero at $x = 0$ and $x = a$). The other two wave functions, $A\sin^3(\pi x/a)$ and $A\left[\sqrt{2/5}\sin(\pi x/a) + \sqrt{3/5}\sin(2\pi x/a)\right]$ with suitable normalization constants, are both smooth functions that satisfy the boundary conditions (each of them goes to zero at $x = 0$ and $x = a$). Thus, each can be written as a linear superposition of the stationary states. More than three-fourths of the students could identify that the wave function written as a linear combination is a possible wave function because it was explicitly written in the form of a linear superposition of stationary states but only one-third gave the correct answer for all three wave functions. About half of the students claimed that $A\sin^3(\pi x/a)$ is not a possible wave function but that $A\left[\sqrt{2/5}\sin(\pi x/a) + \sqrt{3/5}\sin(2\pi x/a)\right]$ is possible. The interviews suggest that a majority of students did not know that any smooth, single-valued wave function that satisfies the boundary conditions can be written as a linear superposition of stationary states. Interviews and written explanations also suggest that many students incorrectly thought that any possible wave function must satisfy both of the following constraints: 1) it must be a smooth, single-valued function that satisfies the boundary conditions; and 2) it must either be possible to write it as a linear superposition of stationary states or it must satisfy the Time-Independent Schrödinger Equation. Some students who correctly realized that $A\sin^3(\pi x/a)$ satisfies the boundary conditions incorrectly claimed that it is still not a possible wave function because it does not satisfy the TISE. Many students claimed that only pure sinusoidal wave functions are possible, thus functions involving $\sin^2$ or $\sin^3$ are not possible wave functions. Many students thought that $A\sin^3(\pi x/a)$ cannot be written as a linear superposition of stationary states and hence it is not a possible wave function while others claimed that $A\sin^3(\pi x/a)$ works for three electrons but not one.

Difficulties with diverse representations of a wave function: In another multi-university investigation, students were given a valid and reliable survey with multiple-choice questions [64]. On one question, graphs (or diagrams) of three possible wave functions for a one-dimensional infinite square well were provided in which two graphs displayed stationary state wave functions and one showed a non-stationary state wave function. All wave functions were possible because they were smooth and satisfied the boundary conditions for a one-dimensional infinite square well. Students were asked to choose all wave functions that are possible for the infinite square well. In response, half of the students incorrectly claimed that only the stationary state wave functions are possible. On the same survey, more than one-third of the students incorrectly claimed that a possible wave function must be an even or odd function if the potential energy is a symmetric function due to a confusion with the energy eigenstates for familiar problems. Also, on another question on the same survey, many students correctly noted that a linear superposition of stationary states is a possible wave function for a one-dimensional infinite square well. However, students did not answer different questions about the same system consistently. In particular, many students who noted that the possible wave function must be an even or odd function if the potential energy is a symmetric function also noted that a linear superposition of stationary states is a possible wave function for a one-dimensional infinite square well which is contradictory since a linear combination of energy eigenstates for this system is not necessarily an even or odd function. Similarly, those who only selected even or odd functions as possible wave functions in the diagrammatic representation often claimed that a linear superposition of stationary states is a possible wave function for a one-dimensional infinite square well, which is also contradictory. On the same survey [64], in the context of a finite square well, students were given diagrammatic representation of a possible wave function which is non-zero only in the well (it goes to zero outside the well), and they were asked if it is a possible wave function. Less than half correctly identified it as a possible wave function for a finite square well. More than half incorrectly claimed that it is not a possible wave function because it does not satisfy the boundary conditions (it goes to zero inside the well) and the probability of finding the particle outside the finite square well is zero but quantum mechanically it must be nonzero. Thus, many students incorrectly thought that any possible wave function for a finite square well must have a non-zero probability in the classically forbidden region.

Difficulties with bound states and scattering states: When a quantum particle is in an energy eigenstate or a superposition of energy eigenstates such that the energy is less than the potential energy at both plus and minus infinity, the particle is in a bound state. Otherwise, it is in a scattering state. Here, we will only discuss situations in which the bound states and scattering states refer to stationary states since most investigations of student difficulties have focused on those cases. The bound states have a discrete energy spectrum and the scattering states have a continuous energy spectrum. Bound state wave functions go to zero at infinity so they can always be normalized. Scattering state wave functions are not normalizable since the probability of finding the particle is non-zero at infinity, but a normalized wave function can be constructed using their linear superpositions.

Students have difficulties with various aspects of the bound and scattering states of a quantum system [28, 64, 74]. In a multi-university survey [64], on questions focusing on students' knowledge about the bound and scattering state wave functions, many students either claimed that the scattering state wave functions are normalizable or they did not recognize that a linear superposition of the scattering state wave functions can be normalized. Moreover, more than one-third did not recognize that the scattering states have a continuous energy spectrum and claimed that energy is always discrete in quantum mechanics while a comparable percentage of the students claimed that the finite square well only allows discrete energy states (bound states).

On several questions on the same survey that required students to judge whether a given potential energy allows for bound states or scattering states, students had great difficulties [64]. One question uses a graphical representation showing four different potential energy wells. The distractor (incorrect answer) that the students found challenging was a graph in which the potential energy of the well bottom was greater than the potential energy at infinity (which is zero). Therefore, no bound state can exist in this potential energy well. About two-thirds of the students failed to interpret these features. They thought that any potential energy that has the shape of a "well" would allow for bound states if there were classical turning points.

Some questions on the survey focused on the common student difficulty that a given quantum particle may be in a bound or a scattering state depending on its location. This notion often has its origin in students' classical experiences. In particular, some students mistakenly claimed that a particle could have different energies in different regions in a potential energy diagram. However, if a quantum particle is in an energy eigenstate, it has a definite energy and it is not appropriate to talk about different energies in different regions. Students often incorrectly asserted that a particle is in a bound state when it is in the classically allowed region and it is in a scattering state when it is in a classically forbidden region. Responses on other questions also indicate that the students did not realize that whether a state is a bound or a scattering state only depends on the energy of the particle compared to the potential energy at plus and minus infinity.

Difficulties with graphing wave functions: In addition to upper-level studies, studies on introductory and intermediate level quantum mechanics have also found that students have difficulties in sketching the shape of a wave function [20, 24, 28]. Questions related to the shape of the wave function show that students may draw a qualitatively incorrect sketch even if their mathematical form of the wave function is correct, may draw wave functions with discontinuities or cusps, or may confuse a scattering state wave function for a potential energy barrier problem with the wave function for a potential energy well problem.

In a multi-university study [24], upper-level students were given the potential energy diagram for a finite square well. In part (a), they were asked to sketch the ground state wave function and in part (b) they had to sketch any one scattering state wave function. In both cases, students were asked to comment on the shape of the wave function inside and outside the well. In part (a), students had to draw the ground state wave function as a sinusoidal curve inside the well and with exponentially decaying tails in the classically forbidden regions. The wave function and its first derivative should be continuous everywhere and the wave function should be single valued. In part (b), they had to draw a scattering state wave function showing oscillatory behavior in all regions, but because the potential energy is lower in the well, the wavelength is shorter in the well.

For part (b), all graphs of functions that were oscillatory in both regions (regardless of the relative wavelengths or amplitudes in different regions) and showed the wave function and its first derivative as continuous were considered correct. If the students drew the wave function correctly, their responses were considered correct even if they did not comment on the shape of the wave function in the three regions.

We note that this is one of the easiest questions involving the sketching of a wave function that upper-level students can be asked to do. In response to this question, some students incorrectly drew as the ground state wave function for the infinite square well a curve that goes to zero in the classically forbidden region. Others drew an oscillatory wave function in all three regions. Many students drew either the first excited state or a higher excited bound state with many oscillations in the well and exponential decay outside. Some students incorrectly claimed that the particle is bound inside the well but free outside the well. These types of student responses displayed confusion about what a "bound state" means and whether the entire wave function is associated with the particle at a given time or the parts of the wave function outside and inside the well are associated with the particle at different times. In part (b), some students drew a scattering state wave function that had an exponential decay in the well and others drew wave functions with incorrect boundary conditions or that had discontinuities or cusps in some locations. Although students were explicitly given a diagram of the potential energy well, responses suggest that some may be confusing the potential energy well with a potential energy barrier. For example, some students plotted a wave function (without labeling the axes) which looked like a parabolic well with the entire curve drawn below the horizontal axis and claimed that the wave function must follow the sign of the potential energy.

2.4.3 Difficulties with the time-dependence of a wave function

The time-dependence of a quantum state or wave function is governed by the Time-Dependent Schrödinger Equation (TDSE)

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t}=\hat{H}|\Psi(t)\rangle \text{ or } i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\hat{H}\Psi(x,t)$$

(where the second equation above is the TDSE for a particle confined in one spatial dimension in the position representation for which the Hamiltonian $\hat{H}=\hat{p}^2/2m+\hat{V}$ in the position representation is $\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\hat{V}(x)$.

The TDSE shows that the time evolution of a wave function $\Psi(x,t)$ is governed by the Hamiltonian $\hat{H}$ of the system and therefore the eigenstates of the Hamiltonian are special with respect to the time-evolution of a state.

When the Hamiltonian does not have an explicit time dependence, an equivalent way to represent the time evolution of the wave function is via $\Psi(x,t)=e^{-i\hat{H}t/\hbar}\Psi(x,0)$. In general, one can write $\Psi(0)=\Psi(x,t=0)=\sum_{n=1}^{\infty}C_n\phi_n$, where ϕ_n are the stationary state wave functions for the given Hamiltonian with a discrete energy eigenvalue spectrum and $C_n=\langle\phi_n|\Psi\rangle$ are the expansion coefficients. Then, given any initial state of the system $\Psi(x,t=0)$, one can write $\Psi(x,t)=e^{-i\hat{H}t/\hbar}\Psi(x,0)=\sum_{n=1}^{\infty}C_n e^{-iE_n t/\hbar}\phi_n$, where E_n are the possible energies. It is clear from this form of $\Psi(x,t)$, which does not involve the Hamiltonian operator (but instead involves possible energies of the system, which are numbers), that only in the case in which the initial state is an energy eigenstate will the time-dependence of the system be trivial (because the wave function after a time t will differ from the initial wave function only via an overall phase factor which does not alter measurement probabilities). For all other initial state wave functions, the time-dependence of the wave function will be non-trivial and, in general, the probabilities of measuring different observables will be time-dependent.

The following difficulties with the time-dependence of the wave function were commonly found via research.

Incorrect belief that the Time-Independent Schrödinger Equation is the most fundamental equation in quantum mechanics: The most common difficulties with quantum dynamics are coupled with a focus on the Time-Independent Schrödinger Equation (TISE). The time evolution of a wave function $\Psi(x,t)$ is governed by the Hamiltonian $\hat{H}$ of the system via the TDSE, and thus, the TDSE is considered the most fundamental equation of quantum mechanics. Since there are no dynamics in the TISE, focusing on the TISE as the most fundamental equation in quantum mechanics leads to difficulties. For example, in Ref. [24], students were asked to write down the most fundamental equation of quantum mechanics. Approximately one-third of the students provided a correct response while half of them claimed that the TISE is the most fundamental equation of quantum mechanics. It is true that if the potential energy is time-independent, one can use separation of variables to obtain the TISE, which is an eigenvalue equation for the Hamiltonian. The eigenstates of $\hat{H}$ obtained by solving the TISE are stationary states which form a complete set of states so that any general wave function can be written as a linear superposition of the stationary states. However, overemphasis on the TISE and de-emphasis on the TDSE in quantum mechanics courses result in many students struggling with the time-dependence of a wave function.

Incorrect belief that the time-evolution of a wave function is always via an overall phase factor of the type "$e^{-iEt/\hbar}$": Due to excessive focus on the TISE and stationary state wave functions, many students claim that given any $\Psi(x, t = 0)$, one can find the wave function after time t using "Ψ(x,t)= $e^{-iEt/\hbar}\Psi(\mathrm{x},0)$" where E is a constant. For example, in Ref. [24], students from seven universities were given a linear superposition of the ground and first excited state wave function as the initial wave function $\Psi(x,0)=\sqrt{2/7}\,\phi_1(x)+\sqrt{5/7}\,\phi_2(x)$ for an electron in a one-dimensional infinite square well and asked to find the wave function $\Psi(x,t)$ after a time t.

Instead of the correct response, $\Psi(x,t)=\sqrt{2/7}\,\phi_1(x)e^{-iE_1t/\hbar}+\sqrt{5/7}\,\phi_2(x)e^{-iE_2t/\hbar}$, in which the ground state wave function is $\phi_1(x)$ and the first excited state wave function is $\phi_2(x)$, approximately one-third of students wrote common phase factors for both terms, e.g., "$\Psi(x,t)=e^{-iEt/\hbar}\Psi(\mathrm{x},0)$." Interviews suggested that these students were having difficulty differentiating between the time-dependence of stationary and non-stationary state wave functions. Students struggled with the fact that since the Hamiltonian operator governs the time-development of the system, the time- dependence of a stationary state wave function is via a simple phase factor but non-stationary state wave functions, in general, have a non-trivial time-dependence because each term in a linear superposition of stationary states evolves via a different phase factor. Apart from using "$e^{-iEt/\hbar}$ " as the common phase factor, other common choices include "$e^{-i\omega t}$", "$e^{-i\hbar t}$," "e^{-it}," "e^{-ixt}," "e^{-ikt}," etc.

In the context of a non-stationary state wave function which is not explicitly written as a linear superposition of stationary states, similar difficulties are observed. For example, in a study involving ten different universities, students were asked to select the correct probability density after a time t for an initial normalized wave function $A\sin^5(\pi x/a)$ in an infinite square well potential. In response to this question, half of the students incorrectly claimed that the probability density is time-independent because of the overall time-dependent phase factor in the wave function which cancels out in probability density [64].

Inability to differentiate between $e^{-i\hat{H}t/\hbar}$ and $e^{-iEt/\hbar}$: In Ref. [24], in response to the question asking for $\Psi(x,t)$ given an initial state which is a linear superposition of the ground and first excited states, $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$, some students wrote incorrect intermediate steps; e.g., "$\Psi(x,t) = \Psi(\mathrm{x},0)e^{-iEt/\hbar} = \sqrt{2/7}\,\phi_1(x)e^{-iE_1t/\hbar} + \sqrt{5/7}\,\phi_2(x)e^{-iE_2t/\hbar}$." Probing during the individual interviews showed that these students had difficulty differentiating between the Hamiltonian operator and its eigenvalue and incorrectly used "$\hat{H} = E$" where E is a number instead of $\Psi(x,t) = e^{-i\hat{H}t/\hbar}\Psi(x,0) = \sqrt{2/7}\,\phi_1(x)e^{-iE_1t/\hbar} + \sqrt{5/7}\,\phi_2(x)e^{-iE_2t/\hbar}$ where the Hamiltonian $\hat{H}$ acting on the stationary states gives the corresponding energies [75]. The inability to differentiate between the Hamiltonian operator and energy can reinforce the difficulty that all wave functions evolve via an overall phase factor of the type "$e^{-iEt/\hbar}$."

Incorrect belief that for a time-independent Hamiltonian, the wave function does not depend on time: Some students claimed that $\Psi(x,t)$ should not have any time dependence whatsoever if the Hamiltonian does not have an explicit time-dependence. For example, in response to the question about the time-dependence of the wave function given an initial state which is a linear superposition of the ground and first excited states ($\Psi(x,t) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$), some students claimed that there is no time dependence and typically justified their answer by pointing to the TISE and adding that the Hamiltonian is not time-dependent so there cannot be any time-dependence to the wave function [24].

Incorrect belief that the time-dependence of a wave function is represented by a real exponential function: Some students claimed that the time dependence of a wave function, e.g., an initial wave function $\Psi(x,t) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ is a decaying exponential, e.g., of the type "$\Psi(x,0)e^{-xt}$," "$\Psi(x,0)e^{-Et}$," "$\Psi(x,0)e^{-ct}$," "$\Psi(x,0)e^{-t}$," etc. During the interviews, some of these students explained their choices by insisting that the wave function must decay with time because "this is what happens for all physical systems" [24].

2.4.4 Difficulties in distinguishing between three-dimensional Euclidian space and Hilbert space

In quantum theory, it is necessary to interpret the outcomes of real experiments performed in real space by making a connection with an abstract Hilbert space (state space) in which the state of the system or wave function lies. The physical observables that are measured in the laboratory correspond to Hermitian operators in the Hilbert space in which the state of the system lies. Knowing the initial wave function and the Hamiltonian of the system allows one to determine the time-evolution of the wave function unambiguously and the measurement postulate can be used to determine the possible outcomes of individual measurements and ensemble averages (expectation values) at a given time. Research suggests that students have the following types of difficulties about these issues:

Difficulties in distinguishing between vectors in real space and Hilbert space: It is difficult for students to distinguish between vectors in real space and Hilbert space. For example, S_x, S_y and S_z denote the orthogonal components of the spin angular momentum vector of an electron in three dimensions, each of which is a physical observable that can be measured in the laboratory. However, the Hilbert space corresponding to the spin degree of freedom for a spin-1/2 particle is two-dimensional (2D). In this Hilbert space, $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ are operators whose eigenstates span the 2D space [67]. The eigenstates of $\hat{S}_x$ are vectors which span the 2D space and are orthogonal to each other (but not orthogonal to the eigenstates of $\hat{S}_y$ or $\hat{S}_z$). Also, $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ are operators and not orthogonal components of a vector in 2D space. If the electron is in a magnetic field with a gradient in the z-direction in the laboratory (real space) as in a Stern-Gerlach experiment, the magnetic field is a vector field in three-dimensional (3D) space and not in 2D Hilbert space. It does not make sense to compare vectors in 3D space with vectors in the 2D space as in statements such as "the magnetic field gradient is perpendicular to the eigenstates of $\hat{S}_x$." However, these distinctions are difficult for students to make and such difficulties are common as discussed in Refs. [24, 66].

For example, in a multi-university study in Ref. [24], these types of difficulties were found in student responses to a question related to the Stern-Gerlach experiment. Students were told that the notation $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ represents the orthonormal eigenstates of $\hat{S}_z$ (the z component of the spin angular momentum) of a spin-1/2 particle. In the situation in the question, a beam of electrons propagating along the y-direction (into the page) in spin state $|\uparrow_z\rangle$ is sent through an apparatus with a horizontal magnetic field gradient in the $-x$-direction. Students were asked to sketch the electron cloud pattern they expect to see on a distant phosphor screen in the $x - z$ plane and explain their reasoning. This question is challenging because students have to realize that the eigenstate of $\hat{S}_z$, $|\uparrow_z\rangle$, can be written as a linear superposition of the eigenstates of $\hat{S}_x$, that is, $|\uparrow_z\rangle = (|\uparrow_x\rangle + |\downarrow_x\rangle)/2$. Therefore, the magnetic field gradient in the $-x$-direction will split the beam along the x-direction corresponding to the electron spin components in $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$ states and cause two spots on the phosphor screen. The most common difficulty was assuming that there should not be any splitting since the magnetic field gradient (in the $-x$-direction) and the spin state (an eigenstate of $\hat{S}_z$) are orthogonal to each other. It can be inferred from the responses that students incorrectly relate the direction of the magnetic field in real space with the “direction” of the state vectors in Hilbert space.

Difficulties in distinguishing between the dimension of physical space and Hilbert space: The dimension of a Hilbert space is equal to the number of linearly independent basis vectors. The linearly independent eigenstates of an operator corresponding to an observable may be used as basis vectors. For example, for a particle in a one-dimensional (1D) infinite square well, the infinitely many energy eigenstates $|\phi_n\rangle$ of the Hamiltonian operator form a complete set of basis vectors for the infinite-dimensional Hilbert space. However, students have great difficulty in distinguishing between the dimensions of the Hilbert space and the dimensions of the physical space. For example, in a multiple choice question about the dimensionality of the Hilbert space for a 1D infinite square well [84], less than half of the students provided the correct answer. The rest of the students claimed that the Hilbert space for this system is 1D and that the position eigenstates and energy eigenstates of the system form a basis for the one-dimensional Hilbert space (students did not realize that they were making contradictory statements because there is not only one but infinitely many energy eigenstates or position eigenstates) for this quantum system.

2.4.5 Difficulties with measurements and expectation values

If the wave function is known right before a measurement, quantum theory only provides the probability of measurement outcomes when an observable is measured. After the measurement, the state of the system collapses into an eigenstate of the operator corresponding to the observable measured. The expectation value of an observable Q in a state is the average value of a large number of measurements of Q on identically prepared systems. Since measurement outcomes are probabilistic if the state is not in an eigenstate of $\hat{Q}$, an ensemble average is useful because it is deterministic for a given quantum state of a system. Research suggests that students have great difficulties with quantum measurement [7, 23, 24, 54, 76-79].

Difficulties with the probability of a particular outcome of a measurement: When calculating the probability of obtaining a certain value in the measurement of a physical observable, students often incorrectly claim that the operator corresponding to that observable must be explicitly involved in the expression [20]. For example, in a multi-university multiple-choice survey [64], students were asked to suppose that a particle in a one-dimensional infinite square well is in the ground state with wave function $\phi_1(x)$ and they had to find the probability that the particle will be found in a narrow range between x and $x + dx$. In response to this question, approximately one-third of the students chose the distractor "$\int_x^{x+dx} x|\phi_1(x)|^2 dx$" as the probability of finding the particle in the region between x and $x + dx$. They did not recognize that $|\phi_1(x)|^2 dx$ is the probability of finding the particle between x and $x + dx$. In another question on the same survey [64], students were given a non-stationary state wave function $\Psi(x, 0) = Ax(a - x)$ for an infinite square well and they were asked to select the correct expression, $\left|\int_0^a \phi_n^*(x)\Psi(x, 0)dx\right|^2$, for the probability of measuring energy E_n. Less than half of the students provided the correct response and one-third of the students incorrectly claimed that "$\left|\int_0^a \phi_n^*(x)\hat{\mathrm{H}}\Psi(\mathrm{x}, 0)dx\right|^2$" is the probability of measuring the energy. Students often did not realize that the required information about the energy measurement is obtained by projecting the state of the system along the energy eigenstate (multiplication of the wave function by $\phi_n^*(x)$ before integrating).

Difficulties with the possible outcomes of a measurement: According to the Copenhagen interpretation, the measurement of a physical observable instantaneously collapses the state to an eigenstate of the corresponding operator and the corresponding eigenvalue is measured. In Ref. [64], some questions on the survey investigated students' understanding of the energy measurement outcomes, e.g., for a superposition of two stationary states $\Psi(x, 0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ of a 1D infinite square well. The only possible results of the energy measurement are the ground state energy E_1 and the first excited state energy E_2. When the energy E_2 is obtained, the wave function of the system collapses to $\phi_2(x)$ and remains there. However, students often incorrectly claimed that the normalized collapsed wave function should be "$\sqrt{5/7}\,\phi_2(x)$" which has an incorrect normalization. Also, one-third incorrectly claimed that the wave function would collapse first but finally evolve back to the initial state. Other students did not realize that the wave function would collapse and claimed that the system will remain in the initial state even after the measurement.

Difficulties in distinguishing between eigenstates of operators corresponding to different observables: A very common difficulty is assuming that eigenstates of operators corresponding to all physical observables are the same [7, 23, 24]. The measurement of a physical observable collapses the wave function of a quantum system into an eigenstate of the corresponding operator. Many students had difficulties in distinguishing between energy eigenstates and the eigenstates of other physical observables. In a multi-university survey [64], half of the students claimed that the stationary states refer to the eigenstates of any operator corresponding to a physical observable because they had difficulty in differentiating between the related concepts of stationary states and eigenstates of other observables. Many students claimed that in an isolated system, if a particle is in a position eigenstate (has a definite value of position) at time $t = 0$, the position of the particle is well-defined at all times $t > 0$. Students did not relate the stationary state with the special nature of the time evolution in that state (the state evolves via an overall phase factor so that the measurement probabilities for observables do not depend on time). In another study [24], some students claimed that the wave function will become peaked about a certain value of position and drew a delta function in position when asked to draw the wave function after an energy measurement.

Confusion between the probability of measuring position and the expectation value of position: Born's probabilistic interpretation of the wave function can also be confusing for students. In a multi-university investigation [24], students were told that for an electron in a 1D infinite square well, immediately after an energy measurement which yields the first excited state energy $4\pi^2\hbar^2/(2ma^2)$, the position of the electron is measured. They were asked to qualitatively describe the possible values of position one can measure and the probability of measuring them. The correct answer involves noting that it is possible to measure position values between $x = 0$ and $x = a$ (except at $x = 0$, $a/2$, and a where the wave function is zero), and according to Born's interpretation, $|\phi_2(x)|^2 dx$ gives the probability of finding the particle between x and $x + dx$ if $\phi_2(x)$ is the first excited state. Less than half of the students provided the correct response. Many students tried to find the expectation value of position $\langle x \rangle$ instead of the probability of finding the electron at a given position. They wrote the expectation value of position in terms of an integral involving the wave function. Others explicitly wrote that "Probability = $(2/a)\int_0^a x\sin^2(2\pi x/a)dx$" and claimed that instead of $\langle x \rangle$ they were calculating the probability of measuring the position of the electron. Some students justified their response by incorrectly claiming that $|\Psi|^2$ gives the probability of the wave function being at a given position and if you multiply it by x you get the probability of measuring the position x.

Difficulties with measuring energy after position measurement: In a multi-university investigation [64], one question examined students' understanding of consecutive quantum measurements, e.g., measuring the energy of a quantum system immediately after a position measurement. For a one-dimensional infinite square well with an initial state which is a superposition of the ground and first excited states, the position measurement will collapse the wave function of the system to a delta function which is a superposition of infinitely many energy eigenfunctions. Therefore, one can obtain higher order energy values ($n > 2$) for the energy measurement after the position measurement. However, less than one-third of the students correctly answered the question and realized that the state of the system changed after the position measurement. More than one-third mistakenly claimed that they can only obtain either energy E_1 or E_2, which correspond to the initial state before the position measurement.

Difficulties with measuring position after energy measurement: In another multi-university study [24], one question asked students to qualitatively describe the possible values of the position of an electron that one can measure if the position measurement follows an energy measurement which yields the first excited state energy. In response to this question, some students tried to use the generalized uncertainty principle between energy and position or between position and momentum, but most of their arguments led to incorrect inferences. According to the generalized uncertainty principle, if σ_A and σ_B are the standard deviations in the measurement of two observables A and B, respectively, in a state $|\Psi\rangle$, and $[\hat{A}, \hat{B}]$ is the commutator of the operators corresponding to A and B, respectively, then $\sigma_A^2 \sigma_B^2 \geq \left(\frac{\langle\Psi|[\hat{A}, \hat{B}]|\Psi\rangle}{2i}\right)^2$.

Although the generalized uncertainty principle implies that position and energy are indeed incompatible observables since their corresponding operators do not commute, students often made incorrect inferences to answer the question posed. For example, several students noted that because the energy is well-defined immediately after the measurement of energy, the uncertainty in position must be infinite according to the uncertainty principle. Some students even went on to argue that the probability of measuring the particle's position is the same everywhere using the generalized uncertainty principle. Others restricted themselves only to the inside of the well and noted that the uncertainty principle says that the probability of finding the particle is the same everywhere inside the well and for each value of position inside the well this constant probability is "$1/a$." These students typically claimed that the particle must be between $x = 0$ and $x = a$ but by knowing the exact energy, we can know nothing about position so the probable position is spread uniformly within in $0 < x < a$ region. Some students thought that the most probable values of position were the only possible values of the position that can be measured. The following statement was made by a student who thought that it may not be possible to measure the position after measuring the energy: "Can you even do that? Doesn't making a measurement change the system in a manner that makes another measurement invalid?" The fact that the student felt that making a measurement of one observable can make the immediate measurement of another observable invalid sheds light on the student's epistemology about quantum theory.

Difficulties with interpreting the expectation value as an ensemble average: Many students have difficulty in interpreting the expectation value as an ensemble average. For example, in a multi-university survey [24], students were given the wave function of an electron in a one-dimensional infinite square well as a particular linear superposition of ground and first excited states ($\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$). They were asked to write down the possible outcomes of energy measurement and their probabilities in part (I) and then calculate the expectation value of the energy in state $\Psi(x,t)$ in part (II).

In part (I), two-thirds of the students correctly stated that the only possible values of the energy in state $\Psi(x,0)$ are E_1 and E_2 and their respective probabilities are $2/7$ and $5/7$. But only slightly more than one-third provided the correct response for part (II). The discrepancy in percentages is due to the fact that many students who could calculate probabilities for the possible outcomes of energy measurement were unable to use that information to determine the expectation value of the energy. Since the expectation value of the energy is time-independent, if $\Psi(x,t) = C_1(t)\phi_1(x) + C_2(t)\phi_2(x)$, then the expectation value of the energy in this state is $\langle E\rangle = P_1E_1 + P_2E_2 = |C_1(t)|^2E_1 + |C_2(t)|^2E_2 = 2/7\,E_1 + 5/7\,E_2$, where $P_i = |C_i(t)|^2$ is the probability of measuring the energy E_i at time *t*. However, many students who answered part (II) correctly calculated $\langle E\rangle$ by "brute-force": first writing $\langle E\rangle = \int_{-\infty}^{\infty}\Psi\hat{H}\Psi dx$, expressing $\Psi(x,t)$ in terms of the linear superposition of two energy eigenstates, then acting with the operator $\hat{H}$ on the eigenstates, and finally using orthogonality to obtain the answer. Some got lost early in this process. Others did not remember some steps, for example, taking the complex conjugate of the wave function, using the orthogonality of stationary states, or recognizing the proper limits of the integral. The interviews revealed that many students did not know or recall the interpretation of expectation value as an ensemble average and did not recognize that expectation values could be calculated more simply in this case by taking advantage of their answer to part (I).

Confusion between individual measurements vs. expectation value: In response to the question discussed in the preceding section [24], some students who were asked about possible values of an energy measurement and their probabilities in a particular superposition of the ground and first excited state wave functions became confused between individual measurements of the energy and its expectation value. Almost none of them calculated the correct expectation value of the energy.

Incorrect assumption that all energies are possible when the state is in a superposition of only the ground and first excited states: In response to the question discussed in the preceding section [24], another mistake students made was assuming that all allowed energies for the infinite square well were possible if the measurement of energy was performed when the system was in state $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ and that the ground state energy is the most probable measurement outcome because it is the lowest energy state.

Difficulties with time development of the wave function after measurement of an observable: In a multi- university investigation [64], students were told that a measurement of the position of the particle is performed when it is in the first excited state of a one-dimensional finite square well and were asked about the time development of the wave function after the measurement. More than one-third of the students incorrectly claimed that the wave function of the system after a position measurement will go back to the first excited state (which was the state before the measurement was performed) after a long time. Other students who provided incorrect responses often claimed that the wave function was stuck in the collapsed state after the measurement. In one-on-one interview situations, when these students were told explicitly that their initial responses were not correct and they should think about what quantum mechanics predicts about what should happen to the wave function after a long time, students often switch from stating “it goes back to the original wave function before measurement” to “it remains stuck in the collapsed state” and vice versa. When students were told that neither of the possibilities is correct and that they should think about what quantum mechanics actually predicts, some of them explicitly asked the interviewer how there can be any other possibility. Thus, students have great difficulty with this three-part problem in which 1) the particle is initially in the first excited state of a 1D infinite square well, 2) a measurement of position collapses the wave function of the particle at the instant the measurement is performed, and 3) the wave function evolves again according to the TDSE. Connecting the different parts of this situation is extremely challenging for advanced students.

In the same multi-university investigation [64], students were told that the wave function for the system is $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ when a measurement of energy is performed. They were asked about the wave function a long time after the measurement if the energy measurement yields $4\pi^2\hbar^2/(2ma^2)$. Less than half of the students provided the correct response and an equal percentage claimed that a long time after the measurement, the system will be in the original superposition state $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$.

In response to a similar question [24], some students claimed that the answer to the question depends upon how much time you wait after the measurement. They claimed that at the instant you measure the energy, the wave function will be $\phi_2(x)$, but if you wait long enough it will go back to the state before the measurement. The notion that the system must go back to the original state before the measurement was sometimes deep-rooted. For example, when an interviewer said to a student that it was not clear why that would be the case, the student said, “The collapse of the wave function is temporary . . . something has to happen to the wave function for you to be able to measure energy or position, but after the measurement the wave function must go back to what it *actually* (student’s emphasis) is supposed to be.” When probed further, the student continued, “I remember that if you measure position you will get a delta function, but it will stay that way only if you do repeated measurements . . . if you let it evolve it will go back to the previous state (before the measurement).” Some students confused the measurement of energy with the measurement of position and drew a delta function for what the wave function will look like after the energy measurement. They claimed that the wave function will become very peaked about a given position after the energy measurement. As for the time evolution after that, students with these types of responses either incorrectly claimed that the system would be stuck in that peaked state or will evolve back to the original state of the system.

Incorrect belief that the Hamiltonian acting on a state represents energy measurement: In a multi-university investigation [23], students were asked to argue whether or not “$\hat{H}\Psi = E\Psi$” is always true for any possible Ψ of the system. Many students incorrectly claimed that any statement involving a Hamiltonian operator acting on a state is a statement about the measurement of energy. Some of the students who incorrectly claimed that “$\hat{H}\Psi = E\Psi$” is a statement about energy measurement agreed that the statement “$\hat{H}\Psi = E\Psi$” is always true, while others disagreed. Those who disagreed often claimed that “$\hat{H}\Psi = E_n\phi_n$” because as soon as $\hat{H}$ acts on Ψ, the wave function will collapse into one of the energy eigenstates ϕ_n and the corresponding energy E_n will be obtained. For example, one student stated: “Agree. $\hat{H}$ is the operator for an energy measurement. Once this measurement takes place, the specific value E of the energy will be known.” The interviews and written answers suggest that these students thought that the measurement of a physical observable in a particular state is achieved by acting with the corresponding operator on the state. These incorrect notions are overgeneralizations of the fact that the Hamiltonian operator corresponds to energy and after the measurement of energy, the system is in a stationary state so $\hat{H}\Psi = E_n\phi_n$. This example illustrates the difficulty students have in relating the formalism of quantum mechanics to the measurement of a physical observable.

In other investigations [61, 80], over half of the students claimed that either "$\hat{Q}\Psi = q_n\Psi$," "$\hat{Q}\Psi = q_n\Psi_n$," or both expressions are correct for a system in a state Ψ which is not an eigenstate of $\hat{Q}$. Neither of the aforementioned expressions is correct in terms of linear algebra. The response rates are very similar when the question is asked explicitly about the Hamiltonian operator. Thus, in this case, when "$\hat{H}\Psi = E_n\phi_n$" is explicitly brought to students' attention, more students are primed to select "$\hat{H}\Psi = E_n\phi_n$" as true compared to the case when they are asked the question in an open ended format (i.e., when they are asked if "$\hat{H}\Psi = E\Psi$" is always true for all possible wave functions) [23]. This difference in the percentages of students who select a particular incorrect response depending on whether some common difficulty was explicitly mentioned to prime students was discussed at the beginning of this section. This type of context dependence of responses is a sign of the fact that students do not have a robust knowledge structure of quantum mechanics.

Incorrect belief that "$\hat{Q}\Psi = \lambda\Psi$" is true for all possible Ψ of the system for any physical observable Q: In general, $\hat{Q}\Psi \neq \lambda\Psi$ unless Ψ is an eigenstate of $\hat{Q}$ with eigenvalue λ. A generic state Ψ can be represented as $\Psi = \sum_{n=1}^{\infty} D_n\psi_n$, where ψ_n are the eigenstates of $\hat{Q}$ and $D_n = \langle\psi_n|\Psi\rangle$. Then, $\hat{Q}\Psi = \sum_{n=1}^{\infty} D_n\lambda_n\psi_n$ (for an observable with a discrete eigenvalue spectrum). In Ref. [24], individual interviews suggest that some students thought that if an operator $\hat{Q}$ corresponding to a physical observable Q acts on any state Ψ, it will yield the corresponding eigenvalue λ and the same state back, that is, "$\hat{Q}\Psi = \lambda\Psi$" [24]. Some of these students were overgeneralizing their incorrect "$\hat{H}\Psi = E\Psi$" reasoning and attributing "$\hat{Q}\Psi = \lambda\Psi$" to the measurement of an observable Q.

Incorrect belief that an operator acting on a state represents a measurement of the corresponding observable: In Ref. [24], some students overgeneralized their incorrect notion that "$\hat{H}\Psi = E_n\phi_n$" to conclude that "$\hat{Q}\Psi = \lambda_n\psi_n$" must be true. They claimed that this equation is a statement about the measurement of Q which collapses the wave function into an eigenstate of $\hat{Q}$ corresponding to the eigenvalue λ_n measured [24].

2.4.6 Difficulties with the time-dependence of expectation values

Generally, the expectation value of an observable Q evolves in time because the state of the system evolves in time in the Schrödinger formalism. If an operator $\hat{Q}$ corresponding to an observable Q has no explicit time dependence (assumed throughout), taking the time derivative of the states in the expectation value and making use of the TDSE where appropriate yields Ehrenfest's theorem: $\frac{d}{dt}\langle Q(t)\rangle = \frac{\langle\Psi(t)|[\hat{Q},\hat{H}]|\Psi(t)\rangle}{i\hbar}$. Two major results can be deduced from this theorem: (1) The expectation value of an operator that commutes with the Hamiltonian is time-independent regardless of the initial state; and (2) If the system is initially in an energy eigenstate, the expectation value of any operator $\hat{Q}$ will be time-independent. The following student difficulties were commonly found via research [7, 81, 82]:

Difficulties in recognizing the relevance of the commutator of an operator corresponding to an observable and the Hamiltonian: A consequence of Ehrenfest's Theorem is that if an operator $\hat{Q}$ corresponding to an observable Q commutes with the Hamiltonian, the time derivative of $\langle Q \rangle$ is zero, regardless of the state. However, approximately half of students [81] did not realize that since the Hamiltonian governs the time-evolution of the system, any operator $\hat{Q}$ that commutes with it must correspond to an observable which is a constant of motion and its expectation value must be time-independent.

Difficulties in recognizing the special properties of stationary states: In the context of Larmor precession, if the magnetic field is along the z-axis, all expectation values are time independent if the initial state is an eigenstate of $\hat{S}_z$ because it is a stationary state. However, half of students [81] incorrectly stated that $\langle S_x \rangle$ and $\langle S_y \rangle$ depend on time in this case. One common difficulty includes reasoning such as "since the system is not in an eigenstate of $\hat{S}_x$, the associated expectation value must be time dependent," even in a stationary state. Another very common difficulty is reasoning such as "since $\hat{S}_x$ does not commute with $\hat{H}$, its expectation value must depend on time," even in a stationary state.

Difficulties in distinguishing between stationary states and eigenstates of operators corresponding to observables other than energy: Any operator corresponding to an observable has an associated set of eigenstates, but only eigenstates of the Hamiltonian are stationary states because the Hamiltonian plays a central role in the time-evolution of the state. However, many students were unable to differentiate between these concepts. For example, for Larmor precession with the magnetic field in the z-direction, half of the students [81] claimed that if a system is initially in an eigenstate of $\hat{S}_x$ or $\hat{S}_y$, the system will remain in that eigenstate. A related common difficulty is exemplified by the following comment from a student: "if a system is initially in an eigenstate of $\hat{S}_x$, then only the expectation value of S_x will not depend on time."

These difficulties related to the time-dependence of expectation values were often due to the following types of overgeneralizations or confusions:

- An eigenstate of any operator is a stationary state.
- If the system is initially in an eigenstate of $\hat{Q}$, then the expectation value of that operator is time independent.
- If the system is initially in an eigenstate of any operator $\hat{Q}$, then the expectation value of another operator $\hat{Q}'$ will be time independent if $[\hat{Q}, \hat{Q}'] = 0$.
- If the system is in an eigenstate of any operator $\hat{Q}$, then it remains in the eigenstate of $\hat{Q}$ forever unless an external perturbation is applied.
- The statement “the time dependent exponential factors cancel out in the expectation value” is synonymous with the statement “the system does not evolve in any eigenstate.”
- The expectation value of an operator in an energy eigenstate may depend upon time.
- If the expectation value of an operator $\hat{Q}$ is zero in some initial state, the expectation value cannot have any time dependence.
- Individual terms in a time-independent Hamiltonian involving a magnetic field can cause transitions from one energy eigenstate to another. Therefore, being in a stationary state of a harmonic oscillator potential energy system is different from being in a stationary state of a system in which an electron is at rest in a uniform magnetic field. In the latter case, the expectation values will depend on time in a stationary state but not for the former (because there is no field to cause a transition).
- Time evolution of a state cannot change the probability of obtaining a particular outcome when any observable is measured regardless of the initial state because the time evolution

operator is of the form $e^{-i\hat{H}t/\hbar}$, so time-dependent terms cancel out. Also, since $|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle$, the expectation value of any observable Q in a generic state $\langle\Psi(t)|\hat{Q}|\Psi(t)\rangle$ is time-independent.

2.4.7 Difficulties with the addition of angular momentum

For a system consisting of two spin-1/2 particles, the Hilbert space is four dimensional. There are two common ways to represent the basis vectors for the product space. Since the spin quantum numbers $s_1 = 1/2$ and $s_2 = 1/2$ are fixed, we can use the "uncoupled representation" and express the orthonormal basis vectors for the product space as $|s_1, m_1\rangle \otimes |s_2, m_2\rangle = |\, m_1\rangle \otimes |m_2\rangle$. In this uncoupled representation, the operators related to each particle (subspace) act on their own states, e.g., $\hat{S}_{1z}|1/2\rangle_1 \otimes |-1/2\rangle_2 = \frac{\hbar}{2}|1/2\rangle_1 \otimes |-1/2\rangle_2$ and $\hat{S}_{2z}|1/2\rangle_1 \otimes |-1/2\rangle_2 = -\frac{\hbar}{2}|1/2\rangle_1 \otimes |-1/2\rangle_2$. On the other hand, we can use the "coupled representation" and find the total spin quantum number for the system of two particles together. The total spin quantum number for the two spin-1/2 particle system, s, is either $1/2 + 1/2 = 1$ or $1/2 - 1/2 = 0$. When the total spin quantum number s is 1, the quantum number m_s for the z-component of the total spin, S_z, can be 1, 0, and -1. When the total spin is 0, m_s can only be 0. Therefore, the basis vectors of the system in the coupled representation are $|s = 1, m_s = 1\,\rangle$, $|s = 1, m_s = 0\,\rangle$, $|s = 1, m_s = -1\,\rangle$ and $|s = 0, m_s = 0\,\rangle$. In the coupled representation, the state of a two-spin system is not a simple product of the states of each individual spin although we can write each coupled state as a linear superposition of a complete set of uncoupled states. The following is a summary of the common difficulties students have with the addition of angular momentum [83, 84].

Difficulties with the dimension of a Hilbert space in product space: Students often incorrectly assumed that the dimension D of a product space consisting of two subspaces of dimensions D_1 and D_2 is $D = D_1 + D_2$, stating that this was true for the following reasons: (1) We are "adding" angular momentum; and (2) For two spin-one-half systems, the dimension is four which is both 2 × 2 and 2 + 2.

Difficulties in identifying different basis vectors for the product space: Students often displayed the following difficulties in identifying different basis vectors for the product space: (1) Some had difficulties with choosing a convenient basis to represent an operator as an $N \times N$ matrix in an N-dimensional product space; and (2) Some incorrectly claimed that if the operator matrix is diagonal in one representation, it must also be diagonal in another representation.

Difficulties in constructing an operator matrix in the product space and realizing that the matrix corresponding to an operator could be very different in a different basis: Students displayed the following difficulties in constructing an operator matrix in the product space: (1) Mistakenly adding the operators in different Hilbert spaces algebraically to construct the operator for the product space as if they act in the same Hilbert space; (2) Incorrectly claiming that the dimension of the operator matrix depends on the choice of basis vectors and it is lower for the un-coupled representation compared to the coupled representation; (3) Incorrectly assuming, e.g., that if $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$ is diagonal in the coupled representation, then $\hat{S}_{1z} + \frac{1}{2}\hat{S}_{2z}$ must also be diagonal in that representation; (4) Incorrectly assuming, e.g., for two spin-1/2 systems, that $\hat{S}_{1z} + \hat{S}_{2z}$ is a two-by-two matrix in a chosen basis but $\hat{S}_{1z}\hat{S}_{2z}$ is a four- by-four matrix; and (5) The Hamiltonian of the system must be known in order to construct a matrix for an operator other than the Hamiltonian operator.

2.4.8 Difficulties involving the uncertainty principle

The uncertainty principle is a foundational principle in quantum mechanics and is due to the incompatibility of operators corresponding to observables. In particular, if the operators corresponding to two observables do not commute, there will be an uncertainty relation between them. For example, the uncertainty principle between position and momentum is a particular example of the generalized uncertainty principle and says that the product of the standard deviations in the measurement of position and momentum for a given state of the system (wave function) must be greater than or equal to $\hbar/2$. Students have great difficulty with the uncertainty principle. Some major reasons for the difficulty are due to students' misunderstanding of the word uncertainty in this context. In particular, students often incorrectly associate the uncertainty principle with measurement errors or they mistake the concepts of standard deviations and average values (e.g., of position and momentum in the case of the position and momentum uncertainty principle). For example, in one study [85], many students incorrectly claimed that when a particle is moving fast, the position measurement has uncertainty because one cannot determine the particle's position precisely. They used this incorrect reasoning to infer that the uncertainty principle is due to the fact that if the particle has a large speed, the position measurement cannot be very precise. This type of reasoning is incorrect because it is not the speed of the particle, but rather, the uncertainty in the particle's speed that is related to the uncertainty in position. Further discussions with some students with these types of responses indicate that they were confused about measurement errors and/or attributed the uncertainty principle to something related to the expectation values of the different observables. In another multi-university study, students were asked a question about position and momentum uncertainty [64]. Many students incorrectly claimed that according to the uncertainty principle, the uncertainty in position is smaller when the expectation value of momentum is larger. Others incorrectly claimed that the expectation value of position is larger when the expectation value of momentum is smaller.

2.4.9 Difficulties with Dirac notation and issues related to quantum mechanics formalism

Because Dirac notation is used so extensively in upper-level quantum mechanics, it is important that students have a thorough understanding of this notation. However, research suggests that students have great difficulties with it [7, 73]. Below, we give examples of some difficulties found via research.

Difficulties in consistently recognizing the position space wave function in Dirac notation: In an investigation on students' facility with this notation, students displayed inconsistent reasoning in their responses to consecutive questions [73]. For example, on a multiple-choice survey, three consecutive conceptual questions were posed about the quantum mechanical wave function in position representation, with and without Dirac notation. In the first question, almost all of the students correctly noted that the position space wave function is $\Psi(x) = \langle x|\Psi\rangle$. The second question asked about a generic quantum mechanical operator $\hat{Q}$ (which is diagonal in the position representation) acting on the state $|\Psi\rangle$ in the position representation, i.e., $\langle x|\hat{Q}|\Psi\rangle$. Two of the answer choices were $\hat{Q}(x)\Psi(x)$ and $\hat{Q}(x)\langle x|\Psi\rangle$, which are both correct since $\Psi(x) = \langle x|\Psi\rangle$. However, more than one-third of the students incorrectly claimed that only one of the answers ($\hat{Q}(x)\Psi(x)$ or $\hat{Q}(x)\langle x|\Psi\rangle$) is correct, but not both. In the third question, more than a third of the students claimed that "$\langle x|\Psi\rangle = \int_{-\infty}^{\infty} x\Psi(x)dx$" is correct. However, it is incorrect because if $\Psi(x) = \langle x|\Psi\rangle$, then the expression "$\langle x|\Psi\rangle = \int_{-\infty}^{\infty} x\Psi(x)dx$" does not make sense. In a fourth consecutive question, more than a third of the students claimed that $\langle x|\Psi\rangle = \int_{-\infty}^{\infty} \delta(x - x')\Psi(x')dx'$ is incorrect. However, it is a correct equality because the integral results in $\Psi(x) = \langle x|\Psi\rangle$. We note that the integrals of the type shown above are easy for an advanced student taking quantum mechanics if the problem is given as a math problem without the quantum mechanics context.

Difficulties with the probability of obtaining a particular outcome for the measurement of an observable in Dirac notation: Students also struggled to find the probability of obtaining a particular outcome for a measurement of an observable in a given quantum state when they were asked the question in Dirac notation, even when they correctly identified the same probability in position representation (not written in Dirac notation) [73]. For example, in one question, they were told that an operator $\hat{Q}$ corresponding to a physical observable Q has a continuous non-degenerate spectrum of eigenvalues and the states $|q\rangle$ are the eigenstates of $\hat{Q}$ with eigenvalues q. They were also told that at time $t = 0$, the state of the system is $|\Psi\rangle$ and asked to select correct expressions for the probability of obtaining an outcome between q and $q + dq$ if they measure Q at time $t = 0$. The probability of obtaining an outcome between q and $q + dq$ can be written as $|\langle q|\Psi\rangle|^2 dq$ or $\left|\int_{-\infty}^{\infty} e_q^*(x)\Psi(x)dx\right|^2 dq$ in which $e_q(x)$ and $\Psi(x)$ are the wave functions corresponding to the states $|q\rangle$ and $|\Psi\rangle$, respectively. Some students thought that only the first expression is correct while others claimed that only the second expression is correct. Pertaining to this issue, one common difficulty revealed in the interviews was related to confusion about projection of a state vector. Projecting state vector $|\Psi\rangle$ along an eigenstate $|q\rangle$ or a position eigenstate $|x\rangle$ gives the probability density amplitude for measuring an eigenvalue q or probability density amplitude for measuring x, respectively, in a state $|\Psi\rangle$. These students often incorrectly claimed that an expression for the probability of measuring an observable in an infinitesimal interval must involve integration over q or x even when written in the Dirac notation.

Difficulties with expectation value, measured values, and their probabilities in Dirac notation: In a multi- university study [7], students were asked to find a mathematical expression for $\langle\phi|\hat{Q}|\phi\rangle$, where $|\phi\rangle$ is a general state and the eigenvalue equation for an operator $\hat{Q}$ is given by $\hat{Q}|\psi_i\rangle = \lambda_i|\psi_i\rangle$, $i = 1, \ldots, N$. The correct response is the following: $\langle\phi|\hat{Q}|\phi\rangle = \sum_i |\langle\psi_i|\phi\rangle|^2\lambda_i$, or simply $\sum_i |C_i|^2\lambda_i$, where $C_i = \langle\psi_i|\phi\rangle$. Less than half of the students provided the correct response. Some students had difficulty with the principle of linear superposition and with Dirac notation. They could not expand a general state in terms of the complete set of eigenstates of an operator. The common mistakes include writing incorrect expressions such as "$|\phi\rangle = |\psi\rangle$." "$|\phi\rangle = \sum_i |\psi_i\rangle$, "$\langle\phi|\psi_i\rangle = 1$," writing "$\lambda$" without any subscript in the answers, making mistakes with summation indices, etc. Also, many students in the written test and interviews could retrieve from memory that a general state $|\phi\rangle$ can be expanded as $\sum_n C_n|\psi_n\rangle$ but thought that $\langle\phi|\psi_n\rangle$ is unity. This dichotomy suggests that many students lack a clear understanding of what the expansion $|\phi\rangle = \sum_n C_n|\psi_n\rangle$ means and that $C_i = \langle\psi_i|\phi\rangle$ (which implies $\langle\phi|\psi_i\rangle = C_i^*$). In addition, some students thought that the eigenvalue λ_i gives the probability of obtaining a particular eigenstate and expanded the state as "$|\phi\rangle = \sum_i \lambda_i|\psi_i\rangle$."

Other difficulties with Dirac notation: In the investigation described in Ref. [73], some students also incorrectly claimed that one can always exchange the bra and ket states in the Dirac notation without changing its value if the operator sandwiched between them is a Hermitian operator corresponding to an observable, i.e., $\langle x|\hat{Q}|\Psi\rangle = \langle\Psi|\hat{Q}|x\rangle$ if $\hat{Q}$ is Hermitian. While some of them correctly reasoned that the eigenvalues of a Hermitian operator are real, they erroneously concluded that this implies that one can exchange the bra and ket states without complex conjugation if the scalar product involves sandwiching a Hermitian operator. Students also had difficulties explaining why the scalar product $\langle\Psi|\Psi\rangle = 1$ is dimensionless whereas $\langle x|\Psi\rangle$, which is also a scalar product of two states, has the dimensions of square root of inverse length. Moreover, similar to the difficulties with the position space wave function, students also had difficulties with the momentum space wave function.

2.5 INADEQUATE PROBLEM SOLVING, REASONING, AND SELF-MONITORING SKILLS

Although the studies discussed so far focused on the difficulties with specific topics while solving non-algorithmic problems, they also reveal that students in upper-level quantum mechanics courses often have inadequate problem-solving, reasoning, and self-monitoring skills. For example, some of these studies show that many students are inconsistent in their reasoning about a particular topic in quantum mechanics across different problems. Their responses are often context dependent and they are unable to transfer their learning from one situation to another appropriately. They often overgeneralize concepts learned in one situation to another in which they are not applicable. They also have difficulty distinguishing between related concepts and often make use of memorized facts and algorithms to solve problems. Moreover, they often have difficulty solving multi-part problems. The theoretical frameworks discussed earlier suggest that instructors must not only know students' difficulties with various topics, but also their current level of expertise in problem-solving, reasoning, and self-monitoring in order to tailor instruction and build on these skills. For example, according to Hammer's resource model, students' resources include not only their content knowledge, but also the skills they bring to bear to solve problems [55]. To tailor instruction appropriately, instructors should take into account students' resources effectively. In the same manner, in order to provide students an "optimal mismatch" [56] or to help students remain in the "zone of proximal development" [59], instruction must build on students' initial knowledge and skills in order to "stretch" their learning and develop useful skills. Similarly, to help students remain in the "optimal adaptability corridor" as suggested by Bransford and Schwartz [58], students must be given tasks that are appropriate to their skill level and are neither too efficient nor too innovative. All of these theoretical frameworks point to the fact that instructors must not only know students' difficulties with content, but also their level of expertise in their problem-solving, reasoning, and self-monitoring skills in order to help them learn effectively. An understanding of these student difficulties can enable instructors to design instruction to help students learn quantum mechanics content while developing their problem-solving, reasoning, and self-monitoring skills.

While the studies discussed so far have focused explicitly on investigating students' difficulties with various topics in upper-level quantum mechanics, fewer studies have focused explicitly on students' problem-solving and self- monitoring skills. The following two studies [13, 14] shed light on the problem-solving and self-monitoring skills of students in upper-level quantum mechanics.

2.5.1 Difficulties with categorizing quantum physics problems

Categorizing or grouping together problems based upon similarity of solution is often considered a hallmark of expertise. Chi et al. [86] used a categorization task to assess introductory students' expertise in physics. Unlike experts who categorized problems based on the physics principles, introductory students categorized problems involving inclined planes in one category and pulleys in a separate category. Lin et al. [14] extended this type of study and performed an investigation in which physics professors and students from two traditionally taught junior/senior level quantum mechanics courses were asked to categorize 20 quantum mechanics problems based upon the similarity of the solution. Professors' categorizations were overall rated higher than those of students by three faculty members who evaluated all of the categorizations without the knowledge of whether those categories were created by the professors or students. The distribution of scores obtained by the students on the categorization task was more or less evenly distributed with some students scoring similar to the professors while others obtained the lowest scores possible. This study suggests that there is a wide distribution in students' performance on a quantum mechanics categorization task, similar to the diversity in students' performance on a categorization of introductory physics problems. Therefore, the study suggests that it is inappropriate to assume that, because they have made it through the introductory and intermediate physics courses, all students in upper-level quantum mechanics will develop sufficient expertise in quantum mechanics after traditional instruction. In fact, the diversity in student performance in categorization of quantum mechanics problems suggests that many students are getting distracted by the "surface features" of the problem and have difficulty recognizing the deep features which are related to how to solve the problem. The fact that many students are struggling to build a robust knowledge structure in a traditionally taught quantum mechanics course suggests that it is inappropriate to assume that teaching by telling is effective for most of these students because it worked for the professors when they were students.

2.5.2 Not using problem solving as a learning opportunity automatically

Reflection and sense-making are integral components of expert behavior. Experts monitor their own learning. They use problem solving as an opportunity for learning by repairing, extending, and organizing their knowledge. One related attribute of physics experts is that they learn from their own mistakes in solving problems. Instructors often take for granted that advanced physics students will learn from their own mistakes in problem solving without explicit prompting or incentive, especially if students are given access to clear solutions. It is implicitly assumed that, unlike introductory students, advanced physics students have become independent learners and will take the time to learn from their mistakes–even if the instructors do not reward them for correcting them, for example, by explicitly asking them to turn in, for course credit, a summary of the mistakes they made and writing how those mistakes can be corrected. Mason et al. [13, 87] investigated whether advanced students in quantum mechanics have developed these self-monitoring skills and the extent to which they learn from their mistakes. They administered four problems in the same semester twice, both in the midterm and final exams, in a junior/senior level quantum mechanics course. The performance on the final exam shows that while some students performed equally well or improved compared to their performance on the midterm exam on a given question, a comparable number performed poorly both times or regressed (performed well on the midterm exam but performed poorly on the final exam). The wide distribution of students' performance on problems administered a second time points to the fact that many advanced students may not automatically exploit their mistakes as an opportunity for repairing, extending, and organizing their knowledge structure. Mason et al. [13, 87] also conducted individual interviews with a subset of students to delve deeper into students' attitudes towards learning and the importance of organizing knowledge. They found that some students focused on selectively studying for the exams and did not necessarily look at the solutions provided by the instructor for the midterm exams to learn partly because they did not expect those problems to show up again on the final exam and found it painful to confront their mistakes.

2.6 IMPLICATIONS OF THE RESEARCH ON STUDENT DIFFICULTIES

The research on student difficulties summarized here can help instructors, researchers, and curriculum designers design approaches to help students improve their content knowledge and skills and develop a functional understanding of upper-level quantum mechanics. These research studies can also pave the way for future research directions.

2.6.1 Research-based instructional approaches to reduce student difficulties

The scaffolding supports that are currently prevalent in research on upper-level quantum mechanics learning involve approaches similar to those that have been found successful at the introductory level [88-91]. These tools and approaches include: 1) tutorials [67, 79, 84, 85], which provide a guided inquiry approach to learning; 2) peer- instruction tools [92] such as reflective problems and concept-tests, which have been very effective in introductory physics courses; 3) collaborative problem solving; and 4) kinesthetic explorations [54, 93].

Several Quantum Interactive Learning Tutorials (QuILTs) that use a guided inquiry-based approach to learning have been developed to reduce student difficulties [23, 67, 70, 71, 74, 79, 82, 84, 85]. They are based on systematic investigations of difficulties students have in learning various concepts in quantum physics. They consistently keep students actively engaged in the learning process by asking them to predict what should happen in a particular situation and then providing appropriate feedback. They often employ visualization tools to help students build physical intuition about quantum processes. QuILTs help students develop content knowledge and skills by attempting to bridge the gap between the abstract, quantitative formalism of quantum mechanics and the qualitative understanding necessary to explain and predict diverse physical phenomena. They can be used by instructors in class to supplement lectures. Several students can work on them in groups. QuILTs consist of self-sufficient modular units that can be used in any order that is convenient. The development of a QuILT goes through a cyclical, iterative process which includes the following stages: (1) development of a preliminary version based on a theoretical analysis of the underlying knowledge structure and research on student difficulties; (2) implementation and evaluation of the QuILT by administering it individually to students; (3) determining its impact on student learning and assessing what difficulties were not remedied to the extent desired; and (4) refinements and modifications based on the feedback from the implementation and evaluation. The topics of these QuILTs include the time-dependent and time-independent Schrödinger equation, the time-development of the wave function, the time-dependence of an expectation value, quantum measurement, expectation values, bound and scattering state wave functions, the uncertainty principle, which-path information and double-slit experiments, a Mach-Zehnder interferometer (including the delayed choice experiment, interaction free measurement, quantum eraser, etc.), Stern Gerlach experiments, Larmor precession of spin, quantum key distribution (distribution of a key over a public-channel for encoding and decoding information using single photon states), the basics of a single spin system, and product space and addition of angular momentum (two separate QuILTs on coupled representation and uncoupled representation).

A pedagogical approach that has been used extensively in introductory physics courses is peer instruction [90, 91]. Similar approaches have been effective in helping students learn quantum mechanics [92]. In this approach, the instructor poses conceptual, multiple-choice questions to students periodically during the lecture. The focal point of the peer instruction method is the discussion among students based on the conceptual questions. The instructor polls the class after peer interaction to learn about the fraction of students with the correct answer and the types of incorrect answers that are common. Students learn about the course goals and the level of understanding that is desired by the instructor. The feedback obtained by the instructor is also valuable because the instructor determines the fraction of the class that has understood the concepts at the desired level. This peer instruction strategy helps students both learn content knowledge since students must answer conceptual questions and also develop reasoning and self-monitoring skills by asking them to explain their answers to their peers. The method keeps students actively engaged in the learning process and allows them to take advantage of each other’s strengths. It helps both the low and high performing students at a given time because explaining and discussing concepts with peers helps even the high performing students organize and solidify concepts in their minds. Recent data suggests that the peer instruction approach is effective in quantum mechanics [92].

Moreover, for introductory physics, Heller et al. [89] have shown that collaborative problem solving is valuable for learning physics and for developing effective problem-solving strategies. Prior research [94] has shown that even with minimal guidance from the instructors, introductory physics students can benefit from peer collaboration. In that study, students who worked with peers on conceptual electricity and magnetism questions not only outperformed an equivalent group of students who worked alone on the same task, but collaboration with a peer led to "co-construction" of knowledge in 29% of the cases. Co-construction of knowledge occurs when neither student who engaged in peer collaboration was able to answer the questions before the collaboration, but both were able to answer them after working with a peer on a post-test given individually to each person. Similar to the introductory physics study involving co-construction [94], a study was conducted in which conceptual questions on the formalism and postulates of quantum mechanics were administered individually and in groups of two to 39 upper-level students. It was found that co-construction occurred in 25% of the cases in which both students individually had selected an incorrect answer [95].

Developing a functional knowledge is closely connected to having appropriate epistemological views of the subject matter. Epistemological beliefs can affect students' motivation, enthusiasm to learn, time on task, approaches to learning, and ultimately, learning. Motivation can play a critical role in students' level and type of cognitive engagement in learning quantum mechanics. What types of instructional strategies can help improve students' epistemological views? Similar to students' views about learning in introductory mechanics, students' epistemological views about learning quantum mechanics can be improved if instructional design focuses on sense making and learning rather than on memorization of facts and accepting the instructor as authority. These effective instructional strategies should include encouraging students to work with peers to make sense of the material and providing problems in contexts that are interesting and appealing to students. Kinesthetic explorations [54, 93] can also be effective in this regard. Both formative assessments (e.g., peer instruction with concept tests, tutorial pre-tests/post-tests, collaborative problem-solving, homework assignments) and summative assessments (e.g., exams) should include problems that help students with conceptual reasoning and sense-making. Problems involving interesting applications such as quantum key distribution, Mach-Zehnder interferometer with single photons, and quantum eraser can be beneficial. Otherwise, students may continue to perform well on exams without developing a functional understanding, e.g., by successfully solving algorithmic problems involving solutions of the time-independent Schrödinger equation with complicated boundary conditions and potential energies.

2.6.2 Concluding remarks and future directions

Mathematically skilled students in a traditional introductory physics course focusing on mastery of algorithms can "hide" their lack of conceptual knowledge behind their mathematical skills [90]. However, their good performance on algorithmic physics problems does not imply that they have engaged in self-regulatory activities throughout the course or have built a hierarchical knowledge structure. In fact, most physics faculty, who teach both introductory and advanced courses, agree that the gap between conceptual and quantitative learning gets wider in a traditional physics course from the introductory to advanced level. Therefore, students in a traditionally taught and assessed quantum mechanics course can hide their lack of conceptual knowledge behind their mathematical skills even better than students in introductory physics. Closing the gap between conceptual and quantitative problem-solving by assessing both types of learning is essential to helping students in quantum mechanics develop functional knowledge. Interviews with faculty members teaching upper-level quantum mechanics [96, 97] suggest that some assign only quantitative problems in homework and exams (e.g., by asking students to solve the time-independent Schrödinger equation with complicated boundary conditions) because they think students will learn the concepts on their own. Nevertheless, as illustrated by the examples of difficulties in this paper, students may not adequately learn about quantum mechanics concepts unless course assessments value conceptual learning, sense-making, and the building of a robust knowledge structure. Therefore, to help students develop a functional knowledge of quantum mechanics, formative and summative assessments should emphasize the connection between conceptual understanding and mathematical formalism.

Further research comparing traditional and transformed upper-level quantum mechanics courses should be conducted to shed light on the extent to which students are making an effort to extend, organize, and repair their knowledge structure and develop a functional understanding. It would be valuable for future research studies to also investigate the extent to which students in these courses are making a connection between mathematics and physics, whether it is to interpret the physical significance of mathematical procedures and results, convert a real physical situation into a mathematical model, or apply mathematical procedures appropriately to solve the physics problems beyond memorization of disconnected pieces for exams. Students' ability to estimate physical quantities and evaluate limiting cases in different situations as appropriate and their physical intuition for the numbers across different content areas in traditional and transformed courses can be useful for evaluating their problem-solving, reasoning, and metacognitive skills. Although tracking the same student's learning and self-monitoring skills longitudinally is a difficult task, taking snapshots of physics majors' learning and self-monitoring skills across different physics content areas and across contexts within a topic can be very valuable. It would also be useful to explore the impact of traditional and non-traditional homework (e.g., reflective problems which are conceptual in nature) on student learning. More research on traditional and transformed courses is also needed to investigate the facility with which upper-level students transfer what they learned in one context to another context in the same course, whether students retain what they have learned when the course is over, and whether they are able to transfer their learning from one course to another (e.g., from quantum mechanics to statistical mechanics) or whether such transfer is rare. It will be useful to investigate the types of scaffolding supports that may significantly improve students' problem-solving, reasoning, and metacognitive skills in upper-level quantum mechanics and how and when such support should be decreased.

Finally, research should also focus on how community building affects how students learn quantum mechanics and on effective strategies for making students part of a learning community. It will also be useful to investigate the quality of students' communication about course content with their peers and the instructor in transformed upper-level quantum mechanics courses and learn about the extent to which students are more advanced compared to introductory physics students in the level of sophistication displayed by their word usage, terminology, and related semantics. We hope that this review of student difficulties will be helpful for developing learning tools and approaches to improve student learning of quantum mechanics.

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3.0 A FRAMEWORK FOR UNDERSTANDING THE PATTERNS OF STUDENT DIFFICULTIES IN QUANTUM MECHANICS

3.1 INTRODUCTION

A solid grasp of the fundamental principles of quantum physics is essential for many scientists and engineers. However, quantum physics is technically difficult and abstract. The subject matter makes instruction quite challenging, and even capable students constantly struggle to develop expertise and master basic concepts.

In order to help students develop expertise in quantum mechanics, one must first ask how experts compare to novices in terms of their knowledge structure and their problem-solving, reasoning, and metacognitive skills. According to Sternberg [1], some of the characteristics of an expert in any field include: 1) having a large and well organized knowledge structure about the domain; 2) spending more time in determining how to represent problems than searching for a problem strategy (i.e., more time spent analyzing the problem before implementing the solution); 3) working forward from the given information in the problem and implementing strategies to find the unknowns; 4) developing representations of problems based on deep structural similarities between problems; 5) efficient problem-solving; when under time constraints, experts solve problems more quickly than novices, and 6) accurately predicting the difficulty in solving a problem. Additionally, experts are more flexible than novices in their planning and actions [2].

Experts also have more robust metacognitive skills than novices. Metacognitive skills, or self-regulatory skills, refer to a set of activities that can help individuals control their learning [3].

The three main self-regulatory skills are planning, monitoring, and evaluation [4]. Planning involves selecting appropriate strategies to use before beginning a task. Monitoring is the awareness of comprehension and task performance. Evaluation involves appraising the product of the task and re-evaluating conclusions [4]. Self-regulatory skills are crucial for learning in knowledge-rich domains. For example, in physics, students benefit from approaching a problem in a systematic way, such as analyzing the problem (e.g., drawing a diagram, listing knowns/unknowns, and predicting qualitative features of the solution that can be checked later), planning (e.g., selecting pertinent principles/concepts to solve the problem), and evaluating (e.g., checking that the steps are valid and that the answer makes sense) [5]. When experts repeatedly practice problems in their domain of expertise, problem-solving and self-regulatory skills may even become automatic and subconscious [3]. Therefore, unless experts are given a new, "novel" problem, they may go through the problem-solving process automatically without making a conscious effort to plan, monitor, or evaluate their work [5, 6].

How can a student become an expert in physics, whether at an introductory or advanced level? There is a vast amount of research literature focusing on student reasoning difficulties in introductory courses, how students in introductory courses differ from physics experts in their problem-solving and self-regulatory skills, and the strategies that may help students become better problem solvers and independent learners (e.g., see Refs. [7-9]). Relatively few investigations have focused on the nature of expertise of advanced physics students and strategies that can be used in upper-level courses to help them build a robust knowledge structure and develop their problem-solving, reasoning, and metacognitive skills [10-17].

Investigations on the nature of expertise development in upper-level courses can benefit from having a framework, even if rudimentary, on which to develop research studies and interpret results. The framework can be refined further as more empirical evidence becomes available. Here, we describe a framework for understanding patterns of student reasoning difficulties and how students develop expertise in quantum mechanics. The framework proposes that the challenges many students face in developing expertise in upper-level quantum mechanics are analogous to the challenges students face in developing expertise in introductory classical mechanics. These analogous patterns of difficulties are often associated with the diversity in the goals, motivation, and prior preparation of upper-level students (i.e., the facts that even in an upper-level physics course, students may be inadequately prepared, have unclear goals, and may not have sufficient motivation to excel) as well as the "paradigm shift" from classical mechanics to quantum mechanics. The framework is based on research demonstrating that the patterns of difficulties in the context of quantum mechanics bear a striking resemblance to those found in introductory classical mechanics.

Why is it useful to have a framework for understanding the patterns of student difficulties and how students develop expertise in quantum mechanics? One common assumption of many physics instructors is that a majority of upper-level physics students are like them, having developed significantly better problem-solving, reasoning, and metacognitive skills than students in introductory physics. Instructors may also presume that, even without guidance and scaffolding support, upper-level students will automatically focus on building a robust knowledge structure of physics. In particular, many instructors assume that most upper-level physics students have developed good learning strategies, are eager and "primed" to learn in all their courses, and are unlikely to struggle in the same manner as students in introductory courses. However, research suggests that there is a large diversity in the preparation of students even in upper-level courses, both in terms of students' content knowledge and their problem-solving and self-regulatory skills

[18, 19]. If an instructor of an upper-level course targets instruction at a certain level, many underprepared students will struggle to learn. Furthermore, students have various motivations and goals for enrolling in a course and what they want to get out of a course. Many students will not necessarily be able to learn if the level of instruction is too advanced based on their current knowledge state. This problem is likely exacerbated in a traditionally taught course that does not accommodate the inadequate prior preparation of students and mainly involves lectures that are targeted assuming a certain level of expertise. Moreover, classical mechanics and quantum mechanics are two significantly different paradigms. Therefore, learning quantum mechanics can be challenging even for students who have developed a good knowledge structure of classical mechanics [20, 21]. Adopting such a framework and contemplating the analogous patterns of student difficulties in quantum mechanics and introductory classical mechanics can aid researchers in utilizing the extensive literature about introductory physics education in the design of teaching and learning tools for helping students develop expertise in quantum mechanics.

In the following sections, we first give an overview of the framework. We discuss the reasons for the diversity in the student population (which implies that there are students with inadequate preparation, unclear goals, and insufficient motivation for excelling in the course) and describe how the novel nature of the quantum paradigm make learning challenging in ways that are analogous to the challenges introductory students face in developing expertise in classical mechanics. Then, we describe how introductory physics students and upper-level students may face similar patterns of difficulty as they learn to unpack the respective principles and grasp the formalism in each knowledge domain during the development of expertise. We discuss empirical research data that provide evidence to support the framework and use concrete examples to illustrate how the patterns of student reasoning, problem-solving, and self-monitoring difficulties are analogous in these two sub-domains of physics. We also discuss how students' inadequate preparation, unclear goals, and insufficient motivation along with the paradigm shift can result in, e.g., a lack of a robust knowledge structure and effective problem-solving skills, transfer difficulties, lack of self-regulation, cognitive overload, and unproductive epistemologies. The concluding section focuses on the implications of this framework for quantum mechanics instruction and research-based instructional design. We discuss how the analogous patterns of difficulties in the two sub-domains of physics can inspire suitable adaptation of research-based strategies. In particular, research-based strategies for helping students develop expertise in introductory mechanics may also be effective in helping upper-level students learn quantum mechanics.

3.2 OVERVIEW OF THE FRAMEWORK

The framework of quantum mechanics student expertise and difficulties (FoQuSED) posits that the challenges many students face in upper-level quantum mechanics are analogous to the challenges introductory students face in classical mechanics. Figure 3-1 summarizes how the increased diversity in the student population, which implies that students who enroll in a course do not necessarily have adequate prior preparation, clear goals, and sufficient motivation to excel, combined with the "paradigm shift" can result in analogous patterns of learning difficulties in introductory mechanics and quantum mechanics. These factors can lead to difficulties in building a robust knowledge structure, developing effective problem-solving, reasoning, and metacognitive skills, transferring knowledge from one context to another, managing cognitive load, and developing productive epistemological views in each of these sub-domains of physics.

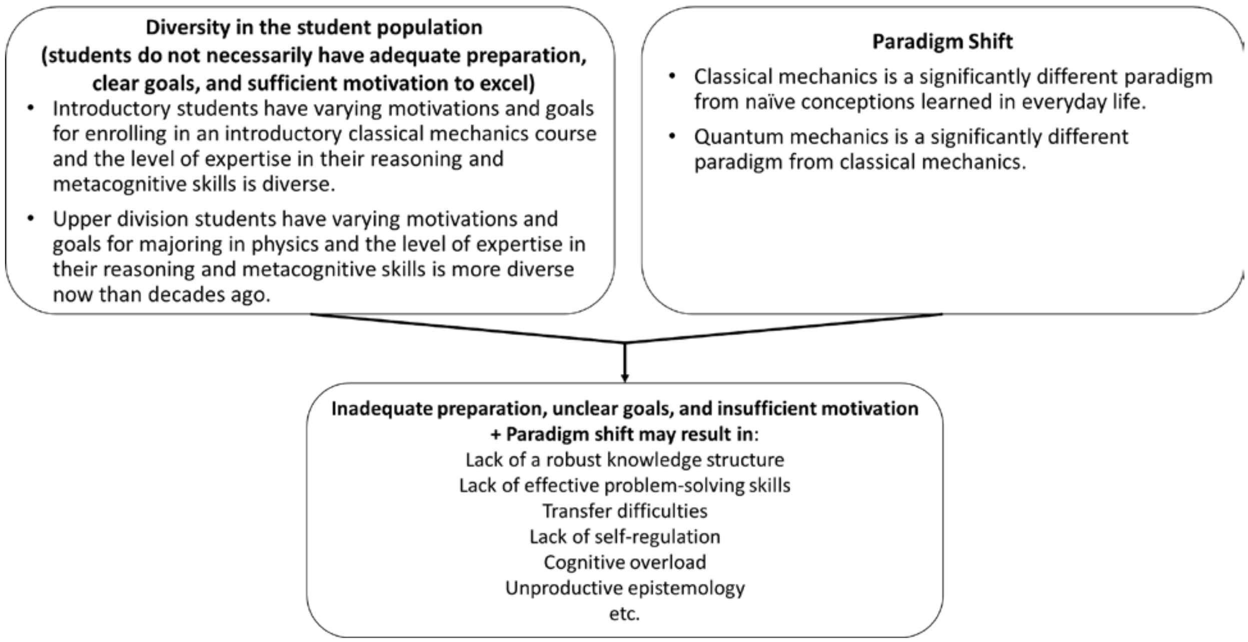

Figure 3-1. Framework of Quantum mechanics Student Expertise and Difficulties (FoQuSED) for understanding why patterns of difficulties in quantum mechanics are analogous to those in introductory classical mechanics

3.2.1 Diversity in students' prior preparation, goals, and motivation

Introductory physics is highly abstract and requires logical problem-solving, formal reasoning, and mathematical skills [22]. Many students have not mastered these types of skills by the time they enroll in an introductory college physics course and face difficulties in developing expertise. McDermott points out that the introductory student cannot be thought of as a "younger version" of the instructor [26]. She says that traditional introductory physics courses worked well for instructors, as they do for typically only 1 out of every 30 students in the class [23]. She emphasizes that "a large number of introductory students are inadequately prepared for the level of instruction. Unfortunately, a disproportionate percentage of minority students falls into this category" ([23], p. 302). Halloun and Hestenes developed a composite index, called the competence index, which is determined by students' prior preparation in physics and mathematics (as determined by the performance on diagnostic tests in physics and mathematics administered at the beginning of the course) and showed that the competence index has a significant correlation with students' performance at the end of the course [34]. Based upon the competence index, they state that "with probabilities greater than 0.60 in the large student population we have studied, high competence students were likely to receive an A or B course grade, average competence students were likely to receive a C grade, and low competence students were likely to receive a D or E grade" in traditionally taught algebra or calculus-based introductory physics courses ([34], p. 1047).

In fact, between the years 2003-2009, approximately 42% of beginning postsecondary students took remedial coursework in mathematics [24]. In 2000, approximately 20% of freshmen intending to major in science and engineering reported needing remedial work in mathematics and approximately 10% of them reported needing remedial work in science [24]. These percentages increase for women and minorities—of all freshmen science and engineering majors, approximately 26% of women and 40% of minorities reported needing remedial work in math in 1995 [25]. Students also have various goals and motivations for taking a physics course. They may enroll in a physics course because it is required for their major or they may have an intrinsic interest in the subject. Majors for students taking introductory physics include, for example, computer and information science, biology, medicine, mathematics, chemistry, and engineering. Students in these majors are likely to have diverse goals which can affect their motivation to develop a coherent knowledge structure of introductory physics.

Similar to the diversity of introductory students which makes teaching and learning challenging as McDermott, Halloun and Hestenes point out [23, 26, 34], there is also considerable diversity in upper-level students' preparation, motivation, and goals. Prior investigations have shown that there is a large diversity in both the content knowledge and in the problem-solving, reasoning, and self-regulatory skills of upper-level physics students in quantum mechanics [18, 19]. The goals and motivations for majoring in physics and the preparation of students in upper-level physics courses have gradually become more diverse [27]. A variety of statistics available from the American Institute of Physics (AIP) on undergraduate and graduate education point to the diverse goals and motivations of students enrolling in physics courses [27]. According to AIP data, the percentage of physics Ph.D. students pursuing an academic career (including all types of post-secondary institutions) has steadily decreased over time to approximately 20% currently [27]. AIP data also show that upper-level students' career plans have become more diverse in recent decades, which can impact their motivation to engage deeply with the material [27].

On the other hand, instructors of upper-level physics courses often assume that a majority of their students have already developed robust problem-solving, formal reasoning, mathematical, and self-regulatory skills. They may also believe that upper-level students will automatically make an effort to build a robust knowledge structure, engage in sense-making, and learn from their mistakes without guidance and scaffolding support. Instructors may also assume that all students have goals similar to their own when they were students and are intrinsically motivated to learn. Thus, instructors may teach the way they were taught, i.e., using the traditional approach, assuming that all students are "primed" to learn. Most do not take into account the diversity in students' prior preparation, goals, and motivation. This traditional approach is in contrast to the central tenets of PER-based instructional approaches, which focus on in-class and out-of-class activities and self-paced tools to build on the prior knowledge of a diverse group of students to help them develop expertise.

There is no doubt that some upper-level students are well prepared, have clear goals, and are sufficiently motivated to excel. While the percentage of such students in an upper-level course may be more than 1 out of 30 students as in an introductory physics course [23], a significant portion of students even in an upper-level course are neither intrinsically motivated to learn physics like their instructors nor are prepared or "primed" to learn from a traditional "lecture only" approach [18, 19]. This situation is similar to students in introductory physics courses failing to learn from traditional lectures alone [21, 28, 29]. Figure 3-2 summarizes the connections between the diversity in students' backgrounds and the final state of expertise in a traditional course (either introductory classical mechanics or quantum mechanics). For an individual student at the beginning of instruction, his/her prior preparation, goals, and motivation (PGM) can be thought of as components which can be weighted appropriately for an individual student to yield a composite PGM score (or "PGM," in short) to determine where he/she initially falls on the PGM spectrum (see Figure 3-2). Similar to each student's composite PGM in introductory physics, each student's PGM in an upper-level course can affect the extent and manner in which the student engages while learning quantum mechanics. In both introductory and upper-level courses, there is a distribution of individual student's PGM scores. Some students are highly prepared, motivated, and have clear goals while others are underprepared, have unclear goals, and lack sufficient motivation to excel. Traditional instruction may only benefit students above a threshold PGM at which instruction is targeted. In fact, highly prepared and motivated upper-level students may become experts in quantum mechanics regardless of the type of instruction. Some students who are not adequately prepared but are motivated to learn and have clear goals may also manage to develop expertise even in a traditionally taught course. However, underprepared students lacking clear goals and motivation who fall below the threshold PGM score (based upon the level at which the instruction is targeted in a traditional course) will struggle to develop expertise in a traditionally taught physics course that does not take into account individual student's prior knowledge and builds on it. These types of students may display learning difficulties which are analogous to the difficulties displayed by students learning introductory classical mechanics.

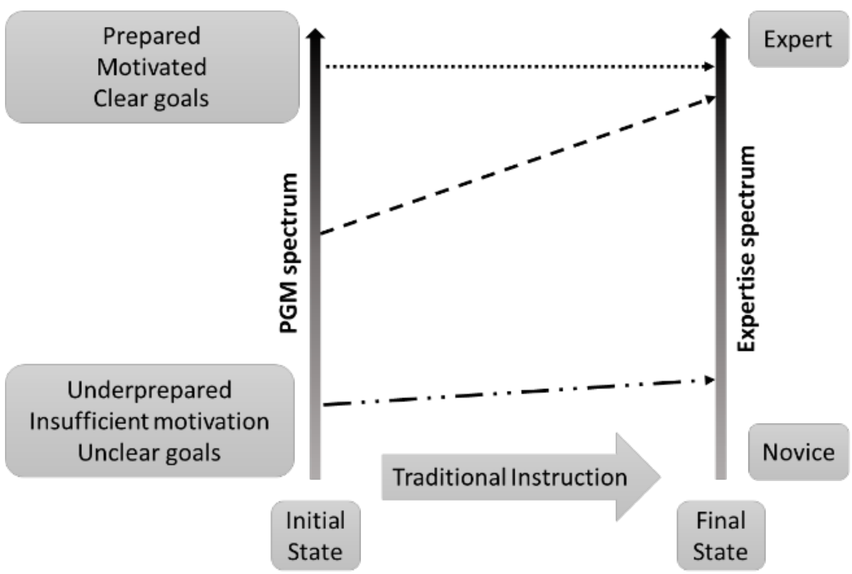

Figure 3-2. A student's initial preparation, goals, and motivation, when weighted appropriately, can yield a composite PGM score (or PGM). If a student's PGM is below a certain threshold, it can result in learning difficulties and impact the student's performance.

3.2.2 The paradigm shift

While the diversity in students' preparation, goals, and motivations (specifically, the fact that there are students with a PGM score below a certain threshold at which instruction is targeted) may partly account for the difficulties in learning classical mechanics and quantum mechanics, difficulties may be exacerbated by the fact that the paradigms of classical mechanics and quantum mechanics are significantly different than the paradigms that students in the respective courses have previously learned. Therefore, the very nature of a new paradigm causes additional difficulties for students. In his book *The Structure of Scientific Revolutions,* Thomas Kuhn focuses on the concept of a "paradigm shift," i.e., how insurmountable problems lead scientists to question a traditional paradigm's assumptions and a new paradigm emerges [30]. He states that "the reception of a new paradigm often necessitates a redefinition of the corresponding science" ([30], p. 103). He discusses how new paradigms are born from older paradigms and, as such, they often incorporate elements such as vocabulary, concepts, and experiments of the prior paradigm. However, the new paradigm does not utilize these elements in the traditional way, which can result in misunderstandings between the two paradigms and lead to learning difficulties. Kuhn discusses the example of the paradigm shift from classical mechanics to quantum mechanics to demonstrate how difficult it is to reconcile the old and new paradigms. He notes that as individuals begin learning a new paradigm, they may continue to apply their knowledge of the older paradigm onto the new paradigm, and this is not surprising. He states that, at least partly, "the source of resistance is the assurance that the older paradigm will ultimately solve all its problems, that nature can be shoved into the box the paradigm provides" ([30], pp. 151-152).

Kuhn’s work influenced science education research and inspired the theory of conceptual change [31, 32]. Research suggests that introductory physics students constantly try to make sense of the world around them. The mental models they build of how things work in everyday life are based on naïve reasoning and limited expertise and are often inconsistent with the laws of physics [33]. Moreover, everyday terms such as velocity, acceleration, momentum, energy, work, etc., do not have the same precise meaning as in physics and students must learn to differentiate between how those terms are used in physics vs. how they are used in everyday life. Students in introductory physics must shift from their adherence to their naïve mental models to the models consistent with the new paradigm of classical mechanics. Clement notes that students’ resistance in shifting from their naïve mental models to the classical mechanical model is not surprising, since “pre-Newtonian concepts of mechanics had a strong appeal, and scientists were at least as resistant to change as students are” ([22], p. 70]). Similarly, McDermott emphasizes that “the student mind is not a blank slate on which new information can be written without regard to what is already there. If the instructor does not make a conscious effort to guide the student into making the modifications needed to incorporate new information correctly, the student may do the rearranging. In that case, the message inscribed on the slate may not be the one the instructor intended to deliver” ([23], p. 305). Halloun and Hestenes also note that each student possesses beliefs and “common sense” intuitions about physical phenomena that are derived from their personal experience and they use these “common sense theories” to interpret what is taught in a physics course [34]. In fact, Clement emphasizes that a student possessing robust mathematical skills can “mask his or her misunderstanding of underlying qualitative concepts” ([22], p. 66). Having robust problem-solving skills does not guarantee success in developing a conceptual understanding of introductory physics—the students must revise their own "common sense theories" and build a coherent knowledge structure [22, 23, 34].

Similarly, students learning quantum mechanics must shift their adherence from the concepts and principles learned in classical mechanics to the new quantum paradigm in order to predict and explain quantum phenomena. Because the quantum mechanics paradigm is radically different from the classical paradigm, students must build a knowledge structure for quantum mechanics essentially from scratch, even if they have built a robust knowledge structure of classical mechanics. It is true that students are unlikely to have unproductive mental models about quantum mechanics concepts before formal instruction in quantum mechanics because one does not routinely encounter situations that require reasoning about quantum processes in everyday life. Therefore, one might assume that learning quantum mechanics may be easier than classical mechanics in this regard. However, as Kuhn suggests, the physics content knowledge that students learned in earlier courses, including classical mechanics, can interfere with building a robust knowledge structure of quantum mechanics. Similar to the possibility of naïve notions about velocity, momentum, or work from everyday experience interfering with learning classical mechanics, concepts of position, momentum, angular momentum, etc., are embedded so differently in the classical mechanics and quantum mechanics formalisms that intuition about these concepts developed in classical mechanics can actually interfere with learning quantum mechanics. For example, in quantum mechanics, the connection between quantum formalism and phenomena is made through measurement and inferences about physical observables, e.g., position, momentum, energy, and angular momentum. But unlike classical mechanics, a particle does not, in general, have a definite position, momentum, or energy in quantum mechanics. In quantum mechanics, all information about a system is contained in the state vector or wave function, which lies in an abstract vector space. The measurement of an observable collapses the wave function to an eigenstate of the operator corresponding to the observable measured, and the probability of measuring a particular value can be calculated from the knowledge of the wave function. These novel quantum concepts have no analogs in classical mechanics even though position, momentum, energy, angular momentum, etc., are common terms in both paradigms. Similar to introductory students' difficulties, upper-level students' difficulties with quantum concepts can be masked if they have developed robust mathematical skills. Indeed, the gap between conceptual and quantitative learning can continue to get wider at the advanced level in the traditional mode of instruction that focuses on "plug and chug" approaches to teaching and assessment. Unless upper-level students construct a coherent knowledge structure of quantum mechanics, difficulties at the conceptual level will persist.

3.2.3 Analogous patterns of difficulty in the development of expertise in classical mechanics and quantum mechanics

As discussed in the previous sections, in both introductory physics and quantum mechanics, the large diversity in students' goals, motivations, and prior preparation (specifically, a sufficient number of students with a PGM score below a threshold at which instruction is targeted) coupled with the paradigm shift can result in learning difficulties as students develop expertise in each of these sub-domains of physics. As introductory and upper-level students start to build a knowledge structure about classical mechanics and quantum mechanics, respectively, their knowledge will initially be in disconnected pieces [33, 35] and their reasoning about their respective domains will only be locally consistent and lack global consistency. In fact, there is nothing unusual about students going through this stage. Those who begin their pursuit of developing expertise in any knowledge-rich domain must go through a phase in which their knowledge is in small, disconnected pieces which are only locally consistent, and this “knowledge in pieces” phase causes reasoning difficulties [33, 35, 36-38]. While students struggle to manage many small, disconnected pieces of knowledge, they can experience cognitive overload [39] and may not have the cognitive capacity to engage in self-regulatory activities. Additionally, students may possess relevant knowledge to solve a problem, but they may not invoke or apply relevant knowledge pieces appropriately in certain contexts. Cognitive overload and failure to invoke or apply relevant knowledge may lead to inconsistent reasoning and difficulties in the transfer of knowledge. Each student must go through the process of gradually building a knowledge structure and pass through the “knowledge in pieces” phase [33] while learning classical mechanics and quantum mechanics separately because the conceptual paradigms are sufficiently different in these sub-domains of physics as discussed (even though the same terminology is used, e.g., momentum, energy, etc.).

Instructors of upper-level courses may inadvertently teach students at a level which is not aligned with many students’ prior preparation, goals, and motivation because they often assume that a majority of their students have already developed robust problem-solving, reasoning, and metacognitive skills and that they are intrinsically motivated to learn. However, if instruction in quantum mechanics is not aligned with students’ prior preparation, many students will struggle to learn because they may not have developed robust problem-solving, reasoning, and metacognitive skills. Furthermore, students have various goals for enrolling in a quantum mechanics course and many of them are not necessarily intrinsically motivated to learn [19]. Even if students are prepared, have clear goals, and are intrinsically motivated to learn, they may bring to bear prior classical conceptions within the new paradigm of quantum mechanics. Thus, students’ mastery of classical mechanics does not imply that they will be able to master quantum mechanics without a conscious effort on the part of the students to build a knowledge structure of quantum mechanics and assimilate and accommodate new ideas (and make lateral connections between the classical mechanics and quantum mechanics schema to understand the differences between these formalisms explicitly and when and how they come together, e.g., by taking the classical limit). Therefore, students learning classical mechanics and quantum mechanics are likely to show similar patterns of reasoning difficulties as they move up along the expertise spectrum in each of these sub-domains of physics. In each case, if students continue their efforts to repair, reorganize, and extend their knowledge structure [36-38] they will reach a point where their knowledge structure becomes robust enough that they become a nominal expert. Then, they will be able to make predictions and inferences which are globally consistent within the respective formalisms and their reasoning difficulties will be significantly reduced. Even after becoming a nominal expert, a student's expertise in the respective sub-domain of physics can keep evolving. In the knowledge schema of classical mechanics or quantum mechanics, the strengthening of nodes and building of additional links between nodes (even if there are redundancies in the links) can make students transition from nominal to adaptive experts who can solve more complex problems [36-38, 40].

3.3 EXAMPLES OF ANALOGOUS PATTERNS OF STUDENT DIFFICULTIES IN QUANTUM MECHANICS AND INTRODUCTORY CLASSICAL MECHANICS

Upper-level physics students typically display expert-like behavior when solving problems in introductory classical mechanics because they possess a large amount of compiled knowledge about introductory physics due to repetition of the basic content in various courses [41]. They may not need to do much self-regulation while solving introductory problems [36, 41]. However, they may fail to use these skills when solving problems in the domain of quantum mechanics in which they are not experts and may display patterns of difficulties analogous to those of students learning introductory classical mechanics.

Below, we discuss empirical evidence for the framework based upon research on student difficulties in quantum mechanics and introductory classical mechanics. In particular, we discuss concrete examples of difficulties involving: 1) categorization of problems based upon how they are solved; 2) not using problem solving as an opportunity for learning; 3) inconsistent and/or context-dependent reasoning; 4) inappropriate or negative transfer from one situation to another; 5) lack of transfer of knowledge; 6) "gut-feeling" responses inconsistent with the laws of physics; 7) solving multi-part problems; and 8) epistemological issues. Each of these types of difficulties are symptoms of ineffective problem solving, a lack of self-regulation, an incoherent knowledge structure, cognitive overload, an inability to transfer knowledge appropriately, or unproductive epistemologies. It is impossible to disentangle the contributions of the paradigm shift and the inadequate preparation, unclear goals, and insufficient motivation of students to each example of difficulty discussed below. However, each difficulty is an indication of how these factors can result in impediments to learning. We note that many of the examples of student difficulties in introductory classical mechanics and quantum mechanics discussed below could be placed into multiple categories of difficulties, but we have typically chosen to place them in one of the categories mentioned earlier since they are used to illustrate a particular type of analogous difficulty in introductory mechanics and quantum mechanics. In particular, we place each example in one category which clearly represents the difficulty.

3.3.1 Categorization of physics problems

3.3.1.1 In quantum mechanics

Categorization of problems refers to grouping problems together based upon how one would solve the problems. Lin and Singh [18] performed an investigation in which physics professors and students from two junior/senior level quantum mechanics courses were asked to categorize twenty quantum mechanics problems based upon the similarity of the solutions. Students completed the categorization task after instruction in relevant concepts. Professors' categorizations were overall rated higher than those of students by three faculty members who evaluated all of the categorizations blindly (without the knowledge of whether the categories were created by the professors or students). Many students categorized quantum mechanics problems based on the surface features of the problems, such as "infinite square well problem," "free particle problem," or "Stern-Gerlach problem." The scores obtained by the students on the categorization task were more or less evenly distributed with some students scoring similar to the professors while other students scored extremely low.

3.3.1.2 In introductory physics

Chi et al. used a categorization task to assess introductory physics students' expertise in classical mechanics after instruction in relevant concepts [42]. Unlike physics experts who categorized problems based on the physics principles (e.g., conservation of mechanical energy, conservation of momentum, etc.), introductory students categorized problems based on surface features, such as "inclined plane problems" and "pulley problems" [42].

3.3.1.3 Possible causes for poor categorization in quantum mechanics and introductory classical mechanics

Categorizing problems based upon the similarity of solution is often considered a hallmark of expertise [42, 43]. The wide distribution in students' performance on the categorization tasks in introductory classical mechanics and quantum mechanics suggests that students are still developing expertise in the respective sub-domains of physics. Students' prior preparation, goals, and motivation as well as the paradigm shift can affect the extent to which students develop expert-like approaches to problem categorization. If students have not developed expertise in the respective sub-domains of physics, they may focus on the "surface features" rather than "deep features" of the problems with a negative impact on their performance in categorizing problems. Furthermore, students' goals and motivations for enrolling in a course can impact the extent to which they develop a coherent knowledge structure of classical mechanics or quantum mechanics and are able to group together problems with differing surface features but equivalent deep features. Students may also incorrectly categorize problems based upon their "common sense theories" in classical mechanics or prior classical mechanics knowledge in quantum mechanics, depending on the type of problem posed.

3.3.2 Not using problem solving as a learning opportunity

3.3.2.1 In quantum mechanics

One attribute of physics experts is that they learn from their own mistakes while solving problems. Mason and Singh [19] investigated the extent to which upper-level students in quantum mechanics learn from their mistakes. In this investigation, they administered four problems in the same semester twice, on the midterm and final exams in an upper-level quantum mechanics course. The performance on the final exam shows that while some students performed equally well or improved compared to their performance on the midterm exam on a given question, a comparable number performed poorly both times or regressed (i.e., performed well on the midterm exam but performed poorly on the final exam). The wide distribution of students' performance on problems administered a second time points to the fact that many advanced students may not automatically exploit their mistakes as an opportunity for repairing, extending, and organizing their knowledge structure. Mason and Singh [19] also conducted individual interviews with a subset of students to delve deeper into students' attitudes toward learning and the importance of organizing knowledge. They found that many students focused on selectively studying for the exams and did not necessarily look at the solutions provided by the instructor for the midterm exams to learn, partly because they did not expect those problems to be repeated on the final exam and/or found it painful to confront their mistakes. When students were given grade incentives to fix their mistakes on a midterm exam, they did significantly better on similar final exam problems than students who were not given a grade incentive to fix their mistakes on the midterm exam [99].

3.3.2.2 In introductory classical mechanics

Yerushalmi et al. [44] investigated the extent to which diagnosing one's own mistakes in multi-part recitation quiz problems (by rewarding students for completing a self-diagnosis task during a following recitation class) helped students in introductory classical mechanics perform better on similar exam problems given later. Students in the three intervention groups diagnosed their mistakes by either 1) using a detailed solution provided by the teaching assistant (TA); 2) having the TA outline the main features of the solutions; or 3) consulting their own books and notes. The students in an equivalent comparison group were not explicitly asked to diagnose their mistakes. It was found that, compared to the comparison group, the performance on challenging follow-up exam problems was 46% better for students who diagnosed their mistakes by consulting their books and notes compared to those who were provided a detailed solution. The students in this intervention group were generally more engaged and struggled more to diagnose their mistakes than those in the intervention group in which the TA provided a detailed solution. The study suggests that introductory students do not use problem solving as a learning opportunity unless they are given an incentive (e.g., via grades) to diagnose their mistakes and become cognitively engaged with the material.

3.3.2.3 Possible causes for not automatically using problem solving as a learning opportunity in quantum mechanics and introductory physics

Students' goals, motivation, and prior preparation may affect whether they use problem solving as a learning opportunity without an explicit reward system. Students may not automatically use problem solving as a learning opportunity because they have not necessarily developed robust self-monitoring skills. Furthermore, many introductory students and upper-level students have not become independent learners and they do not necessarily have intrinsic motivation to learn from their mistakes. Also, as students are developing expertise in a new paradigm, they may be in a "knowledge in pieces" phase [33] and may not necessarily have the cognitive capacity to automatically learn from their mistakes.

3.3.3 Inconsistent and/or context-dependent reasoning

3.3.3.1 In quantum mechanics

Inconsistent reasoning about the time dependence of an expectation value of an observable in the context of Larmor precession: Eighty-nine students from multiple universities were asked the following question about the time-dependence of the expectation value of an electron spin component [20]:

An electron is in a uniform magnetic field B that is pointing in the z-direction. The Hamiltonian for the spin degree of freedom for this system is given by $\hat{H} = -\gamma B \hat{S}_z$ where γ is the gyromagnetic ratio and $\hat{S}_z$ is the z component of the spin angular momentum operator. If the electron is initially in an eigenstate of $\hat{S}_x$, does the expectation value of $\hat{S}_y$ depend on time? Justify your answer.

Some students correctly stated that the expectation value of $\hat{S}_y$ is zero if the initial state is an eigenstate of $\hat{S}_x$. However, they incorrectly claimed that the time dependence of the expectation value of $\hat{S}_y$ is also zero. For example, one interviewed student argued that the expectation value is zero when the initial state is not an eigenstate of the spin component whose time dependence of expectation value is desired. His argument was that all eigenstates of $\hat{S}_x$ are orthogonal to all eigenstates of $\hat{S}_y$ (which is actually not true although the expectation value of $\hat{S}_y$ is zero for the given initial state which is an eigenstate of $\hat{S}_x$). The interviewer reminded him that the eigenstate of $\hat{S}_x$ is only the initial state and he had to find the time dependence of the expectation value of $\hat{S}_y$. The student immediately responded: "I understand that ... [but] since the expectation value of $\hat{S}_y$

is zero in the initial state ... so is its time dependence." In the context of an electron which is initially in an eigenstate of $\hat{S}_x$ in a uniform magnetic field, the student was unable to differentiate between the expectation value and rate of change of the expectation value. Students often display inconsistent reasoning in different contexts, e.g., students may recognize the difference between the expectation value and the rate of change of the expectation value in a particular context but are unable to recognize the difference in another context.

Inconsistency in identifying a quantum state in position representation: Students in quantum mechanics courses often display inconsistent reasoning in their responses to consecutive questions. For example, a conceptual, multiple-choice survey was administered to 39 upper-level students to determine the extent to which they use appropriate problem-solving, reasoning, and self-regulatory skills while solving quantum mechanics problems [45]. In addition, think-aloud interviews were conducted with 23 students to observe how they reasoned about the quantum mechanics problems. On the multiple-choice survey, three consecutive conceptual questions were posed about the quantum mechanical wave function in position representation with and without Dirac notation. In the first question, 90% of the students correctly noted that the position space wave function is $\Psi(x) = \langle x|\Psi\rangle$. However, the second question asked about a generic quantum mechanical operator $\hat{Q}$ acting on the state $|\Psi\rangle$ in the position representation, i.e., $\langle x|\hat{Q}|\Psi\rangle$. Students were told that $\hat{Q}$ was a diagonal operator in position representation. Two of the answer choices were $Q(x)\langle x|\Psi\rangle$ and $Q(x)\Psi(x)$, which are both correct since $\Psi(x) = \langle x|\Psi\rangle$. A student who is self-monitoring would note that the two statements are the same since $\Psi(x) = \langle x|\Psi\rangle$. However, 41% of the students claimed that only one of the answers ($Q(x)\langle x|\Psi\rangle$ or $Q(x)\Psi(x)$) is correct, but not both. In the third question, 36% of the students claimed that $\langle x|\Psi\rangle = \int x\Psi(x)dx$ is correct.

However, it is incorrect because if $\Psi(x) = \langle x|\Psi\rangle$, then $\langle x|\Psi\rangle = \int x\Psi(x)dx = \Psi(x)$ does not make sense. In a fourth consecutive question, 39% of the students claimed that $\langle x|\Psi\rangle = \int \delta(x - x')\Psi(x')dx'$ is incorrect (it is a correct equality because the integral results in $\Psi(x)$). In one interview, a graduate student who noted correctly that $\Psi(x) = \langle x|\Psi\rangle$ but who incorrectly claimed that $\langle x|\Psi\rangle = \int \delta(x - x')\Psi(x')dx'$ is incorrect reasoned as follows "… it just doesn't seem correct, that $\Psi(x)$ should just pop out [of the integral]. It's giving you just a wave function of x and I just don't like that. I think [the inner product] should just give you a number." He correctly reasoned that the inner product is a number, but did not make the connection that $\Psi(x)$ is also a number for any particular value of x. He was so focused on his concern that the inner product is a number that he did not notice the inconsistency between the responses to this question and question 1 in which he appeared quite confident that $\Psi(x) = \langle x|\Psi\rangle$. We note that the integrals of the type shown above are simple to solve for an advanced student taking quantum mechanics if the problem is given as a math problem without the quantum mechanics context. However, in the context of quantum mechanics, the integral involving a delta function was enough to make this student (and many others) concerned about whether the physical content of that statement made sense from the point of view of quantum mechanics when the integral was nothing more than $\Psi(x) = \langle x|\Psi\rangle$.

Inconsistency in determining possible wave functions for an infinite square well: Research suggests that many students are inconsistent in their responses to whether a specific wave function is allowed for an infinite square well [46]. For example, the following question was administered to students in quantum mechanics courses at many different universities:

Which of the following wave functions are allowed for an electron in a one dimensional infinite square well of width a with boundaries at $x = 0$ and $x = a$? In each of the three cases, A is a suitable normalization constant. You must provide clear reasoning for each case.

I. $Asin^3(\pi x/a)$

II. $A(\sqrt{2/5}\,sin(\pi x/a) + \sqrt{3/5}\,sin(2\pi x/a))$

III. $Ae^{-((x-a/2)/a)^2}$

The wave function $Ae^{-((x-a/2)/a)^2}$ is not allowed because it does not satisfy the boundary conditions. The first two wave functions are both smooth functions which satisfy the boundary conditions, so each can be written as a linear superposition of the stationary states. Therefore, they are both possible wave functions. However, 45% of the students claimed that $Asin^3(\pi x/a)$ is not an allowed wave function but $A(\sqrt{2/5}\,sin(\pi x/a) + \sqrt{3/5}\,sin(2\pi x/a))$ is an allowed wave function. The most common reason for claiming that $Asin^3(\pi x/a)$ is not allowed was that it does not satisfy the time-independent Schrödinger equation, $\hat{H}\Psi(x) = E\Psi(x)$. Students incorrectly claimed that the time-independent Schrödinger equation was the equation that all allowed wave functions should satisfy. Many of the students asserted that $Asin^3(\pi x/a)$ does not satisfy $\hat{H}\Psi(x) = E\Psi(x)$ but $A(\sqrt{2/5}\,sin(\pi x/a) + \sqrt{3/5}\,sin(2\pi x/a))$ does, which is incorrect (because neither satisfies the time-independent Schrödinger equation). In their reasoning, many students explicitly wrote the Hamiltonian as $(-\hbar^2/2m)\,\partial^2/\partial x^2$ and showed that the second derivative of $Asin^3(\pi x/a)$ would not yield the same wave function back multiplied by a constant, which is a correct statement (although it does not imply that $Asin^3(\pi x/a)$ is not a possible wave function, which is what they were trying to prove). On the other hand, the same students did not attempt to explicitly take the second derivative of $A(\sqrt{2/5}\, sin(\pi x/a) + \sqrt{3/5}\, sin(2\pi x/a))$, which also does not yield the same wave function back multiplied by a constant. For this wave function, a majority claimed that it is a possible wave function because it is a linear superposition of the functions $sin(n\pi x/a)$. Many students used incorrect inconsistent reasoning, claiming that a linear superposition of stationary states would satisfy the time-independent Schrödinger equation $\hat{H}\Psi(x) = E\Psi(x)$ but that $Asin^3(\pi x/a)$ would not satisfy it (even though $Asin^3(\pi x/a)$ can also be written as a linear superposition of two stationary states). Furthermore, in interviews, when students were asked whether or not $sin^3(x)$ can be written as a sum of sine functions, some of them remembered that it can be written as a sum of sine functions (i.e., $sin^3(x) = (3\, sin(x) - sin(3x))/4$). But even with this realization, some students did not change their previous answer that $Asin^3(\pi x/a)$ is not a possible wave function but $A(\sqrt{2/5}\, sin(\pi x/a) + \sqrt{3/5}\, sin(2\pi x/a))$ is. Thus, while many students explicitly showed that $Asin^3(\pi x/a)$ did not satisfy the time-independent Schrödinger equation and recalled that $Asin^3(\pi x/a)$ can be written as a linear superposition of sine functions, they did not use this knowledge to interpret that linear combinations of stationary states with different energies do not satisfy the time-independent Schrödinger equation (contrary to their claim).

Inconsistent reasoning about a possible wave function for a finite square well: Another instance of inconsistent reasoning in quantum mechanics is displayed in the following example. The following question about a particle in a finite square well was administered to 226 students from multiple universities [47]:

Choose all of the following statements that are correct about the wave function for a particle in a one-dimensional finite square well shown below at time $t = 0$. $\Psi(x,0)$ and $d\Psi(x,0)/dx$ are continuous and single-valued everywhere. The wave function $\Psi(x,0)$ is zero in the regions $x < b_1$ and $x > b_2$. Assume that the area under the $|\Psi(x,0)|^2$ curve is 1.

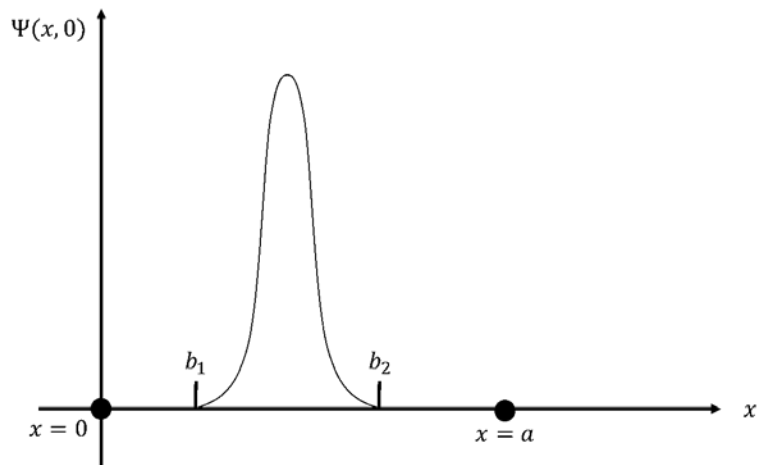

Figure 3-3. A possible wave function for a particle in a finite square well.

(1) It is a possible wave function.

(2) It is not a possible wave function because it does not satisfy the boundary conditions. Specifically, it goes to zero inside the well.

(3) It is not a possible wave function because the probability of finding the particle outside the finite square well is zero but quantum mechanically it must be nonzero.

A. 1 only B. 2 only C. 3 only D. 2 and 3 only E. None of the above

Forty percent of the students selected the correct response (A). Fifty-five percent of the students incorrectly responded that it is not a possible wave function. Students correctly reasoned that for a finite square well, the particle has a non-zero probability of being in the classically forbidden region in a stationary state. However, they incorrectly overgeneralized this knowledge and claimed that any possible wave function for this system must also have a nonzero probability in the classically forbidden region [47]. In individual interviews, students who answered the above question incorrectly were asked if a highly localized function (approximately a delta function in position) could represent a possible wave function because that is what one obtains after a position measurement. Some students readily responded that a delta function could represent a possible wave function because you can obtain a delta function wave function after a position measurement. However, some of them failed to reason that if a delta function can be a possible wave function for a finite square well, then the wave function in Figure 3-3 can also be a possible wave function. Students did not note the inconsistency in their statements that a delta function is a possible wave function but the wave function in the question discussed above does not represent a possible wave function for a finite square well. For the wave function shown in Figure 3-3, students focused on the fact that the stationary state wave functions of a finite square well have non-zero values in the classically forbidden region.

3.3.3.2 In introductory classical mechanics

Inconsistent reasoning about velocity and acceleration: Similar to upper-level students in quantum mechanics claiming that if the expectation value of an operator is zero in an initial state, then the time dependence of the expectation value of that operator is also zero, introductory students often claim that if the velocity of a particle is zero, the particle must have zero acceleration (rate of change of velocity is zero). This type of inconsistent reasoning about a physical quantity and rate of change of that physical quantity has been found in other introductory physics contexts as well.

Inconsistent reasoning about Newton's Second Law: A lack of consistency in student responses is well-documented in introductory physics. In introductory mechanics, a student may correctly reason in a simple context that a larger net force on an object would imply a larger acceleration (as opposed to a larger constant velocity), but incorrectly claim that the net force is larger on an object moving at a constant velocity of $2\vec{v}_o$ compared to one that is moving at $\vec{v}_o$ [48].

Inconsistent reasoning in applying Newton's Third Law: On the Force Concept Inventory [48], there are many questions involving Newton's Third Law. Typically, the percentage of students at a typical state university who answer these questions correctly is quite varied, with approximately 80% of the students providing correct responses in some contexts while only approximately 20% provide correct responses for other questions [48].

3.3.3.3 Possible causes for inconsistent reasoning and/or context-dependent reasoning in quantum mechanics and introductory classical mechanics

The above examples indicate that students in both introductory classical mechanics and quantum mechanics may fail to use appropriate problem-solving and self-regulatory skills while solving problems in a domain in which they are still developing expertise. This may be due, in part, to students' inadequate prior preparation. Students who have not developed robust problem-solving, reasoning, and metacognitive skills will display inconsistent reasoning while solving problems. Furthermore, the examples illustrate that students learning a new paradigm may discern the applicability of appropriate concepts in one context, but in another context they may overgeneralize and fail to consistently apply or interpret a concept. When students are developing expertise in a new paradigm, they may be in a "knowledge in pieces" phase [33] and are more likely to overgeneralize concepts and apply principles that are inapplicable in a particular context.

3.3.4 Inappropriate or negative transfer

Transfer of learning is defined as the application of knowledge and skills acquired in one context to another context [49]. Transfer occurs when learning in one context either enhances or undermines a related performance in another context. Negative transfer occurs when learning in one context negatively impacts performance in another context, and it commonly occurs in the early stages of learning in a new domain [50]. In introductory physics, students often have naïve notions about velocity, momentum, or work from everyday experience that can negatively transfer into their learning of classical mechanics. Similarly, concepts learned in classical mechanics, such as position and momentum, are embedded differently in the context of quantum mechanics and students may negatively transfer these concepts to quantum mechanics while developing expertise [51]. We discuss examples of these types of transfer difficulties in quantum mechanics and classical mechanics.

3.3.4.1 In quantum mechanics

Difficulties with the physical, laboratory space vs. Hilbert space: The following example demonstrates negative transfer in quantum mechanics from previous courses. One common difficulty that upper-level students in quantum mechanics have is that they assume that an object with a label "x" is orthogonal to or cannot influence an object with a label "y." This difficulty is evident from responses in a multi-university study in the context of Larmor precession in which students provided responses such as "the magnetic field is in the z-direction so the electron is not influenced if it is initially in an eigenstate of $\hat{S}_x$" or "eigenstates of $\hat{S}_x$ are orthogonal to eigenstates of $\hat{S}_y$" [51]. In introductory physics, x, y, and z are conventional labels for orthogonal components of a vector. These types of difficulties indicate that upper-level students in quantum mechanics courses negatively transferred knowledge acquired in previous courses and were confused about the significance of the labels x, y, and z to denote orthogonal spin states in a Hilbert space in quantum mechanics. In particular, students who claimed that the magnetic field is orthogonal to the eigenstate of a spin component did not realize that the magnetic field is a vector in the three-dimensional laboratory space but eigenstates of spin components are vectors in an abstract Hilbert space in which the state of the system lies.

Difficulties with successive measurements of an observable whose corresponding operator has a continuous vs. discrete eigenvalue spectrum: Another difficulty involving negative transfer in upper-level quantum mechanics courses involves measurement of an observable whose corresponding operator has continuous vs. discrete eigenvalues. Students incorrectly claimed that successive measurements of observables whose corresponding operators have a continuous eigenvalue spectrum produce somewhat deterministic outcomes whereas successive measurements of observables whose corresponding operators have a discrete eigenvalue spectrum produce very different outcomes [51]. For example, in an individual interview, one student stated: "If an observable has a continuous spectrum … the next measurement won't be very different from the first one. But if the spectrum is discrete then you will get very different outcomes." When asked to elaborate, the student added, "For example, imagine measuring the position of an electron. It is a continuous function so that time dependence is gentle and after a few seconds you can only go from A to its neighboring point (pointing to an

x vs. t graph that he sketched on the paper). You cannot go from this without going through this intermediate space. Think of discrete variables like spin … they can give you very different values in a short time because the system must flip from up to down. I find it strange that such large changes can happen almost instantaneously. But that's what quantum mechanics predicts" [51].

Difficulties with the uncertainty principle: Another example of negative transfer from classical mechanics to quantum mechanics involves the uncertainty principle. The following question was administered to students after traditional instruction on the uncertainty principle [10]:

Consider the following statement: "The uncertainty principle makes sense. When the particle is moving fast, the position measurement has uncertainty because you cannot determine the particle's position precisely. It's a blur and that's exactly what we learn in quantum mechanics. If the particle has a large speed, the position measurement cannot be very precise." Explain why you agree or disagree with the statement.

The statement is incorrect because it is not the particle's speed, but rather, the uncertainty in the particle's speed that is related to the uncertainty in position. Fifty-eight percent of the students provided incorrect responses. One student stated: "I agree because when a particle has a high velocity, it is difficult to measure the position accurately." Another student agreed with the statement and provided the following reasoning: "When a particle is moving fast, we cannot determine its position exactly—it resembles a wave—at fast speed, its momentum can be better determined." Further discussions with these students indicate that students may have negatively transferred ideas from classical mechanics into quantum mechanics.

Difficulties with quantum tunneling: Students also have difficulty with the concept of quantum tunneling. Research has shown that students often transfer classical reasoning when thinking about quantum tunneling [52]. Many students state that a particle "loses energy" when it tunnels through a rectangular potential barrier. This reasoning is incorrect because the particle does not lose energy when tunneling through the barrier, although the wave function of the particle inside the potential barrier is described by exponential decay. During interviews with students, common responses regarding tunneling involve statements such as: "the particle collides with and loses energy in the barrier" and "it requires energy to go through the barrier" [52]. These types of responses indicate that many students attempt to apply classical concepts to quantum mechanical situations.

3.3.4.2 In classical mechanics

Difficulties with the definition of work: Physics education research is filled with investigations of alternative conceptions of students due to negative transfer of knowledge (see, e.g., Refs. [22, 23, 34]). For example, according to the definition of work in physics, there is no work done by a force if there is no component of force along an object's direction of motion. Introductory physics students have a naïve mental model that non-zero work must be done by the gravitational force if a person holds an object in his/her hand at rest because the person holding it gets tired. They transfer this naïve mental model into their learning of Newtonian concepts, resulting in learning difficulties.

Difficulties with the net force on an object in circular motion: When an object is moving in a circle at a constant speed, it has a net force acting on it that gives rise to the centripetal acceleration. However, many students in introductory physics courses claim that there is no net force on an object in uniform circular motion because they overgeneralize concepts and associate "constant speed with no net force" even if the direction of the velocity is changing in uniform circular motion.

3.3.4.3 Possible causes for negative transfer in quantum mechanics and introductory classical mechanics

All of the above examples demonstrate that students are applying their knowledge of an older paradigm in the new paradigm. Introductory students inappropriately transfer naïve notions about motion when learning classical mechanics, and upper-level students inappropriately transfer concepts learned in classical physics to quantum mechanics. Students are attempting to fit their prior conceptions in the new paradigm's "box." Furthermore, students' prior preparation, goals, and motivation impacts their reasoning and self-regulatory skills, which can affect the extent to which they transfer knowledge appropriately. Students with limited problem-solving, reasoning, and self-regulatory skills may have difficulty in determining how a particular concept can be applied in various contexts, or they may lack the motivation to do so because they have differing goals for the course.

3.3.5 Lack of transfer

3.3.5.1 In quantum mechanics

Students often have difficulty transferring knowledge from one context to another. For example, students who had previously learned about the time dependence of a non-stationary state wave function in the context of problems involving an infinite square well were asked to find the wave function after a time t, given that the initial wave function was a non-stationary state wave function for a harmonic oscillator potential energy. Many students were unable to solve the problem correctly and complained that the time dependence of wave functions was only discussed in class in the context of an infinite square well so they were not sure how to solve such problems in the context of a harmonic oscillator potential energy [53].

3.3.5.2 In introductory classical mechanics

In one study, 81 students in an introductory mechanics class were given a problem involving a ballerina that is commonly used by instructors in the context of angular momentum conservation [54]. In a multiple-choice format, students were asked what happens to the ballerina's angular momentum and her angular speed when she pulls her arms close to herself. In response to this question, 53% of the students provided the correct answer. An equivalent group of 65 students was given an isomorphic problem (i.e., a problem that can be mapped onto another problem in terms of the physics principle involved, although the contexts are different) in which a spinning neutron star is collapsing under its gravitational force and asked to determine what happens to the angular momentum and angular speed of the neutron star. Only 23% of the students provided the correct response. Many students did not discern the relevance of the ballerina problem that they had learned in class to the neutron star problem.

3.3.5.3 Possible causes for lack of transfer in quantum mechanics and introductory classical mechanics

The above examples indicate that students in introductory physics and quantum mechanics are often unable to transfer knowledge from one context to another. They are unable to see the deeper, underlying principles used to solve the problems. This may be due, in part, to the lack of preparation in students' problem-solving, reasoning, and metacognitive skills. Students may not have robust abstract reasoning skills to identify how different situations are isomorphic. Furthermore, students developing expertise in a new paradigm are in a "knowledge in pieces" phase [33], and so they may be unable to determine the relationship between different types of isomorphic problems.

3.3.6 "Gut-feeling" responses inconsistent with the laws of physics

3.3.6.1 In quantum mechanics

A common difficulty in quantum mechanics (analogous to introductory physics) is manifested by the fact that many students resist writing down quantum mechanical principles explicitly, and instead, answer questions based on their "gut-feeling." For example, in a multi-university study, 48% of students incorrectly claimed that $\hat{H}\Psi(x) = E\Psi(x)$ is the most fundamental equation of quantum mechanics and 39% incorrectly claimed that it is true for all possible wave functions [21]. In individual interviews, students were explicitly asked whether this equation is true for a linear superposition of the ground and first excited states of a one-dimensional infinite square well. Many students incorrectly claimed that it is indeed true in that case primarily because they incorrectly thought that the time-independent Schrödinger equation is the most fundamental equation of quantum mechanics. When these students were asked to explicitly show that this equation is true in this given context, most of them verbally argued without writing down any equations that $\hat{H}\Psi_1(x) = E_1\Psi_1(x)$ and $\hat{H}\Psi_2(x) = E_2\Psi_2(x)$ implied that their addition will give $\hat{H}\Psi(x) = E\Psi(x)$. Even when students were told that $\hat{H}\Psi(x) = E\Psi(x)$ is not obtained by summing the two individual equations, many had difficulty believing the interviewer until they explicitly wrote these equations on paper after additional encouragement to do so from the interviewer (and checked that since E_1 and E_2 are not equal, $\hat{H}\Psi(x) \neq E\Psi(x)$ for a linear superposition of energy eigenstates).

3.3.6.2 In introductory classical mechanics

Students in introductory classical mechanics often use their "gut-feeling" to solve qualitative problems instead of explicitly writing down a physics principle and checking its applicability in a particular situation. If the same question is asked in a quantitative format, students are more likely to think about the applicable laws of physics. For example, 138 introductory students were asked to find a mathematical expression for the magnitude of the momentum of a boat that started from rest and had a constant horizontal force of magnitude F acting on it for a time t (and in which that force was used to tow the boat a distance d) [54]. Students were asked the following quantitative question:

A tugboat pulls a ship of mass M into the harbor with a constant tension force F in the horizontal tow cable. Both the tugboat and the ship start from rest. After the ship has been towed a distance d in time t, the magnitude of its momentum will be

(a) Fd

(b) $(1/2)(F/M)t^2$

(c) $(F/M)t^2/d$

(d) $(1/2)(F/M)dt^2$

(e) Ft

Another equivalent group of 215 introductory students was asked a similar but conceptual question in which two boats started from rest and had the same constant net horizontal force acting on each for the same period of time [54]. They were asked the following conceptual question:

Two identical tugboats pull other ships starting from rest. The Queen Mary is a much more massive ship than the Minnow. Both tugboats pull with the same horizontal force. Neglect other forces. After both tugboats have been pulling for the same amount of time, which one of the following is true about the Queen Mary and the Minnow?

(a) The Queen Mary will have a greater magnitude of momentum.

(b) The Minnow will have a greater magnitude of momentum.

(c) Both ships will have the same magnitude of momentum.

(d) Both ships will have the same kinetic energy.

(e) The Queen Mary will have a greater kinetic energy

Many introductory students used their incorrect "gut-feeling" rather than applying the appropriate physics principle (impulse-momentum theorem) to answer the conceptual question. The percentage of students providing the correct response for the qualitative question was roughly half of the percentage of students who correctly answered the quantitative problem. When a third equivalent group of 289 students (different from the first two groups) was given both questions with the quantitative question first and the qualitative question second, they performed equally well on both. Interviews suggest that introductory students who solved the quantitative problem took advantage of their expression (Ft) to answer the qualitative question. However, during interviews, introductory students who were only given a qualitative question wanted to use their "gut-feeling" and were very reluctant to convert the problem into a quantitative expression in order to solve it [54].

3.3.6.3 Possible causes for incorrect "gut-feeling" responses in quantum mechanics and introductory classical mechanics

The reluctance of introductory students to use their cognitive resources for quantitative analysis of qualitative problems is similar to the reluctance of advanced students in quantum mechanics to verify the validity of $\hat{H}\Psi(x) = E\Psi(x)$ explicitly by writing it down in the given situation. One possible explanation for students using their "gut-feeling" is that many students lack robust problem-solving, reasoning, and self-regulatory skills. Furthermore, students are still developing expertise in a significantly new paradigm (the classical mechanics paradigm is different from students' naïve mental models and the quantum mechanics paradigm is different from the classical mechanics paradigm). Consequently, writing down each step explicitly and converting a conceptual question to a quantitative question in order to solve it are cognitively demanding tasks and may cause cognitive overload [55]. This may lead some students to solve problems based on their "gut-feeling" rather than by engaging in the cognitively demanding task of generating systematic solutions using physics principles.

3.3.7 Difficulties in solving multi-part problems

3.3.7.1 In quantum mechanics

The following example demonstrates student difficulties with solving multi-part problems in quantum mechanics. Upper-level students were first given an initial wave function of a particle in an infinite square well which was not a stationary state. They were then told that a measurement of position was performed. Students were asked to describe the quantum wave function of the particle a long time after the position measurement. According to the Copenhagen interpretation of quantum mechanics (the most widely-held view of the nature of measurement in quantum mechanics and the most commonly taught interpretation of quantum mechanics), a particle in a generic superposition of states is forced into a single state by the act of measurement. After a position measurement, the particle will become localized in space and the corresponding position space wave function will collapse into a delta function centered about the measured position. With time, the highly-peaked wave function will evolve according to the Hamiltonian, but the wave function is neither "stuck" in the collapsed state nor will it go back to the original state before the position measurement. However, many students who had already taken an upper-level quantum mechanics course claimed that a long time after a position measurement, the wave function of the system will go back to the state before the measurement was performed [56]. Other students who provided incorrect responses often claimed that the wave function "gets stuck" in the collapsed state after a position measurement [56]. In individual interviews, these students were explicitly told that their initial responses were not correct and that they should think about what quantum mechanics predicts about the wave function a long time after the position measurement. Then, students who initially claimed that the wave function reverts to the original wave function a long time after the position measurement typically changed their response, saying that the wave function gets stuck in the collapsed state. The students who initially claimed that the wave function gets stuck also typically changed their response, saying that the wave function reverts to the original wave function. When the students were told that neither of the possibilities are correct and that they should think about what quantum mechanics actually predicts, some of them explicitly asked the interviewer how any other possibility exists for this situation because these are the only two possibilities they could generate. The fact that the delta function will start evolving according to the time-dependent Schrödinger Equation (TDSE) based upon the Hamiltonian of the system was something these advanced students were unable to take into account.

3.3.7.2 In introductory classical mechanics

A similar difficulty in introductory physics is observed with a three-part problem involving a ballistic pendulum in which a piece of putty is raised to a certain height and released. It then collides with another piece of putty, the two pieces of putty stick together, and then the merged pieces of putty rise together [57]. In a multi-university study, students were asked for the final height of the merged pieces of putty in terms of the initial height of one of the pieces of putty. Even after instruction, only 27% of the introductory students noted that both conservation of energy and conservation of momentum should be used to answer this question. A majority of students incorrectly claimed that only one of these principles is sufficient to find the final height of the merged putties in terms of the initial height because they either focused on the change in height of the putty or the collision [57].

3.3.7.3 Possible causes for difficulties in solving multi-part problems in quantum mechanics and introductory classical mechanics

The difficulties in solving multi-part problems may be caused by students' inadequate problem-solving, reasoning, and self-regulatory skills—many students may not have a sufficient skill set to break the problem into sub-problems and coordinate different principles and concepts in which the outcomes of the different sub-problems are coupled to each other. Furthermore, students who are still developing expertise in a new paradigm may only focus on some parts of the problem while solving a complex problem. Since students in each sub-domain of physics are still developing expertise and their knowledge is in pieces [33], it is often difficult for them to solve complex, multi-part problems.

3.3.8 Difficulties related to students' epistemological views

According to Hammer [35], a student's epistemology regarding physics includes three components: 1) beliefs about the structure of physics knowledge as a collection of isolated pieces or a single coherent system; 2) beliefs about the content of physics knowledge as formulas or concepts that underlie the formulas; and 3) beliefs about learning physics, whether it entails receiving information or actively reconstructing one's understanding. Students' epistemologies can impact whether they engage in self-regulation, sense-making, and building a robust, conceptual knowledge structure. Similar to students in introductory physics [35], students' inadequate preparation, unclear goals, and insufficient motivation and the fact that the paradigm of quantum mechanics is significantly different from classical mechanics can influence students' epistemological views of quantum mechanics, e.g., whether they check for mathematical consistency and strive to develop a good knowledge structure instead of memorizing algorithms. Below, we discuss examples of students' epistemological views on reconciling physical models with their mental models, checking for consistency in their answers, reliance on memorizing algorithms, ambiguous or careless language, and the learning process in quantum mechanics and introductory mechanics. Finally, we discuss some possible causes that may explain why students exhibit difficulties in developing expert-like epistemological views.

3.3.8.1 Difficulties reconciling physical models with one's own mental model

In quantum mechanics

Students often have difficulty describing the measurement process in quantum mechanics. For example, in a multi-university study, the following problem was administered to 202 students [21]:

The wave function of an electron in a one-dimensional infinite square well of width a *at time t=0 is given by* $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ *, where* $\phi_1(x)$ *and* $\phi_2(x)$ *are the ground state and first excited stationary state of the system.* ($\phi_n(x) = \sqrt{2/a}\,sin(n\pi x/a)$, $E_n = n^2\pi^2\hbar^2/2ma^2, where\ n = 1,2,3 \ldots$).

a) *You measure the energy and the measurement yields* $4\pi^2\hbar^2/(2ma^2)$. *Write an expression for the wave function right after the measurement.*
b) *Immediately after this energy measurement, you measure the position of the electron. Qualitatively describe the possible values of position you can measure and the probability of measuring them.*

In response to part a), some students claimed that the system should remain in the original state which is a linear superposition of the ground and first excited states after the energy measurement. One student stated: "… the collapse of the wave function is temporary … . Something has to happen to the wave function for you to be able to measure energy or position, but after the measurement the wave function must go back to what it *actually* (student's emphasis) is supposed to be." Students with this type of reasoning often felt that the collapse of the wave function during a measurement is a "trick" used in the Copenhagen interpretation to find the possible outcomes and their probabilities but the wave function must revert back to what it *actually* represents (which is the wave function right before the measurement). Some students claimed that their instructor had explicitly mentioned that the collapse of the wave function is not real but just a "trick." They incorrectly interpreted it to mean that the collapse does not really change the wave function. In response to part b), some students incorrectly noted that because the energy is well defined immediately after the measurement of energy, the uncertainty in position must be infinite according to the generalized uncertainty principle. When a student with this type of response was asked to plot the wave function after the energy measurement, the student was able to do that correctly but he still continued to claim that the uncertainty in position must be infinite in this state. When the student was explicitly asked about how one would calculate the uncertainty in position, he was unable to articulate it correctly although he noted that it has something to do with how accurately you can measure the position. He admitted that he had difficulty forming good pictures in his mind about quantum measurement. In response to part b), one student argued that it may not be possible to measure the position after measuring the energy, stating: "Can you even do that? Doesn't making a measurement change the system in a manner that makes another measurement invalid?" This student was struggling with what the incompatibility of observables means and whether incompatibility implies that it is impossible to measure one incompatible observable after another (which seems absurd from an experimental point of view). These types of statements shed light on students' epistemological views about quantum theory. Advanced students learning quantum mechanics struggle to come up with good mental models of quantum measurements and some of them may have difficulty reconciling their own mental models with the appropriate physical model.

In classical mechanics

Difficulties in interpreting situations for which mechanical energy of a system is not conserved: Similar to upper-level students, students in introductory physics often develop their own mental models of classical concepts. They may have difficulty reconciling their mental model with the appropriate physical model in a given context. In a survey on energy and momentum [57], the following situation was posed to students:

Three bicycles approach a hill as described below:

(1) Cyclist 1 stops pedaling at the bottom of the hill, and her bicycle coasts up the hill.

(2) Cyclist 2 pedals so that her bicycle goes up the hill at a constant speed.

(3) Cyclist 3 pedals harder, so that her bicycle accelerates up the hill.

Ignoring the retarding effects of friction, select all the cases in which the <u>total mechanical energy</u> of the cyclist and bicycle is conserved.

(a) (1) only

(b) (2) only

(c) (1) and (2) only

(d) (2) and (3) only

(e) (1), (2), and (3).

In this scenario, going up a hill at a constant speed implies that mechanical energy is not conserved because mechanical energy must be put into the system by a non-conservative force in order to make the bicycle go up at a constant speed. One interviewed student who chose the incorrect option (e) explained: "if you ignore the retarding effects of friction ... mechanical energy will be conserved no matter what.” Other interviewed students who chose option (e) also suggested that the retarding effect of friction was the only force that could change the mechanical energy of the system. Although some students may have chosen (b) because they could not distinguish between the kinetic and mechanical energies, the following interview excerpt shows why that option was chosen by a student despite the knowledge that kinetic and mechanical energies are different: “if she goes up at constant speed then kinetic energy does not change ... that means potential energy does not change so the mechanical energy is conserved ... mechanical energy is kinetic plus potential.” When asked to explain what the potential energy is, the student continued: “isn’t it *mgh*?” When asked to explain why it is not changing, the student first paused and then added: “*h* is the height ... I guess *h* does change if she goes up the hill ... maybe that means that potential energy changes. I am confused ... I thought that if the kinetic energy does not change, then potential energy cannot change ... aren’t the two supposed to compensate each other ... is it a realistic situation that she bikes up the hill at constant speed or is it just an ideal case?” The student was convinced that the mechanical energy is conserved because he was asked to ignore the retarding effects of friction (which he thought was the only non-conservative force that can do work on the system and change mechanical energy). Thus, he used his mental model that mechanical energy was conserved in that case to claim that both the kinetic and potential energies must remain unchanged (even though potential energy must be changing as the bike goes up the hill). When he confronted the fact that the potential energy is changing, he failed to reason that the mechanical energy must be changing if the kinetic energy is constant. Instead, he questioned whether it is realistic to bike up the hill at a constant speed and suggested that this is only possible in the idealized physics world. Although he ignored the work done by the non-conservative force applied on the pedal to keep the speed constant, his statements shed light on students’ epistemological beliefs about how much one can trust physics to explain everyday phenomena and his difficulty in reconciling his mental model with the physics model.

Difficulties with normal force: The following example involving the normal force on an inclined plane demonstrates how introductory students have difficulties in reconciling their own mental models with appropriate physics models. When learning about normal force, many students create a mental model in which the force due to gravity is always antiparallel to the normal force. This model is only appropriate for objects on a horizontal surface. However, in the context of an inclined plane, many students incorrectly claim that the normal force is not perpendicular to the inclined plane, but rather, antiparallel to the force due to gravity. When questioned about their answer, students often state that this is what their instructor told them. Students are interpreting what their instructor taught them to conform to their mental model. Similar difficulties are displayed when children learn about the shape of Earth. Since children often have the mental model that Earth is flat, when they are told that Earth is round, they often claim that the earth is round like a flat pancake or that it is shaped like a hemisphere and humans live on the flat side [58]. In these cases, students are coming up with mental models that may take into account some elements of what they are taught but are modified to make them consistent with their own world view.

3.3.8.2 Difficulties involving overlooking consistency

In quantum mechanics

Another type of difficulty in reasoning and self-monitoring is displayed when students explicitly violate mathematical rules of linear algebra in the context of quantum mechanics. For example, students were asked the following question about a quantum mechanical operator $\hat{Q}$ acting on a generic state $|\Psi\rangle$:

Consider the following conversation between Andy and Caroline about the measurement of an observable Q for a system in a state $|\Psi\rangle$ which is not an eigenstate of $\hat{Q}$:

***Andy**: When an operator $\hat{Q}$ corresponding to a physical observable Q acts on the state $|\Psi\rangle$, it corresponds to a measurement of that observable. Therefore, $\hat{Q}\,|\Psi\rangle = q_n|\Psi\rangle$ where q_n is the observed value.*

***Caroline**: No. The measurement collapses the state so $\hat{Q}\,|\Psi\rangle = q_n|\Psi_n\rangle$ where $|\Psi_n\rangle$ on the right hand side of the equation is an eigenstate of $\hat{Q}$ with eigenvalue q_n.*

With whom do you agree?

a) Agree with Caroline only

b) Agree with Andy only

c) Agree with neither

d) Agree with both

e) The answer depends on the observable Q.

Fifty-two percent of the students claimed that $\hat{Q}|\Psi\rangle = q_n|\Psi_n\rangle$, $\hat{Q}|\Psi\rangle = q_n|\Psi\rangle$, or both equations are correct [59]. Actually, neither of the above equations is correct because they both violate basic rules of linear algebra. In one-on-one interviews, students were so focused on thinking about how a single equation should describe the measurement process and the collapse of the wave function that none of them felt the need to verify that the above equations are both incorrect in terms of linear algebra. Upper-level students are unlikely to make such mistakes if this question is asked in a linear algebra course without the quantum mechanics context. However, in the context involving quantum measurement, their incorrect conception that an operator corresponding to an observable acting on a quantum state corresponds to the measurement of the observable was so strong that they did not consistently apply tenets of linear algebra. When the interviewed students were explicitly asked how the right hand side (RHS) of an equation can change when the left hand side (LHS) remains the same, many students appeared not to be concerned about such an anomalous situation in linear algebra where, depending upon the context, the same LHS yields a different RHS. Students were often very focused on the context. They were convinced that the collapse of a wave function upon the measurement of an observable in quantum mechanics must be represented by an equation and Caroline's equation must correspond to the equation after the collapse of the wave function has occurred. They often reiterated that such changes occur only to the RHS (and the LHS is the same for both Andy and Caroline) because the RHS corresponds to the "output" and the LHS corresponds to the "input." According to their reasoning, it is only the output that is affected by the measurement process (and not the input) so the LHS for Andy and Caroline are the same. When students were asked to explicitly choose the observable to be energy so that the operator is the Hamiltonian operator, their qualitative responses were unchanged even in that concrete case. Some interviewed students were explicitly asked to explain how, on the RHS, a linear combination of the eigenfunctions of the operator that Andy proposes can be the same as only one term in the sum proposed by Caroline in her equation. These students often explained their reasoning by claiming that an operator acting on the wave function corresponds to the measurement of the observable as Caroline proposes. They incorrectly added that Andy's equation is true only before the measurement of the observable has actually taken place and Caroline's statement is true right after the measurement of the observable has taken place and has therefore led to the collapse of the wave function. Many students explicitly stated that at the instant the measurement takes place both Caroline and Andy are correct because the wave function undergoes an instantaneous collapse and the RHS of the equation changes. As noted, in the interviews, when students were explicitly reminded that the equation they thought was correct violated linear algebra and the RHS of an equation cannot change when the left hand side remains the same, some students became worried. However, some students noted that they were unsure about the rules of quantum mechanics and that they were not sure whether quantum mechanics not only violates the principles of Newtonian mechanics but also violates the rules of linear algebra.

The above example shows how difficult the measurement postulate (based upon the Copenhagen interpretation) is from an epistemological point of view and how students have built a locally coherent knowledge structure (inconsistent with the quantum postulate) to represent the measurement process with equations. It is also interesting to note that since students were often convinced about the physical process of the wave function collapse being represented by the equations that Andy and Caroline wrote, they overlooked the linear algebra involved and did not question the anomaly regarding the same LHS yielding different RHS. Unproductive epistemological views, e.g., “quantum mechanics is not supposed to make sense” or “perhaps linear algebra is not necessarily supposed to work as expected in quantum mechanics” may lead to serious difficulties in reasoning and can impede sense-making.

In introductory classical mechanics

Similar overlooking of mathematical or other types of consistency, especially due to strong alternative conceptions, is common in introductory physics. For example, in one investigation, introductory students were given two isomorphic problems involving Newton's second law in an equilibrium situation on an inclined plane [54]. The two questions are shown below:

A car that weighs 15,000 N is at rest on a frictionless 30° incline. The car is held in place by a light strong cable parallel to the incline. Find the magnitude of tension force T in the cable.

a) 7,500 N

b) 10,400 N

c) 11,700 N

d) 13,000 N

e) 15,000 N

A car that weighs 15,000 N is at rest on a 30° incline. The coefficient of static friction between the car's tires and the road is 0.90, and the coefficient of kinetic friction is 0.80. Find the magnitude of the frictional force on the car.

a) 7,500 N

b) 10,400 N

c) 11,700 N

d) 13,000 N

e) 15,000 N

The second problem elicits a strong incorrect conception that static frictional force is always at its maximum value. Many introductory students ignored the similarity between the adjacent problems (including the fact that the free-body diagrams provided were identical except that the tension force in one problem was replaced by the frictional force in the other problem, which would logically imply that the desired quantities, tension and friction, had the same magnitude). While 72% of the students answered the tension problem correctly, only 28% of the students provided the correct response to the friction problem. A majority did not recognize the mathematical consistency between the isomorphic problems—despite doing the tension problem correctly—and launched into a calculation of maximum static friction although it was not at the maximum value in the problem. Asking students to explicitly focus on the free body diagrams for each isomorphic problem did not help [54]. Even when students' attention was explicitly brought to the fact that the free body diagrams were similar except that the tension force was replaced by the friction force, students continued to stick with their initial answer, claiming that one does not need to use the free body diagram for the friction force for which there is a formula but one must use the free body diagram for the tension force for which there is no formula. These types of epistemological views about learning introductory physics can lead to a lack of incentive to look for coherence and a unified nature of physics knowledge and can impact how much effort students make to build a robust knowledge structure.

3.3.8.3 Difficulties due to reliance on memorized algorithms

In quantum mechanics

Many upper-level students in quantum mechanics use memorization tactics over conceptual understanding—preferring to "plug and chug" without understanding the underlying concepts. For example, in a multi-university survey, the following problems were administered to 202 students [21]:

The wave function of an electron in a one-dimensional infinite square well of width a at time t=0 is given by $\Psi(x,0) = \sqrt{2/7}\,\phi_1(x) + \sqrt{5/7}\,\phi_2(x)$ *, where* $\phi_1(x)$ *and* $\phi_2(x)$ *are the ground state and first excited stationary states of the system.* ($\phi_n(x) = \sqrt{2/a}\,sin(n\pi x/a)$, $E_n = n^2\pi^2\hbar^2/(2ma^2)$, $where\ n = 1,2,3\ ...$). *Answer the following questions about this system:*

a) *Write down the wave function* $\Psi(x,t)$ *at time t in terms of* $\phi_1(x)$ *and* $\phi_2(x)$.

b) *You measure the energy of an electron at time t=0. Write down the possible values of the energy and the probability of measuring each.*

c) *Calculate the expectation value of the energy in the state* $\Psi(x,t)$ *above.*

For part c), the expectation value of energy is time independent because the Hamiltonian does not depend on time. The expectation value of energy in this state is $\langle E\rangle = 2/7\,E_1 + 5/7\,E_2$. Only 39% of the students provided the correct response to part c) although 67% of students answered part b) correctly. Many students did not discern the relevance of part b) for part c) and did not exploit what they found for part b) in answering part c). Consequently, many of the students worked out the expectation value of energy from scratch by explicitly writing $\langle E\rangle = \int \Psi^*(x,t)\hat{H}\Psi(x,t)dx$. Then, they wrote the wave function as a linear superposition of the ground state and first excited state and were able to show that the Hamiltonian operator $\hat{H}$ acting on the stationary states will give the corresponding energy and the same state back. They further demonstrated that the time-dependent phase factors for the two terms that survive will vanish due to complex conjugation. However, many students who tried to solve the problem using the memorized algorithm for calculating expectation value got lost along the way. They often forgot to take the complex conjugate of the wave function, use orthogonality of stationary states, or did not realize the proper limits of the integral. This example sheds light on the epistemology of students in upper-level quantum mechanics and suggests that sometimes even they rely on memorized knowledge and employ complicated algorithmic approaches instead of focusing on the significantly simpler approach that exploits the underlying quantum concepts to solve problems.

In introductory classical mechanics

Research in introductory physics teaching and learning suggests that introductory students often use a “plug and chug” approach to problem solving [23]. Research suggests that introductory students are able to solve seemingly difficult problems because they can apply an algorithm to get the correct final answer but fail to answer simpler conceptual questions related to the same problem. Mazur illustrates this with examples and states, “it is possible for students to do well on conventional problems by memorizing algorithms without understanding the underlying physics” ([60], p. 6). In solving quantitative problems, students often look for a formula consistent with the givens and variables in the problem and proceed with an algorithmic approach without thinking about the physics principles involved. For example, a student who knows how to use the algorithm for conservation of mechanical energy can derive an expression for the speed of a person at the bottom of a slide who started at rest from the top but may be unable to answer whether the speed at the bottom of the slide depends on the mass of the person if asked as a qualitative question [57].

3.3.8.4 Difficulties due to the interpretation of ambiguous or careless language

In quantum mechanics

Difficulties with the wave-particle duality: The terminology of quantum mechanics incorporates some of the vocabulary and concepts used in classical mechanics, e.g., position, momentum, and energy, but these concepts are not utilized or interpreted in the classical way. As an example, the double-slit experiment demonstrates the wave-particle duality of single electrons. An electron passes through both slits while traveling toward a screen due to its wave-like nature. However, when the electron arrives at the detecting screen, a flash is seen at one location on the screen due to the collapse of the wave function. These types of experiments are epistemologically challenging even for advanced students. The wave-particle duality of a single electron that becomes evident at different times in the same experiment is very difficult for students to rationalize. Students may have used vocabulary such as "particle" to describe a localized entity in their classical mechanics courses. Consequently, they may find it very difficult to think of the electron as a wave in part of the experiment and as a particle in another part of the experiment (when it lands on the detecting screen and the wave function collapses). To reduce this difficulty, some researchers coined the term "wavicle" [61] for a quantum entity such as an electron. However, this terminology did not become popular.

Difficulties with terminology involving the Mach-Zehnder Interferometer with single photons: The use of careless vocabulary by experts and novices alike is a challenge students face in learning quantum mechanics. A new paradigm may require new vocabulary to explain radically different concepts. However, the concepts in quantum mechanics are often expressed using classical terminology. For example, in quantum mechanical gedanken (thought) experiments, terminology such as "which-path" or "which-slit" information was popularized by Wheeler [62]. One experiment which often elicits careless vocabulary by instructors is the Mach-Zehnder interferometer. Similar to the double-slit experiment, the Mach-Zehnder interferometer with single photons is an experiment which has been conducted in undergraduate laboratories to illustrate fundamental principles of quantum mechanics (see Figure 3-4) [63]. In this experiment, a large number of single photons are emitted from the source. After propagating through beam-splitter 1 (BS1), a photon is in a superposition of the upper (U) and lower (L) path states. Beam-splitter 2 (BS2) mixes the path states of a single photon and the detectors (D1 and D2) can project both components of the photon path state, which interfere at the detectors. The single photon path states from the two paths arriving at detector 1 (D1) undergo a total phase shift of 2π, arriving in phase at D1 and displaying constructive interference. If the photon source emits a large number of photons, all photons will arrive at D1. The single photon path states from the two paths arriving at detector 2 (D2) arrive out of phase, displaying destructive interference. If the source emits a large number of single photons, no photons will arrive at D2. Changing the thickness of the phase shifter will affect how many photons arrive at the detectors.

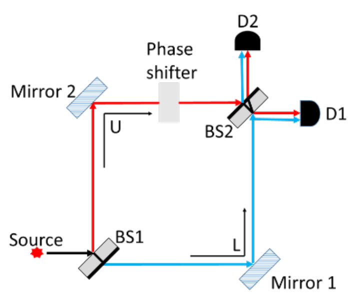

Figure 3-4. Mach-Zehnder Interferometer setup with a phase shifter in the upper path

Wheeler suggested that observing interference of a single photon with itself at D1 and D2 when a large number of single photons are emitted from the source can be interpreted in terms of not having "which-path" information about the single photon [62]. In the Mach-Zehnder interferometer experiment, following Wheeler, it is often stated that "which-path" information is unknown if the photon "took both paths" and displays interference effects at the detectors (see

Figure 3-4). However, if beam-splitter 2 is removed after the photon has already propagated through beam-splitter 1 as in the delayed-choice experiment (see Figure 3-5), it is said that "which-path" information is known because the photons arriving at D1 must have propagated through the upper path only and the photons arriving at D2 must have propagated through the lower path only [62]. When discussing the delayed-choice experiment in the Mach-Zehnder interferometer, many instructors use Wheeler's terminology and state that "all photons reaching D2 took the lower path and all photons reaching D1 took the upper path." However, this type of terminology may indicate that one can retro-cause the photon to go through both paths or one path by inserting or removing beam-splitter 2 after the photon has propagated through beam-splitter 1 [64]. Students may develop unproductive epistemologies that quantum mechanics phenomena can violate causality. In the situation in which beam-splitter 2 is inserted after the photon has already propagated through beam-splitter 1, students have additional difficulties. For example, some students claim that detector 1 would register a photon 50% of the time and detector 2 would never register a photon because, although the photon arrives at detector 2, destructive interference "kills" the photon and it is lost. These types of statements shed light on students' epistemology and the challenges in the development of expertise in quantum mechanics.

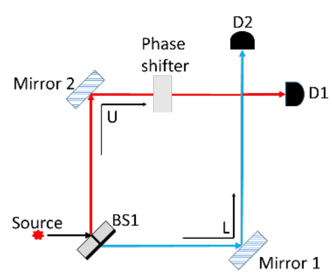

Figure 3-5. Mach-Zehnder Interferometer with beam-splitter 2 removed

To avoid this confusing terminology, we have developed a quantum interactive learning tutorial about a Mach-Zehnder interferometer with single photons [65]. In this tutorial, students learn about how a photon is in a superposition of both the upper and lower path states after propagating through beam-splitter 1. The photon is in a superposition of path states until it arrives at the detectors, regardless of whether beam-splitter 2 is inserted or removed. Once the photon is detected at D1 or D2, the superposition state collapses. "Which-path" information is "known" about the photon if D1 and D2 can only project one component of the photon path state (as opposed to the photon "taking *either* the upper or lower path"). For example, in Figure 3-5, "which-path" information is known for single photons arriving at the detectors because only the component of a photon state along the upper path can be projected in D1 and only the component of a photon state along the lower path can be projected in D2. On the other hand, "which-path" information is unknown about single photons arriving at the detectors in the setup shown in Figure 3-4 because beam-splitter 2 mixes the path states of the single photon. Thus, D1 and D2 can project both components of the photon path state and the projection of both components at each detector leads to interference.

In introductory physics

Difficulties with everyday terminology vs. physics terminology: In introductory physics, even before formal instruction, many students have common notions from everyday experience, e.g., a larger constant velocity implies a larger net force, momentum is equivalent to force, velocity is equivalent to speed, acceleration is equivalent to force, and work is done by a force even if there is no displacement. However, since these concepts are defined differently in physics, their incorrect notions impede their learning. If instruction is not designed appropriately to help students explicitly resolve issues involving terminology and concepts in the new paradigm, they may conclude that physics does not make sense and physics is about idealized situations that cannot be used to understand real-world phenomena. Students may try to memorize what they are taught and combine their own mental models with physics models to come up with something that is not consistent with the laws of physics as discussed in the examples earlier.

Difficulties with defining the system when angular momentum is conserved: In introductory physics, an instructor may state that angular momentum is conserved when a ballerina holding a barbell pulls her arms close to her body or extends her arms far from her body. However, instructors may not clarify for which system the angular momentum is conserved, assuming it is obvious to the students. Nevertheless, knowing what happens to the ballerina's angular speed if she drops the barbell requires an understanding of the fact that the angular momentum is conserved for the ballerina-barbell system. This type of ambiguity about the appropriate system also exists for mechanical energy conservation, linear momentum conservation, etc. In both classical mechanics and quantum mechanics, instructional design should explicitly focus on clarity of language to guide students to learn the concepts in a new paradigm.

3.3.8.5 Difficulties associated with unproductive beliefs about active engagement during the learning process

While learning quantum mechanics

Reliance on rote learning strategies vs. active construction of a coherent knowledge structure: Interviews suggest that, even in upper-level quantum mechanics, many students do not use their mistakes as an opportunity for learning and for building a robust knowledge structure and they resort to rote learning strategies for getting through the course [19]. For example, instead of focusing on developing a robust knowledge structure of quantum mechanics, students employed test-taking strategies (which have nothing to do with developing conceptual understanding and a coherent knowledge structure) by focusing only on fragments of the material that the instructor was likely to ask on exams and skipping the material that was on the midterm examination while studying for the final exam (because they did not expect that material from the midterm exam to be repeated on the final exam) [19].

Reliance on the instructor as the authority: In addition, students in quantum mechanics courses often make statements in interviews similar to introductory physics students [35] indicating that they believe the instructor is an authority on the subject and therefore they accept what the instructor says without questioning it. These types of attitudes can lead to students not making an effort to develop a robust knowledge structure or engage in sense-making. For example, in a multi-university survey with more than 200 students, on a question regarding whether the time-independent Schrödinger equation is the most fundamental equation of quantum mechanics, 39% of students incorrectly claimed that $\hat{H}\Psi(x) = E\Psi(x)$ is unconditionally true whereas it is only true for stationary states for a given system. Interviews with a subset of students suggest that, typically, they felt that this is what their instructor had taught them. For example, one student who was confident that this is what his instructor had taught stated: "This is what 80 years of experiment has proven. If future experiments prove this statement wrong, then I'll update my opinion on this subject." These students incorrectly interpreted what the instructor had said. Another interviewed student who was told later in an interview situation that possible wave functions need not satisfy $\hat{H}\Psi = E\Psi$ and any normalized smooth function that satisfies the boundary conditions is a possible wave function for a system threw up his hands and argued that "if possible wave functions can be that generic, then what is the point of the Schrödinger equation?" He stated that what he was being told by the interviewer did not sound like what his instructor had taught, and he did not know what to make of it. The student did not realize that the purpose of the time-dependent Schrödinger equation, which is the most fundamental equation of quantum mechanics, is to govern the time-evolution of the wave function (it is analogous to Newton's second law in classical mechanics). Responses of this type indicate that students may take the instructor's words without questioning but internalize the instruction by adapting it to achieve consistency with their own mental models. In turn, they may not make the effort to self-regulate or build a robust knowledge structure [21].

We note that instructors may also inadvertently hinder students' sense-making in the new paradigm of quantum mechanics by echoing the statement of Richard Feynman: "I think I can safely say that nobody understands quantum mechanics" [66]. Feynman or the instructor is referring to the fact that they do not understand the origin of the postulates and interpretations, but interviews suggest that the students often misinterpret them to mean that they do not know how to "do" quantum mechanics. Interviews with individual students also suggest that they reason that if their instructor does not understand quantum mechanics formalism, it will be impossible for them to understand it. This viewpoint can hinder students' self-regulation of learning. They may not engage deeply with the basic tenets of quantum mechanics to build a coherent knowledge structure but rather assume, e.g., that quantum mechanics is so strange that it can also violate mathematical rules of linear algebra as discussed earlier. To counteract this viewpoint, students should be made aware of the distinction between understanding the "origin" of the postulates and interpretations of quantum mechanics vs. "doing" quantum mechanics. While there are many interpretations of quantum mechanics and the underlying reasons for why the postulates of quantum mechanics work are difficult to understand (even within the Copenhagen interpretation that is taught to students), learning and applying the Copenhagen interpretation can allow students to calculate what is desired relatively easily. While it is true that many quantum phenomena are not yet fully understood (e.g., the mechanisms for exotic behavior in some highly correlated electron systems such as high temperature superconductors), quantum formalism has been highly successful in explaining and predicting outcomes of experiments. Similarly, some instructors use phrases such as "the collapse of the wave function is just a trick," but students misinterpret it to imply that the collapse does not change the state of the system even if the system was not in an eigenstate of the operator corresponding to the observable measured (as in the example discussed earlier). Indeed, misinterpretations of this type can have detrimental effects on students' epistemology and ultimately their learning.

While learning introductory physics

Similar to upper-level students' epistemological views about learning quantum mechanics, research also suggests that many introductory physics students believe that physics is simply a collection of facts and formulas and that the teacher is the authority on the subject [35, 67]. Thus, they take meticulous notes and memorize knowledge imparted rather than engaging in sense-making [35, 67]. These beliefs can hinder students' self-regulation and the building of a robust knowledge structure. Similarly, Schoenfeld emphasizes that when students are taught basic mathematics in the traditional method, they may come to believe that school mathematics consists of memorizing formal procedures taught by instructors that are completely divorced from real life [68].

3.3.8.6 Possible causes for difficulties in developing expert-like epistemological views

The above examples and discussions suggest that students in quantum mechanics and introductory physics often display unproductive epistemologies that can hinder learning. The paradigm shift may partly cause difficulties and make it difficult for them to reconcile their mental models with correct physical models, make them overlook inconsistency, and make it difficult for them to clarify for themselves the ambiguous or careless language used. It can negatively impact students' views of the structure of physics knowledge and lead them to think that it is a collection of isolated pieces of information (as opposed to a single coherent system) and that the content of physics knowledge is a collection of formulas (as opposed to concepts that underlie the formulas) that comes from an authority. In addition, students' prior preparation, goals, and motivation can affect the extent to which they hold productive beliefs about active participation in the learning process, impacting their perception of how to learn physics (receiving information vs. active processing). The paradigm shift coupled with students' unclear goals, insufficient motivation, and inadequate prior preparation can greatly influence the development of expert-like epistemological views in both introductory physics and quantum mechanics.

3.4 DISCUSSION AND IMPLICATIONS OF THE FRAMEWORK FOR LEARNING QUANTUM MECHANICS

It is widely assumed that a majority of upper-level physics students have not only learned significantly more physics content, but have also developed significantly better reasoning, problem-solving, and self-regulatory skills than introductory physics students. However, expertise is domain-specific—it is unclear how readily skills transfer across domains [36-38]. Classical mechanics and quantum mechanics are two significantly different paradigms. Learning quantum mechanics can be challenging even for advanced students who have developed a good knowledge structure of classical mechanics. These challenges are similar to the challenges faced by students in introductory mechanics who are transitioning from their naïve views about force and motion to those consistent with Newtonian physics [20, 21].

As discussed earlier, many physics education researchers, e.g., McDermott, Halloun and Hestenes, Clement, etc. [22, 23, 26, 34] have emphasized that students in introductory mechanics courses often struggle because they have inadequate prior preparation and diverse goals and motivations for excelling in a course in addition to the fact that the paradigm of classical mechanics is very different from the common sense conceptions students develop trying to rationalize their everyday experiences. Although these researchers may not have explicitly attributed these reasons for introductory student difficulties to a framework, they essentially describe a framework explaining why many introductory physics students struggle in these courses.

In this paper, we described a framework that posits that the patterns of difficulties that students face in developing expertise in quantum mechanics are analogous to what many students face in learning introductory physics. The framework incorporates the facts that many students have inadequate preparation, unclear goals, and insufficient motivation and that the paradigms of classical mechanics and quantum mechanics are significantly different. In particular, students in both introductory classical mechanics and upper-level quantum mechanics have varying goals, motivations, and preparation including a range in the proficiency of their problem-solving, reasoning, mathematical, and self-regulatory skills. In addition, students in both introductory mechanics and quantum mechanics encounter a paradigm shift in which they must assimilate and accommodate radically different concepts from what they are used to. Because of these similarities, the patterns of student difficulties in quantum mechanics are analogous to those of introductory students learning classical mechanics. The framework helps explain analogous patterns of various types of difficulties, e.g., lack of a robust knowledge structure and effective problem-solving skills, failure to transfer knowledge, lack of self-regulation, cognitive overload, and unproductive epistemological views. This framework can be used to help instructors further contemplate possible patterns of student reasoning and metacognitive difficulties in learning quantum mechanics. It can also enable physics education researchers and curriculum developers to leverage the extensive literature for introductory physics education research and adapt promising approaches to help guide the design of effective teaching and learning strategies for quantum mechanics.

3.4.1 Development of research-based curricula and pedagogies for quantum mechanics

Research in introductory physics suggests that in order to help all students with diverse goals and preparation build a robust knowledge structure of introductory mechanics, appropriately connect mathematics and physics, and learn to apply physics principles in diverse situations to explain and predict phenomena, instructional design should conform to the field-tested cognitive apprenticeship model [69]. Our framework suggests that a similar model may be useful for helping students develop a functional understanding of quantum mechanics. The cognitive apprenticeship model of learning involves three major components: “modeling,” “coaching and scaffolding,” and “weaning.” This approach has also been found to be effective in helping students learn effective problem-solving heuristics and developing their reasoning and metacognitive skills. In this approach, “modeling” means that the instructor demonstrates and exemplifies the skills that students should learn. “Coaching and scaffolding” refer to providing students suitable practice, guidance, and feedback so that they learn the skills necessary for good performance. “Weaning” means gradually fading the support and feedback with a focus on helping students develop self-reliance.

In many traditionally taught, “lecture-only” physics classes at all levels, instructors model criteria of good performance. Modeling is often done implicitly in lectures, which is not very effective. As adaptive experts [40], instructors are unaware of some of the cognitive processes they engage in and do not model these explicitly for the students. However, what is truly lacking in the traditional instructional approach is coaching and scaffolding. In that sense, the traditional model of teaching physics is akin to asking students to watch the instructor or the TA play a piano (solve physics problems for them) and then telling them to practice playing piano on their own (solve physics problems in homework) [70]. Based upon the framework, students with a wide variety of goals and backgrounds in both introductory mechanics and quantum mechanics may struggle to develop a functional understanding in a novel domain and may fail to develop useful skills. Therefore, in both domains, effective instructional design should include appropriate coaching and scaffolding to help all students learn.

In order to provide appropriate scaffolding in introductory physics courses, effective instructional approaches have been based, e.g., on Piaget’s model of “optimal mismatch [71-75], Vygotsky’s notion of the “zone of proximal development” [76-78], and the preparation for future learning model focusing on “innovation vs. efficiency” by Bransford and Schwartz [79]. Piaget’s optimal mismatch model is similar to the “Conceptual Change” model of Posner et al. [31] and suggests that students will benefit if instruction provides a cognitive conflict which makes them understand that there is a mismatch between their naïve, everyday model and what the laws of physics predict in a particular context. Then, students are provided appropriate guidance and feedback for the "assimilation and accommodation" of new ideas consistent with classical physical laws. In line with Piaget's ideas, Posner et al. encourage instructional designers to develop learning activities which allow students to accommodate ideas within the new paradigms with their prior knowledge. They suggest that learning activities should involve creating a state of disequilibrium in students' minds as well as helping them discern anomalies in their knowledge structure, diagnose errors in their thinking, make sense of scientific content by presenting it in multiple representations (verbal, mathematical, graphical, etc.), and translate between representations [31]. The zone of proximal development attributed to Vygotsky is a dynamic zone defined by what a student can accomplish on his/her own at a given time vs. with the help of a guide who is familiar with the student's initial knowledge and targets instruction somewhat above it continuously for effective learning [76-78]. Similarly, Bransford and Schwartz recommend that balanced instruction should include opportunities to learn how to rapidly retrieve and accurately apply appropriate knowledge and skills to solve a problem (efficiency) and to adapt knowledge to new situations (innovation). Students learn most optimally when they follow the "optimal adaptability corridor" in which there are elements of both efficiency and innovation concurrently which helps them be cognitively engaged and prevents them from becoming bored or frustrated [79]. All of these models are synergistic in that one can provide an optimal mismatch by ensuring that instruction is in the zone of proximal development and by designing instructional tasks that are in the "optimal adaptability corridor." Our framework suggests that, similar to instructional strategies in introductory physics, instructional tasks in quantum mechanics that include these types of scaffolding supports and provide sense-making and learning opportunities may help students organize their knowledge coherently and hierarchically while helping them acquire useful skills.

3.4.2 Design of scaffolding supports to help students develop a functional knowledge of quantum mechanics

3.4.2.1 Creation of “a time for telling” to activate prior knowledge and prime students to learn

In order to make the lecture of the instructional design effective, Schwartz and Bransford suggest that instructors create a “time for telling” by first giving students the opportunity to struggle while solving problems and activate relevant prior knowledge before attending the lecture [80]. They suggest that struggling and activating prior knowledge “primes” students to utilize lecture time as a learning opportunity [80]. Due to the facts that many students are inadequately prepared, have unclear goals, and insufficient motivation to excel and there is a paradigm shift from classical to quantum mechanics, our framework suggests that instruction in quantum mechanics should also focus on priming students in order to help all of them learn. Instructional designers can create “a time for telling” [80] by developing research-based learning activities that provide opportunities to activate relevant prior knowledge and make students struggle before lectures in quantum mechanics.

3.4.2.2 Research-based active learning tools to improve students' conceptual understanding of quantum mechanics

Research-based active-learning tools such as tutorials [26], peer-instruction [60], group problem-solving [81], and exploiting computers for pedagogical purposes, e.g., the "Just-In-Time Teaching method" [82] are scaffolding tools that help students develop a functional knowledge. They build on students' prior knowledge and explicitly address common difficulties students have in reconciling their naïve mental models with those consistent with the laws of physics. These learning tools give students an opportunity to assimilate and accommodate new ideas while building and organizing their knowledge structure. The guided approach also promotes collaboration and helps students take advantage of each other's strengths and learning styles. Another activity which may help students develop a functional knowledge is asking students in small groups to categorize problems based upon how those problems are solved. While research has shown that students have difficulty categorizing quantum mechanics problems [18], asking them to categorize problems and discuss why certain groupings are better than others may help students look beyond the surface features of the problem, consider the applicability of a physics principle in diverse situations, and "chunk" [42, 83] conceptual knowledge pieces in a hierarchical manner. Based upon the framework, it is likely that research-based active learning strategies like those that have been successful for improving learning in introductory physics (e.g., see Refs. [9, 26, 60, 81, 82, 84]) may be effective for helping students learn quantum mechanics. Indeed, existing research corroborates the implications of the framework to learning quantum mechanics, and research-based pedagogies such as tutorials and peer-instruction tools are proving to be effective in helping students learn quantum mechanics (e.g., see Refs. [11, 20, 85-93]).

Since the patterns of student difficulties in developing expertise in quantum mechanics are analogous to those in introductory mechanics, scaffolding involving research-based active-learning tools that have proven to be successful in introductory courses are likely to be effective in teaching quantum mechanics [10, 11, 85, 86]. Moreover, research has shown that, similar to introductory students, students in quantum mechanics courses can also “co-construct” knowledge when they solve problems with peers [94]. Co-construction of knowledge while working in pairs occurs when neither student in a discussion group can solve the problem individually, but they are able to solve the problem together [95]. In a study by Singh [95], the Conceptual Survey of Electricity and Magnetism [96] was administered to introductory students, both individually and in groups of two. It was found that co-construction occurred in 29% of the cases in which both students had selected an incorrect answer individually. Similarly, a conceptual, multiple-choice test on the formalism and postulates of quantum mechanics was administered to 39 upper-level students, and it was found that co-construction occurred in 25% of the cases in which both students had selected an incorrect answer individually [94]. Thus, even upper-level students benefit from working with peers. Research has already shown that research-based active learning instructional strategies which have been developed for introductory physics such as peer instruction [60] are also effective in the teaching and learning of quantum mechanics [87].

3.4.2.3 Explicit guidance to engage students in self-regulatory activities

Similar to introductory physics students, students in upper-level quantum mechanics display varying levels of proficiency in their problem-solving, reasoning, and metacognitive skills. What types of activities may help students improve these skills in upper-level quantum mechanics? Similar to introductory students, upper-level students need explicit guidance to engage in self-regulatory activities. Schoenfeld proposes a few scaffolding methods that explicitly help students develop their problem-solving, reasoning, and metacognitive skills. He suggests that presenting "polished" solutions to the class may hide the problem-solving processes that the instructor engaged in while solving the problem [68]. Instead, Schoenfeld recommends presenting "problem resolutions" in which the instructor models the problem-solving process explicitly by looking through a few examples, making tentative explorations, and asking questions such as "Am I making reasonable progress? Does this seem like the right thing to do?" After the instructor solves the problem, he should assist students in reviewing and evaluating the entire solution, helping them to learn why reflection is an important component of learning from problem solving. This method of teaching may focus students' attention on metacognitive behaviors, even if it is only used in some of the classes. Another method Schoenfeld uses in his mathematics courses is to conduct whole-class discussions of problems while he acts as a scribe or moderator. The entire class decides which methods to pursue while solving a problem, and Schoenfeld asks questions such as "Do things seem to be going pretty well? If not, we might want to reconsider. Are there ideas we want to return to?" These types of sessions are primarily aimed to focus students' attention on their control of learning and self-regulation [68]. Another approach involving reciprocal teaching was used by Reif and Scott [97] to help students learn introductory mechanics. In self-paced computer tutorials called Personal Assistants to Learning (PALs), computers and students took turns to help each other solve physics problems. This approach was found to be effective in improving students' self-regulatory skills.

Another instructional approach that explicitly encourages students to view problem-solving as a learning opportunity is requiring students to correct their mistakes on homework, quizzes, and exams [43, 44, 98]. Introductory students who self-diagnosed their mistakes performed significantly better on a follow-up exam [44]. Based upon our framework, students taking quantum mechanics may not automatically learn from their mistakes and may also benefit from self-diagnosing their mistakes on homework, quizzes, and exams similar to introductory students. Students taking quantum mechanics should be rewarded appropriately for self-diagnosis activity; otherwise, they may not engage with the material deeply. In fact, research has already shown that when students in quantum mechanics were given grade incentives to fix their mistakes on a midterm exam, they did significantly better on similar final exam problems than students who were not given a grade incentive to fix their mistakes on the midterm exam [99].

3.4.2.4 Instructional strategies to improve students' epistemological views

Developing a functional knowledge is closely connected to appropriate epistemological views of the subject matter. What types of instructional strategies can help improve students' epistemological views? Based upon the framework, analogous to instructional strategies that improve students' epistemological views in introductory mechanics, students' epistemological views about learning quantum mechanics can be improved if instructional design focuses on sense-making and learning rather than on memorization of facts and accepting the instructor as the authority. These effective instructional strategies should include students working with peers to make sense of the material and providing problems in contexts that are interesting and appealing to students. Both formative assessments (e.g., homework, in-class conceptual questions, group problem-solving, etc.) and summative assessments (e.g., exams) should include context-rich problems and sense-making problems to evaluate whether students can apply quantum mechanical principles to a real-world setting. Otherwise, students will continue to "game" exams by successfully solving complex algorithmic problems involving, e.g., solutions of the time-independent Schrödinger equation with complicated boundary conditions and potential energies without having developed a functional understanding of quantum mechanics. Additionally, similar to instructors of introductory physics, instructors of quantum mechanics should choose their terminology carefully and be consistent to avoid negatively impacting student learning. For example, it is important that students become aware of the difference between "doing" quantum mechanics and "understanding" quantum mechanics (as alluded to by Feynman). In particular, the curriculum should help students understand that while there are many interpretations of quantum mechanics, there are interpretations with well-established postulates and procedures for predicting quantum mechanical outcomes in diverse situations (e.g., the Copenhagen interpretation). Instructors should guide students to make sense of these postulates and procedures to evaluate outcomes of experiments. These activities may further improve students' epistemological views about quantum mechanics, encourage them to engage in self-regulatory activities, and help them organize their knowledge structure of quantum mechanics.

3.4.2.5 Types of assessment to encourage students to develop a functional understanding

Mathematically skilled students in a traditional introductory physics course focusing on mastery of algorithms without conceptual understanding can "hide" their lack of conceptual knowledge behind their mathematical skills [60]. However, their good performance on algorithmic physics problems does not imply that they have engaged in self-regulation throughout the course or have built a hierarchical knowledge structure. In fact, most physics faculty, who teach both introductory and advanced courses, agree that the gap between conceptual and quantitative learning gets wider in a traditional physics curriculum from the introductory to advanced level [100]. Therefore, students in a traditionally taught and assessed quantum mechanics course can “hide” their lack of conceptual knowledge behind their mathematical skills even better than students in introductory physics. Based upon the framework, research on student learning in introductory physics suggests that closing the gap between conceptual and quantitative problem-solving by assessing both types of learning is essential in helping students in quantum mechanics develop functional knowledge [10]. Interviews with faculty members teaching upper-level quantum mechanics suggest that some assign only quantitative problems in homework and exams (e.g., by asking students to solve the time-independent Schrödinger equation with complicated boundary conditions) because they think students will learn the concepts on their own [100]. Nevertheless, a majority of students may not learn much about quantum mechanics concepts including the formalism unless course assessments value conceptual learning, sense-making, and the building of a robust knowledge structure. Therefore, to help students develop a functional knowledge of quantum mechanics, formative and summative assessments should emphasize the connection between conceptual understanding and mathematical formalism. Since assessment drives learning (i.e., students will learn what they are tested on), formative assessment can be an effective way to coach and scaffold students [101]. Students who are assessed on both conceptual and quantitative understanding of quantum mechanics throughout the semester are more likely to acquire a functional knowledge similar to the findings from research in introductory physics teaching and learning.

Instructors should also assess students’ self-regulation. One way this can be done is by requiring students to explicate their reasoning while solving problems. Research has shown that students in introductory physics (and other introductory science courses) who articulate their reasoning, or “self-explain,” while studying worked physics examples can detect conflicts in their knowledge structure and they can be coached explicitly on effective self-explanation processes while learning on their own [43, 98, 102]. It is recommended that instructors provide students with prompts that encourage students to detect conflicts [43, 98]. Based upon our framework, students in quantum mechanics courses display difficulties in self-regulation similar to introductory physics students, so quantum mechanics instructors should also assess students' explication and reasoning while solving problems. Further, assessments should evaluate students' self-regulatory skills by considering the consistency and sense-making in their responses. These types of assessments may explicitly focus on coaching and scaffolding student learning to help students self-regulate and engage in sense-making while solving quantum mechanics problems.

3.4.3 Concluding remarks

Consistent with the framework, the existing research-based instructional tools for helping students learn quantum mechanics that are inspired by similar tools for introductory physics are already proving to be effective [10, 11, 65, 85-87]. As further research is conducted in quantum mechanics teaching and learning, we will learn more about the patterns of difficulties and the nature of expertise so that the framework presented here can be refined further.

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4.0 DEVELOPMENT AND VALIDATION OF A CONCEPTUAL SURVEY ON THE FORMALISM AND POSTULATES OF QUANTUM MECHANICS

4.1 INTRODUCTION

Learning quantum mechanics is challenging partly because it is non-intuitive and students often transfer ideas from classical mechanics to quantum mechanics inappropriately. Developing a robust understanding of quantum mechanics at the upper-division undergraduate level also requires a solid grasp of linear algebra, differential equations, and special functions. Students must develop a coherent knowledge structure of the formalism and postulates of quantum mechanics before they can solve novel complex problems. Without conceptual understanding, students may resort to "plug and chug" methods to solve problems without connecting what they are supposed to learn from the problems with their prior knowledge appropriately and developing a functional understanding of the quantum mechanics principles used to solve the problem.

Research-based conceptual surveys (whether involving free response or multiple-choice questions) are useful tools for evaluating student understanding of various topics and carefully developed and validated surveys can play an important role in measuring the effectiveness of a curriculum and instruction. If well-designed multiple-choice pretests and posttests are administered before and after instruction in relevant concepts, they can provide one objective means to measure the effectiveness of a curriculum and instructional approach in a particular course. When compared to free response, multiple choice is free of grader bias and such tests can be graded with great efficiency. Furthermore, the results are objective and amenable to statistical analysis so that different instructional methods or different student populations can be compared. Also, good instructional design requires taking into account the prior knowledge of the students. An effective way to assess the prior knowledge of students, i.e., what the students know before instruction in a particular course, is to administer conceptual surveys as pre-tests. When pre-tests are compared with post-tests, the comparison can give us one objective measure of the effectiveness of instruction.

Multiple-choice surveys have been developed for introductory physics which help instructors determine the initial and final knowledge states of the students at the beginning and end of instruction in a particular topic, e.g., the Force Concept Inventory, Conceptual Survey of Electricity and Magnetism, Rotational and Rolling Motion Survey, Energy and Momentum Survey, etc. [1-4]. Similarly, in quantum mechanics, surveys have been developed which help instructors determine the initial and final knowledge states of the students, e.g., the Quantum Mechanics Survey covers topics in quantum mechanics in one spatial dimension typically covered in the first semester of an upper-level undergraduate course [5]. Research-based instructional strategies have been shown to significantly improve students' conceptual understanding of both introductory and advanced concepts as measured by the conceptual surveys [1-6].

Here, we discuss the development and validation of the Quantum Mechanics Formalism and Postulates Survey (QMFPS) appropriate for an upper-level quantum mechanics course. It is a 34 item multiple-choice test. The survey can be used to identify upper-level undergraduate students' initial and final knowledge states related to the formalism and postulates of quantum mechanics at the beginning and end of a course to assess the effectiveness of a quantum mechanics curriculum in which relevant concepts are covered. The results of the survey can also be used to guide the development of instructional strategies to help students learn these concepts better. It should not be administered as a high-stakes test, but rather, some credit should be given to students who complete the survey in order for students to take it seriously. For example, in an upper-level undergraduate course, if the survey is given as a pretest, students should be given full credit (e.g., for a quiz) for trying their best, but on a posttest, it can count as a graded quiz. In addition, the survey may also be used as a diagnostic for beginning graduate students to determine if they have mastered relevant concepts (in addition to displaying a mastery of technical skill).

4.2 SURVEY DEVELOPMENT AND VALIDATION

The survey focuses on assessing students' conceptual understanding of the formalism and postulates of quantum mechanics rather than assessing their mathematical skills. Students can answer the questions without performing complex calculations, although they do need to understand the basics of linear algebra. The survey is appropriate for a junior/senior level undergraduate quantum mechanics course (at the level of the first four chapters in Griffiths' textbook [7]), as long as students have learned Dirac notation. While designing the survey, we focused on making sure that it is valid and reliable [8,9]. Validity refers to the appropriateness of interpreting the test scores, and reliability refers to the degree of consistency between individual scores if someone immediately repeats the test. As noted earlier, the survey is appropriate for making interpretations about the effectiveness of instruction on relevant topics in a particular course and it is not supposed to be used for high stakes testing of individual students.

To ensure that the survey is valid, we consulted with 6 faculty members regarding the goals of their quantum mechanics courses and topics their students should have learned related to the formalism and postulates of quantum mechanics. In addition to carefully looking through the coverage of these topics in several upper-level undergraduate quantum mechanics classes, we also browsed over several homework, quiz and exam problems that faculty in these courses at the University of Pittsburgh (Pitt) had given to their students in the past when we started the development of the survey. After these preliminary activities, before developing the survey questions, we first developed a test blueprint to provide a framework for deciding the desired test attributes. The specificity of the test plan helped us to determine the extent of content covered and the complexity of the questions. The preliminary distribution of questions from various topics was discussed and agreed upon with several course instructors at Pitt. Many of the concepts identified via interactions with the instructors and their course artifacts were included in the survey questions such as properties of the states of a quantum system and their time-development, issues related to the measurement of observables, expectation values and their time dependence, compatible and incompatible observables, Dirac notation and spin angular momentum (see the enclosed survey, Appendix A).

The alternative choices for the multiple-choice questions were developed based on prior research on student difficulties in quantum mechanics [10-14]. In addition, free-response questions were developed and administered to students as appropriate. The answers to these open-ended questions were summarized and categorized, and many of the incorrect responses were developed into alternative choices for the multiple-choice questions. Common difficulties observed were incorporated into the different versions of the survey. We developed good distractor choices based upon students' common incorrect conceptions. As preliminary versions of the survey were developed, statistical analysis was performed on the multiple choice questions to refine the question statements as well as the answer options.

We also conducted individual interviews with 23 students using a think-aloud protocol [15] at various phases of test development to better understand students' reasoning processes while they answered the open-ended and multiple-choice questions. Within this interview protocol, students were asked to talk aloud while they answered the questions so that the interviewer could understand their thought processes. The interviews often revealed unnoticed difficulties, and these were incorporated into new versions of the survey. Faculty members also reviewed different versions of the survey several times to ensure the appropriateness and relevance of test questions and to detect ambiguities in wording. This allowed us to refine the survey further to ensure that the questions were relevant and clearly worded. The final version of the survey has 34 multiple choice questions. Each question has one correct choice and four incorrect choices. Since we want QMFPS to be administered in one 50 minute long class period, the final version of the survey has 34 multiple-choice questions. We find that almost all of the students are able to complete the survey in one 50 minute class period.

As noted, in addition to developing good distractors by giving free-response questions to students and interviewing students, ongoing expert feedback is essential. We not only consulted with faculty members initially before the development of the questions, but also iterated different versions of the open-ended and multiple-choice questions with several instructors at Pitt at various stages of the development of the survey. Four professors at Pitt reviewed the different versions of the survey several times to examine its appropriateness and relevance for the upper-level quantum mechanics courses and to detect any possible ambiguity in item wording. These valuable comments and feedback were used to fine-tune the survey.

4.3 SURVEY ADMINISTRATION IN CLASSES

The QMFPS was administered to 378 students from 6 institutions.* Of the 378 students, 311 were undergraduate students and 67 were graduate students. The undergraduate students had taken at least a one-semester quantum mechanics course at the junior/senior level. The graduate students were enrolled in a graduate level quantum mechanics course. The undergraduate students completed the survey at the end of their first semester in quantum mechanics in one class period, and the graduate level students completed the survey after approximately two months into the first semester of graduate level quantum mechanics. Two of the junior/senior level classes used research-based learning tools such as concept tests and quantum interactive learning tutorials ($N = 43$). The survey was given to a subset of these students twice, once at the end of the first semester ($N = 18$) and then again at the beginning of the second semester after the winter break ($N = 16$).

4.4 OTHER MEASURES OF RELIABILITY AND VALIDITY

The average score on the survey was 40% (including only the first score of the students who took the survey twice). The standard deviation was 20%, with the highest score being 100%. The Kuder-Richardson reliability index (KR-20) is a measure of the self-consistency of the entire test. If a test is administered twice at different times to the same sample of students, then one would expect a highly significant correlation between the two test scores (test-retest reliability), assuming that the students' performance is stable and that the test environmental conditions are the same on each occasion [8]. According to the standards of test design [8], the KR-20 should be higher than 0.7 to ensure that the test is reliable. The KR-20 for the QMFPS is 0.88, indicating that the survey is quite reliable.

The average score for graduate students is 52% and the average score for undergraduates is 37%. There is a significant difference between the graduate and undergraduate students' scores (p-value on t-test<0.001). We note that even though graduate students perform significantly better than undergraduate students, their average overall score is not very high. This may partly be due to the fact that graduate students may have developed algorithmic skills to solve problems on their exams which often reward plug and chug approaches but lack a conceptual understanding of quantum mechanics.

The average score for the upper-level students who used concept tests and quantum interactive learning tutorials during the semester ($N = 43$) was 58% (S.D.=20%). The average score for other undergraduate students who did not use research-based learning tools ($N = 175$) was 32% (S.D.=16%). There is a significant difference between the scores of students who used research-based learning tools and those who did not (p-value on t-test<0.001). This difference in performance indicates that students benefit from the research-based instructional strategies used in the course.

Performing item analysis can provide important insight into the survey. According to the standards of test design, the item difficulty (percentage of students answering the question correctly) should be above 0.2. On the QMFPS, the item difficulty ranges from approximately 0.2 to 0.7 (see Figure 4-1), which indicates that item difficulty for each item is reasonable.

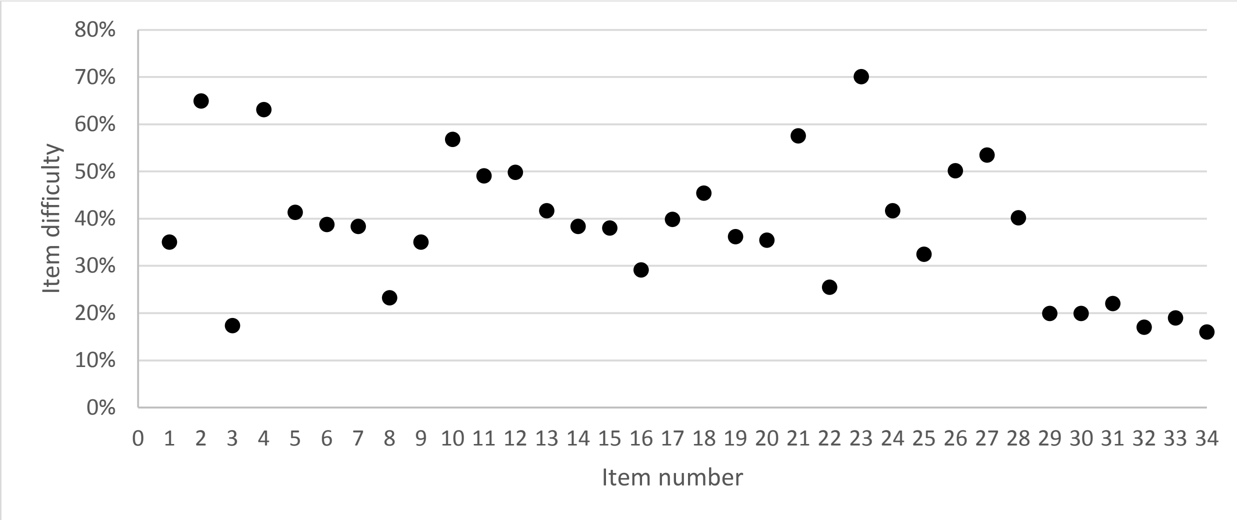

Figure 4-1. Item difficulty (percentage of students answering the question correctly) for each item on the QMFPS.

It is also important to calculate item discrimination for each item on the survey to ensure that the test is reliable. One way to measure item discrimination is by calculating the point-biserial coefficient. It is a measure of consistency of a single test item with the whole test [8] because it reflects the correlation between a student's score on an individual item and their score on the entire test. The point-biserial coefficient has a possible range of −1 to +1. If an item is highly positively correlated with the entire test, then students with high total scores are more likely to answer the item correctly than are students with low total scores. A negative value indicates that students with low overall scores were more likely to get a particular item correct than those with a high overall score and is an indication that the particular test item is probably defective (it could even be due to the fact that the answer of a multiple-choice question was listed incorrectly inadvertently). Ideally, point-biserial coefficients should be above 0.2 [8]. The point-biserial coefficients for each item on the QMFPS are shown in Figure 4-2. The average point-biserial is 0.44 and ranges from

0.3 – 0.6. All of the items are above 0.2, so the standards of test design [8] indicate that the survey questions have reasonably good item discrimination.

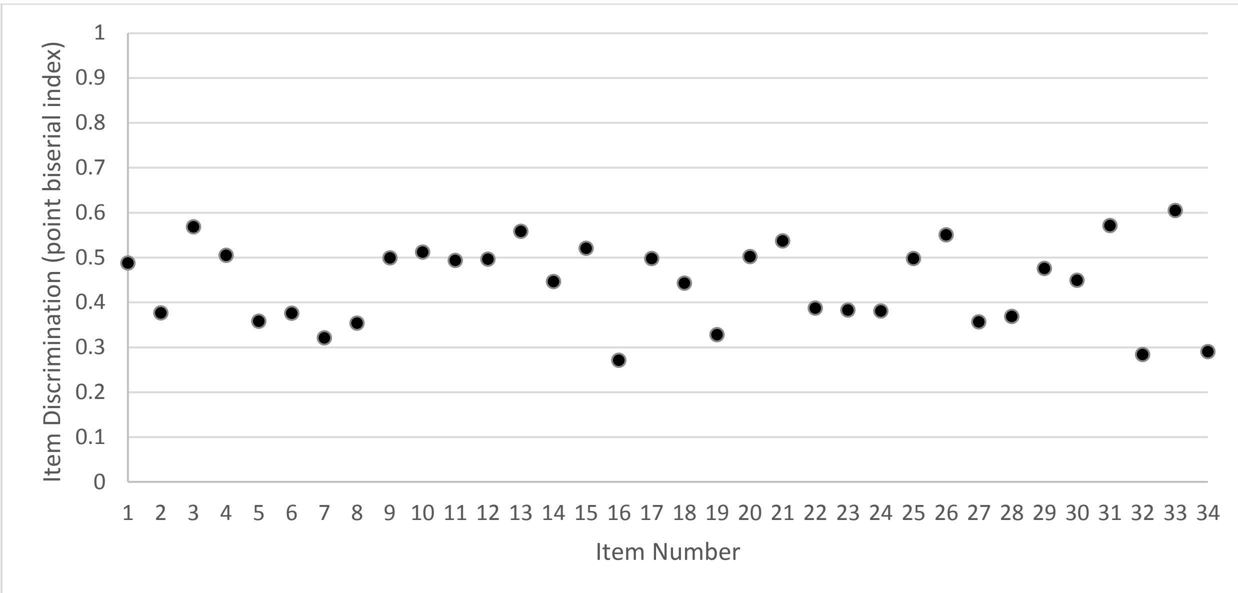

Figure 4-2. Item discrimination for each item on the QMFPS.

The survey is included in Appendix A. Table 4-1 shows one possible categorization of the questions on the survey based upon the concepts although the categorization may be done in other ways. In the following sections, we describe the common difficulties found in each of the categories.

Table 4-1. A possible categorization of the survey questions, the number of questions that fall in each category, and the question numbers belonging to each category. The number of questions in different categories do not add up to 34 because some questions fall into more than one category.

Topic	**Number of Questions**	**Item number**
Quantum states	10	1,4,7,11,12,13,14,15,18,20
Eigenstates of operators corresponding to physical observables	8	1,4,7,14,15,17,18, 20
Time development of quantum states	8	3,4,5,6,7,26,32,34
Measurement	19	2,3,4,5,7,8,9,13,19,21,23,24,25,27, 28,31,32,33,34
Expectation value of observables	3	5,10,22
Time dependence of expectation value of observables	5	15,16,17,29,30
Commutators/compatibility	6	16,17,19,20,27,28
Spin angular momentum	11	20,21,22,23,24,25,26,27,28,29,30
Dirac notation	8	4,9,10,11,12,13,14,18
Dimensionality of the Hilbert space	1	1

4.5 STUDENT DIFFICULTIES WITH DIFFERENT TOPICS

Tables 4-2 through 4-9 show the percentages of students selecting the choices (a)-(e) on the problems in different categories shown in Table 4-1, for example, quantum states. The correct answers are in bold face. In some columns, the percentages of students selecting the choices (a)-(e) do not sum to 100% because some students left the question blank.

4.5.1 Quantum states

On the survey, students exhibit difficulties with quantum states. Table 4-2 shows the percentages of students choosing answer options (a) – (e) on questions related to quantum states.

Proficiency with writing a generic quantum state vector in Dirac notation in terms of energy eigenstates: Questions 4 and 13 assess students' understanding of how to write a generic state vector $|\Psi\rangle$ in terms of energy, position, and momentum eigenstates in Dirac notation. On question 4, students were told that $|\Psi\rangle$ is a generic state and the energy eigenstates $|n\rangle$ are such that $\hat{H}|n\rangle = E_n|n\rangle$, where $n = 1,2,3 \ldots \infty$. In this context, students performed well. In particular, 85% of them recognized that $|\Psi\rangle$ can be written as a linear superposition of energy eigenstates, i.e., $|\Psi\rangle = \sum_n \langle n|\Psi\rangle\, |n\rangle$.

Inconsistencies in writing $|\Psi\rangle$ as a linear superposition of position eigenstates or momentum eigenstates. Question 13 investigates students' understanding of how to write a generic state $|\Psi\rangle$ as a linear superposition of position eigenstates or momentum eigenstates. While 82% of the students recognized that $|\Psi\rangle = \int \langle p|\Psi\rangle|p\rangle dp$, a lower percentage (70%) recognized that $|\Psi\rangle = \int \Psi(x)|x\rangle dx$ in question 13. Even though writing $|\Psi\rangle$ as a linear superposition of position eigenstates or momentum eigenstates are analogous tasks, 50% of the students choose an answer option that includes $|\Psi\rangle = \int \Psi(x)|x\rangle dx$ but not $|\Psi\rangle = \int \langle p|\Psi\rangle|p\rangle dp$ and vice versa. Responses of this type indicate that many upper-level students are in an intermediate level of expertise and apply concepts and procedures correctly in one context but not in another context.

Table 4-2. Distribution of students' responses for questions related to quantum states. Correct responses are in bold.

	Q1(%)	Q4(%)	Q7(%)	Q11(%)	Q12(%)	Q13(%)	Q14(%)	Q15(%)	Q(18%)	Q20(%)
(a)	**35**	**63**	21	32	6	7	**38**	13	10	23
(b)	7	9	8	1	26	9	11	**38**	**45**	**35**
(c)	14	13	4	**49**	**50**	24	28	17	26	10
(d)	7	6	**38**	8	12	19	13	13	4	8
(e)	37	9	28	10	6	**42**	9	19	14	22

4.5.2 Eigenstates of operators corresponding to physical observables

Students exhibit difficulties when reasoning about eigenstates of operators which correspond to physical observables. Table 4-3 shows the percentages of students choosing answer options (a)-(e) on questions related to eigenstates.

Confusion between stationary states and eigenstates of any observable. Question 15 assesses students' understanding of energy eigenstates (stationary states) vs. position eigenstates and whether students can differentiate between the two. We find that many students had difficulty with the concept of what a stationary state is and 49% of the students incorrectly claimed that the stationary states refer to the eigenstates of any operator corresponding to any physical observable. This type of response indicates that students have difficulty differentiating between the related concepts of stationary states and eigenstates of observables other than energy.

Difficulty differentiating between energy eigenstates and eigenstates of other operators that do not commute with the Hamiltonian. On question 17, which is related to student understanding of a conserved quantity, 49% of the students incorrectly claimed that if a quantum system is in an eigenstate of the momentum operator at initial time $t = 0$, momentum is a conserved quantity. Individual interviews suggest that students thought that if the system is in an eigenstate of an operator, the corresponding observable is a conserved quantity. They did not differentiate between the eigenstates of the Hamiltonian operator (and other Hermitian operators corresponding to observables that commute with the Hamiltonian) and eigenstates of other Hermitian operators that do not commute with the Hamiltonian. During the clarification phase of the individual interviews, some students explicitly claimed that it does not make sense for an operator to have time dependence in its own eigenstate.

Table 4-3. Distribution of students' responses for questions related to eigenstates. Correct responses are in bold.

	Q1(%)	**Q4(%)**	**Q7(%)**	**Q14(%)**	**Q15(%)**	**Q17(%)**	**Q18(%)**	**Q20(%)**
(a)	**35**	**63**	21	**38**	13	**40**	10	23
(b)	7	9	8	11	**38**	11	**45**	**35**
(c)	14	13	4	28	17	7	26	10
(d)	7	6	**38**	13	13	21	4	8
(e)	37	9	28	9	19	21	14	22

Difficulty writing a generic operator $\hat{Q}$ in Dirac notation in terms of its eigenvalues and eigenstates. Question 18 investigates students' understanding of how to write a generic operator $\hat{Q}$ in terms of its eigenvalues and eigenstates. Students were told that $\{|q_n\rangle, n = 1,2,3 \ldots N\}$ form a complete set of orthonormal eigenstates of an operator $\hat{Q}$ with eigenvalues q_n. We find that 54% of the students chose an incorrect answer choice for the expression for $\hat{Q}$. The most popular incorrect answer choice was writing $\hat{Q}$ as a double sum over two indices, i.e., $\hat{Q} = \sum_{n,m} q_n|q_n\rangle\langle q_m|$. Even though the majority of students (87%) did recognize the identity operator in terms of the eigenstates of a generic operator $\hat{Q}$, i.e., $\sum_n|q_n\rangle\langle q_n| = \hat{I}$ in question 10, they had difficulty applying this knowledge to determine how to write $\hat{Q}$ in terms of its eigenvalues and eigenstates.

4.5.3 Time development of quantum states

Students exhibit various difficulties when reasoning about the time development of a quantum state. Table 4-4 shows the percentages of students choosing answer options (a)-(e) on questions related to the time development of a quantum state.

Proficiency with how a generic quantum state evolves in time: On question 4, students were told that $|\Psi\rangle$ is a generic state and the energy eigenstates $|n\rangle$ are such that $\hat{H}|n\rangle = E_n|n\rangle$, where $n = 1,2,3 \ldots \infty$. We find that 78% of the students recognize that the expression $e^{-i\hat{H}t/\hbar}|\Psi\rangle = \sum_n e^{-iE_n t/\hbar}\langle n|\Psi\rangle\, |n\rangle$ is correct. This type of response indicates that many students know that the operator $e^{-i\hat{H}t/\hbar}$ is the time evolution operator which acts on the state $|n\rangle$ to give $e^{-iE_n t/\hbar}$ and governs the time evolution of a quantum state $|\Psi\rangle$.

Difficulties with describing the time evolution operator $e^{-i\hat{H}t/\hbar}$. Question 6 investigates student difficulties with the operator $e^{-i\hat{H}t/\hbar}$. We find that 92% of students correctly recognize how the time evolution of a state can be determined, i.e., the state of the system at time $t > 0$ is $|\Psi(\mathrm{t})\rangle = e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle$. However, 56% incorrectly claim that $e^{-i\hat{H}t/\hbar}$ is a Hermitian operator. During interviews with students, some tried to prove that $e^{-i\hat{H}t/\hbar}$ is Hermitian by expanding it in terms of a power series, i.e., $e^X = \sum_{j=0}^{\infty} \frac{1}{j!} X^j$ where X is an $n \times n$ matrix. They claimed that the time-evolution operator must be Hermitian (some even thought that all operators one encounters in quantum mechanics are Hermitian). This type of response indicates that some students do not recognize that a Hermitian operator corresponds to a physical observable, and not all operators including $e^{-i\hat{H}t/\hbar}$ are Hermitian since they do not correspond to a physical observable.

Furthermore, 27% did not recognize that $e^{-i\hat{H}t/\hbar}$ is a unitary operator (which preserves the norm of the state).

Difficulties with determining how the coefficients of a quantum state evolve in time. Question 5 assesses students' understanding of how the coefficients of a quantum state expanded as a linear superposition of eigenstates of a generic operator corresponding to an observable evolve in time. Students were told that $|q_n\rangle$ are the eigenstates of a generic operator $\hat{Q}$ corresponding to a physical observable with a discrete spectrum of non-degenerate eigenvalues q_n where $n = 1, 2, \ldots \infty$. At time $t = 0$, the state of the system is $|\Psi\rangle = \sum_n c_n(t = 0)|q_n\rangle$. We find that 41% of students incorrectly claimed that the coefficients will evolve in time similar to their time evolution for the Hamiltonian operator, i.e., $c_n(t) = e^{-iq_n t/\hbar}c_n(0)$ at time $t > 0$.

Difficulties with qualitatively describing how a quantum state evolves after a position measurement. Question 7 investigates students' understanding of what happens after the measurement of position in the context of a one-dimensional simple harmonic oscillator potential energy well. 38% of students correctly recognized that the wave function will be peaked about a particular value of position after the measurement AND that the wave function will not go back to the first excited state wave function, even if one waits for a long time after the position measurement. Eighty-seven percent of the students recognized that the wave function becomes peaked about a particular value of position immediately after the position measurement. However, 32% of the students incorrectly chose an answer option that stated that the wave function will go back to the first excited state wave function a long time after the position measurement.

Table 4-4. Distribution of students' responses for questions related to time development of a quantum state. Correct responses are in bold.

	Q3 (%)	Q4 (%)	Q5 (%)	Q6 (%)	Q7 (%)	Q26 (%)	Q32 (%)	Q34 (%)
(a)	7	**63**	7	5	21	12	38	39
(b)	24	9	9	3	8	25	15	15
(c)	3	13	9	27	4	7	**17**	**16**
(d)	48	6	**42**	**39**	**38**	**50**	11	9
(e)	**17**	9	32	26	28	3	13	14

Incorrectly assuming that probability density for measuring position is time independent. Question 3 investigates students' understanding of probability density at a time t > 0. Students were told that the initial wave function is $\Psi(x,0) = Ax(a-x)$ for $0 \le x \le a$, where A is a suitable normalization constant and were asked to choose the correct expression for probability density $|\Psi(x,t)|^2$ at time $t > 0$. Forty-eight percent of the students incorrectly chose answer option $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2$, which is time-independent. Interviews suggest that many students reasoned that the probability density is time-independent and is found by taking the absolute square of the initial wave function, even if the quantum state is not initially an energy eigenstate. Another 34% of students chose answer options which included mention of the expectation value of energy, e.g., $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2 \cos^2\left(\frac{Et}{\hbar}\right)$, where E is the expectation value of energy.

Incorrectly assuming that probability for measuring position does not depend on time. Students also display difficulties in determining whether the probability of measuring position between x and $x + dx$ depends on time. On questions 32 and 34, approximately 20% of students incorrectly claimed that if one measures the position of the particle <u>after a time t</u>, the probability of obtaining a value between x and $x + dx$ is $\int_x^{x+dx} x|\Psi(x,0)|^2\, dx$. Not only is the expression for probability incorrect for time $t = 0$, the probability of measuring the position of the particle between x and $x + dx$ is time-dependent because: 1) the initial state of the system is not an energy eigenstate, and 2) the position operator does not commute with the Hamiltonian for this system.

Inconsistent responses to questions about probability density of measuring position at time $t > 0$. Questions 32 and 34 assess students' understanding of position measurements after a quantum state evolves in time. Students were given that the particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \le x \le a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1,2,3 \ldots$. In question 32, students were told that the wave function at time $t = 0$ is $\Psi(x, 0) = Ax(a - x)$ for $0 \le x \le a$, where A is a suitable normalization constant. Question 34 is the same as question 32 except that the initial wave function is $\Psi(x, 0) = \frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}$. On both questions, approximately 30% of the students incorrectly claimed that the probability density for measuring x after a time t is the absolute square of the initial wave function, i.e., $|Ax(a - x)|^2$ or $\left|\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right|^2$. Question 3 was a very similar question because students were told that the initial wave function is $\Psi(x, 0) = Ax(a - x)$ for $0 \le x \le a$, where A is a suitable normalization constant and were asked to choose the correct expression for probability density $|\Psi(x, t)|^2$ at time $t > 0$. Forty-eight percent of the students incorrectly chose answer option $|\Psi(x, t)|^2 = |A|^2 x^2 (a - x)^2$ in question 3. The discrepancy between the percentages of students selecting an incorrect answer option in questions 32 and 34 vs. question 3 may be due to the fact that in question 3, the expression for probability density was explicitly stated, i.e., $|\Psi(x, t)|^2$. Students may have been cued to find the absolute square of the expression and many simply selected the option involving squared initial wave function, i.e., $|A|^2x^2(a-x)^2$. In questions 32 and 34, students were less likely to choose expressions for probability density at time t such as $|Ax(a-x)\ |^2$ because they were not cued with the expression for probability density, $|\Psi(x,t)|^2$. These types of discrepancies demonstrate how sensitive students' responses are based upon the question statement. An expert in quantum mechanics would not be distracted by the fact that the expression for probability density, $|\Psi(x,t)|^2$, was included in the problem statement. However, students who are still developing expertise in quantum mechanics may respond differently to questions which are worded slightly differently because they have not yet developed a coherent knowledge structure. Their knowledge structure is only locally consistent and certain cues may prime them to answer incorrectly.

Difficulty with recognizing that the probability of measuring an energy eigenvalue is time independent if the Hamiltonian operator does not depend on time. Questions 32 and 34 also investigated students' understanding of the probability of measuring energy after a time t. Less than 20% of students correctly responded that if one measures the energy of the system <u>after a time t</u>, the probability of obtaining E_1 is $\left|\int_0^a \psi_1^*(x)Ax(a-x)dx\right|^2$ (or $\left|\int_0^a \psi_1^*(x)\left(\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right)dx\right|^2$). The probability of obtaining energy E_1 does not depend on time because it is a constant of motion. Many students have difficulty with how energy is conserved for a quantum state and that the probability of measuring a particular energy is time-independent.

Difficulties with the time evolution of a state in the context of Larmor precession. Question 26 assesses students' understanding of time development in the context of a spin-1/2 particle. Students were told that at time $t=0$, the particle is in an initial normalized spin state $|\chi\rangle = a|1/2\,,1/2\rangle + b|1/2\,,-1/2\rangle$ where a and b are suitable constants and the Hamiltonian is

$\hat{H} = -\gamma B_0 \hat{S}_z$ where the uniform field B_0 is along the z-direction and γ is the gyromagnetic ratio (a constant). Students were asked to find the state of the system after time t. Only 50% of the students correctly answered the question ($|\chi(t)\rangle = ae^{\frac{i\gamma B_0 t}{2}}|1/2\,,1/2\rangle + be^{\frac{-i\gamma B_0 t}{2}}|1/2\,,-1/2\rangle$). The most common incorrect answer choice (44% of students) was an option which included an overall phase factor in the form of $e^{\frac{i\gamma B_0 t}{2}}$, e.g., $|\chi(t)\rangle = e^{\frac{i\gamma B_0 t}{2}}(a|1/2\,,1/2\rangle + b|1/2\,,-1/2\rangle)$.

Difficulties with measurement of observables after a time t in the context of Larmor precession. Question 28 examines students' understanding of time development and successive measurements in the context of a spin-1/2 particle. Students are told that at time $t = 0$, the particle is in an initial state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$. The Hamiltonian is $\hat{H} = -\gamma B_0 \hat{S}_z$ where the uniform field B_0 is along the z-direction and γ is the gyromagnetic ratio (a constant). Students were asked to choose correct expressions about measurements performed on the system after a long time t. Fifty-three percent of the students incorrectly claim that if one measures S_x immediately following another measurement of S_x, both measurements of S_x will yield the same value $\frac{\hbar}{2}$ with 100% probability. This statement is incorrect because after a long time t, the particle will no longer be in a state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$ and successive measurements of S_x will not yield $\frac{\hbar}{2}$ with 100% probability. Similarly, 24% of the students incorrectly claimed that if one first measures $\vec{S}^2$ and then measures S_x in immediate succession, the measurement of S_x will yield the value $\frac{\hbar}{2}$ with 100% probability. This statement is also incorrect because after a long time t, the particle will no longer be in a state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$ and successive measurements of $\vec{S}^2$ and S_x will not yield $\frac{\hbar}{2}$ with 100% probability. Twenty-nine percent of the students did not recognize that if one first measures S_z and then measures S_x in immediate succession, the measurement of S_x will yield the value $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$ with equal probability (this is a correct statement). These types of difficulties indicate that students have much difficulty reasoning about how a quantum state evolves according to the Hamiltonian.

4.5.4 Measurement/Hermitian Operators/Observables

Table 4-5 includes the distribution of students' responses to questions involving measurement. The following difficulties involving measurement, Hermitian operators, and observables were observed:

Proficiency with measurement outcomes: Question 9 investigates students' understanding of measurement and probability of measuring an outcome of a generic operator corresponding to a physical observable. It is encouraging that 97% of students recognized that a measurement of a physical observable must return one of the eigenvalues of the operator corresponding to the physical observable.

Incorrectly assuming that $\hat{H}$ acting on a quantum state corresponds to an energy measurement. Question 8 elicits a common difficulty that the Hamiltonian operator acting on a generic state corresponds to a measurement of energy. Students were asked the following question: "*Consider the following conversation between Andy and Caroline about the measurement of energy in a state $|\Psi\rangle$ which is not an energy eigenstate.*

***Andy**: When an operator $\hat{H}$ corresponding to energy acts on a generic state $|\Psi\rangle$, it corresponds to* *a measurement of energy. Therefore, $\hat{H}|\Psi\rangle = E_n|\Psi\rangle$, where E_n is the observed value of energy.*

***Caroline**: No. The measurement collapses the state so $\hat{H}|\Psi\rangle = E_n|n\rangle$, where $|\Psi\rangle$ on the left hand side is the original state before the measurement and $|n\rangle$ on the right hand side of the equation is the state in which the system collapses after the measurement and it is an eigenstate of $\hat{H}$ with eigenvalue E_n.*

With whom do you agree?"

Only 23% of the students disagreed with both Andy and Caroline, which is the correct response. Sixty-six percent of students agreed with Caroline, Andy, or both. Responses of this type indicate that, even after instruction, students have a deeply held conception that the measurement process and collapse of the state are represented by an equation of the type discussed by Andy and Caroline.

Table 4-5. Distribution (in percentages) of students' responses for questions related to measurement of physical observables. Correct responses are in bold.

	Q2	Q3	Q4	Q5	Q7	Q8	Q9	Q13	Q19	Q21	Q23	Q24	Q25	Q27	Q28	Q31	Q32	Q33	Q34
(a)	**65**	7	**63**	7	21	36	10	7	11	1	18	**42**	19	29	12	14	38	16	39
(b)	1	24	9	9	8	20	29	9	22	18	**70**	12	13	4	**40**	12	15	13	15
(c)	14	3	13	9	4	**23**	23	24	24	7	4	14	17	**54**	17	**22**	**17**	**19**	**16**
(d)	13	48	6	**42**	**38**	10	3	19	7	**57**	3	26	**33**	5	19	25	11	23	9
(e)	6	**17**	9	32	28	11	**35**	**42**	**36**	14	3	4	13	4	7	22	13	21	14

Confusing expectation value of position with probability distribution for measuring position at time $t = 0$: According to Born's interpretation, the probability of measuring the particle's position between x and $x + dx$ is $|\Psi(x,0)|^2\,dx$. Question 13 assesses students' understanding of the probability of measuring position of a particle between x and $x + dx$, given that the particle is in the generic quantum state $|\Psi\rangle$ given in Dirac notation. We find that 88% of the students correctly recognized that the probability to find the particle between x and $x + dx$ is

$|\langle x|\Psi\rangle|^2 dx$. Questions 31 and 33 examine students' understanding of the probability of measuring position between x and $x + dx$ given that the initial wave function at time $t = 0$ is not an energy eigenstate. Students were told that a particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1,2,3\ldots$. In question 31, the wave function at time $t = 0$ is $\Psi(x,0) = Ax(a-x)$ for $0 \leq x \leq a$, where A is a suitable normalization constant. In question 33, the wave function at time $t = 0$ is $\Psi(x,0) = \frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}$. Approximately 80% of the students correctly recognized that the probability density for measuring x is $|Ax(a-x)\,|^2$ (or $\left|(\psi_1(x)+\psi_2(x))/\sqrt{2}\right|^2$). However, approximately 60% of the students incorrectly responded that the probability of measuring position is $\int_x^{x+dx} x|\Psi(x,0)|^2 dx$. This dichotomy indicates that many students do not discern the connection between probability density and the probability of measuring position between x and $x + dx$, i.e., one can multiply the probability density $|\Psi(x,0)|^2$ by infinitesimal interval dx to obtain the probability of measuring the position in a narrow range between x and $x + dx$. Interviews suggest that some students who thought that the expression $\int_x^{x+dx} x|\Psi(x,0)|^2 dx$ in questions 31 and 33 is correct confused the probability of measuring position with the expectation value of position (although the integral $\int_x^{x+dx} x|\Psi(x,0)|^2 dx$ is not from $x = 0$ to $x = a$, necessary for the expectation value), and they chose answer choices which involved the position operator in position representation, x.

Incorrect assumption that the probability density for measuring x is time-independent: Questions 32 and 34 examine students' understanding of the probability distribution for measuring position given that the initial wave function at time $t = 0$ is not an energy eigenstate. Students were told that a particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1,2,3\ldots.$ In question 32, the wave function at time $t = 0$ is $\Psi(x, 0) = Ax(a - x)$ for $0 \leq x \leq a$, where A is a suitable normalization constant. In question 34, the wave function at time $t = 0$ is $\Psi(x, 0) = \frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}$. In both questions, approximately 30% of the students claimed that the probability density for measuring x at time $t > 0$ is time independent. This type of response indicates that students have difficulty reasoning about how the wave function will evolve in time according to the Hamiltonian $\hat{H}$ of the system in a non-trivial manner and the probability of measuring an observable such as position whose corresponding operator does not commute with $\hat{H}$ will depend on time.

Context-dependent responses involving probability density at time $t > 0$: Although there is no explicit mention of a position measurement in question 3, students were explicitly asked to select the probability density $|\Psi(x,t)|^2$ at time $t > 0$ for the same initial wave function as in question 32 (i.e., $\Psi(x, 0) = Ax(a - x)$). Thus, while questions 3 and 32 are posed differently, an expert would recognize that the two questions are conceptually very similar. On question 3, 48% of the students incorrectly selected the answer choice (D) $|\Psi(x,t)|^2 = |A|^2x^2(a - x)^2$, which is time-independent, as the probability density for measuring x at time $t > 0$. This type of response indicates that students incorrectly assumed that the probability density is found by taking the absolute square of the initial wave function, even if the quantum state is not initially an energy eigenstate. The percentage of students (48%) who incorrectly assumed that the probability density for measuring x does not depend on time on question 3 is significantly higher than the percentage of students (28%) who made the same incorrect assumption on question 32 and selected the expression $|Ax(a-x)\ |^2$ as the probability density for measuring x at time $t > 0$. Interviews suggest that since the expression for the probability density was explicitly stated in question 3, i.e., $|\Psi(x,t)|^2$, some students used it as a cue to find the answer by simply squaring the initial wave function, i.e., $|A|^2 x^2 (a-x)^2$. On question 32 (and even on question 34), students were less likely to choose expressions such as $|Ax(a-x)\ |^2$ as correct for the probability density at time $t > 0$ because they were not cued with the expression for the probability density, $|\Psi(x,t)|^2$. Moreover, since question 3 did not explicitly mention position measurement, some interviewed students did not realize that the probability density $|\Psi(x,t)|^2$ in question 3 is the probability density *for measuring position* in statement (1) of question 32: "If you measure the position of the particle <u>after a time t</u>, the probability density for measuring x is $|Ax(a-x)\ |^2$." These types of discrepancies demonstrate how student responses are sensitive to the context and how the questions are posed. An expert in quantum mechanics would not be distracted by the fact that the expression for probability density, $|\Psi(x,t)|^2$, was included in the problem statement for question 3. However, students who are developing expertise in quantum mechanics may respond differently to questions which are worded slightly differently since they have not developed a coherent knowledge structure [16]. Their knowledge structure is locally consistent and certain cues may prime them to answer incorrectly.

Difficulties with the probability distribution for an energy measurement at time $t = 0$: The probability for measuring energy E_1 given an initial wave function $\Psi(x,0)$ is $\left|\int_0^a \psi_1{}^*(x)\Psi(x,0)dx\right|^2$. On question 31, the wave function at time $t = 0$ is $\Psi(x,0) = Ax(a-x)$

for $0 \leq x \leq a$, where A is a suitable normalization constant. Approximately 50% of students did not recognize that the probability of measuring energy E_1 is $\left|\int_0^a \psi_1^*(x) Ax(a-x)\,dx\right|^2$. On question 33, the initial wave function is $\Psi(x,0) = (\psi_1(x) + \psi_2(x))/\sqrt{2}$. An expert would immediately recognize that the probability of measuring E_1 is ½ and can be obtained using $\left|\int_0^a \psi_1^*(x)\big((\psi_1(x) + \psi_2(x))/\sqrt{2}\big)dx\right|^2$. However, half of the students did not recognize that the expression $\left|\int_0^a \psi_1^*(x)\left(\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right)dx\right|^2$ is a correct expression for the probability for measuring energy E_1. Interviews suggest that even students who recognize that the probability of measuring energy E_1 is ½ for this wave function, which is an equal superposition of ground and first excited states, did not recognize that the integral $\int_0^a \psi_1^*(x)\left(\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right)dx$ gives the component of the quantum state along the ground state and is related to the energy measurement amplitude.

Incorrect assumption that the probability distribution for an energy measurement depends on time: Questions 32 and 34 also investigated student understanding of the probability of measuring an energy eigenvalue at time $t > 0$ given that the initial wave function at time $t = 0$ is not an energy eigenstate. Students were told that a particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1,2,3\ldots$. Seventy-seven percent of the students claimed that the probability for measuring energy E_1 depends on time and did not select the expression $\left|\int_0^a \psi_1^*(x) Ax(a-x)\,dx\right|^2$ or $\left|\int_0^a \psi_1^*(x)\big((\psi_1(x) + \psi_2(x))/\sqrt{2}\big)dx\right|^2$ as true. Responses of this type indicate that students have difficulty with the fact that energy is conserved for a quantum system for which the

Hamiltonian does not depend on time. In other words, the probability of obtaining energy E_1 does not depend on time because energy is a constant of motion. Interviews suggest that students have difficulty with why the probability density for measuring position depends on time but the probability of measuring a particular value of energy is time-independent for these systems.

Giving consistently incorrect responses to analogous questions for measurements made at time $t = 0$: Questions 31 and 33 are analogous because the initial wave function is not an eigenstate of the Hamiltonian operator and the measurements of position and energy are made at time $t = 0$. Seventy-two percent of the students answered questions 31 and 33 consistently (e.g., if a student selected answer choice "C" in question 31, he/she also selected answer choice "C" in question 33). This consistency indicates that they recognize the analogous nature of questions 31 and 33. However, only 17% of them answered questions 31 and 33 both consistently and correctly. Of those who answered questions 31 and 33 consistently but incorrectly, 45% incorrectly claimed that the probability of measuring position is $\int_x^{x+dx} x|\Psi(x,0)|^2 dx$ and 22% did not recognize that the probability of measuring E_1 is $\left|\int_0^a \psi_1{}^*(x) Ax(a-x)\, dx\right|^2$ or $\left|\int_0^a \psi_1{}^*(x)\big((\psi_1(x)+\psi_2(x))/\sqrt{2}\big)dx\right|^2$ in question 31 and 33, respectively.

Giving consistently incorrect responses to analogous questions for measurements made at time $t > 0$: Questions 32 and 34 are analogous because the initial wave function is not an eigenstate of the Hamiltonian operator and the measurements of position and energy are made at time $t > 0$. Sixty-nine percent of the students provided consistent answers on questions 32 and 34. However, only 10% answered questions 32 and 34 consistently and correctly. The most common incorrect but consistent answer was (A), none of the above (see Appendix A). This choice indicates that these students correctly recognize that the probability distribution for measuring position depends on time but do not realize that probability distribution for measuring energy does not depend on time since energy is a constant of motion.

Difficulty with determining the measurement probability of spin component S_y if the state is in an eigenstate of $\hat{S}_z$. Question 23 involves measurements performed on a spin-1/2 particle. Students were told that at time $t = 0$, the initial state of a spin-1/2 particle is $|1/2\,,1/2\rangle$ so that $\hat{S}_z|1/2\,,1/2\rangle = \frac{\hbar}{2}|1/2\,,1/2\rangle$. Twenty-two percent of the students claimed that if you measure S_y, you will obtain zero with 100% probability. This type of response indicates that they did not understand that an eigenstate of $\hat{S}_y$ is a linear superposition of eigenstates of $\hat{S}_z$, i.e., $|\uparrow\rangle_y = \frac{|1/2,1/2\rangle + i|1/2,-1/2\rangle}{\sqrt{2}}$ or $|\downarrow\rangle_y = \frac{|1/2,1/2\rangle - i|1/2,-1/2\rangle}{\sqrt{2}}$. Thus, if a measurement of S_y is made, one would obtain either spin-up y or spin-down y with probability ½.

Difficulties with determining how a Stern-Gerlach apparatus affects the spin states of particles. Questions 23-25 involve sending a beam of neutral silver atoms through a Stern-Gerlach apparatus. In question 23, the beam consists of atoms in a linear superposition of the eigenstates of S_z, i.e., $|\chi\rangle = 1/\sqrt{2}\,(|1/2,\ 1/2\rangle + |1/2,\ -1/2\rangle$, and the magnetic field gradient in the Stern-Gerlach apparatus is aligned in the –z-direction. Seventy-percent of the students correctly recognized how the neutral silver atoms would behave in this Stern-Gerlach apparatus. However, in question 24, students were told that the atoms are now all in spin state $|\chi\rangle = |1/2,\ 1/2\rangle$ (spin up-z) and were asked to determine how they behave in a Stern-Gerlach apparatus with a magnetic field gradient in the –y-direction. The atoms in state $|\chi\rangle = |1/2,\ 1/2\rangle$ would be deflected in the +y-direction or –y-direction in a magnetic field gradient in the –y-direction. Thus, one would see two dots where the atoms are detected on a distant screen. Only 42% recognized that the atoms in state $|\chi\rangle = |1/2,\ 1/2\rangle$ would be deflected in the +y-direction or –y-direction in a magnetic field gradient in the –y-direction. Twenty-six percent of the students responded that atoms in state $|\chi\rangle = |1/2,\ 1/2\rangle$ would all go in the same direction in the Stern-Gerlach apparatus with a magnetic field gradient in the –y-direction, and there would only be one dot on the distant screen in the +y-direction.

Difficulties distinguishing between a mixture of atoms and atoms in a linear superposition of eigenstates of a spin component in the context of a Stern-Gerlach apparatus. Question 25 assesses students' understanding of a mixture of atoms (mixture with either $|\chi\rangle = |1/2,\ 1/2\rangle$ or $|\chi\rangle = |1/2,\ -1/2\rangle$) and atoms in a superposition state ($|\chi\rangle = 1/\sqrt{2}\,(|1/2,\ 1/2\rangle + |1/2,\ -1/2\rangle)$). Only 33% of the students correctly responded that the state of each silver atom in the superposition beam will become a superposition of two spatially separated components after passing through a Stern-Gerlach apparatus with a magnetic field gradient in the $-z$-direction and that one can distinguish between the mixture and the superposition by analyzing the pattern on a distant screen after each beam is sent through a Stern-Gerlach apparatus with a magnetic field gradient in the $-x$-direction. Forty-three percent incorrectly responded that passing either the mixture or superposition through a Stern-Gerlach apparatus with a magnetic field gradient in the -z-direction would distinguish between the beams.

4.5.5 Expectation value of observables

Students have difficulties with determining the expectation value of an observable. Questions 5, 10, and 22 assess students' understanding of the expectation value of an observable. Table 4-6 shows the percentages of students choosing answers related to expectation value of observables.

Difficulty with determining the expectation value of a generic operator in Dirac notation. Question 10 assesses students' understanding of the expectation value in Dirac notation. Students were told that $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n and $\hat{I}$ is the identity operator. Students had difficulty determining the expectation value of a generic operator $\hat{Q}$ in a generic state $|\Psi\rangle$. Thirty-four percent of the students did not choose the correct answer option for expectation value, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$, and 25% of students chose the incorrect option $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n \langle q_n|\Psi\rangle$ as the expectation value of $\hat{Q}$. This difficulty indicates that students do not have a conceptual understanding of expectation value as the probability of measuring a particular eigenvalue of an operator multiplied by the eigenvalue, summed over all possible values.

Difficulties involving the expectation value of a spin component. Question 22 assesses students' understanding of the expectation value of S_x, given that the initial state of the spin-1/2 particle is a linear superposition of the eigenstates of S_z, i.e., $|\chi\rangle = a|1/2,\ 1/2\rangle + b|1/2,\ -1/2\rangle$. 75% of students were unable to determine the expectation value of S_x in a generic spin-1/2 state. Students were told that the eigenstates of $\hat{S}_x$ were $|\uparrow\rangle_x = \frac{|1/2,1/2\rangle + |1/2,-1/2\rangle}{\sqrt{2}}$ and $|\downarrow\rangle_x = \frac{|1/2,1/2\rangle - |1/2,-1/2\rangle}{\sqrt{2}}$. One way to answer this question correctly is to recognize that one can write the eigenstates of $\hat{S}_z$ as a linear superposition of eigenstates of $\hat{S}_x$. The state $|\chi\rangle$ can be written in terms of eigenstates of $\hat{S}_x$ as $|\chi\rangle = \frac{a+b}{\sqrt{2}}|1/2,\ 1/2\rangle_x + \frac{a-b}{\sqrt{2}}|1/2,\ -1/2\rangle_x$. Once the state $|\chi\rangle$ is written in terms of the eigenstates of $\hat{S}_x$, determining the expectation value of $\hat{S}_x$ requires multiplying the probabilities of measuring the eigenstates of $\hat{S}_x$ with the corresponding eigenvalues of $\hat{S}_x$ and summing them.

Table 4-6. Distribution of students' responses for questions related to expectation value of observables. Correct responses are in bold.

	Q5(%)	Q10(%)	Q22(%)
(a)	7	9	11
(b)	9	8	17
(c)	9	4	16
(d)	**42**	**57**	27
(e)	32	21	**25**

4.5.6 Time dependence of expectation values of observables

Students have many difficulties with determining whether the expectation value of an observable is time-dependent. Questions 15, 16, 17, 29, and 30 assess students' understanding of the time dependence of expectation value of observables. Table 4-7 shows the percentages of students choosing answers related to time dependence of expectation value of observables.

Table 4-7. Distribution of students' responses for questions related to the time dependence of the expectation values of observables. Correct responses are in bold.

	Q15 (%)	Q16 (%)	Q17 (%)	Q29 (%)	Q30 (%)
(a)	13	13	**40**	11	**20**
(b)	**38**	19	11	4	4
(c)	17	19	7	**20**	9
(d)	13	20	21	42	48
(e)	19	**29**	21	17	12

Difficulty with steps involved in deriving Ehrenfest's theorem. On question 16, only 49% correctly reasoned that $\frac{d}{dt}\langle Q\rangle = \langle \partial\Psi/\partial t\,|\hat{Q}|\Psi\rangle + \langle\Psi|\hat{Q}|\,\partial\Psi/\partial t\rangle$, which one of the steps in deriving Ehrenfest's theorem. Interviews revealed that students thought that $\frac{d}{dt}\langle Q\rangle =$

$\langle\partial\Psi/\partial t\,|\hat{Q}|\Psi\rangle + \langle\Psi|\hat{Q}|\,\partial\Psi/\partial t\rangle$ was designed to trick them into thinking that the chain rule for derivatives in calculus can be applied to write the partial derivative with time of the bra and ket states in an expectation value. One student said, "$\frac{d}{dt}\langle Q\rangle = \langle\partial\Psi/\partial t\,|\hat{Q}|\Psi\rangle + \langle\Psi|\hat{Q}|\,\partial\Psi/\partial t\rangle$ just seems weird. It doesn't seem like something you can do…it's not a multiplication of states…you can't apply the chain rule." The fact that many students explicitly noted that $\frac{d}{dt}\langle Q\rangle = \langle\partial\Psi/\partial t\,|\hat{Q}|\Psi\rangle + \langle\Psi|\hat{Q}|\,\partial\Psi/\partial t\rangle$ did not seem technically correct but claimed that $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$ is correct suggests that they can recall Ehrenfest's theorem as a memorized fact but they do not understand how it is derived mathematically.

Difficulty with using Ehrenfest's theorem to determine whether the expectation value of an observable depends on time. Question 16 examines students' understanding of Ehrenfest's Theorem, $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$ (assuming that neither the Hamiltonian operator nor $\hat{Q}$ depend on time). Eighty-one percent of the students correctly recognized that $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$. In interviews, students often recalled this relationship by memory. For example, one interviewed student, said, "it is just like a definition. That's how you figure out…how a state evolves in time is based on how it commutes with the Hamiltonian." However, a smaller percentage of students (67%) recognized that the expectation value of observables will not depend time if the system is in a stationary state (i.e., $\frac{d}{dt}\langle Q\rangle = 0$ in a stationary state for all observables Q). One interviewed student, when explaining why he didn't choose the statement $\frac{d}{dt}\langle Q\rangle = 0$ in a stationary state for all observables Q as correct, stated, "I don't understand how the fact that the state is in a stationary state is connected to how the expectation value of an observable depends on time. What if it's not in a stationary state, what changes? I would think that it depends on the observable, because if it's in a stationary state of that observable, then…." When the interviewer asked what he meant by "a stationary state of that observable", he replied, "Observables have certain eigenstates, right? So if it's in an eigenstate of that observable…that's what I mean [by a stationary state of that observable]." He then continued, "So if it's in an eigenstate of an observable Q I would think then maybe it [the expectation value for that operator $\hat{Q}$] doesn't depend on time." Several other interviewed students also incorrectly claimed that an eigenstate of an operator corresponding to a physical observable is a stationary state of that observable. They did not realize that a stationary state is an eigenstate of the Hamiltonian and expectation values of all observables are time independent in a stationary state.

C**onfusion about whether an observable without explicit time dependence is a conserved quantity.** Question 17 investigates student difficulties with the time-dependence of expectation values of observables. Eighty-two percent of the students correctly recognized that an observable whose corresponding time-independent operator commutes with the time-independent Hamiltonian of the system, $\hat{H}$, corresponds to a conserved quantity (constant of motion). However, 32% incorrectly reasoned that if an observable Q does not depend explicitly on time, Q is a conserved quantity.

Difficulty recognizing that if the initial state is in an eigenstate of the Hamiltonian, then the expectation values of all observables are time independent. On question 30, students were told that a spin-1/2 particle was initially in an eigenstate of the z-component of spin angular momentum $\hat{S}_z$ and the Hamiltonian of the particle at rest in an external uniform magnetic field is $\hat{H} = -\gamma B_0 \hat{S}_z$. We find that 12% of the students claimed that all of the expectation values $\langle S_x \rangle$, $\langle S_y \rangle$, and $\langle S_z \rangle$ would depend on time. This type of reasoning suggests that students did not recognize that since the particle is initially in an eigenstate of the Hamiltonian operator, the expectation values of all observables will be time independent. In particular, in order to answer question 30 correctly, students must understand what a stationary state is and what that entails for the time dependence of expectation values of the observables.

Interviews suggest that many students struggled to explain what a stationary state is. Moreover, even those who realized that they should use the equation $\frac{d}{dt}\langle \mathrm{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$ (given in question 16) to answer both questions 29 and 30 were often not able to answer question 30 correctly because they did not understand how this equation would yield no time dependence of the expectation value of any observable in a stationary state. In order to utilize this equation to interpret that the expectation value of all observables will be time independent in a stationary state, they had to realize that the Hamiltonian in the commutator acting on the bra and ket state would give the energy corresponding to that stationary state (which is a constant) and hence the expectation value of the commutator becomes zero. When interviewees were explicitly asked whether the initial conditions should matter for answering questions 29 and 30, i.e., whether it should matter whether the particle starts off in an eigenstate of $\hat{S}_x$ or $\hat{S}_z$, one student said, "The fact that it's in an eigenstate of one or the other doesn't change anything. So it's only the expectation value of $\hat{S}_z$ that doesn't depend on time in both cases. It doesn't matter because $\hat{S}_x$ doesn't commute with the Hamiltonian. When you're finding the expectation value of $\hat{S}_x$, you sandwich it between two $|\Psi(t)\rangle$ states. Either way you can't commute the operator that's in the middle of two exponentials that have Hamiltonians in them. [but] $\hat{S}_z$…you can commute it over." While he did reason that the commutator of the Hamiltonian and $\hat{S}_x$ was non-zero, he didn't recognize that the initial state was an eigenstate of the Hamiltonian and thus the system was in a stationary state and all expectation values would be time-independent. Another student stated, "If it starts out in $\hat{S}_z$, I don't feel like that matters still, as long as the Hamiltonian still has the z dependence. I still feel like you would still have $\langle S_x \rangle$ and $\langle S_y \rangle$ depending on time. The magnetic field would cause it to rotate in the x-y plane and have no component along z." This student tried to visualize what was happening but concluded that the x and y components should precess if the system started out in an eigenstate of $\hat{S}_z$. When explicitly asked whether the system was in a stationary state in question 30, he replied, "The Hamiltonian will evolve it. Because you have $e^{-i\hat{H}t/\hbar}$ and that will evolve it in time." One student said that it didn't make sense that the initial states did not change his responses to questions 29 and 30, but he did not know how to make sense of the effect of the initial states mathematically. Similar to several other students, he concluded that since $\hat{S}_x$ and $\hat{S}_y$ do not commute with the Hamiltonian, their expectation values would depend on time in both questions 29 and 30 by incorrectly using the equation for the time dependence of expectation value in question 16.

Incorrectly assuming that if a particle is initially in an eigenstate of a spin component (e.g., $\hat{S}_x$), then the expectation value of the corresponding observable (e.g., S_x) will not depend on time in the context of Larmor precession. Questions 29 and 30 investigated students' understanding of how expectation values of different components of the spin angular momentum evolve in time. Students were told that the Hamiltonian of a charged particle with spin-1/2 at rest in an external uniform magnetic field is $\hat{H} = -\gamma B_0 \hat{S}_z$ where the uniform field B_0 is along the z-direction and γ is the gyromagnetic ratio (a constant). Question 29 refers to a particle initially in an eigenstate of the x-component of spin angular momentum operator, $\hat{S}_x$. Forty-eight percent of the students correctly stated that the expectation value $\langle S_x \rangle$ depends on time, 79% of the students correctly claimed that $\langle S_y \rangle$ depends on time, and 63% of the students incorrectly claimed that $\langle S_z \rangle$ depends on time. Forty-two percent of the students reasoned that only $\langle S_y \rangle$ and $\langle S_z \rangle$ depend on time, suggesting that these students incorrectly thought that if the particle is initially in an eigenstate of the x component of spin, then the expectation value of $\hat{S}_x$ will not depend on time.

Question 30 refers to a particle initially in an eigenstate of the z-component of spin angular momentum $\hat{S}_z$. Only 20% of the students correctly responded that none of the expectation values $\langle S_x \rangle$, $\langle S_y \rangle$, or $\langle S_z \rangle$ would depend on time. On the other hand, 60% of the students claimed that $\langle S_x \rangle$ and $\langle S_y \rangle$ would depend on time. These types of responses suggest that students incorrectly reasoned that if the particle is initially in an eigenstate of the z-component of spin, then the expectation values of $\langle S_x \rangle$ and $\langle S_y \rangle$ would depend on time.

4.5.7 Commutators/Compatibility

Students exhibit various difficulties with compatibility of operators. Questions 16, 17, 19, 20, 27, and 28 assess students' understanding of compatibility and commutators. Table 4-8 shows the distribution of students' responses on questions related to compatibility of operators.

Difficulty with eigenstates of incompatible operators. Question 19 involves differentiating between compatible and incompatible operators. Students were told that Hermitian operators $\hat{A}$ and $\hat{B}$ are compatible when the commutator $[\hat{A}, \hat{B}] = 0$ and incompatible when $[\hat{A}, \hat{B}] \neq 0$. We find that 35% of the students thought that one can find a complete set of simultaneous eigenstates for incompatible operators.

Difficulties with compatible operators and inferences about outcomes of measurements. Question 19 also assesses students' understanding of the relationship between compatible operators and inferences about measurement outcomes. We find that 33% of the students did not recognize that for two compatible operators $\hat{A}$ and $\hat{B}$ whose eigenvalue spectra have no degeneracy, one can infer the value of an observable B after a measurement of observable A returns a particular value for A.

Table 4-8. Distribution of students' responses for questions related to commutators and compatibility of operators. Correct responses are in bold.

	Q16 (%)	Q17 (%)	Q19 (%)	Q20 (%)	Q27 (%)	Q28 (%)
(a)	13	**40**	11	23	29	12
(b)	19	11	22	**35**	4	**40**
(c)	19	7	24	10	**54**	17
(d)	20	21	7	8	5	19
(e)	**29**	21	**36**	22	4	7

Difficulty with determining whether $\hat{S}_+$ and $\hat{S}_z$ are compatible operators. Question 20 involves compatibility of spin operators in the context of a spin-1/2 particle. Students were given the relationships for the raising the lowering spin operators, i.e., $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ and $S_\pm|s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}|s, m_s \pm 1\rangle$. They were told that for a spin-1/2 particle, $|s, m_s\rangle = |1/2, -1/2\rangle$ is a simultaneous eigenstate of $\hat{S}^2$ and $\hat{S}_z$ with quantum numbers $s = \frac{1}{2}$, and $m_s = -\frac{1}{2}$. A majority of students (90%) correctly respond that $\hat{S}_+|1/2, -1/2\rangle$ is an eigenstate of both $\hat{S}^2$ and $\hat{S}_z$. However, 40% of the students incorrectly reasoned that $\hat{S}_z$ and $\hat{S}_+$ are compatible, i.e, they claim that if $\hat{S}_z\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = -\frac{\hbar}{2}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, then $\hat{S}_+\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ is an eigenstate of $\hat{S}_z$ with eigenvalue $-\frac{\hbar}{2}$. Interviews suggest that some students provided this type of response because they overgeneralized the fact that $\hat{S}_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle$ is an eigenstate of both $\hat{S}^2$ and $\hat{S}_z$ to incorrectly infer that the operators $\hat{S}_z$ and $\hat{S}_+$ are compatible.

Difficulties with determining whether $\hat{S}^2$ and $\hat{S}_+$ are compatible operators. Question 20 also assesses students' understanding of the compatibility of $\hat{S}^2$ and $\hat{S}_+$. We find that 33% of the students did not choose the correct answer option that stated "if $\hat{S}^2\left|\frac{1}{2},-\frac{1}{2}\right\rangle=\frac{3}{4}\hbar^2\left|\frac{1}{2},-\frac{1}{2}\right\rangle$, then $\hat{S}_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle$ is an eigenstate of $\hat{S}^2$ with eigenvalue $\frac{3}{4}\hbar^2$." Interviews with students suggest that those with this type of response often did not recognize that $\hat{S}^2$ and $\hat{S}_+$ commute with each other.

Difficulties with successive measurements of compatible and incompatible operators. Question 27 involves immediate, successive measurements in the context of a spin-1/2 system. Students were told that at time $t=0$, the particle is in an initial state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$. The majority of students (88%) recognized that if one measures S_x immediately following a measurement of S_x at time $t=0$, both measurements would yield the same value $\frac{\hbar}{2}$. Similarly, 83% of students recognized that if a measurement of S_z is made and then a measurement of S_x is made in immediate succession at time $t=0$, one would *not* obtain the value $\frac{\hbar}{2}$ with 100% probability. Interviews suggest that students with this type of response often recognize that if two operators whose eigenvalue spectra have no degeneracy commute, e.g., $\hat{S}_x$ and $\hat{S}_x$ in this problem, they share a complete set of eigenstates and one can infer the value of an observable S_x immediately after a measurement of observable S_x returns a particular value for S_x. Similarly, if two operators whose eigenvalue spectra have no degeneracy do not commute, e.g., $\hat{S}_x$ and $\hat{S}_z$, one cannot infer the value of S_x after a measurement of observable S_z returns a particular value for S_z. It is interesting to note that in the abstract case of this question (question 19), 67% of the students recognized that for two compatible operators $\hat{A}$ and $\hat{B}$ whose eigenvalue spectra have no degeneracy, one can infer the value of an observable B after a measurement of observable A returns a particular value for A. In the concrete case, a greater percentage of students (88%) recognized that one can infer the value of observable S_x after a measurement of observable S_x returns a particular value ($\frac{\hbar}{2}$) although in this particular case it is a very special case since S_x is measured twice here in immediate succession. However, students had difficulty with the compatibility of operators $\hat{S}^2$ and $\hat{S}_x$. We find that 38% of the students did not recognize that if one first measures $\vec{S}^2$ at $t = 0$ and then measures S_x in immediate succession, the measurement of S_x will yield the value $\frac{\hbar}{2}$ with 100% probability. Interviews suggest that students with this type of response often did not recognize that operators $\hat{S}^2$ and $\hat{S}_x$ commute with each other. They often incorrectly thought that if operators $\hat{S}^2$ and $\hat{S}_z$ commute then operators $\hat{S}^2$ and $\hat{S}_x$ cannot commute because different components of the spin angular momentum do not commute with each other.

4.5.8 Dirac notation

Having a robust understanding of Dirac notation is important especially if students will advance to graduate level quantum mechanics since Dirac notation is considered a pre-requisite in such a course. We find that students display many difficulties with Dirac notation. Questions 4, 9, 10, 11, 12, 13, 14, and 18 assess students' understanding of Dirac notation involving position and momentum space. Table 4-9 includes the percentages of students who selected different answer choices for questions related to Dirac notation.

Difficulty recognizing that the inner product $\langle x|\Psi\rangle$ is a number. Question 13 is related to writing a generic state $|\Psi\rangle$ using a complete set of position or momentum eigenstates and the probability of finding the particle between x and $x + dx$. Seventy percent of the students recognized that $|\Psi\rangle = \int \Psi(x)|x\rangle dx$. During the clarification phase in student interviews, asking the students to expand the state vector in terms of the identity operator written in terms of a complete set of position eigenstates, i.e., $|\Psi\rangle = \int |x\rangle\langle x|\Psi\rangle dx$, and to make use of $\Psi(x) = \langle x|\Psi\rangle$ to judge the validity of $|\Psi\rangle = \int \Psi(x)|x\rangle dx$, did not help and some students still had difficulty. Interviews suggest that some students did not realize that the inner product $\langle x|\Psi\rangle$ is not an operator and can be moved around inside the integral (since it is just a number).

Difficulties with determining probability of measuring an observable corresponding to an operator with a continuous eigenvalue spectrum in an infinitesimal region. In question 13, 88% of the students recognized that the probability to find the particle between x and $x + dx$ is $|\langle x|\Psi\rangle|^2 dx$. However, some students were confused about the validity of $|\langle x|\Psi\rangle|^2 dx$ in interview situations. For example, one interviewed student said, "I wasn't sure if $|\langle x|\Psi\rangle|^2 dx$ was right, because when you say the probability of finding the particle somewhere, that should be a number, so it was throwing me off that there was a *dx* in there …how can the probability depend on *x*?"

Difficulty involving confusing the position operator with the position bra state $\langle x|$. Question 12 investigates common difficulties students have with the inner products $\langle x|\Psi\rangle$ and $\langle p|\Psi\rangle$. Forty-four percent of the students claimed that $\langle x|\Psi\rangle = \int x\Psi(x)dx$, even though 91% of them recognized that $\Psi(x) = \langle x|\Psi\rangle$ in the previous question 11. This difficulty stems from the fact that many students treated the bra state $\langle x|$ as the operator $\hat{x}$. Twenty-four percent of the students did not recognize that $\langle p|\Psi\rangle = \int \langle p|x\rangle\langle x|\Psi\rangle dx = \int e^{-ipx/\hbar}\Psi(x)dx$ and 38% of students did not recognize that $\langle x|\Psi\rangle = \int \delta(x-x')\Psi(x')dx'$. The integral with a delta function is in general easy for students but 38% had difficulty in this context.

Table 4-9. Distribution of students' responses for questions related to Dirac notation and position/momentum representation. Correct responses are in bold.

	Q4 (%)	**Q9 (%)**	**Q10 (%)**	**Q11 (%)**	**Q12 (%)**	**Q13 (%)**	**Q14 (%)**	**Q18 (%)**
(a)	**63**	10	9	32	6	7	**38**	10
(b)	9	29	8	1	26	9	11	**45**
(c)	13	23	4	**49**	**50**	24	28	26
(d)	6	3	**57**	8	12	19	13	4
(e)	9	**35**	21	10	6	**42**	9	14

Difficulty with differentiating between a momentum eigenstate and a momentum operator. Question 11 involves writing a generic state vector in position and momentum representation. 91% of the students recognize that $\Psi(x) = \langle x|\Psi\rangle$ and 82% of the students recognize that $\widetilde{\Psi}(p) = \langle p|\Psi\rangle$. However, 50% of the students incorrectly claim that $\widetilde{\Psi}(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$ is correct. Interviews suggest that some students inserted a complete set of position eigenstates into $\langle p|\Psi\rangle$, but confused the momentum eigenstate in position representation with the momentum operator $i\hbar\frac{\partial}{\partial x}$. An interviewed student who claimed that $\widetilde{\Psi}(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$ is correct said, "…this inner product $\langle p|\Psi\rangle$ is like an integral, so if you think about it… as p is the momentum operator in one dimension… that would just be $\frac{\hbar}{i}\frac{\partial}{\partial x}$ and then $\Psi(x)dx$ [gets] integrated. So I believe $\widetilde{\Psi}(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$ … is true." Further discussion suggests that the student was having difficulty in differentiating between the momentum eigenstate in dual space and the momentum operator. In particular, the student noted that the momentum eigenstate in the dual space was like the momentum operator acting on state $|\Psi\rangle$. Students who had this type of difficulty generally did not realize that the wave functions in momentum and position are related by Fourier transform.

Inconsistencies in responses to questions about the probability distribution for measuring a concrete observable (e.g., position) vs. a generic observable. Question 13 asks students about the probability distribution of measuring position, and 88% of the students recognized that the probability to find the particle between x and $x + dx$ is $|\langle x|\Psi\rangle|^2 dx$. However, fewer students answer a question involving probability correctly in the abstract context (e.g., in question 9, 67% of the students recognize that the probability for measuring observable Q corresponding to an operator with continuous eigenvalues between q and $q + dq$ is $|\langle q|\Psi\rangle|^2 dq$). These types of difficulties indicate that students are at an intermediate level of expertise and often answer questions correctly in one context but not in another analogous context.

Dirac notation can be used to scaffold student learning of probability of measurements: Question 9 assesses students' understanding of Dirac notation in the context of a generic operator $\hat{Q}$. Sixty-seven percent of the students correctly recognized that the probability of obtaining an outcome between q and $q + dq$ *is* $|\langle q|\Psi\rangle|^2 dq$ and 61% of the students correctly recognized that the probability for measuring values of the observable Q corresponding to an operator with continuous eigenvalues in the interval between q and $q + dq$ in the position representation is $\left|\int_{-\infty}^{\infty} e_q^*(x)\Psi(x)dx\right|^2 dq$ ($e_q(x)$ and $\Psi(x)$ are the wave functions in position representation corresponding to states $|q\rangle$ and $|\Psi\rangle$, respectively). Interviews suggest that students sometimes took advantage of the expression $|\langle q|\Psi\rangle|^2 dq$ in Dirac notation to determine that the expression $\left|\int_{-\infty}^{\infty} e_q^*(x)\Psi(x)dx\right|^2 dq$ in position representation was correct. The fact that comparable large percentages of students in written surveys also recognize that both $|\langle q|\Psi\rangle|^2 dq$ and $\left|\int_{-\infty}^{\infty} e_q^*(x)\Psi(x)dx\right|^2 dq$ are correct (i.e., 67% and 60%) further indicates that students may use statements posed in Dirac notation as a scaffold to determine probability distribution for measurements in position representation.

Inconsistent responses to questions involving writing a momentum eigenvalue equation in position representation. Question 14 involves writing a momentum operator acting on a momentum eigenstate in position and momentum representation. Ninety percent of the students recognize that $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$. Seventy-five percent of the students recognize that $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$ and 60% recognize that $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$. Only 38% of the students recognize that all three of the expressions are correct. Students are also inconsistent in their responses; 41% of students select an answer which involves $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$ but not $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$ and vice versa. Interviews suggest that students with this type of response often do not recognize the connection between the two expressions, i.e., one can act with momentum operator first and pull out the momentum eigenvalue or one can write the momentum operator in position representation and act on the momentum eigenstate in position representation.

4.5.9 Dimensionality of the Hilbert Space

Question 1 deals with the dimensionality of the Hilbert space. Students were told that a particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and

$V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$. The appropriate Hilbert space for this system is infinite dimensional and there are infinitely many energy eigenstates and position eigenstates. The eigenstates corresponding to physical observables span the Hilbert space. Forty-four percent of the students incorrectly claimed that the appropriate Hilbert space for this system is one dimensional. Fifty-one percent of the students claimed that the energy eigenstates of the system form a basis in a one dimensional Hilbert space and 44% of the students claimed that the position eigenstates of the system form a basis in a one dimensional Hilbert space. These types of responses indicate that students have difficulty separating the dimensionality of the physical space in which the particle is confined and the dimensionality of the Hilbert space.

4.6 RETENTION

Eighteen students in an upper-level quantum mechanics course were given the QMFPS after instruction in relevant concepts. The course used research-based learning tools and built on students' common difficulties throughout the semester. The average score on the QMFPS for these students was 66%. After approximately two months, many of these same students ($N = 17$) were given the QMFPS again. The average score was 69%. This finding indicates that students who used research-based learning tools both performed better on the QMFPS compared to students who had traditional instruction and performed equally well on the QMFPS after two months, indicating good retention of concepts.

4.7 COMPARISON TO QUANTUM MECHANICS SURVEY (QMS)

There is a strong correlation between students' scores on the Quantum Mechanics Survey (QMS) [5] and the QMFPS. This correlation provides further content validity to the survey because students who do well on the QMS are generally likely to have a better foundation in quantum mechanics and perform better on the QMFPS (see Fig. 4-3). The QMFPS tends to be more difficult for students than the QMS, possibly because it covers more advanced topics as opposed to the QMS which covers quantum mechanics in one spatial dimension. The students who took both the QMS and the QMFPS were in a course which used research-based instructional strategies to build on students' prior knowledge and help them develop expertise. Since these strategies are likely to be effective for concepts covered in both surveys, students perform reasonably well on both QMS and QMFPS surveys.

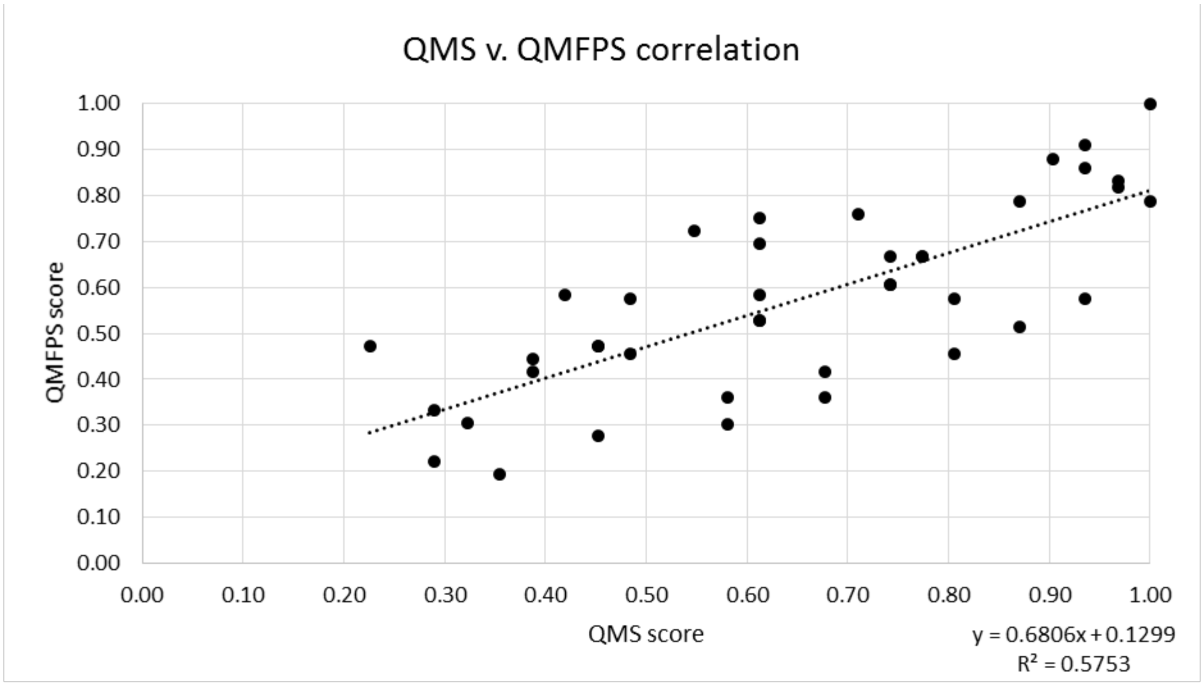

Figure 4-3. Correlation between 41 students' QMFPS scores and their QMS scores. The coefficient of determination is R^2 and the correlation coefficient is R=0.7585.

4.8 SUMMARY

Identification of student difficulties can guide the design of instructional strategies and learning tools to improve students' understanding. The QMFPS serves to assess students' conceptual understanding of the formalism and postulates of quantum mechanics. We found that advanced undergraduate and graduate students have many common difficulties with various topics covered in the survey. We also found that students who used research-based instructional tools such as quantum interactive learning tutorials and concept tests performed significantly better on the QMFPS than students who had traditional instruction. This survey can administered to undergraduate students after instruction in the relevant concepts to evaluate the effectiveness of the course. It can also be given to graduate students as a preliminary test to evaluate their preparation for a graduate level quantum mechanics course. It can serve as a tool for instructors who want to determine students' initial knowledge states in quantum mechanics and tailor instruction for their students.

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4.10 CHAPTER REFERENCES

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APPENDIX A

A.1 QUANTUM MECHANICS FORMALISM AND POSTULATES SURVEY

Definitions, notation, and instructions:

* For a spinless particle confined in one spatial dimension, the expectation value of a time-independent physical observable Q in a state $|\Psi(t)\rangle$ at time t in position space is $\langle Q\rangle = \left\langle\Psi(t)\middle|\hat{Q}\middle|\Psi(t)\right\rangle = \int_{-\infty}^{\infty}\Psi^*(x,t)Q\left(x,-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)dx$. For the special case $t=0$, we will write simply $|\Psi\rangle \equiv |\Psi(0)\rangle$ and $\Psi(x) \equiv \Psi(x,0)$.

* Notation $\left(\hat{Q}|\Psi\rangle\right)^\dagger = \left(|\hat{Q}\Psi\rangle\right)^\dagger = \langle\Psi|\hat{Q}^\dagger = \langle\hat{Q}^\dagger\Psi|$

* $\hat{x}, \hat{p}, \hat{H}$ are generic symbols for the position, momentum and Hamiltonian operators, respectively, for a given quantum system.

* $|x\rangle$, $|p\rangle$, and $|n\rangle$ are eigenstates of position, momentum and Hamiltonian operators with eigenvalues x, p, and E_n, respectively. The eigenvalue equation for a generic hermitian operator $\hat{Q}$ with discrete and continuous eigenvalue spectra is given by $\hat{Q}|q_n\rangle = q_n|q_n\rangle$ and $\hat{Q}|q\rangle = q|q\rangle$, respectively.

* For a particle confined in one spatial dimension, the momentum eigenfunction in position space is $Ae^{ipx/\hbar}$ with eigenvalue p, where A is a constant.

* Ignore the normalization issues of the position eigenstates and momentum eigenstates.

* The Schrödinger representation is used throughout; there is NO explicit time dependence to any of the observables in any question in the survey.

* When the summation or integration limits are not given explicitly, the summation/integration is over all possible values of the summation/integration variable.

* All measurements are ideal (i.e., they are projective measurements).

*$\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ are the x, y, and z components of the spin angular momentum operator (or spin) and $\hat{S}^2$ is the square of the spin angular momentum operator.

Questions 1-3 refer to the following system: A particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1, 2, 3 \ldots \infty$.

1. Choose all of the following statements that are correct for a particle interacting with a one dimensional (1D) infinite square well.
   (1) The appropriate Hilbert space for this system is one dimensional.
   (2) The energy eigenstates of the system form a basis in a 1D Hilbert space.
   (3) The position eigenstates of the system form a basis in a 1D Hilbert space.

   A. none of the above B. 1 only C. 2 only D. 3 only E. all of the above

2. The wave function at time $t = 0$ is $\sqrt{\frac{2}{5}}\psi_1(x) + \sqrt{\frac{3}{5}}\psi_2(x)$ when you perform a measurement of the energy. Choose all of the following statements that are correct.
   (1) The measurement of the energy will yield either E_1 or E_2.
   (2) The spatial part of the **normalized** wave function (excluding the time part) after the energy measurement is either $\sqrt{\frac{2}{5}}\psi_1(x)$ or $\sqrt{\frac{3}{5}}\psi_2(x)$.
   (3) The measurement of the energy will yield $\frac{2}{5}E_1 + \frac{3}{5}E_2$.

   A. 1 only B. 2 only C. 3 only D. 1 and 2 only E. 1 and 3 only

3. Consider the following wave function at time $t = 0$: $\Psi(x, 0) = Ax(a - x)$ for $0 \leq x \leq a$, where A is a suitable normalization constant. Which one of the following is the probability density $|\Psi(x,t)|^2$, at time $t > 0$?

   A. $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2 \cos^2\left(\frac{Et}{\hbar}\right)$, where E is the expectation value of energy.

   B. $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2 e^{\frac{-2iEt}{\hbar}}$, where E is the expectation value of energy.

   C. $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2 \sin^2\left(\frac{Et}{\hbar}\right)$, where E is the expectation value of energy.

   D. $|\Psi(x,t)|^2 = |A|^2 x^2 (a-x)^2$, which is time-independent.

   E. None of the above.

4. Suppose $|\Psi\rangle$ is a generic state and the energy eigenstates $|n\rangle$ are such that $\hat{H}|n\rangle = E_n|n\rangle$, where $n = 1,2,3 \ldots \infty$. Choose all of the following statements that are correct.

   (1) $|\Psi\rangle = \sum_n \langle n|\Psi\rangle\, |n\rangle$

   (2) $e^{-i\hat{H}t/\hbar}|\Psi\rangle = \sum_n e^{-iE_n t/\hbar} \langle n|\Psi\rangle\, |n\rangle$

   (3) If you measure the energy of the system in the state $|\Psi\rangle$, the probability of obtaining E_n and collapsing the state to $|n\rangle$ is $|\langle n|\Psi\rangle|^2$.

   A. all of the above   B. 1 and 2 only   C. 1 and 3 only   D. 2 and 3 only   E. 3 only

5. Suppose $|q_n\rangle$ are the eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with a discrete spectrum of non-degenerate eigenvalues q_n where $n = 1, 2, \ldots \infty$. At time $t = 0$, the state of the system is $|\Psi\rangle = \sum_n c_n(t = 0)|q_n\rangle$. Choose all of the following statements that are necessarily correct.

   (1) $\langle Q\rangle = \sum_n |c_n(0)|^2 q_n$ at time $t = 0$.

   (2) $c_n(t) = e^{-iq_n t/\hbar} c_n(0)$ at time $t > 0$.

   (3) Experimentally, $|c_n(0)|^2$ for various n can be estimated by measuring Q in an ensemble of identically prepared systems in state $|\Psi\rangle$ at time $t = 0$.

   A. 1 only   B. 2 only   C. 3 only   D. 1 and 3 only   E. all of the above

Questions 6-7 refer to the following system: A particle with mass m interacts with a one-dimensional simple harmonic oscillator well $V(x) = \frac{Kx^2}{2}$. The stationary states are $\psi_n(x)$ and the allowed energies are $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, where $n = 0, 1, 2 \ldots \infty$ and $\omega = \sqrt{\frac{K}{m}}$.

6. $|\Psi(0)\rangle$ is the initial state of the system at time $t = 0$ and $\hat{H}$ is the Hamiltonian operator. Choose all of the following statements that are necessarily correct for all times $t > 0$.
   (1) $e^{-i\hat{H}t/\hbar}$ is a hermitian operator.
   (2) $e^{-i\hat{H}t/\hbar}$ is a unitary operator.
   (3) The state of the system at time $t > 0$ is $|\Psi(\mathrm{t})\rangle = e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle$
   A. 2 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. all of the above

7. Suppose you perform a measurement of the position of the particle when it is in the first excited state of a one dimensional simple harmonic oscillator potential energy well. Choose all of the following statements that are correct about this experiment:
   (1) Right after the position measurement, the wave function will be peaked about a particular value of position.
   (2) The wave function will not go back to the first excited state wave function, even if you wait for a long time after the position measurement.
   (3) A long time after the position measurement, the wave function will go back to the first excited state wave function.
   A. 1 only B. 2 only C. 3 only D. 1 and 2 only E. 1 and 3 only

8. Consider the following conversation between Andy and Caroline about the measurement of energy in a state $|\Psi\rangle$ which is not an energy eigenstate.

Andy: When an operator $\hat{H}$ corresponding to energy acts on a generic state $|\Psi\rangle$, it corresponds to a measurement of energy. Therefore, $\hat{H}|\Psi\rangle = E_n|\Psi\rangle$, where E_n is the observed value of energy.

Caroline: No. The measurement collapses the state so $\hat{H}|\Psi\rangle = E_n|n\rangle$, where $|\Psi\rangle$ on the left hand side is the original state before the measurement and $|n\rangle$ on the right hand side of the equation is the state in which the system collapses after the measurement and it is an eigenstate of $\hat{H}$ with eigenvalue E_n.

With whom do you agree?

A. Agree with Caroline only

B. Agree with Andy only

C. Agree with neither

D. Agree with both

E. The answer depends on the details of the state $|\Psi\rangle$, which is a linear superposition of energy eigenstates.

For a spinless particle confined in one spatial dimension, the state of the quantum system at time $t = 0$ is denoted by $|\Psi\rangle$ in the Hilbert space. $|x\rangle$ and $|p\rangle$ are the eigenstates of position and momentum operators. Answer questions 9 to 19.

9. An operator $\hat{Q}$ corresponding to a physical observable Q has a continuous non-degenerate spectrum of eigenvalues. The states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with eigenvalues q. At time $t = 0$, the state of the system is $|\Psi\rangle$. Choose all of the following statements that are correct.

   (1) A measurement of the observable Q must return one of the eigenvalues of the operator $\hat{Q}$.

   (2) If you measure Q at time $t = 0$, the probability of obtaining an outcome between q and $q + dq$ is $|\langle q|\Psi\rangle|^2 dq$.

   (3) If you measure Q at time $t = 0$, the probability of obtaining an outcome between q and $q + dq$ is $\left|\int_{-\infty}^{\infty} e_q^*(x)\Psi(x)dx\right|^2 dq$ in which $e_q(x)$ and $\Psi(x)$ are the wave functions in position representation corresponding to states $|q\rangle$ and $|\Psi\rangle$ respectively.

   A. 1 only   B. 1 and 2 only   C. 1 and 3 only   D. 2 and 3 only   E. all of the above

10. Suppose $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n. $\hat{I}$ is the identity operator. Choose all of the following statements that are correct.

    (1) $\sum_n |q_n\rangle\langle q_n| = \hat{I}$ (2) $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$ (3) $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n \langle q_n|\Psi\rangle$

    A. 1 only   B. 2 only   C. 3 only   D. 1 and 2 only   E. 1 and 3 only

11. Choose all of the following statements that are correct about the position space and momentum space wave functions for this quantum state.

(1) The wave function in position representation is $\Psi(x) = \langle x|\Psi\rangle$ where x is a continuous index.

(2) The wave function in momentum representation is $\widetilde{\Psi}(p) = \langle p \,|\, \Psi\rangle$ where p is a continuous index.

(3) The wave function in momentum representation is $\widetilde{\Psi}(p) = \int dx(-i\hbar \frac{\partial}{\partial x}\Psi(x))$

A. all of the above B. 2 only C. 1 and 2 only D. 3 only E. 1 and 3 only

12. Choose all of the following equations involving the inner product that are correct.

(1) $\langle x|\Psi\rangle = \int x\Psi(x)dx$

(2) $\langle x|\Psi\rangle = \int \delta(x - x')\Psi(x')dx'$

(3) $\langle p|\Psi\rangle = \int\langle p|x\rangle\langle x|\Psi\rangle dx = \int e^{-ipx/\hbar}\Psi(x)dx$ (Ignore normalization issues.)

A. 1 and 2 only B. 1 and 3 only C. 2 and 3 only D. 1 only E. 2 only

13. Choose all of the following statements that are correct.

(1) $|\Psi\rangle = \int\langle p|\Psi\rangle|p\rangle dp$

(2) $|\Psi\rangle = \int \Psi(x)|x\rangle dx$

(3) If you measure the position of the particle in the state $|\Psi\rangle$, the probability of finding the particle between x and $x + dx$ is $|\langle x|\Psi\rangle|^2 dx$.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. all of the above

14. $|p'\rangle$ is the momentum eigenstate with eigenvalue p' for a particle confined in one spatial dimension. Choose all of the following statements that are correct. Ignore normalization issues.

(1) $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p - p')$

(2) $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$

(3) $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$

A. all of the above B. 1 only C. 1 and 2 only D. 1 and 3 only E. 2 and 3 only

15. Choose all of the following statements that are correct:

(1) The stationary states refer to the eigenstates of any operator corresponding to any physical observable.

(2) In an isolated system, if a particle is in a position eigenstate (has a definite value of position) at time

$t = 0$, the position of the particle is well-defined at all times $t > 0$.

(3) In an isolated system, if a system is in an energy eigenstate (it has a definite energy) at time $t = 0$, the energy of the particle is well-defined at all times $t > 0$.

A. 1 only B. 3 only C. 1 and 3 only D. 2 and 3 only E. All of the above

16. Choose all of the following statements that are correct about the time dependence of the expectation value of an observable Q in a state $|\Psi\rangle$. Neither the Hamiltonian $\hat{H}$ nor the operator $\hat{Q}$ depends explicitly on time. (Notation: $\frac{\partial}{\partial t}|\Psi\rangle = \left|\frac{\partial \Psi}{\partial t}\right\rangle$)

(1) $\frac{d}{dt}\langle \mathrm{Q} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}] \rangle$

(2) $\frac{d}{dt}\langle \mathrm{Q} \rangle = 0$ in a stationary state for all observables Q.

(3) $\frac{d}{dt}\langle \mathrm{Q} \rangle = \left\langle \frac{\partial \Psi}{\partial t} \middle| \hat{Q} \middle| \Psi \right\rangle + \left\langle \Psi \middle| \hat{Q} \middle| \frac{\partial \Psi}{\partial t} \right\rangle$

A. 1 only B. 2 only C. 1 and 2 only D. 1 and 3 only E. all of the above

17. Choose all of the following statements that are <u>necessarily</u> correct.

(1) An observable whose corresponding time-independent operator commutes with the time-independent Hamiltonian of the system, $\hat{H}$, corresponds to a conserved quantity (constant of motion).

(2) If an observable Q does not depend explicitly on time, Q is a conserved quantity.

(3) If a quantum system is in an eigenstate of the momentum operator at initial time $t = 0$, momentum is a conserved quantity.

A. 1 only B. 2 only C. 3 only D. 1 and 3 only E. all of the above

18. Suppose $\{|q_n\rangle, n = 1,2,3 \ldots N\}$ form a complete set of orthonormal eigenstates of an operator $\hat{Q}$ with eigenvalues q_n. Which one of the following relations is correct? All of the summations are over all possible values of n and m.

A. $\hat{Q} = \sum_n q_n \langle q_n | q_n \rangle$ B. $\hat{Q} = \sum_n q_n |q_n\rangle\langle q_n|$

C. $\hat{Q} = \sum_{n,m} q_n |q_n\rangle\langle q_m|$ D. $\hat{Q} = \sum_n q_n |\langle q_n | q_n \rangle|^2$ E. None of the above

19. Hermitian operators $\hat{A}$ and $\hat{B}$ are compatible when the commutator $[\hat{A}, \hat{B}] = 0$ and incompatible when $[\hat{A}, \hat{B}] \neq 0$. Choose all of the following statements that are correct.

(1) You can always find a complete set of simultaneous eigenstates for compatible operators.

(2) You can never find a complete set of simultaneous eigenstates for incompatible operators.

(3) For two compatible operators $\hat{A}$ and $\hat{B}$ whose eigenvalue spectra have no degeneracy, you can infer the value of the observable B after the measurement of the observable A returns a particular value for A.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. all of the above

For questions 20-30:

$|s, m_s\rangle$ denotes a simultaneous eigenstate of $\hat{S}^2$ and $\hat{S}_z$ such that the quantum numbers corresponding to $\hat{S}^2$ and $\hat{S}_z$ are s and m_s, respectively.

Raising and lowering operators for spin angular momentum are defined by $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ and $S_\pm |s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}|s, m_s \pm 1\rangle$. The commutator is defined by $[S_x, S_y] = i\hbar S_z$.

For example, for a spin-1/2 particle:

$$s = \frac{1}{2}, \qquad m_s = \pm\frac{1}{2}$$

$$\hat{S}_z \left|\frac{1}{2}, \frac{1}{2}\right\rangle = +\frac{\hbar}{2}\left|\frac{1}{2}, \frac{1}{2}\right\rangle \qquad \hat{S}_z \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = -\frac{\hbar}{2}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$$

$$\hat{S}_+ \left|\frac{1}{2}, \frac{1}{2}\right\rangle = 0 \qquad \hat{S}_+ \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

$$\hat{S}_- \left|\frac{1}{2}, \frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \qquad \hat{S}_- \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = 0$$

Eigenstates of $\hat{S}_x$: $|\uparrow\rangle_x = \frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle + \left|\frac{1}{2},-\frac{1}{2}\right\rangle}{\sqrt{2}}$ $\qquad |\downarrow\rangle_x = \frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle - \left|\frac{1}{2},-\frac{1}{2}\right\rangle}{\sqrt{2}}$

Eigenstates of $\hat{S}_y$: $|\uparrow\rangle_y = \frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle + i\left|\frac{1}{2},-\frac{1}{2}\right\rangle}{\sqrt{2}}$ $\qquad |\downarrow\rangle_y = \frac{\left|\frac{1}{2},\frac{1}{2}\right\rangle - i\left|\frac{1}{2},-\frac{1}{2}\right\rangle}{\sqrt{2}}$

20. For a spin-1/2 particle, suppose $|s, m_s\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ is a simultaneous eigenstate of $\hat{S}^2$ and $\hat{S}_z$ with quantum numbers $s = \frac{1}{2}$, and $m_s = -\frac{1}{2}$. Choose all of the following statements that are correct.

(1) $\hat{S}_+ \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ is an eigenstate of both $\hat{S}^2$ and $\hat{S}_z$.

(2) If $\hat{S}^2 \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \frac{3}{4}\hbar^2 \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, then $\hat{S}_+ \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ is an eigenstate of $\hat{S}^2$ with eigenvalue $\frac{3}{4}\hbar^2$.

(3) If $\hat{S}_z \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = -\frac{\hbar}{2} \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, then $\hat{S}_+ \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ is an eigenstate of $\hat{S}_z$ with eigenvalue $-\frac{\hbar}{2}$.

A. 1 only B. 1 and 2 only C. 1 and 3 only D. 2 and 3 only E. all of the above

21. At time $t = 0$, the initial state of a spin-1/2 particle is $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ so that $\hat{S}_z \left|\frac{1}{2}, \frac{1}{2}\right\rangle = \frac{\hbar}{2} \left|\frac{1}{2}, \frac{1}{2}\right\rangle$. Choose all of the following statements that are correct at time $t = 0$.

(1) If you measure S_y, you will obtain zero with 100% probability.

(2) If you measure S_z, you will obtain $\frac{\hbar}{2}$ with 100% probability.

(3) If you measure S^2, you will obtain $\frac{3\hbar^2}{4}$ with 100% probability.

A. 1 only B. 2 only C. 1 and 3 only D. 2 and 3 only E. all of the above

22. At time $t = 0$, the initial normalized state of a spin-1/2 particle is $|\chi\rangle = a\left|\frac{1}{2}, \frac{1}{2}\right\rangle + b\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ where a and b are suitable constants. What is the expectation value $\langle S_x \rangle$ at time $t = 0$?

A. $\langle S_x \rangle = 0$

B. $\langle S_x \rangle = \frac{\hbar}{2}(|a|^2 + |b|^2)$

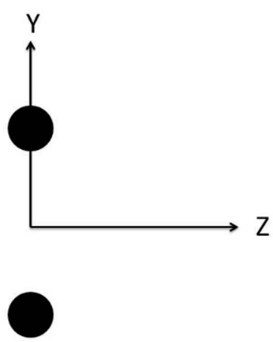
C. $\langle S_x \rangle = \frac{\hbar}{2}(|a|^2 - |b|^2)$

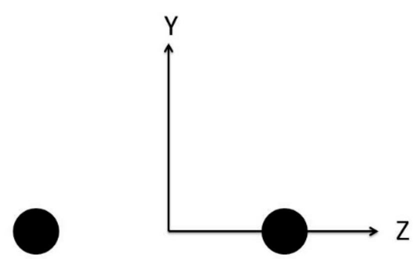
D. $\langle S_x \rangle = \frac{\hbar}{2}\left(\frac{|a+b|^2}{2} + \frac{|a-b|^2}{2}\right)$

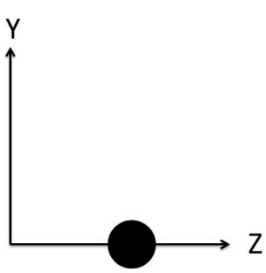
E. $\langle S_x \rangle = \frac{\hbar}{2}\left(\frac{|a+b|^2}{2} - \frac{|a-b|^2}{2}\right)$

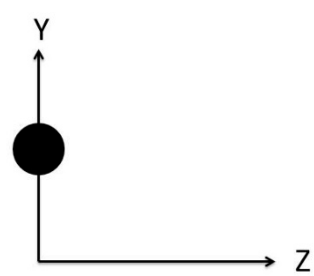
Questions 23-25 refer to Stern-Gerlach experiments with magnetic field gradients in various directions. The neutral silver atoms have zero orbital angular momentum. If an atom in state $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ (or $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$) passes through a Stern-Gerlach apparatus with the magnetic field gradient in the negative-z direction (SGZ-), it will be deflected in the +z (or –z) direction, respectively. Assume that the initial state of each silver atom entering the Stern Gerlach apparatus is spatially localized.

23. A beam of neutral silver atoms, each of which is in a spin state $|\chi\rangle = \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}\right\rangle + \left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right)$, propagates into the paper (x-direction). The beam is sent through a Stern Gerlach apparatus with a magnetic field gradient in the $-z$-direction **(SGZ-)**. Which one of the following schematically represents the pattern you expect to observe on a distant screen in the y-z plane when the atoms hit a screen?

A.


B.


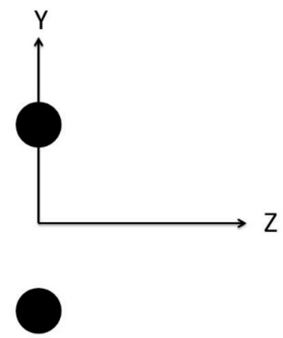
C.


D.


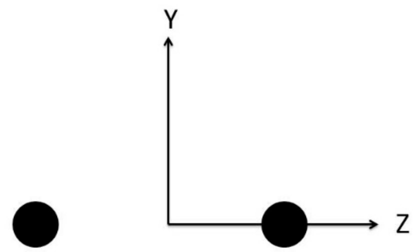
E. None of the above.

24. A beam of neutral silver atoms, each of which is in a spin state state $|\chi\rangle = \left|\frac{1}{2},\ \frac{1}{2}\right\rangle$, propagates into the paper (x-direction). The beam is sent through a Stern Gerlach apparatus with a magnetic field gradient in the $-y$-direction **(SGY-)**. Which one of the following schematically represents the pattern you expect to observe on a distant screen in the y-z plane when the atoms hit a screen?

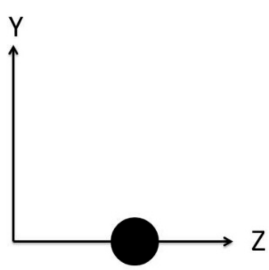
A.



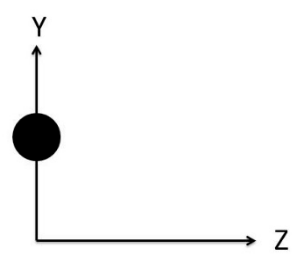
B.



C.



D.



E. None of the above.

25. Suppose Beam A consists of neutral silver atoms, each of which is in the state $|\chi\rangle = \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}\right\rangle + \left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right)$, and Beam B consists of a mixture in which half of the silver atoms are each in state $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ and the other half are each in state $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$. Both beams propagate along the *y* direction. Choose all of the following statements that are correct (Note the magnetic field gradient in each case):

(1) The state of each silver atom in beam A will become a superposition of two spatially separated components after passing through a Stern Gerlach apparatus with a magnetic field gradient in the $-z$-direction **(SGZ-)**.

(2) We can distinguish between Beam A and Beam B by analyzing the pattern on a distant screen after each beam is sent through a Stern Gerlach apparatus with a magnetic field gradient in the $-z$-direction **(SGZ-)**.

(3) We can distinguish between Beam A and Beam B by analyzing the pattern on a distant screen after each beam is sent through a Stern Gerlach apparatus with a magnetic field gradient in the $-x$-direction **(SGX-)**.

A. 1 only B. 2 only C. 1 and 2 only D. 1 and 3 only E. All of the above.

In questions 26-30, the Hamiltonian of a charged particle with spin-1/2 at rest in an external uniform magnetic field is $\hat{H} = -\gamma B_0 \hat{S}_z$ where the uniform field B_0 is along the z-direction and γ is the gyromagnetic ratio (a constant). The phrase "immediate succession" implies that the time evolution can be ignored between the first and second measurements.

26. Suppose that at time $t = 0$, the particle is in an initial normalized spin state $|\chi\rangle = a\left|\frac{1}{2}, \frac{1}{2}\right\rangle + b\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ where a and b are suitable constants. What is the state of the system after time t?

A. $|\chi(t)\rangle = e^{\frac{i\gamma B_0 t}{2}}\left(a\left|\frac{1}{2}, \frac{1}{2}\right\rangle + b\left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right)$

B. $|\chi(t)\rangle = e^{\frac{-i\gamma B_0 t}{2}}\left(a\left|\frac{1}{2}, \frac{1}{2}\right\rangle + b\left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right)$

C. $|\chi(t)\rangle = e^{\frac{i\gamma B_0 t}{2}}\left((a+b)\left|\frac{1}{2}, \frac{1}{2}\right\rangle + (a-b)\left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right)$

D. $|\chi(t)\rangle = ae^{\frac{i\gamma B_0 t}{2}}\left|\frac{1}{2}, \frac{1}{2}\right\rangle + be^{\frac{-i\gamma B_0 t}{2}}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$

E. None of the above.

27. Suppose that at time $t = 0$, the particle is in an initial state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$. Choose all of the following statements that are correct about measurements performed on the system starting with this initial state at $t = 0$.

(1) If you measure S_x immediately following another measurement of S_x at $t = 0$, both measurements of S_x will yield the same value $\frac{\hbar}{2}$.

(2) If you first measure $\vec{S}^2$ at $t = 0$ and then measure S_x in immediate succession, the measurement of S_x will yield the value $\frac{\hbar}{2}$ with 100% probability.

(3) If you first measure S_z at $t = 0$ and then measure S_x in immediate succession, the measurement of S_x will yield the value $\frac{\hbar}{2}$ with 100% probability.

A. 1 only B. 3 only C. 1 and 2 only D. 1 and 3 only E. 2 and 3 only

28. Suppose that at time $t = 0$, the particle is in an initial state in which the x-component of spin S_x has a definite value $\frac{\hbar}{2}$ (as in the preceding question). Choose all of the following statements that are correct about measurements performed on the system after a long time t. (The only difference between the problem statement of questions 29 and 30 is that the measurements are performed at time $t = 0$ in question 29 and after a long time t in question 30.)

(1) If you measure S_x immediately following another measurement of S_x, both measurements of S_x will yield the same value $\frac{\hbar}{2}$ with 100% probability.

(2) If you first measure $\vec{S}^2$ and then measure S_x in immediate succession, the measurement of S_x will yield the value $\frac{\hbar}{2}$ with 100% probability.

(3) If you first measure S_z and then measure S_x in immediate succession, the measurement of S_x will yield the value $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$ with equal probability

A. 1 only B. 3 only C. 1 and 2 only D. 1 and 3 only E. 2 and 3 only

29. Suppose the particle is initially in an eigenstate of the x-component of spin angular momentum operator $\hat{S}_x$. Choose all of the following statements that are correct:

(1) The expectation value $\langle S_x \rangle$ depends on time.

(2) The expectation value $\langle S_y \rangle$ depends on time.

(3) The expectation value $\langle S_z \rangle$ depends on time.

A. 1 only B. 3 only C. 1 and 2 only D. 2 and 3 only E. all of the above

30. Suppose the particle is initially in an eigenstate of the z-component of spin angular momentum $\hat{S}_z$. Choose all of the following statements that are correct:

(1) The expectation value $\langle S_x \rangle$ depends on time.

(2) The expectation value $\langle S_y \rangle$ depends on time.

(3) The expectation value $\langle S_z \rangle$ depends on time.

A. none of the above B. 1 only C. 3 only D. 1 and 2 only E. all of the above

A particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$ otherwise). The stationary state wave functions are $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1, 2, 3\ldots$. Answer questions 31-34.

31. The wave function at time $t = 0$ is $\Psi(x, 0) = Ax(a - x)$ for $0 \leq x \leq a$, where A is a suitable normalization constant. Choose all of the following statements that are correct at time $t = 0$:

(1) If you measure the position of the particle at time $t = 0$, the probability density for measuring x is $|Ax(a - x)|^2$.

(2) If you measure the energy of the system at time $t = 0$, the probability of obtaining E_1 is $\left|\int_0^a \psi_1{}^*(x) Ax(a - x)\, dx\right|^2$.

(3) If you measure the position of the particle at time $t = 0$, the probability of obtaining a value between x and $x + dx$ is $\int_x^{x+dx} x|\Psi(x, 0)|^2\, dx$.

A. 1 only B. 3 only C. 1 and 2 only D. 1 and 3 only E. All of the above

32. The wave function at time $t = 0$ $\Psi(x, 0) = Ax(a - x)$ for $0 \leq x \leq a$, where A is a suitable normalization constant. Choose all of the following statements that are correct at a time $t > 0$:

(1) If you measure the position of the particle after a time t, the probability density for measuring x is $|Ax(a - x)|^2$.

(2) If you measure the energy of the system after a time t, the probability of obtaining E_1 is $\left|\int_0^a \psi_1{}^*(x) Ax(a - x) dx\right|^2$.

(3) If you measure the position of the particle after a time t, the probability of obtaining a value between x and $x + dx$ is $\int_x^{x+dx} x|\Psi(x, 0)|^2\, dx$.

A. None of the above B. 1 only C. 2 only D. 3 only E. 1 and 3 only

33. The wave function at time $t = 0$ is $\Psi(x, 0) = \frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}$. Choose all of the following statements that are correct at time $t = 0$:

(1) If you measure the position of the particle at time $t = 0$, the probability density for measuring x is $\left|\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right|^2$.

(2) If you measure the energy of the system at time $t = 0$, the probability of obtaining E_1 is $\left|\int_0^a \psi_1{}^*(x) \left(\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right) dx\right|^2$.

(3) If you measure the position of the particle at time $t = 0$, the probability of obtaining a value between x and $x + dx$ is $\int_x^{x+dx} x|\Psi(x, 0)|^2\, dx$.

A. 1 only B. 3 only C. 1 and 2 only D. 1 and 3 only E. All of the above

34. The wave function at time $t = 0$ is $\Psi(x, 0) = \frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}$. Choose all of the following statements that are correct at a time $t > 0$:

(1) If you measure the position of the particle after a time t, the probability density for measuring x is $\left|\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right|^2$.

(2) If you measure the energy of the system after a time t, the probability of obtaining E_1 is

$\left|\int_0^a \psi_1{}^*(x)\left(\frac{\psi_1(x)+\psi_2(x)}{\sqrt{2}}\right)dx\right|^2$.

(3) If you measure the position of the particle after a time t, the probability of obtaining a value between x and $x + dx$ is $\int_x^{x+dx} x|\Psi(x,0)|^2\, dx$.

A. None of the above B. 1 only C. 2 only D. 3 only E. 1 and 3 only

5.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON DIRAC NOTATION

5.1 INTRODUCTION

Learning quantum mechanics concepts can be challenging for advanced undergraduate and graduate students in physics. Student difficulties in learning different quantum mechanics concepts have been investigated in prior studies [1-18]. Several research-based learning tools have been developed to improve students' understanding of quantum concepts [19-26]. We have been investigating student difficulties with Dirac notation [14]. Dirac notation is a representation used extensively in quantum mechanics and it is important that students have a thorough understanding of this notation. They should learn how to translate quantum states in Dirac notation to wave functions in the position and momentum representations before they advance to the graduate quantum mechanics courses. Although Dirac notation representation is the one of the most elegant of all representations students learn in upper-level undergraduate quantum mechanics course, many students including those who go on to do graduate study in physics have difficulties with the Dirac notation.

Here, we investigate student difficulties with Dirac notation, e.g., difficulties with the notation itself, difficulties with translating quantum state vectors in Dirac notation to wave functions in position and momentum representations, difficulties with quantum operators, difficulties with the probabilities of measuring a particular value of an observable, and difficulties with the expectation values of observables.

Based upon the investigation of student difficulties with Dirac notation, we have developed a Dirac notation Quantum Interactive Learning Tutorial (QuILT) which uses a guided, inquiry-based approach to learning and helps students build on their prior knowledge. The Dirac notation QuILT can be used in-class, during which students can work on it in small groups as the instructor gives appropriate feedback. The QuILT can also be given as a homework supplement. We discuss the development of the Dirac notation QuILT that helps students develop a functional understanding of Dirac notation. To determine the effectiveness of the Dirac notation QuILT, we examine student performance on pre/posttests on Dirac notation and compare the performance of students who learned from the Dirac notation QuILT with the performance of students who had traditional instruction on free-response and multiple-choice questions related to Dirac notation on midterm exams, retention quizzes, final exams, and conceptual surveys.

5.2 FRAMEWORKS INFORMING THE INVESTIGATION OF STUDENT DIFFICULTIES WITH DIRAC NOTATION AND THE ROLE OF REPRESENTATIONS IN PROBLEM SOLVING

How can a student become an expert in physics, whether at an introductory or advanced level? There is a vast amount of research literature focusing on student reasoning difficulties in introductory courses, how students in introductory courses differ from physics experts in their problem-solving and self-regulatory skills, and the strategies that may help students become better problem solvers and independent learners (e.g., see Refs. [7-9]). Relatively few investigations have focused on the nature of expertise of advanced physics students and strategies that can be used in upper-level courses to help them build a robust knowledge structure and develop their problem-solving, reasoning, and metacognitive skills [10-17]. Here, we discuss an investigation focused on the nature of expertise of advanced physics students in upper-level and graduate-level quantum mechanics, in particular, in the context of Dirac notation, an elegant representation used commonly in upper-level quantum mechanics.

In the investigation of student difficulties involving Dirac notation, differences in upper-level undergraduate and graduate students' abilities to recognize vs. recall vs. generate concepts in various situations were examined. These differences shed light on the development of expertise and the role of "chunking" [27] in problem solving in quantum mechanics. Furthermore, we also explored how upper-level undergraduate and graduate students translate between different representational modes (i.e., translating quantum states in Dirac notation representation to wave functions in position and momentum representations). The findings can clarify the level of proficiency that students have with different representations and their deficiencies in translating between representations. The investigation of difficulties informed the development of the Dirac notation QuILT, which focuses on strategies that can be used to help advanced students build a robust knowledge structure and develop their problem-solving, reasoning, and metacognitive skills. Below, we discuss frameworks based on cognitive science that inform the investigation of student difficulties in Dirac notation.

5.2.1 General Characteristics of Experts and Novices: Knowledge Structure and Performance

In order to help students develop expertise in quantum mechanics, e.g., Dirac notation, one must first ask how experts compare to novices in terms of their knowledge structure and their problem-solving, reasoning, and metacognitive skills. According to Sternberg [28], some of the characteristics of an expert in any field include: 1) having a large and well organized knowledge structure about the domain; 2) spending more time in determining how to represent problems than searching for a problem strategy (i.e., more time spent analyzing the problem before implementing the solution); 3) working forward from the given information in the problem and implementing strategies to find the unknowns; 4) developing representations of problems based on deep, structural similarities between problems; 5) efficient problem-solving; when under time constraints, experts solve problems more quickly than novices, and 6) accurately predicting the difficulty in solving a problem. Additionally, experts are more flexible than novices in their planning and actions [29].

Experts also have more robust metacognitive skills than novices. Metacognitive skills, or self-regulatory skills, refer to a set of activities that can help individuals control their learning [30]. The three main self-regulatory skills are planning, monitoring, and evaluation [31]. Planning involves selecting appropriate strategies to use before beginning a task. Monitoring is the awareness of comprehension and task performance. Evaluation involves appraising the product of the task and re-evaluating conclusions [31]. Self-regulatory skills are crucial for learning in knowledge-rich domains. For example, in physics, students benefit from approaching a problem in a systematic way, such as analyzing the problem (e.g., drawing a diagram, listing knowns/unknowns, and predicting qualitative features of the solution that can be checked later), planning (e.g., selecting pertinent principles/concepts to solve the problem), and evaluating (e.g., checking that the preceding steps are valid and that the answer makes sense) [32]. When experts repeatedly practice problems in their domain of expertise, problem-solving and self-regulatory skills may even become automatic and subconscious [30]. Therefore, unless experts are given a "novel" problem, they may go through the problem-solving process automatically without making a conscious effort to plan, monitor, or evaluate their work [32,33].

On the other hand, novices' knowledge structure is incoherent and consists largely of miscellaneous bits of knowledge, which are unrelated to any general conception [34]. Novices' problem solving usually consists of searching for an appropriate equation without first analyzing the problem and planning a solution [35]. Novices often reason backward, beginning with the unknown variable and solving various sets of equations to finally solve for the unknown variable. This type of backward reasoning is difficult because it requires setting goals and sub-goals and keeping track of them, putting a strain on working memory and leading to errors [36]. Furthermore, novices often lack metacognitive skills. They may reason correctly in one context but not in another context and fail to check for consistency. After solving a problem, novices typically do not check the limiting cases or reason about the deeper meaning of the problem.

5.2.2 Experts' vs. Novices' Retrieval of Knowledge in Different Situations: Recognition, Recall vs. Generating a Solution

Because of the differences between experts' and novices' knowledge structure, experts perform better at solving problems than novices. Chase and Simon [27] compared novice and master chess players' abilities to reproduce game positions from memory (i.e., the chess piece positions on the board of an actual game) and random positions (i.e., the chess piece positions that were randomly placed on the board). They found that masters showed a considerable advantage for reproducing the positions of the chess pieces on the board for actual games. Chase and Simon also used a chess-board reproduction task to examine the nature of the patterns, or chunks, used by the chess masters. The chess masters' task was to reproduce the positions of pieces of a target chessboard (i.e., a chess board with pieces placed on it as would be in an actual game) on a test chessboard. The chess masters glanced at the target board, placed some pieces on the test board, glanced back at the target board, placed some more pieces on the target board, and so on. Each group of chess pieces which were placed on the target board after one glance was considered to be a "chunk." Chunks tended to define meaningful game relations among pieces. These findings demonstrate that experts recognize patterns of elements that repeat in many problems, i.e., chunks [37]. Physics experts are not only good at recognizing or recalling whether knowledge has been applied correctly in a given situation, they are also adept at generating solutions to problems because they have developed knowledge chunks in their domain of expertise which have been organized hierarchically. This type of knowledge structure allows experts to consolidate their knowledge into a few key ideas which can be remembered easily and flexibly elaborated to solve problems [34].

In contrast, novices' incoherent knowledge structure [34] inhibits them from being able to generate solutions to free response questions. They may be able to recognize the correctness of a concept in a multiple-choice question. Students may also be able to recall some bits of knowledge from memory in various situations while solving problems. However, it is often difficult for them to generate a proof that a concept is correct or use the concept to solve other free-response problems because their knowledge structure is fragmented and they have not "chunked" [27,37] enough related knowledge to solve the problem.

Experts also have compiled knowledge, i.e., a repertoire of knowledge about special cases in which to apply a concept [34]. Compiled knowledge can often be used to interpret a concept intuitively without the need for deliberate processing [34]. A student at an intermediate level of expertise may possess some compiled knowledge but lack the ability to elaborate on it in a new situation. For example, many students may quickly recall that the expression in Dirac notation, $\langle p|p'\rangle$, is a wavefunction in the momentum representation, i.e., $\delta(p-p')$. However, the same students may have difficulty generating an expression for a momentum eigenstate with eigenvalue p' in momentum representation (which is representationally equivalent to $\langle p|p'\rangle$ in the Dirac notation representation and $\delta(p-p')$ without the Dirac notation representation). Expert and novice use of representational modes is discussed further in the next section.

5.2.3 Experts' vs. Novices' Problem Solving: Representational Modes

Experts in physics employ a variety of representations when solving problems, e.g., verbal, mathematical, graphical, tabular, etc. [38]. A robust understanding of a concept requires the ability to recognize and manipulate that concept in a variety of representations to solve problems [38]. However, traditional physics instruction often uses quantitative modes of description focusing on "plug and chug" (algorithmic) approaches as opposed to integrating quantitative and qualitative modes of description, e.g., words and pictures, with a focus on functional understanding [34]. Algorithmic problem solving does not result in deep understanding of concepts nor in development of robust problem-solving, reasoning and metacognitive skills [39]. Students often become proficient in quantitative reasoning but display difficulties when reasoning qualitatively. To help students develop knowledge "chunks" and a hierarchically organized knowledge, students need to be asked more than just algorithmic problems. Students should be guided to develop both content knowledge and skills via integrating qualitative and quantitative questions that focus on functional understanding. To accomplish this goal, Reif [34] suggests embedding quantitative discussions in qualitative frameworks (e.g., discuss properties of acceleration before deriving quantitative expressions for the acceleration), solving qualitative as well as quantitative problems, and using qualitative checks (e.g., checking solutions of quantitative problems by assessing whether the results agree with qualitative predictions in special cases).

These frameworks provide a basis for the investigation of student difficulties with Dirac notation and the development of the Dirac notation QuILT.

5.3 METHODOLOGY FOR THE INVESTIGATION OF STUDENT DIFFICULTIES

Student difficulties with Dirac notation were investigated by administering open-ended questions and multiple-choice surveys to upper-level undergraduate and graduate students, observing common difficulties on in-class quizzes and exams, and conducting individual interviews with students in quantum mechanics courses. Data, which included open-ended questions and multiple choice surveys from seven semesters of quantum mechanics I courses at the University of Pittsburgh, were collected and analyzed. Multiple-choice questions were also administered to undergraduate and graduate students from five universities in the U.S.

The open-ended questions on quizzes and exams were graded using rubrics which were developed by two of the investigators together (E.M. and C.S.). A subset of the open-ended questions was graded separately by the investigators. After comparing the grading of the open-ended questions first, the investigators discussed any disagreements in grading and resolved them with a final inter-rater reliability of 90% .

The individual interviews used a think-aloud protocol to better understand the rationale for student responses before, during, and after the development of different versions of the Dirac notation QuILT and the associated pretest and posttest. During the semi-structured interviews, students were asked to verbalize their thoughts while they answered questions. Students were provided a pen and paper and asked to "think aloud" [40] 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 issues that they had not clearly addressed earlier.

We examined the extent to which students: 1) recognize expressions written in Dirac notation (e.g., evaluate the correctness of the statement that a generic wave function $\Psi(x) = \langle x|\Psi\rangle$); 2) recall how to translate expressions written using Dirac notation in the position or momentum representation to those without Dirac notation and vice versa (e.g., given $\langle x|\Psi\rangle$, recall that it can be written as $\Psi(x)$ without Dirac notation); and 3) generate expressions for wave functions in position or momentum representation given a quantum state in Dirac notation (e.g., given a generic state $|\Psi\rangle$, generate an expression for the wave function in position representation). While there are other ways to categorize these types of questions, the researchers jointly agreed that "recognize, recall, generate" is one way to code these types of questions. We discuss difficulties of undergraduate and graduate students with these topics.

5.4 STUDENT DIFFICULTIES

5.4.1 Student difficulties with Dirac notation in the context of a three-dimensional space

An open-ended survey on Dirac notation in the context of a three-dimensional space was administered to 27 upper-level students in a quantum mechanics course after traditional instruction in relevant concepts. The following difficulties were displayed:

Difficulty writing the components of a three dimensional vector. Students display difficulties with Dirac notation in the context of a three-dimensional space (which is similar to the one students learn in introductory physics). For example, 27 upper-level undergraduate students were asked the following question:

Assume that $|i\rangle, |j\rangle,$ and $|k\rangle$ form a complete set of orthonormal basis vectors. For vector $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ (a vector in a three-dimensional vector space), write the components $a, b,$ and c in Dirac notation.

Thirty-seven percent of the students correctly wrote the components as $a = \langle i|\chi_1\rangle$, $b = \langle j|\chi_1\rangle$, and $c = \langle k|\chi_1\rangle$. However, Table 5-1 shows that 33% of the students simply rewrote the vector $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ which was given in the problem statement as their response.

On the other hand, when students were asked to represent $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ as a column vector in the given basis $|i\rangle, |j\rangle,$ and $|k\rangle$, students performed better. We find that 85% of the students correctly wrote $|\chi_1\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ in the basis $|i\rangle, |j\rangle,$ and $|k\rangle$. This type of difficulty indicates that while students are familiar with writing vectors in matrix representation, they do not understand conceptually how one would obtain the components of the vector in Dirac notation.

Table 5-1. Percentages of students displaying difficulties with Dirac notation in the context of a three-dimensional space.

Difficulty	**Percentage of students** ($N = 27$ undergraduate students)
Difficulty with writing the components of a three dimensional vector, e.g., rewriting the vector $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ (which was given in the problem statement)	33%
Incorrectly describing the outer product as a scalar	19%
Incorrectly describing the outer product as a column vector	15%
Writing incorrect matrix forms of bra and ket vectors, e.g., writing ket vectors as row matrices and bra vectors as column matrices	11%
Correctly writing the identity operator in matrix form, i.e., $\hat{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ but not in Dirac notation, i.e., $\hat{I} = |i\rangle\langle i| + |j\rangle\langle j| + |k\rangle\langle k|$	22%
Incorrectly writing that the projection operator that projects vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$ is $\langle i|\chi_1\rangle$	30%

Incorrectly describing the outer product as a scalar or column matrix. Students also had difficulty with describing whether or not the outer product is a scalar, column vector, row vector, or a 3×3 matrix. 27 upper-level undergraduate students were asked the following question:

Assume that $|i\rangle, |j\rangle,$ and $|k\rangle$ form a complete set of orthonormal basis vectors. $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ and $|\chi_2\rangle = d|i\rangle + e|j\rangle + f|k\rangle$ are vectors in a three dimensional vector space. Write the outer product of "ket" vector $|\chi_1\rangle$ with "bra" vector $\langle\chi_2|$ in the given basis. Is this outer product a scalar (number), a column vector, a row vector, or a 3×3 matrix in the given basis?"

63% of the students correctly stated that the outer product is a 3×3 matrix. However, Table 5-1 shows that 19% of the students incorrectly claimed that the outer product is a scalar and 15% of the students incorrectly claimed that the outer product is a column vector. These types of difficulties indicate that some students have not developed understanding of outer products.

Confusing the inner product with the outer product in Dirac notation. The following question was administered to 27 upper-level undergraduate students to investigate student difficulties with determining the outer product:

Assume that $|i\rangle, |j\rangle,$ and $|k\rangle$ form a complete set of orthonormal basis vectors. $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ and $|\chi_2\rangle = d|i\rangle + e|j\rangle + f|k\rangle$ are vectors in a three dimensional vector space. Write the outer product of "ket" vector $|\chi_1\rangle$ with "bra" vector $\langle\chi_2|$ in the given basis.

Forty-eight percent of the students wrote the correct expression for the outer product, i.e., $|\chi_1\rangle\langle\chi_2| \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}(d^* \quad e^* \quad f^*) = \begin{pmatrix} ad^* & ae^* & af^* \\ bd^* & be^* & bf^* \\ cd^* & ce^* & cf^* \end{pmatrix}$. Students were not penalized if they did not complex conjugate the components of the vector $\langle\chi_2|$. The most common difficulty involved writing the outer product as the inner product $\langle\chi_2|\chi_1\rangle$. Nineteen percent of the students wrote the outer product of ket vector $|\chi_1\rangle$ with bra vector $\langle\chi_2|$ *as* $\langle\chi_2|\chi_1\rangle$. Their final answers were typically of the form $\langle\chi_2|\chi_1\rangle = ((\langle i|d^* + \langle j|e^* + \langle k|f^*)(a|i\rangle + b|j\rangle + c|k\rangle) = d^*a + e^*b + f^*c$. This type of difficulty indicates that many students are not adept at writing the outer product in Dirac notation and have difficulty differentiating between the outer product and the inner product.

Incorrectly writing ket vectors as row vectors and bra vectors as column vectors. The following question was administered to 27 upper-level undergraduate students.

Assume that $|i\rangle, |j\rangle,$ and $|k\rangle$ form a complete set of orthonormal basis vectors. $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ and $|\chi_2\rangle = d|i\rangle + e|j\rangle + f|k\rangle$ are vectors in a three dimensional vector space. Write the outer product of "ket" vector $|\chi_1\rangle$ with "bra" vector $\langle\chi_2|$ in the given basis.

Table 5-1 shows that 11% of the students wrote the correct expression for the outer product, i.e., $|\chi_1\rangle\langle\chi_2|$ but wrote incorrect matrix forms of the bra and ket vectors. For example, one student wrote the outer product as $|\chi_1\rangle\langle\chi_2| = (a^* \quad b^* \quad c^*)\begin{pmatrix} d \\ e \\ f \end{pmatrix}$. Others wrote incorrect answers such as $|\chi_1\rangle\langle\chi_2| = (a|i\rangle + b|j\rangle + c|k\rangle)\begin{pmatrix} d^*|i\rangle \\ e^*|j\rangle \\ f^*|k\rangle \end{pmatrix}$ or $|\chi_1\rangle\langle\chi_2| = \begin{pmatrix} a \\ b \\ c \end{pmatrix}\begin{pmatrix} d \\ e \\ f \end{pmatrix}$. These types of responses shed light on students' difficulties with how ket and bra vectors can be represented as column vectors and row vectors, respectively.

Difficulty with the identity operator in Dirac notation representation. The following question was administered to 27 upper-level undergraduate students to investigate their difficulties with the identity operator:

Write the identity operator in terms of $|i\rangle,\ |j\rangle,$ and $|k\rangle$, which form a complete set of orthonormal basis vectors for a three-dimensional vector space.

Forty-eight percent of the students correctly wrote that the identity operator is $\hat{I} = |i\rangle\langle i|+|j\rangle\langle j| + |k\rangle\langle k|$. Table 5-1 shows that 22% of the students correctly wrote the identity operator in matrix form, i.e., $\hat{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ but did not write it in Dirac notation representation. Some students may be more familiar with the identity operator in matrix form, and have difficulty generating the identity operator in Dirac notation. Fifteen percent of the students wrote $\hat{I} = |i\rangle + |j\rangle + |k\rangle$, indicating that they are confusing ket vectors (column matrices) and operators (3×3 matrices). Seven percent of the students wrote that the identity operator is $\hat{I} = \langle i|i\rangle + \langle j|j\rangle + \langle k|k\rangle$, which demonstrates that students are not differentiating between operators and scalar products (numbers).

Difficulty with the projection operator in Dirac notation representation. The following question was administered to 27 upper-level undergraduate students in a quantum mechanics course to investigate common difficulties with the projection operator:

For the vector $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$,

a) Write down the projection operator that projects vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$.

b) Using the projection operator from part a, show what happens to the vector $|\chi_1\rangle$ when the projection operator acts on it.

c) Summarize your result in part b in one sentence.

Only 18% of the students correctly wrote that the projection operator that projects vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$ is $|i\rangle\langle i|$. Table 5-1 shows that the most common incorrect answer was writing that the projection operator that projects vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$ is $\langle i|\chi_1\rangle$ (30% of the students). In response to part b, many students wrote the expression $\langle i|\chi_1\rangle = a$, which is a correct statement. However, the students did not recall that the projection operator returns both the component and the direction of the projection of $|\chi_1\rangle$ along unit vector $|i\rangle$, i.e., $|i\rangle\langle i|\chi_1\rangle = a|i\rangle$. In response to part c, many students correctly stated that a projection of vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$ would give the component of $|\chi_1\rangle$ along $|i\rangle$. However, they did not state that the projection operator returns another vector, i.e., the component of $|\chi_1\rangle$ along $|i\rangle$ and the direction of the projection of $|\chi_1\rangle$ along unit vector $|i\rangle$. This indicates that students recognize that the projection operator involves the component of the vector along the basis state, but they do not realize that the projection operator returns another state, i.e., it yields the component along the basis state multiplied by the basis vector.

5.4.2 Student difficulties with quantum states

Proficiently translating between different representations is considered a hallmark of expertise [27-30]. To develop expertise in quantum mechanics, students should be able to translate quantum states in Dirac notation representation to wave functions in position and momentum representations. Students often display difficulties translating from Dirac notation representation to other representations, e.g., in the context of writing quantum state vectors in position and momentum representation. To explore students' difficulties with writing quantum state vectors in position and momentum representation, we administered open-ended and multiple-choice questions to advanced students in quantum mechanics after traditional instruction.

The generic quantum state $|\Psi\rangle$ in Dirac notation contains all information about the system. To represent the generic state $|\Psi\rangle$ as a wave function in the position representation, one must project $|\Psi\rangle$ along position eigenstates $|x\rangle$, i.e., $\langle x|\Psi\rangle$, where x is a continuous index. Similarly, a generic state $|\Psi\rangle$ can be represented as a wave function in momentum representation by projecting $|\Psi\rangle$ along momentum eigenstates $|p\rangle$, i.e., $\langle p|\Psi\rangle$, where p is a continuous index. To represent position eigenstates $|x'\rangle$ with eigenvalues x' and momentum eigenstates $|p'\rangle$ with eigenvalues p' in the position and momentum representation, one must project them along position eigenstates $|x\rangle$ or momentum eigenstates $|p\rangle$. For example, ignoring normalization issues, a position eigenstate in position representation is a (highly localized) delta function $\langle x|x'\rangle = \delta(x - x')$. On the other hand, a position eigenstate $|x'\rangle$ in momentum representation is a delocalized function of momentum $\langle p|x'\rangle = e^{-ipx'/\hbar}$.

5.4.2.1 Difficulties with a generic quantum state $|\Psi\rangle$

Difficulty writing a generic state vector $|\Psi\rangle$ in position or momentum representation. Table 5-2 shows that a majority of students performed well when they were asked to recognize whether a generic state vector $|\Psi\rangle$ in position representation is $\Psi(x) = \langle x|\Psi\rangle$ and in momentum representation is $\Phi(p) = \langle p|\Psi\rangle$ ($\Phi(p)$ is commonly denoted as $\widetilde{\Psi}(p)$). In particular, upper-level students ($N = 184$) were asked to evaluate the correctness of the following statement after traditional instruction given a generic state vector $|\Psi\rangle$: *"The wave function in position representation is* $\Psi(x) = \langle x|\Psi\rangle$ *where* x *is a continuous index."* Table 5-2 shows that 89% of the students agreed with this statement, indicating that they recognize that the wave function in position representation is $\Psi(x) = \langle x|\Psi\rangle$. The same students also evaluated the correctness of the following statement: *"The wave function in momentum representation is* $\Phi(p) = \langle p|\Psi\rangle$ *where* p *is a continuous index."* Table 5-2 shows that 77% of the students agreed with this statement, which indicates that they correctly recognize that the wave function in momentum representation is $\Phi(p) = \langle p|\Psi\rangle$ (although this percentage is smaller than the percentage of students who correctly recognized $\Psi(x) = \langle x|\Psi\rangle$).

Table 5-2. Percentages of undergraduate students who correctly answered questions related to writing the quantum state $|\boldsymbol{\Psi}\rangle$ in position representation ($\boldsymbol{N}$ = number of students)

Recognize: Evaluate the correctness of the statement: "The wave function in position representation is $\Psi(x) = \langle x|\Psi\rangle$ where x is a continuous index" ($N = 184$)	89
Recognize: Evaluate the correctness of the statement: "The wave function in momentum representation is $\Phi(p) = \langle p|\Psi\rangle$ where p is a continuous index." ($N = 184$)	77
Recall: What is the physical significance of $\langle x|\Psi\rangle$? ($N = 127$)	86
Recall: What is the physical significance of $\langle p|\Psi\rangle$? ($N = 127$)	85
Generate: How would you obtain the wave function in position representation from $|\Psi\rangle$? ($N = 46$)	52

Table 5-2 also shows that when upper-level students ($N = 127$) were asked to describe the physical significance of $\langle x|\Psi\rangle$ on a midterm exam after traditional instruction, 86% of them correctly recalled that $\langle x|\Psi\rangle = \Psi(x)$ and that $\Psi(x)$ is also known as the wave function in position representation (some even related it to the probability density for measuring position). Similarly, when these students were asked to describe the physical significance of $\langle p|\Psi\rangle$ on the same midterm exam, 85% of them correctly recalled that $\langle p|\Psi\rangle = \Phi(p)$ and $\Phi(p)$ is known as the wave function in momentum representation (see Table 5-2).

In contrast, Table 5-2 shows that students had difficulty generating on their own how to write a generic state vector $|\Psi\rangle$ in the position representation. For example, 46 upper-level students were asked the following question after traditional instruction: *You are given a generic state vector*

$|\Psi\rangle$. *How would you obtain the wave function in position representation from* $|\Psi\rangle$*?* Answers were considered correct if students wrote $\langle x|\Psi\rangle$, $\Psi(x)$, or stated that one needs to project the generic state $|\Psi\rangle$ onto the position basis, i.e., $\langle x|\Psi\rangle = \Psi(x)$. Only 52% provided the correct response.

These types of responses indicate that students may be adept at recognizing and recalling answers to questions about translating a generic state vector between Dirac notation and position and momentum representations. However, many struggle to generate the wave function in the position and momentum representation given state vector $|\Psi\rangle$. In other words, depending on the cues or scaffolding provided in the problem statement (e.g., whether the question asked is in the recognize, recall or generate category), students may have different levels of difficulties in translating a state vector from Dirac notation to wave functions in the position and momentum representations. The difference in the difficulty level in recognizing, recalling and generating indicates that students are still developing expertise and their knowledge structure is not robust [7].

Confusing a state with an operator in the context of a generic state vector $|\Psi\rangle$. As noted, many students had difficulty generating the wave function in position representation given the generic state vector $|\Psi\rangle$. One of the most common difficulties was confusing a position eigenstate with an operator and generating a response which included the position operator. Table 5-3 row 1 shows that of the 46 upper-level students, 28% provided responses which involved the position operator when asked to obtain the wave function in position representation from a generic state $|\Psi\rangle$. Common incorrect responses of this type included, e.g., $\hat{x}|\Psi\rangle = x|\Psi\rangle$, $\hat{x}|\Psi\rangle = \langle x|\Psi\rangle$, $\langle x|\Psi\rangle = \int \hat{x}^*\Psi dx = \int x\,\Psi dx$, and $\hat{x}\,\Psi(x) = \langle x|\hat{x}|\Psi\rangle$. Students displayed similar difficulties with a generic state $|\Psi\rangle$ in momentum representation, with common incorrect responses of the form $\langle p|\Psi\rangle = \int \hat{p}^*\Psi dx = \int i\hbar\,\partial/\partial x\,\Psi dx$.

Table 5-3. Percentages of students displaying difficulties with quantum states in position and momentum representations.

Difficulty		Question statement	%
Confusing a state with an operator in the context of a generic state vector $\|\Psi\rangle$	1	You are given a generic state vector $\|\Psi\rangle$. How would you obtain the wave function in position representation from $\|\Psi\rangle$? $(N = 46)$	28
	2	What is the physical significance of $\langle x\|\Psi\rangle$? $(N = 127)$	25
	3	Evaluate the correctness of the statement: "The wave function in momentum representation is $\Psi(\mathrm{p}) = \int \mathrm{dx}(-\mathrm{i}\hbar\frac{\partial}{\partial \mathrm{x}}\Psi(\mathrm{x}))$." $(N = 184)$	61
Confusing a state with an operator in the context of position or momentum eigenstates $\|x'\rangle$ or $\|p'\rangle$	4	$\langle x\|x'\rangle = ?$ $(N = 46)$	13
	5	$\langle p\|p'\rangle = ?$ $(N = 46)$	9
Assuming $\langle x\|x'\rangle =$ 1 or 0 (or $\langle p\|p'\rangle =$ 1 or 0)	6	$\langle x\|x'\rangle = ?$ $(N = 46)$	6
	7	$\langle p\|p'\rangle = ?$ $(N = 46)$	7
Assuming $\langle x\|p'\rangle =$ 0 or $\langle p\|x'\rangle = 0$	8	$\langle x\|p'\rangle = ?$ $(N = 46)$	9
	9	$\langle p\|x'\rangle = ?$ $(N = 46)$	9

Furthermore, many upper-level students $(N = 127)$, who were asked to describe the physical significance of $\langle x|\Psi\rangle$ correctly recalled that $\langle x|\Psi\rangle = \Psi(x)$ and $\Psi(x)$ is also known as the wave function in position representation, often wrote additional incorrect statements in their responses claiming that the position (or momentum) operator is involved in determining the wave function in the position or momentum representation. Table 5-3 row 2 shows that 25% of the students claimed that the position (or momentum) operator is involved in determining the wave function in the position (or momentum) representation. For example, one student stated that "$\langle x|\Psi\rangle$ is just $\int x^*\Psi dx$=Ψ in position basis." Another student incorrectly claimed that "$\langle x|\Psi\rangle$ is the measurement of $|\Psi\rangle$ in position, it yields a position eigenstate of the system at the time of measurement." Similarly, in response to the question about the physical significance of $\langle p|\Psi\rangle$, another student stated "$\langle p|\Psi\rangle = \int \Psi\left(-\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi dx = \frac{\hbar}{i}\int \Psi\left(\frac{\partial}{\partial x}\right)\Psi$." These types of responses indicate that students have difficulty distinguishing between the projection of a state vector $|\Psi\rangle$ along an eigenstate of x or p vs. the position or momentum operator acting on a generic state vector $|\Psi\rangle$. These responses also suggest that students have difficulty with the physical significance of $\langle x|\Psi\rangle$ or $\langle p|\Psi\rangle$, which are the probability density amplitudes for measuring x or p.

When students were asked to evaluate the correctness of a statement in which this type of difficulty is explicitly mentioned (e.g., confusion between representing a generic state in position or momentum representation by projecting a state along an eigenstate of x or p vs. operating on a state with the position or momentum operator), a larger percentage of the students display this type of a difficulty.

Table 5-3 row 3 shows that even when students ($N = 184$) were asked to evaluate the correctness of the statement connecting the wave function in position and momentum representation: "*The wave function in momentum representation is* $\Phi(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$*,*" 61% incorrectly agreed with this statement, indicating that they thought the momentum operator written in the position representation (i.e., $-i\hbar\frac{\partial}{\partial x}$) connects the wave function in momentum and position representations. This response is incorrect. One must use a Fourier transform to obtain $\Phi(p)$ from $\Psi(x)$, $\Phi(p) = \langle p|\Psi\rangle = \int dx\langle p|x\rangle\langle x|\Psi\rangle = \int dx e^{-ipx'/\hbar}\Psi(x)$.

5.4.2.2 Difficulties in representing $|x'\rangle$ and $|p'\rangle$ in the position or momentum representation

In addition to exhibiting difficulties writing a generic state $|\Psi\rangle$ in position and momentum representations, students also struggled to translate position and momentum eigenstates from Dirac notation to the position and momentum representations. Many undergraduate students struggled to recall how to write $\langle x|x'\rangle$, $\langle p|x'\rangle$, $\langle p|p'\rangle$, and $\langle x|p'\rangle$ without using Dirac notation as a function of position or momentum.

Confusing a state with an operator in the context of position or momentum eigenstates: Similar to the difficulty involving confusion between a bra state and an operator in the context of a generic state $|\Psi\rangle$, students confuse a state with an operator in the context of position or momentum eigenstates. For example, in determining $\langle x|x'\rangle$ in position representation without using Dirac notation, students often treated the bra state $\langle x|$ as $\hat{x}$ and incorrectly acted with it on the eigenstate $|x'\rangle$. Upper-level students ($N = 46$) were asked to write $\langle x|x'\rangle$ without Dirac notation as a function of x after traditional instruction. Table 5-3 row 4 shows that 13% of the students often confused a state with an operator and wrote $\langle x|x'\rangle = x'$. Interviews suggest that this type of difficulty sometimes stemmed from the fact that students treated the bra state $\langle x|$ as the position operator $\hat{x}$ and acted with it on $|x'\rangle$ and then incorrectly removed the state $|x'\rangle$ after the operation, e.g., $\langle x|x'\rangle = \hat{x}|x'\rangle = x'$.

Similar difficulties are displayed when 46 upper-level students were asked to write $\langle p|p'\rangle$ without Dirac notation after instruction in relevant concepts. Table 5-3 row 5 shows that 9% of the students confused a state with an operator and wrote $\langle p|p'\rangle = p'$. Interviews suggest that this type of difficulty sometimes stemmed from the fact that students treated the bra state $\langle p|$ as the momentum operator $\hat{p}$ and acted with it on $|p'\rangle$ and then incorrectly removed the state $|p'\rangle$ after the operation, e.g., $\langle p|p'\rangle = \hat{p}|p'\rangle = p'$

Assuming $\langle x|x'\rangle = 1$ or 0 (or $\langle p|p'\rangle = 1$ or 0): Upper-level students ($N = 46$) were asked to write $\langle x|x'\rangle$ and $\langle p|p'\rangle$ without using Dirac notation after traditional instruction. Responses were considered correct if the students wrote $\langle x|x'\rangle = \delta(x - x')$ (or $\langle p|p'\rangle = \delta(p -$

p')). Table 5-4 shows that only 35% answered correctly. Some students incorrectly invoked a "normalization condition" when determining $\langle x|x'\rangle$ or $\langle p|p'\rangle$. For example, 6% wrote that $\langle x|x'\rangle = 1$ and 7% wrote that $\langle p|p'\rangle = 1$ (see Table 5-3 rows 6 and 7). In interviews, students often incorrectly claimed that $\langle x|x'\rangle = 1$ if $x = x'$ (these same students correctly stated that $\langle x|x'\rangle = 0$ if $x \neq x'$). Further discussion with students suggests that this type of difficulty was often the result of confusing the Kronecker delta and the Dirac delta function. The Kronecker delta is appropriate to use, e.g., for orthogonality of eigenstates with discrete eigenvalues (i.e., $\delta_{nm} = 1$ if $n = m$ and $\delta_{nm} = 0$ if $n \neq m$). The Dirac delta function, e.g., $\delta(x - x')$, is appropriate for eigenstates with continuous eigenvalues. When $x = x'$, $\delta(x - x')$ is infinite.

Assuming $\langle \boldsymbol{x}|\boldsymbol{p}'\rangle = \mathbf{0}$ or $\langle \boldsymbol{p}|\boldsymbol{x}'\rangle = \mathbf{0}$: Forty-six upper-level students were also asked to write $\langle p|x'\rangle$ and $\langle x|p'\rangle$ without Dirac notation as a function of position or momentum after instruction in relevant concepts. Table 5-4 shows that 20% correctly recalled that $\langle p|x'\rangle = e^{-ipx'/\hbar}$ and $\langle x|p'\rangle = e^{ip'x/\hbar}$. Students were not penalized if they did not write down a constant pre-factor often used as "normalization" or if they did not have the correct sign in the exponent. A common difficulty involved invoking an orthogonality condition. For example, 9% of the students wrote $\langle p|x'\rangle = 0$ or $\langle x|p'\rangle = 0$ (see Table 5-3 rows 8 and 9). In interviews, some students who had traditional instruction in these issues initially stated that eigenstates of x and p are orthogonal or that since x and p were incompatible, the inner products $\langle p|x'\rangle$ or $\langle x|p'\rangle$ did not make sense. Some students stated that if it was appropriate to have such inner products, they must be zero because x and p have "nothing in common." Prior research shows that even in the context of a two-dimensional vector space for a spin-1/2 system, students often make similar claims, e.g., that eigenstates of $\hat{S}_x$ are orthogonal to eigenstates of $\hat{S}_y$ [25].

5.4.2.3 Performance of graduate students

Graduate students perform significantly better on questions involving recall: Graduate students enrolled in a first year core graduate quantum mechanics course were more proficient than undergraduates at translating between Dirac notation and position and momentum representations. For example, Table 5-4 shows that 45 graduate students, who were asked to write $\langle x|x'\rangle, \langle x|p'\rangle$, $\langle p|x'\rangle$ and $\langle p|p'\rangle$ in position and momentum representation without using Dirac notation, performed significantly better on average than the undergraduate students.

Table 5-4. Percentages of undergraduate (UG) ($\boldsymbol{N = 46}$) and graduate (G) students ($\boldsymbol{N = 45}$) who correctly answered questions related to position and momentum representations.

Question	UG	G
Recall: $\langle x|x'\rangle = ?$	35	91
Recall: $\langle p|x'\rangle = ?$	20	82
Recall: $\langle x|p'\rangle = ?$	20	87
Recall:$\langle p|p'\rangle = ?$	35	91
Generate: "Write a momentum eigenstate with eigenvalue p' in position representation."	13	58
Generate: "Write a momentum eigenstate with eigenvalue p' in momentum representation."	15	49

Graduate students have difficulty in generating answers to questions on these topics although they are good at recall: Table 5-4 shows that when 45 graduate students were asked to write, e.g., $\langle p|p'\rangle$ or $\langle x|p'\rangle$ without Dirac notation, 91% correctly wrote, e.g., that $\langle p|p'\rangle = \delta(p - p')$ which is significantly higher than 35%, the corresponding average undergraduate percentage. However, only 49% of the graduate students correctly answered the question "Write a momentum eigenstate with eigenvalue p' in momentum representation." Responses were considered correct if the student wrote $\langle p|p'\rangle$ or $\delta(p - p')$. What is noteworthy is that on the same survey, 42% of the graduate students correctly recalled but could not generate a related answer, e.g., they correctly wrote $\langle p|p'\rangle = \delta(p-p')$ but answered incorrectly when asked to generate a momentum eigenstate with eigenvalue p' in the momentum representation. Similarly, 29% of the graduate students correctly answered questions asking them to recall a momentum eigenstate with eigenvalue p' in the position representation but could not generate it, i.e., they correctly recalled $\langle x|p'\rangle = e^{ip'x/\hbar}$ but answered incorrectly when asked to generate a momentum eigenstate with eigenvalue p' in the position representation.

This type of dichotomy between recall vs. generate problems shown in Table 5-4 suggests that while most graduate students are proficient at recalling how to convert expressions written in Dirac notation to a form without Dirac notation, almost half of them do not understand the physical meaning of those expressions. The task of generating a momentum eigenstate with eigenvalue p' in momentum or position representation requires understanding of the symbols in Dirac notation and position or momentum representation. If graduate instruction only focuses on problem solving requiring recall of these types of expressions from what was discussed in a particular context and reproducing them on the exams, students are unlikely to develop a functional understanding of these expressions.

Translating between representations is a hallmark of expertise and is important for developing expertise in quantum mechanics. After traditional instruction in relevant concepts, undergraduates and even graduate students, who are proficient at recalling how to write an expression given in Dirac notation without the use of the Dirac notation (or vice versa), have difficulties in generating their own solutions, e.g., when asked to write the position or momentum eigenstates in position and momentum representations. Students must be given multiple opportunities to not only recognize and recall but also generate answers to these types of questions related to translation between the representations discussed here using research-based learning tools to develop a functional understanding of the underlying concepts.

5.4.3 Student difficulties with obtaining the wave function in momentum representation from the wave function in position representation

To investigate student difficulties with obtaining the wave function in momentum representation from the wave function in position representation via a Fourier transform, 184 advanced students were asked to evaluate the correctness of the following statement: "$\langle p|\Psi\rangle = \int \langle p|x\rangle\langle x|\Psi\rangle dx = \int e^{-ipx/\hbar}\Psi(x)dx$." Table 5-5 shows that 69% of the students correctly stated that the statement is true. These same students were asked to evaluate the correctness of the following statement: "The wave function in momentum representation is $\Phi(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$." Table 5-5 shows that only 39% of the students disagreed with this statement, indicating that many students have difficulties in recognizing how the wave function in momentum representation is related to the wave function in position representation via a Fourier transform.

Table 5-5. Percentages of advanced students correctly (or incorrectly) answering questions related to a Fourier transform

Question	
Recognize: $\langle p\|\Psi\rangle = \int \langle p\|x\rangle\langle x\|\Psi\rangle dx = \int e^{-ipx/\hbar}\Psi(x)dx$ (Ignore normalization issues.)	69% ($N = 184$)
Recognize that "the wave function in momentum representation is $\Phi(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$" is an *incorrect* statement	39% ($N = 184$)
Generate: Show that the wave function in position representation is the Fourier transform of the wave function in momentum representation.	17% undergraduate students ($N = 46$) 82% graduate students ($N = 45$)

In addition, 46 undergraduate students and 45 graduate students were asked to prove that the wave function in position representation is the Fourier transform of the wave function in momentum representation. Table 5-5 shows that 17% of the undergraduate students and 82% of the graduate students wrote the correct expression, i.e., $\Phi(p) = \langle p|\Psi\rangle = \int\langle p|x\rangle\langle x|\Psi\rangle dx = \int dx e^{-ipx/\hbar}\Psi(x)$. The common difficulties displayed by the undergraduate students were writing an incorrect expression from memory, e.g., $\Phi(p) = \int e^{ikx} dk$ or $\Phi(p) = \int e^{-ikx} dx$. Some students wrote a correct expression but did not prove it by showing the intermediate steps, i.e., $\langle p|\Psi\rangle = \int\langle p|x\rangle\langle x|\Psi\rangle dx$. This indicates that students have some memorized pieces of knowledge regarding Fourier transforms but are unable to prove the relationship between the wave functions $\Phi(p)$ and $\Psi(x)$.

5.4.4 Student difficulties with quantum operators in Dirac notation

To investigate student difficulties with quantum operators in Dirac notation, we administered both open-ended and multiple-choice questions to advanced students in quantum mechanics after traditional instruction in relevant concepts. The following difficulties were displayed by students:

5.4.4.1 Student difficulties with translating a momentum (or position) operator acting on a momentum (or position) eigenstate from Dirac notation to position or momentum representation and vice versa

Relative difficulty in recalling compared to recognizing the expression $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$. Upper-level students ($N = 184$) from 4 universities were asked to evaluate the correctness of the expression $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$ after traditional instruction in relevant concepts. Table 5-6 shows that eighty percent of the students correctly recognized that $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$ is true.

We also investigated the extent to which students can recall how to write $\langle x|\hat{p}|p'\rangle$ without using Dirac notation in the position representation. Forty-six undergraduate students and 45 graduate students were asked to write $\langle x|\hat{p}|p'\rangle$ without Dirac notation in the position representation. Students were given full credit if they wrote $\langle x|\hat{p}|p'\rangle = p'e^{ip'x/\hbar}$ (ignoring normalization issues). Students were not penalized if they used an incorrect sign in the exponent. Students were given half credit if they wrote $p'\langle x|p'\rangle$. Table 5-6 shows that only 20% of undergraduate students and 68% of graduate students received full credit and were able to correctly recall how to write the expression $\langle x|\hat{p}|p'\rangle$ without using Dirac notation in the position representation. Twenty percent of the undergraduates and 24% of the graduate students wrote $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle$ but did not simplify their expression further.

Relative difficulty in recalling compared to recognizing that $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$. 184 upper-level students from 4 universities were asked to evaluate the correctness of the expression $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$ after traditional instruction in relevant concepts. Table 5-6 shows that eighty-five percent of the students recognized that $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$ is correct.

We also investigated the extent to which students can recall how to write $\langle p|\hat{p}|p'\rangle$ without using Dirac notation in momentum representation. Forty-six undergraduate students and 45 graduate students were asked to write $\langle p|\hat{p}|p'\rangle$ without using Dirac notation in momentum representation. Students received full credit if they wrote $p'\delta(p-p')$ or $p\delta(p-p')$ and half credit if they wrote $p'\langle p|p'\rangle$ or $\delta(p-p')$. Table 5-6 shows that only 30% of the undergraduate students and 82% of the graduate students received full credit and were able to correctly recall how to write $\langle p|\hat{p}|p'\rangle$ without using Dirac notation in the momentum representation. Seven percent of the undergraduates wrote $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle$ but did not simplify their expression further. The large difference in the percentages of students who recognized that $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$ but could not recall how to translate the expression in Dirac notation to an expression without Dirac notation, i.e., $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$ indicates that some students are in an intermediate level of expertise. They may have memorized some knowledge or facts which they can recognize as correct, e.g., $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$. However, they have not yet reached the level of expertise in which they have "chunked" [27] different concepts together and can recognize, recall and generate how to translate an expression between Dirac notation representation to other representations without Dirac notation.

Table 5-6. Percentages of students who correctly recognized and recalled questions related to a momentum operator in position and momentum representation

Question	Percentage of students
Recognize: $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = p'e^{ip'x/\hbar}$	80% ($N = 184$ upper level students)
Recognize: $\langle p\|\hat{p}\|p'\rangle = p'\langle p\|p'\rangle = p'\delta(p-p')$	85% ($N = 184$ upper level students)
Recall: $\langle x\|\hat{p}\|p'\rangle = ?$	20% ($N = 46$ undergraduate students) 68% ($N = 46$ graduate students)
Recall: $\langle p\|\hat{p}\|p'\rangle = ?$	30% ($N = 46$ undergraduate students) 82% ($N = 45$ graduate students)

When translating $\langle \boldsymbol{x}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle$ to position representation, undergraduate students ($\boldsymbol{N} =$ 46) invoke an incorrect orthogonality condition, e.g., $\langle \boldsymbol{x}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'\langle \boldsymbol{x}|\boldsymbol{p}'\rangle = \mathbf{0}$. Forty-six undergraduate students were asked to recall how to write $\langle x|\hat{p}|p'\rangle$ without Dirac notation in the position representation. Table 5-7 shows that one common incorrect answer was writing $\langle x|\hat{p}|p'\rangle$ =0 (7% of undergraduates). Interviews suggest that this difficulty often stems from the difficulty with $\langle p|x'\rangle = 0$ (9% of undergraduate students), indicating that students are incorrectly invoking an orthogonality condition between eigenstates of momentum and position. Similar difficulty has been observed in the context of spin angular momentum for which many students incorrectly think that an eigenstate of one component of spin angular momentum is orthogonal to an eigenstate of another component of spin angular momentum.

When translating $\langle \boldsymbol{p}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle$ to momentum representation, undergraduate students ($\boldsymbol{N} = \mathbf{46}$) invoke an incorrect normalization condition, e.g., $\langle \boldsymbol{p}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \boldsymbol{p}'$ or

$\langle \boldsymbol{p}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \mathbf{1}$. Forty-six undergraduate students were asked to recall how to write $\langle p|\hat{p}|p'\rangle$ without the use of Dirac notation in momentum representation. Table 5-7 shows that one common incorrect answer was writing $\langle p|\hat{p}|p'\rangle = p'$ or ignoring the eigenvalue p' and writing $\langle p|\hat{p}|p'\rangle = 1$ (9% of undergraduates). Other students incorrectly wrote that $\langle p|\hat{p}|p'\rangle = 0$. Interviews suggest that these difficulties often stem from incorrectly assuming that $\langle p|p'\rangle = 1$ or $\langle p|p'\rangle = 0$. In interviews, students often incorrectly claimed that $\langle p|p'\rangle = 1$ if $p = p'$ or $\langle p|p'\rangle = 0$ if $p \neq p'$. Further discussion with students suggests that this type of difficulty was often the result of confusing the Kronecker delta and the Dirac delta function.

Inconsistent responses to equivalent methods to determine $\langle \boldsymbol{x}|\widehat{\boldsymbol{p}}|\boldsymbol{p}'\rangle$ in position representation. A question involving momentum operators was also administered in a multiple-choice format. The following question was administered to 184 upper-level students from 4 universities after traditional instruction in relevant concepts:

$|p'\rangle$ is the momentum eigenstate with eigenvalue p' for a particle confined in one spatial dimension. Choose all of the following statements that are correct. Ignore normalization issues.

1) $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p - p')$

2) $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$

3) $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$

A. all of the above B. 1 only C. 1 and 2 only D. 1 and 3 only E. 2 and 3 only

The correct answer is A. Sixty-seven percent of students correctly chose an answer which included option 2 ($\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'e^{ip'x/\hbar}$) and 52% of students correctly chose an answer which included option 3 ($\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$). However, Table 5-7 shows that 45% of the students chose option 2) but not 3) (and vice versa). In option 2), one can first act on $|p'\rangle$ with the momentum operator, pull the eigenvalue p' out of the braket, and write the momentum eigenstate in position representation. Option 3) is another method to determine the position representation of expression $\langle x|\hat{p}|p'\rangle$--one can write the momentum operator in position representation ($-i\hbar\,\partial/\partial x$) and then write the momentum eigenstate in position representation, i.e., $= \langle x|p'\rangle = e^{ip'x/\hbar}$ (ignoring normalization issues). Interviews suggest that for an upper-level student taking the derivative $-i\hbar\,\partial/\partial x\, e^{ip'x/\hbar}$ to determine that answer options 2) and 3) are equivalent was not the reason why they had difficulty recognizing that option 3) is correct. Rather, they had difficulty recognizing whether $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle$ is true mainly because they did not recognize that the momentum operator acting on momentum eigenstate $|p'\rangle$ can be written in position representation as $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle$.

Table 5-7. Percentages of students displaying difficulties with position and momentum operators in position or momentum representation

Difficulty	Question Statement	% of students
When translating $\langle x\|\hat{p}\|p'\rangle$ to an expression without Dirac notation, students invoke an orthogonality condition, e.g., $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = 0$	$\langle x\|\hat{p}\|p'\rangle = ?$	7% ($N = 46$ undergraduate students)
When translating $\langle p\|\hat{p}\|p'\rangle$ to an expression without Dirac notation, students invoke a normalization condition, e.g., $\langle p\|\hat{p}\|p'\rangle = p'\langle p\|p'\rangle = p'$ or $\langle p\|\hat{p}\|p'\rangle = p'\langle p\|p'\rangle = 1$	$\langle p\|\hat{p}\|p'\rangle = ?$	9% ($N = 46$ undergraduate students)
Inconsistent responses to equivalent methods to determine $\langle x\|\hat{p}\|p'\rangle$ without Dirac notation, e.g., claiming that $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = p'e^{ip'x/\hbar}$ is correct but $\langle x\|\hat{p}\|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x\|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$ is incorrect	Evaluate whether both expressions $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = p'e^{ip'x/\hbar}$ and $\langle x\|\hat{p}\|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x\|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$ are correct	45% ($N = 184$ upper-level students)
When translating $\hat{x}\delta(x-x')$ to an expression in Dirac notation, students treat the Dirac delta function as "picking out" the value x' even when no integration is involved, e.g., writing $\hat{x}\delta(x-x') = x'$	$\hat{x}\delta(x-x') = ?$	20% ($N = 46$ undergraduate students) 11% ($N = 45$ graduate students)

When translating $\hat{x}\delta(x-x')$ to an expression in a different form, students incorrectly treat the Dirac delta function as "picking out" the value x' even when no integration is involved. Students display difficulties when recalling different representations of eigenvalue equations of position. For example, 46 upper-level undergraduate students and 45 graduate students were asked to write $\hat{x}\delta(x-x')$ (or $x\delta(x-x')$) in a different form. Since the question simply asked students to write $\hat{x}\delta(x - x')$ (or $x\delta(x - x')$) in another form, there are various types of responses that were considered correct. Responses were given full credit if they were of the form $x\delta(x - x')$, $x'\delta(x - x')$, $x\langle x|x'\rangle$, $\langle x|x|x'\rangle$, $\langle x|\hat{x}|x'\rangle$. Half credit was given to responses that included $\langle x|x'\rangle$ but were otherwise incorrect. Only 28% of the undergraduate students and 60% of the graduate students answered this question correctly. Table 5-7 shows that the most common incorrect response was $\hat{x}\delta(x - x') = x'$, which was generated by 20% of the undergraduate students and 11% of the graduate students (see Table 5-7). This type of response indicates that students are treating the Dirac delta function as "picking out" the value x' even when no integration is involved as opposed to recognizing that it is an eigenfunction of position in position representation which is being acted on by the position operator.

5.4.4.2 Student difficulties with writing a generic operator $\hat{Q}$ acting on a generic state $|\Psi\rangle$ in position representation, i.e., $\langle x|\hat{Q}|\Psi\rangle$

In addition to investigating student difficulties involving the operators $\hat{x}$ and $\hat{p}$ acting on their respective eigenstates in position and momentum representations, we also investigated students' difficulties with a generic operator $\hat{Q}$ acting on a generic state $|\Psi\rangle$ in position representation. We administered open-ended and multiple-choice questions to advanced students in quantum mechanics after traditional instruction in relevant concepts. The following difficulties were identified:

Relative difficulty with recognizing that in the position representation $\langle x|\hat{Q}|\Psi\rangle = Q(x, -i\hbar\,\partial/\partial x)\Psi(x)$ compared to recalling how to write $\langle x|\hat{Q}|\Psi\rangle$ without Dirac notation. In one study, 184 upper-level students from 4 universities were asked to evaluate the correctness of the expression $\langle x|\hat{Q}|\Psi\rangle = Q(x, -i\hbar\,\partial/\partial x)\Psi(x)$ (given that $\hat{Q}$ is diagonal in the position basis) after instruction in relevant concepts. Table 5-8 shows that eighty-seven percent of students correctly agreed with this statement, indicating that they recognize that the position representation of a generic operator acting on a generic state without using Dirac notation is $Q(x, -i\hbar\,\partial/\partial x)\Psi(x)$.

However, when students were asked to recall how to write $\langle x|\hat{Q}|\Psi\rangle$ without using Dirac notation in position representation in an open-ended format, this question was much more difficult for students. Forty-six undergraduate students and 45 graduate students were asked to write $\langle x|\hat{Q}|\Psi\rangle$ without Dirac notation in position representation after instruction in relevant concepts. Students received full credit if they wrote both the operator and the generic state in position representation, i.e., $\langle x|\hat{Q}|\Psi\rangle = Q(x, -i\hbar\,\partial/\partial x)\Psi(x)$. Half credit was given if the student wrote $\langle x|\hat{Q}|\Psi\rangle = \Psi(x)$, $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\langle x|\Psi\rangle$, or $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\Psi(x)$. Table 5-8 shows that 9% of undergraduates and 31% of the graduate students were able to correctly recall that $\langle x|\hat{Q}|\Psi\rangle = Q(x, -i\hbar\,\partial/\partial x)\Psi$(x). Graduate students attempted other methods to answer the question, such as inserting the identity operator in terms of a complete set of position eigenstates (16% of graduates) and inserting the identity operator in terms of a complete set of eigenstates of $\hat{Q}$ (6% of graduates). However, these methods were not productive for answering the question. This indicates that while graduate students may recognize the importance of using the completeness relation, in this case, it was not helpful in answering the question and it would have been easier had they recognized that the expression $\langle x|\hat{Q}|\Psi\rangle$ is equivalent to writing the operator $\hat{Q}$ acting on a generic state $|\Psi\rangle$ in position representation without using Dirac notation.

Table 5-8. Percentages of undergraduate students (UG) and graduate students (G) who correctly recognized and recalled questions related to a generic operator in position representation with or without Dirac notation

Question	Percentage of students
Recognize: $\langle x\vert\hat{Q}\vert\Psi\rangle = Q(x, -i\hbar\,\partial/\partial x)\Psi(x)$	87% ($N = 184$ upper level students)
Recall: $\langle x\vert\hat{Q}\vert\Psi\rangle = ?$	9% ($N = 46$ undergraduate students) 31% ($N = 45$ graduate students)

5.4.4.3 Student difficulties with the identity operator

We also investigated student difficulties with recognizing, generating, verifying, and applying the identity operator in different contexts.

Relative difficulty in generating the identity operator vs. recognizing the identity operator in Dirac notation: Upper-level students ($N = 184$) from 4 universities were told that $\{|q_n\rangle, n = 1,2,3 \dots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n and $\hat{I}$ is the identity operator. They were asked to evaluate the correctness of the expression $\sum_n |q_n\rangle\langle q_n| = \hat{I}$ after traditional instruction in relevant concepts. Table 5-9 shows that 83% of the students correctly identified that the identity operator shown in option 1 (i.e., $\sum_n |q_n\rangle\langle q_n| = \hat{I}$) is correct. This indicates that many students can recognize the identity operator in this form.

However, students display difficulties in generating different forms of the identity operator. After traditional instruction in the relevant concepts, 46 undergraduate students and 45 graduate students were asked to write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. Students received full credit if they wrote $\int |q\rangle\langle q| dq$ and half credit if they confused continuous and discrete cases and wrote an answer of the form $\sum|q\rangle\langle q|$. Table 5-9 shows that only 13% of undergraduate students and 67% of graduate students were able to correctly generate the identity operator using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$.

We also investigated student difficulties with writing the identity operator using a complete set of eigenstates of an operator with discrete eigenvalues. Undergraduate students ($N = 28$) were asked to prove that the identity operator is $\hat{I} = \sum_{j=1}^{N}|e_j\rangle\langle e_j|$, given that $\{|e_j\rangle\ j = 1, \ldots, N\}$ forms an orthonormal basis for an N-dimensional vector space. This question was asked on two upper-level quantum mechanics midterm exams. Table 5-9 shows that only 18% of the students could successfully show that $\hat{I} = \sum_{j=1}^{N}|e_j\rangle\langle e_j|$, e.g., by acting with $\hat{I}$ on a generic state vector in Dirac notation and writing the generic state vector in terms of the eigenstates $|e_j\rangle$.

Table 5-9. Percentages of students who correctly recognized and recalled questions related to the identity operator

Question	**Percentage of students**
Recognize: $\sum_n|q_n\rangle\langle q_n| = \hat{I}$, given that $\{|\mathrm{q}_n\rangle, n = 1,2,3 \ldots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n and Î is the identity operator	83% ($N = 184$ upper-level students)
Generate: Write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	13% ($N = 46$ undergraduate students) 67% ($N = 45$ graduate students)
Generate: Prove that the identity operator is $\hat{I} = \sum_{j=1}^{N}|e_j\rangle\langle e_j|$, given that $\{|e_j\rangle\ j = 1, \ldots, N\}$ forms an orthonormal basis for an N-dimensional vector space	18% ($N = 28$ undergraduate students)

For an operator with a continuous eigenvalue spectrum, students incorrectly write the identity operator in terms of the eigenstates of an operator with a discrete eigenvalue

spectrum. After traditional instruction in relevant concepts, 46 undergraduate students and 45 graduate students were asked to write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. Students often confused the discrete and continuous cases. Table 5-10 shows that 15% of undergraduates and 18% of graduates wrote a response which included a summation as opposed to an integral.

Confusing the identity operator with a projection operator along a basis vector. After traditional instruction in the relevant concepts, 46 undergraduate students and 45 graduate students were asked to write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. Table 5-10 shows that 9% of the graduate students wrote a projection operator along a basis vector as opposed to the identity operator, e.g., $|q\rangle\langle q|$. These students display novice-like behavior because they fail to differentiate between the related concepts of the identity operator and the projection operator.

Other difficulties with the identity operator: Undergraduate students ($N = 28$) were asked to demonstrate that the identity operator is $\hat{I} = \sum_{j=1}^{N} |e_j\rangle\langle e_j|$, given that $\{|e_j\rangle\ j = 1, \ldots, N\}$ forms an orthonormal basis for an N-dimensional vector space. This question was asked on two upper-level quantum mechanics midterm exams ($N = 28$). Some students were confused regarding the indices of the identity operator $\hat{I} = \sum_{j=1}^{N} |e_j\rangle\langle e_j|$. For example, one student wrote:

$$\sum_{i,j} |e_j\rangle\langle e_i|e_j\rangle = |e_j\rangle\delta_{ij} = \delta_{ij}|e_j\rangle$$

$$\Rightarrow \sum_{i,j} |e_j\rangle\langle e_i| = \underset{\substack{\uparrow \\ \delta_{ii} = 1}}{\delta_{ij}} \Rightarrow \sum_{j} |e_j\rangle\langle e_j| = 1$$

When students write the identity operator as $\sum_{i,j}|e_j\rangle\langle e_i|$, it indicates that they do not conceptually understand what the identity operator represents and it is a sum over all of the projection operators for a given vector space, i.e., a sum over the outer products of all of the basis vectors regardless of what basis is chosen (which yields a square matrix in any given basis with ones along the diagonal).

Table 5-10. Percentages of undergraduate and graduate students displaying difficulties with the identity operator

Difficulty	**Question Statement**	**% of students**
For an operator with a *continuous* eigenvalue spectrum, students incorrectly write the identity operator in terms of the eigenstates of an operator with a *discrete* eigenvalue spectrum	Write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	15% ($N = 46$ undergraduate students) 18% ($N = 45$ graduate students)
Confusing the identity operator with the projection operator	Write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$, given that the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q	9% ($N = 45$ graduate students)

On the same question on the midterm exams, some students arbitrarily switched the bra and ket states within the identity operator and turned an outer product into an inner product, e.g., $\hat{I} = \sum_{j=1}^{N} |e_j\rangle\langle e_j| = \sum_{j=1}^{N} \langle e_j|e_j\rangle$. For example, one student wrote:

$$\sum |e_j\rangle\langle e_j| = \sum \langle e_j|e_j\rangle = \delta_{jj} = 1.$$

Difficulties of this type indicate that some students are unaware of the difference between outer products (operators) and inner products (numbers).

5.4.4.4 Student difficulties with writing a generic operator $\hat{Q}$ in terms of its eigenvalues and eigenstates

We also investigated student difficulties with the spectral decomposition of a generic operator $\hat{Q}$. For example, 184 upper-level students from 4 universities were given the following multiple choice question after traditional instruction in relevant concepts:

Suppose $\{|q_n\rangle, n = 1,2,3 \ldots N\}$ form a complete set of orthonormal eigenstates of an operator $\hat{Q}$ with eigenvalues q_n. Which one of the following relations is correct? All of the summations are over all possible values of n and m.

A. $\hat{Q} = \sum_n q_n \langle q_n|q_n\rangle$

B. $\hat{Q} = \sum_n q_n |q_n\rangle\langle q_n|$

C. $\hat{Q} = \sum_{n,m} q_n |q_n\rangle\langle q_m|$

D. $\hat{Q} = \sum_n q_n |\langle q_n|q_n\rangle|^2$

E. None of the above

The correct answer is B, which was selected by thirty-five percent of the students.

To investigate student difficulties further, 66 students were asked to prove that $\hat{Q}$ can be written in terms of its spectral decomposition: $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, given that $\hat{Q}$ is an operator with a complete set of orthonormal eigenvectors $\hat{Q}|e_j\rangle = \lambda_j |e_j\rangle$ $(j = 1,2,3, \ldots n)$. Only 39% of the students could show that $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$ by acting with $\hat{Q}$ on a generic state vector $|\Psi\rangle$, i.e., $\hat{Q}|\Psi\rangle = \hat{Q} \sum |e_j\rangle\langle e_j|\Psi\rangle = \sum \lambda_j |e_j\rangle\langle e_j|\Psi\rangle \to \hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$. We note that while students are typically better at recognizing correct expressions compared to generating them, students' performance was approximately the same in both the multiple-choice and open-ended questions involving the spectral decomposition of $\hat{Q}$. Interviews suggest that this multiple-choice format cannot be considered as a simple "recognize" question because the incorrect answer options are distracting enough to make the question significantly more difficult for students. In both the multiple-choice and open-ended formats, students must go through intermediate steps to determine the correct answer (e.g., $\hat{Q} = \hat{Q}\hat{I} = \sum \hat{Q}|e_j\rangle\langle e_j| = \sum \lambda_j |e_j\rangle\langle e_j|$ or act with $\hat{Q}$ on a generic state $\hat{Q}|\Psi\rangle = \hat{Q} \sum |e_j\rangle\langle e_j|\Psi\rangle = \sum \lambda_j |e_j\rangle\langle e_j|\Psi\rangle \to \hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$). Thus, it is not surprising that in both the multiple-choice and open-ended questions, approximately the same percentage of students answered the question correctly.

The following difficulties with writing the operator in terms of its spectral decomposition were revealed in students' responses:

In determining how a generic operator $\hat{Q}$ can be written in terms of its spectral decomposition, i.e., $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, students incorrectly claim that $\hat{Q} = \lambda_j$. One common difficulty was students stating that $\hat{Q} = \lambda_j$. For example, one student wrote:

$$\hat{Q}|e_j\rangle = \lambda_j|e_j\rangle$$

Then $\hat{Q}$ *should equal* λ_j

In determining how a generic operator $\hat{Q}$ can be written in terms of its spectral decomposition, i.e., $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, students incorrectly claim that $\hat{Q} = \sum \lambda_j$. Another common difficulty with how $\hat{Q}$ can be written in terms of its spectral decomposition: $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, given that $\hat{Q}$ is an operator with a complete set of orthonormal eigenvectors $\hat{Q}|e_j\rangle = \lambda_j|e_j\rangle$ ($j = 1,2,3, \ldots n$) is that students incorrectly claim that $\hat{Q} = \sum \lambda_j$ because $\hat{I} = |e_j\rangle\langle e_j|$. For example, one student wrote:

If: $\hat{Q}|e_j\rangle = \lambda_j|e_j\rangle$

Start with: $\hat{Q} = \sum \lambda_j$

Multiply each side by $\hat{I} = |e_j\rangle\langle e_j|$

$$\hat{I}\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$$

$$\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$$

These types of difficulties indicate that students have difficulty reasoning about operators in Dirac notation. It does not make sense to reason about an operator as a sum of its eigenvalues, i.e., $\hat{Q} = \sum \lambda_j$. The operators are represented by an outer product (i.e., a square matrix) whereas eigenvalues are numbers.

In determining how a generic operator $\hat{Q}$ can be written in terms of its spectral decomposition, i.e., $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, students confuse the identity operator with a projection operator. Another common difficulty with how $\hat{Q}$ can be written in terms of its spectral decomposition: $\hat{Q} = \sum \lambda_j |e_j\rangle\langle e_j|$, given that $\hat{Q}$ is an operator with a complete set of orthonormal eigenvectors $\hat{Q}|e_j\rangle = \lambda_j|e_j\rangle$ ($j = 1,2,3, \dots n$) is that students confused the identity operator and a projection operator. For example, one student wrote:

$$\hat{Q}|e_j\rangle = \lambda_j|e_j\rangle$$

Multiply both sides on the right by $\langle e_j|$

$$\hat{Q}\underbrace{|e_j\rangle\langle e_j|}_{\text{identity}} = \lambda_j|e_j\rangle\langle e_j|$$

This type of difficulty indicates that even advanced students struggle to make distinctions between related concepts, e.g., discerning the difference between a projection operator and the identity operator.

5.4.5 Student difficulties with expectation value of a generic operator $\hat{Q}$

Students should develop proficiency in calculating the expectation value of an observable because this procedure is used extensively in quantum mechanics since the measurement outcomes are probabilistic. The expectation value is not the outcome of one measurement or most probable value of a measurement of an observable corresponding to an operator $\hat{Q}$, but it is the mean value of an observable when measurements are made on a large number of identically prepared systems. Therefore, it can be written as the probability of measuring a particular eigenvalue of an operator corresponding to the observable measured multiplied by the eigenvalue, summed over all possible values. In order to develop expertise with the expectation value, students should be able to determine expectation values for concrete (e.g., energy or position) as well as generic operators for both generic states and eigenstates of operators corresponding to physical observables. We investigated the extent to which students can both recognize and generate the expectation values of observables in a generic quantum state.

Relative difficulty with generating an expression for expectation value compared to recognizing a correct expression for expectation value: Upper-level students ($N = 184$) from 4 universities were given that $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n and were asked to evaluate the correctness of the expression $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$ after traditional instruction in relevant concepts. Fifty-seven percent of the students correctly recognized that $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$ is a correct expression for the expectation value of the operator $\hat{Q}$.

We also investigated the extent to which students can generate an expression for the expectation value of an operator with <u>discrete</u> eigenvalue spectrum. The following open-ended question was administered to students on quizzes ($N = 46$ undergraduate students, $N = 45$ graduate students) and midterm exams ($N = 82$ undergraduate students) after instruction in relevant concepts:

$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n. Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q_n\rangle$ and eigenvalues q_n. Show your work.

The correct answer is $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n|\langle q_n|\Psi\rangle|^2$. One can find the expectation value of an operator $\hat{Q}$, e.g., by inserting the identity operator in terms of a complete set of eigenstates of the operator $\hat{Q}$,

$$\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi|\hat{Q}\hat{I}|\Psi\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi|\hat{Q}\textstyle\sum_n|q_n\rangle\langle q_n||\Psi\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi|\textstyle\sum_n q_n|q_n\rangle\langle q_n||\Psi\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n\langle\Psi|q_n\rangle\langle q_n|\Psi\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n|\langle q_n|\Psi\rangle|^2$$

Another method to find the expectation value of an operator $\hat{Q}$ is to write $|\Psi\rangle$ as a linear superposition of the eigenstates of operator $\hat{Q}$,

$$|\Psi\rangle = \sum_n\langle q_n|\Psi\rangle|q_n\rangle$$
$$\hat{Q}|\Psi\rangle = \sum_n\langle q_n|\Psi\rangle\hat{Q}|q_n\rangle$$
$$\hat{Q}|\Psi\rangle = \sum_n\langle q_n|\Psi\rangle q_n|q_n\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n\langle q_n|\Psi\rangle\langle\Psi|q_n\rangle$$
$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n|\langle q_n|\Psi\rangle|^2$$

A student earned full credit if the he/she inserted the identity operator, used an expansion of the generic state $|\Psi\rangle = \sum c_n|q_n\rangle$ where $c_n = \langle q_n|\Psi\rangle$, or conceptually reasoned that the expectation value is the sum of the eigenvalues of $\hat{Q}$ multiplied by the probability of obtaining the eigenvalue to obtain the correct final answer. A student earned 83% if he/she wrote the correct expression with no work or explanation provided or used the expansion $|\Psi\rangle = \sum c_n|q_n\rangle$ but forgot to define c_n. A student earned half credit if he/she tried to insert an identity operator or used an expansion of $|\Psi\rangle$ but did not arrive at the correct final result. All other answers were generally irrelevant or inappropriate for the question asked and were considered incorrect (no credit). Table 5-11 shows the percentages of students who correctly were able to generate an expression for expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q_n\rangle$ and eigenvalues q_n.

We also investigated student difficulties with the expectation value of a generic operator $\hat{Q}$ with a continuous eigenvalue spectrum q. The following open-ended quiz question was administered to 46 upper-level undergraduate students and 45 graduate students after traditional instruction in relevant concepts.

$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q\rangle$ and eigenvalues q. Show your work.

The question was graded using the same rubric as for the discrete case, except that in the continuous case, if a student inserted an identity operator involving a summation instead of an integral, he/she received 2/3 credit. Table 5-11 shows the percentages of students who were correctly able to generate an expression for the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q\rangle$ and eigenvalues q.

While over half of the students could correctly recognize the expression for the expectation value, students struggled to generate expressions for the expectation value in both the discrete and continuous cases. Table 5-11 shows that undergraduate students especially had difficulty with this task and only 15% of them could generate a correct expression for the expectation value.

Table 5-11. Percentages of students who correctly recognized and generated expressions for expectation value

Question	Percentage of students
Recognize: $\langle\Psi\|\hat{Q}\|\Psi\rangle = \sum_n q_n \|\langle q_n\|\Psi\rangle\|^2$, given $\{\|q_n\rangle, n = 1,2,3 \dots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n	57% ($N = 184$ upper-level students)
Generate: Find the expectation value of Q for state $\|\Psi\rangle$ using a basis of eigenstates $\|q_n\rangle$ and eigenvalues q_n, given that $\|\Psi\rangle$ is a generic state of a quantum system and the states $\{\|q_n\rangle, n = 1,2,3 \dots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n.	15% ($N = 46$ undergraduate students)
	35% ($N = 82$ undergraduate students, midterm exam question)
	58% ($N = 45$ graduate students)
Generate: Find the expectation value of Q for state $\|\Psi\rangle$ using a basis of eigenstates $\|q\rangle$ and eigenvalues q, given that $\|\Psi\rangle$ is a generic state of a quantum system. The states $\{\|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	15% ($N = 46$ undergraduate students)
	56% ($N = 45$ graduate students)

The following difficulties involving expectation value were revealed:

Writing an incorrect expression for the expectation value when finding the expectation value of an operator $\hat{Q}$. One common difficulty with expectation value involved writing an incorrect expression for the expectation value, e.g., $\langle q_n|\hat{Q}|\Psi\rangle$. Table 5-12 (row 9) shows that 11% of the undergraduate students exhibited this difficulty on an open-ended quiz question and 4% of the students exhibited this difficulty on a midterm exam. For example, one student wrote:

$$\langle q_n|\hat{Q}|\Psi\rangle = \sum_{n=1}^{\infty} q_n \Psi(q)$$

These types of difficulties indicate that many students are not aware of the fact that the expectation value of an observable is found by “sandwiching” the corresponding operator between the state in which the expectation value is evaluated, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle$.

Arbitrarily switching $|\boldsymbol{\Psi}\rangle$ and $|\boldsymbol{q_n}\rangle$ when finding the expectation value of an operator $\hat{\boldsymbol{Q}}$. In finding the expectation value of Q, many students correctly wrote $\langle\Psi|\hat{Q}|\Psi\rangle$ but then arbitrarily wrote the generic state $|\Psi\rangle$ as the eigenstate $|q_n\rangle$ in future steps. Tables 5-12 and 5-13 (row 8) should be consulted for the specific percentages of students displaying this difficulty. For example, one student reasoned:

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{i=1}^{n}\langle q_n'|\hat{Q}|q_n\rangle$$

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{i=1}^{n} q_n\langle q_n'|\hat{Q}|q_n\rangle$$

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{i=1}^{n} q_n\delta(q_n' - q_n)$$

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{i=1}^{n} q_n$$

Another student wrote:

$$\langle\hat{Q}\rangle = \langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{\infty} q_n\langle q_n|q_n\rangle$$

These types of difficulties also shed light on students' reasoning about the generic state $|\Psi\rangle$.

Attempting to use the identity operator or expansion of $|\boldsymbol{\Psi}\rangle$ but getting lost along the way when finding the expectation value of an operator $\hat{\mathbf{Q}}$. Other students were aware of the fact that one could find the expectation value by inserting the identity operator in the expression for the expectation value or by expanding $|\Psi\rangle$ in terms of a complete set of eigenstates of $\hat{Q}$ but they got lost along the way. Tables 5-12 and 5-13 (row 6) should be consulted for the specific percentages of students displaying these difficulties. For example, one student only wrote the following in his response:

$$\hat{I} = \sum_n |q_n\rangle\langle q_n|$$

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum\langle\Psi|\hat{Q}|q_n\rangle\langle q_n|\Psi\rangle = \sum\langle\Psi|\hat{Q}|q_n\rangle\Psi(q_n)$$

Another student wrote the following:

$$\langle\Psi|\hat{Q}|\Psi\rangle \qquad \hat{I} = \textstyle\sum_n |q_n\rangle\langle q_n|$$

$$\hat{I} = \int |q_n\rangle\langle q_n|dq$$

$$\langle\Psi|\hat{Q}\int |q\rangle\langle q|dq\,|\Psi\rangle$$

$$\langle\Psi|\int \hat{Q}|q\rangle\langle q|\Psi\rangle dq$$

$$\langle\Psi|\int q\langle q|\Psi\rangle dq$$

This type of difficulty indicates that students are in an intermediate level of expertise. They have some connected pieces of knowledge (e.g., they recognize that one can use the identity operator to determine expectation value), but they have difficulty utilizing this content knowledge to find the expectation value correctly.

Writing an incorrect expression for the expansion of $|\Psi\rangle$ using a complete set of eigenstates of the operator $\hat{Q}$ when finding the expectation value of an operator $\hat{Q}$: One can find the expectation value of an operator $\hat{Q}$, e.g., by inserting the identity operator in terms of a the complete set of eigenstates of the operator $\hat{Q}$ or writing $|\Psi\rangle$ as a linear superposition of the eigenstates of an operator $\hat{Q}$, $|\Psi\rangle = \sum_n \langle q_n|\Psi\rangle|q_n\rangle$. Some students displayed difficulties such as writing incorrect expressions for the expansion of $|\Psi\rangle$, e.g., $|\Psi\rangle = \sum|q_n\rangle$ or $|\Psi\rangle = \sum q_n|q_n\rangle$. Table 5-12 (row 10) should be consulted for the specific percentages of students displaying this difficulty.

For example, one student reasoned that $|\Psi\rangle = \sum|q_n\rangle$:

$$\langle\Psi|\hat{Q}|\Psi\rangle = \sum\langle\Psi|\hat{Q}|q_n\rangle = \sum\langle\Psi|q_n|q_n\rangle = \sum q_n\langle\Psi|q_n\rangle$$

Another student explicitly stated:

$|\Psi\rangle$ can be explanded as a sum of eigenstates of $\hat{Q}$, $|\Psi\rangle = \sum_n q_n\,|q_n\rangle$.

This type of difficulty demonstrates that students have some correct knowledge, i.e., they know that one can write $|\Psi\rangle$ as a linear superposition of the eigenstates of a generic operator $\hat{Q}$. However, they struggle to determine the appropriate expression for the expansion of $|\Psi\rangle$ or the coefficients of the expansion.

Incorrectly assuming that the operator $\hat{Q}$ acting on $|\Psi\rangle$ yields an eigenvalue of the operator $\hat{Q}$ multiplied by an eigenstate of the operator $\hat{Q}$ (e.g., $\hat{Q}|\Psi\rangle = q_n|q_n\rangle$) or eigenvalue of the operator $\hat{Q}$ multiplied by $|\Psi\rangle$ (e.g., $\hat{Q}|\Psi\rangle = q_n|\Psi\rangle$) when finding the expectation value

of an operator $\hat{Q}$. Some students wrote incorrect expressions for the operator $\hat{Q}$ acting on $|\Psi\rangle$, e.g., $\hat{Q}|\Psi\rangle = q_n|q_n\rangle$, or $\hat{Q}|\Psi\rangle = q_n|\Psi\rangle$ because they reasoned that an operator acting on a generic state will yield an eigenstate or eigenvalue of the operator (see Tables 5-12 and 5-13 row 11). This was often due to the fact that students thought that the measurement process is described by an equation in which there is an operator acting on the state on the left hand side of the equation. One student reasoned:

$\hat{Q}|\Psi\rangle = q_n|q_n\rangle$ because by generalized statistical interpretation, operator on a general state will yield an eigenvalue of that operator with probability $|\langle\Psi|q_n\rangle|^2$. He then wrote:

$$\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi q_n|q_n\rangle = q_n\langle\Psi|q_n\rangle.$$

These students have some correct knowledge, i.e., when a measurement of a physical observable Q is made, the probability of measuring a discrete eigenvalue q_n for the observable Q (corresponding to an operator $\hat{Q}$ with orthonormal eigenstates $\{|q_n\rangle,\ n = 1, 2, 3 \ldots N\}$) is $|\langle q_n|\Psi\rangle|^2$. However, these students overgeneralized this knowledge to incorrectly reason that an operator acting on a general state will yield an eigenvalue of that operator multiplied by the corresponding eigenstate, e.g., $\hat{Q}|\Psi\rangle = q_n|q_n\rangle$.

Table 5-12. Percentages of students answering correctly or displaying difficulties in determining the expectation value of a physical observable with a corresponding operator $\hat{\boldsymbol{Q}}$ with discrete eigenvalues $\boldsymbol{q_n}$.

	Open-ended quiz question		Midterm
	Undergraduates ($N = 46$)	Graduates ($N = 45$)	Undergraduates ($N = 82$)
1. Correct, using identity operator	13	36	21
2. Correct, using expansion of $\|\Psi\rangle$	2	18	13
3. Correct, using conceptual reasoning	2	0	1
4. Correct, no work shown	11	2	0
5. Correct, but did not define c_n	4	13	7
6. Incorrect, using identity operator	7	2	5
7. Incorrect, using expansion of $\|\Psi\rangle$	7	0	7
8. Incorrect, arbitrarily switching $\|\Psi\rangle$ to $\|q_n\rangle$,	9	13	7
9. Incorrect, writing wrong expression for expectation value	11	2	4
10. Incorrect, writing incorrect expansion of $\|\Psi\rangle$, e.g., $\|\Psi\rangle = \sum q_n \|q_n\rangle$, $\|\Psi\rangle = q_n \|q_n\rangle$	0	4	5
11. Incorrect, writing $\hat{Q}\|\Psi\rangle = q_n\|q_n\rangle$, or $\hat{Q}\|\Psi\rangle = q_n\|\Psi\rangle$	0	0	12
12. Incorrect, inserting projection operator instead of identity operator	0	4	7
13. Other difficulties	13	4	13
14. Blank	26	2	0

Table 5-13. Percentages of students answering correctly or displaying difficulties in determining the expectation value of a physical observable with a corresponding operator $\hat{\boldsymbol{Q}}$ with continuous eigenvalues $\boldsymbol{q}$.

	Open-ended quiz question	
	Undergraduates ($N = 46$)	Graduates ($N = 45$)
1. Correct, using identity operator	13	40
2. Correct, using expansion of $\|\Psi\rangle$	0	16
3. Correct, using conceptual reasoning	2	0
4. Correct, no work shown	2	7
5. Correct, but did not define $c = \langle q\|\Psi\rangle$ in expansion	2	0
6. Incorrect, using identity operator	7	4
7. Incorrect, using expansion of $\|\Psi\rangle$	0	2
8. Incorrect, arbitrarily switching $\|\Psi\rangle$ to $\|q\rangle$,	4	11
9. Incorrect, writing wrong expression for expectation value	7	4
10. Incorrect, inserting projection operator instead of identity operator	2	2
11. Incorrect, writing $\hat{Q}\|\Psi\rangle = q\|q\rangle$, or $\hat{Q}\|\Psi\rangle = q\|\Psi\rangle$	4	7
12. Incorrect, used summation instead of integral	2	2
13. Other difficulties	11	2
14. Blank	46	2

Failing to reason about expectation value conceptually. In both the discrete and continuous cases, very few students used conceptual reasoning about how the expectation value is determined. Tables 5-12 and 5-13 (row 3) should be consulted for the specific percentages of students who used conceptual reasoning about the expectation value. While some students were able to correctly insert the identity operator in terms of the eigenstates of the operator or expand the generic state $|\Psi\rangle$ as a linear superposition of the eigenstates of the operator, many students who tried to use these methods got lost along the way. Others did not know that the operator must be "sandwiched" between the generic state $|\Psi\rangle$ to determine expectation value in that state. The fact that so few students reasoned conceptually about how to determine the expectation value points to the fact that even upper-level students may prefer to "plug and chug" as opposed to develop a deeper knowledge of the concepts. While graduate students were somewhat more facile in using the identity operator to determine the expectation value (i.e., they have more robust problem-solving skills in this regard [44]) as shown in Tables 5-12 and 5-13, they may not recognize conceptually that the expectation value can be thought of as the probability of measuring a particular eigenvalue of an operator corresponding to an observable multiplied by the eigenvalue, summed over all possible values because expectation value is the average of a large number of measurements on identically prepared systems (i.e., they may lack a coherent knowledge structure about expectation value [44]). It is important that students are guided to make connections between their content knowledge and problem-solving, reasoning, and metacognitive skills; otherwise, their knowledge structure will remain only locally consistent and they will not become experts.

Finding the expectation value of the Hamiltonian operator $\hat{H}$ by using a memorized procedure as opposed to reasoning conceptually. As discussed earlier, students struggled with determining the expectation value of a generic operator corresponding to a physical observable. However, we also investigated how students respond to questions about the expectation value of a concrete operator, in particular, a Hamiltonian operator. For example, 226 students from 10 universities were asked to answer the following question after traditional instruction in relevant concepts [5]:

A particle interacts with a one-dimensional infinite square well of width a ($V(x) = 0$ for $0 \leq x \leq a$ and $V(x) = +\infty$, otherwise). The stationary states are $\psi_n(x) = \sqrt{2/a}\, sin(n\pi x/a)$ and the allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, where $n = 1,2,3, \ldots + \infty$. Consider the following wave function for the particle: $\Psi(x,t) = \frac{1}{\sqrt{3}}\psi_1(x) + \sqrt{\frac{2}{3}}\psi_2(x)$. Choose all of the following statements that are correct about the expectation value of the energy of the system at time $t = 0$.

(1) $\langle E \rangle = 1/3\, E_1 - 2/3\, E_2$

(2) $\langle E \rangle = 1/3\, E_1 + 2/3\, E_2$

(3) $\langle E \rangle = \int_0^a \Psi^*(x,0)\hat{H}\Psi(x,0)dx$.

A. 1 only B. 2 only C. 3 only D. 1 and 3 only E. 2 and 3 only

The correct answer is option E, selected by 56% of the students. Although this question is not directly related to Dirac notation, it supports the results from the investigation of student difficulties involving expectation value in the abstract context, discussed earlier. While 92% of the students selected an answer choice that involved option 3 ($\langle E \rangle = \int_0^a \Psi^*(x,0)\hat{H}\Psi(x,0)dx$), only 60% of students chose an answer which involved option 2 ($\langle E \rangle = 1/3\, E_1 + 2/3\, E_2$). In individual interviews, when students were asked to find the expectation value of energy, many students correctly calculated $\langle E\rangle$ by "brute-force": first writing $\langle E\rangle = \int_{-\infty}^{\infty}\Psi^*\hat{H}\Psi dx$, expressing $\Psi(x,0)$ in terms of the linear superposition of two energy eigenstates, then acting $\hat{H}$ on the eigenstates, and finally using orthogonality to obtain the answer. Some got lost early in this process. Others did not remember some steps, for example, taking the complex conjugate of the wave function, using the orthogonality of stationary states, or recognizing the proper limits of the integral. The interviews revealed that many students did not know or recall the interpretation of expectation value as an ensemble average [4].

These types of responses indicate that many students may have memorized a procedure for finding the expectation value of an operator (i.e., "sandwiching" the operator between the state in which they have to find the expectation value and writing the expectation value in position representation). However, fewer students have developed a rigorous, connected knowledge network [41, 45] in order to determine that the expectation value can be determined by both methods, i.e., "sandwiching" the operator between the state, writing the expectation value in position representation and evaluating an integral or multiplying the probability of measuring a particular eigenvalue of an operator with the corresponding eigenvalue and summing over all possible values. These results support the previous results and reinforce the fact that students must be guided to develop a robust knowledge structure and enhance their skills.

5.4.6 Student difficulties with probability distribution of measurement outcomes

Quantum mechanics is probabilistic. The results of experiments cannot be predicted precisely, but the probability that a certain result is obtained in a measurement can be predicted. For orthonormal eigenstates $\{|q_n\rangle,\ n = 1, 2, 3 \ldots N\}$ of operator $\hat{Q}$ with discrete eigenvalues q_n, $|\langle q_n|\Psi\rangle|^2$ is the probability of measuring q_n for an observable Q. For orthonormal eigenstates $|q\rangle$ with continuous eigenvalues q, $|\langle q|\Psi\rangle|^2 dq$ is the probability of measuring the observable Q in a narrow range between q and $q + dq$. Since probability distribution of the measurement outcomes is a fundamental concept in quantum mechanics, students should develop proficiency in determining the probability of obtaining an outcome as well as conceptual understanding of these issues. In particular, they should be able to differentiate between the probability of obtaining an outcome, the expectation value of an observable in a given quantum state, and the connection between measurement process and quantum theory. We discuss the differences between students' answers to multiple choice questions about probability distribution and their answers to open-ended questions which require them to generate expressions for probability distribution.

Relative difficulty with generating a correct expression for probability compared to recognizing a correct expression for probability: Students perform well on questions which require recognition of correct expressions for probability of a particular outcome in a given state. For example, after traditional instruction in relevant concepts, Table 5-14 shows that 89% of students ($N = 184$ upper level students) from 4 universities recognized that if $|n\rangle$ is an eigenstate of the Hamiltonian operator, $|\langle n|\Psi\rangle|^2$ is the probability of measuring energy E_n. In addition, 80% of these same students recognized that $|\langle x|\Psi\rangle|^2 dx$ is the probability of measuring position between x and $x + dx$. In the abstract case, in which an operator $\hat{Q}$ corresponding to a physical observable Q has a continuous non-degenerate spectrum of eigenvalues and the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with eigenvalues q, Table 5-14 shows that 58% of these same students recognized that $|\langle q|\Psi\rangle|^2 dq$ is the probability of obtaining an outcome between q and $q + dq$.

However, students' performance is not as good when they are asked to generate an expression for the probability of measuring a particular outcome. For example, 46 upper-level undergraduate students and 45 graduate students were asked the following question:

Write an expression for the probability of measuring observable Q in the interval between q and $q + dq$ in the state $|\Psi\rangle$, given that $|\Psi\rangle$ is a generic state of a quantum system and the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.

Students were given full credit if they wrote $|\langle q|\Psi\rangle|^2 dq$ and half credit if they wrote an answer of the form $|\langle q|\Psi\rangle|^2$ or $|\langle q_n|\Psi\rangle|^2$, i.e., forgot to multiply by dq or treated it as a discrete case. Thirteen percent of undergraduate students and 53% of graduate students correctly wrote an expression for this probability, i.e., $|\langle q|\Psi\rangle|^2 dq$.

For the discrete case, 20 upper-level undergraduate students (different than the students discussed above) were asked the following question on a quiz:

Write an expression for the probability that a general state $|\Phi\rangle$ will collapse into an eigenstate $|\Psi_i\rangle$ of $\hat{Q}$ upon measurement of Q, given that $\hat{Q}|\Psi_i\rangle = \lambda_i|\Psi_i\rangle$, where $i = 1,2,3, \ldots N$.

Students were given full credit if they wrote $|\langle \Psi_i|\Phi\rangle|^2$. Only 10% of the students wrote a correct expression for probability.

Table 5-14. Percentages of students who correctly recognized and generated expressions for probability distribution for measuring an observable

Question	Percentage of students
Recognize: $\lvert\langle n\vert\Psi\rangle\rvert^2$ is the probability of measuring energy E_n if $\vert n\rangle$ is an eigenstate of the Hamiltonian operator	89% ($N = 184$ upper level students)
Recognize: $\lvert\langle x\vert\Psi\rangle\rvert^2 dx$ is the probability of measuring position between x and $x + dx$	80% ($N = 184$ upper level students)
Recognize: $\lvert\langle q\vert\Psi\rangle\rvert^2 dq$ is the probability of obtaining an outcome between q and $q + dq$ in which an operator $\hat{Q}$ corresponding to a physical observable Q has a continuous non-degenerate spectrum of eigenvalues and the states $\{\vert q\rangle\}$ are eigenstates of $\hat{Q}$ with eigenvalues q	58% ($N = 184$ upper level students)
Generate: Write an expression for the probability of measuring observable Q in the interval between q and $q + dq$ in the state $\vert\Psi\rangle$, given that $\vert\Psi\rangle$ is a generic state of a quantum system and the states $\{\vert q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	13% ($N = 46$ undergraduate students) 53% ($N = 45$ graduate students)
Generate: Write an expression for the probability that a general state $\vert\Phi\rangle$ will collapse into an eigenstate $\vert\Psi_\mathrm{i}\rangle$ of $\hat{\mathrm{Q}}$ upon measurement of Q, given that $\hat{\mathrm{Q}}\vert\Psi_\mathrm{i}\rangle = \lambda_\mathrm{i}\vert\Psi_\mathrm{i}\rangle$, where $\mathrm{i} = 1,2,3, \ldots \mathrm{N}$.	10% ($N = 20$ undergraduate students)

The following difficulties were revealed via students' free responses:

Confusing probability of measuring a particular value of the observable $\boldsymbol{Q}$ with expectation value of the observable $\boldsymbol{Q}$. In both the discrete and continuous cases, the common difficulties involved students writing an expression that looked like an expectation value or that involves the operator $\hat{Q}$ in their expression for the probability. In the continuous case, Table 5-15 shows that 28% of the undergraduate students and 15% of the graduate students wrote an expression which involved the operator $\hat{Q}$ (the expression usually somewhat resembled an expression for expectation value). In the discrete case, Table 5-15 shows that 20% of the students wrote an expression which involved the operator $\hat{Q}$.

Table 5-15. Percentages of students displaying difficulties with probability of measurement outcomes for observable $\boldsymbol{Q}$ with a continuous eigenvalue spectrum or a discrete eigenvalue spectrum

Difficulty	**Question**	**Percentage of students**
Expression for probability of a particular outcome involves operator $\hat{Q}$/writing expression for probability of an outcome of an observable which resembles expectation value	Write an expression for the probability of measuring observable Q in the interval between q and $q + dq$ in the state $\|\Psi\rangle$, given that $\|\Psi\rangle$ is a generic state of a quantum system and the states $\{\|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	28% ($N = 46$ undergraduate students) 15% ($N = 45$ graduate students)
	Write an expression for the probability that a general state $\|\Phi\rangle$ will collapse into an eigenstate $\|\Psi_\mathrm{i}\rangle$ of $\hat{\mathrm{Q}}$ upon measurement of Q, given that $\hat{\mathrm{Q}}\|\Psi_\mathrm{i}\rangle = \lambda_\mathrm{i}\|\Psi_\mathrm{i}\rangle$, where $i = 1,2,3, \dots N$.	20% ($N = 20$ undergraduate students)
Not multiplying by dq or confusing probability amplitude with probability	Write an expression for the probability of measuring observable Q in the interval between q and $q + dq$ in the state $\|\Psi\rangle$, given that $\|\Psi\rangle$ is a generic state of a quantum system and the states $\{\|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.	15% ($N = 46$ undergraduate students) 11% (N=45 graduate students)

For example, one student wrote the following expression for the probability of measuring the observable Q in the interval between q and $q + dq$ for the state $|\Psi\rangle$, given that $|\Psi\rangle$ is a generic state of a quantum system and the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q:

$$Probability\ of\ measuring\ observable\ Q = \left|\langle\Psi\middle|\hat{Q}\middle|\Psi\rangle\right|^2 dq$$

Another student reasoned that the probability for measuring an observable Q corresponding to an operator $\hat{Q}$ with a discrete eigenvalue spectrum in a generic state $|\Psi\rangle$ is:

$$Probability\ of\ measuring\ observable\ Q = \langle\psi_i|\hat{Q}|\psi_i\rangle = \langle\psi_i|\lambda_i|\psi_i\rangle$$

Other think-aloud interviews indicated that many students had difficulty distinguishing between the probability of measuring a particular value of an observable in a given state and the measured value or the expectation value. For example, during individual interviews, students were asked to find an expression for the probability of measuring E_n in the general state $|\Psi\rangle$. Students often wrote $\langle\psi_n|\hat{H}|\psi_n\rangle$ or $\langle\Psi|\hat{H}|\Psi\rangle$ as the probability of measuring E_n in the general state $|\Psi\rangle$. When these students were explicitly asked to compare their expressions for the probability of measuring a particular value of energy and the expectation value of energy, some students appeared concerned. They recognized that probability and expectation value were different, but they still struggled to distinguish between these concepts. They could not write an expression for the probability of measuring E_n either using the Dirac notation or in the position space representation using the integral form [6]. Difficulties of this type indicate that students often struggle to differentiate between the concepts of probability and expectation value. This can lead to overgeneralization of concepts and attempts to apply concepts in inappropriate situations.

For an operator with a continuous eigenvalue spectrum, students have difficulty with whether an integral is needed when determining the probability of measuring observable Q in the interval between q and $q + dq$ in the state $|\Psi\rangle$. In interviews, some students had difficulty with whether an integral is needed for continuous cases for the probability of measuring Q between

q and $q + dq$. One student stated, "You would have to integrate between q and $q + dq$, it's not just $|\langle q|\Psi\rangle|^2 dq$. You need to take the integral from q to $q + dq$." These types of difficulties indicate that even some advanced students struggle with reasoning involving calculus in the physics context. They do not realize that an integral is only needed for a finite interval. The physics can put a strain on their working memory and impede their sense-making.

These types of difficulties (e.g., difficulties distinguishing between the concepts of probability distribution for measurement outcomes, operators, and expectation value) can lead to difficulties in generating correct expressions for the probability distribution for measurement of an observable in a given quantum state. They suggest that upper-level undergraduate and graduate students are not yet experts and are exhibiting novice-like behavior (e.g., over-generalizing) in a new domain of quantum mechanics.

5.5 QUILT DEVELOPMENT (WARM-UP, TUTORIAL, HOMEWORK COMPONENTS)

The difficulties discussed above indicate that even after traditional instruction, upper-level undergraduate and graduate students have many common difficulties. They could benefit from a tutorial-based approach to learn about the concepts underlying Dirac notation as well as to develop skills to help them solve problems using Dirac notation. Using the common difficulties exhibited as a guide, we developed a Quantum Interactive Learning Tutorial (QuILT) on Dirac notation. The QuILT includes a warm-up, a tutorial on the basics of Dirac notation, and a homework component which focuses on position and momentum representation. The QuILT can be used in class to give students an opportunity to work together, discuss their answers with a partner, and learn from each other.

The Dirac notation QuILT builds on students' prior knowledge and was developed by taking into account the difficulties discussed above. The development of the QuILT was a cyclical, iterative process which included the following stages: 1) development of a preliminary version of the QuILT based on the research on student difficulties; 2) implementation and evaluation of the QuILT by administering it to individual students and measuring the effectiveness of it via pre-/post-tests; and 3) refinement and modifications based upon the feedback from the implementation and evaluation. The QuILT was also iterated with three faculty members and two graduate students to ensure that the content and wording of the questions were appropriate. When we found that the QuILT was effective in individual administration and students' pre-/post-test performance showed significant improvement, the QuILT (including the warmup, basics QuILT and the homework component) was administered to students in an upper-level undergraduate quantum mechanics course ($N = 46$). The QuILT was also administered to graduate students in a teaching assistant training class who were enrolled in the first semester of a graduate level quantum mechanics course ($N = 45$).

To assess the effectiveness of the Dirac notation QuILT, a Dirac notation pretest was administered to 46 upper-level undergraduate students in a junior/senior level quantum mechanics course and 45 graduate students in a teaching assistant training class who were enrolled in the first semester of a graduate level quantum mechanics course. After the students completed the pretest, they were given one week to work through the QuILT (the part they could not finish in class working in small groups, they completed at home and submitted as homework) and were then given a Dirac notation posttest upon submission of the QuILT. Any student who did not work through the Dirac notation QuILT was omitted from the posttest data. A subset of the undergraduate students ($N = 27$) was also given a Dirac notation warm-up pretest and posttest to assess the effectiveness of the Dirac notation QuILT warm-up.

5.5.1 Dirac Notation QuILT-Warm-Up

The Dirac Notation QuILT-warm-up helps students to get acquainted with Dirac notation in a familiar context of a three-dimensional vector space. It builds on their prior knowledge of working with basis vectors $\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$. Students are guided to translate vectors written in the form $\vec{F} = a\hat{\imath} + b\hat{\jmath} + c\hat{k}$ to Dirac notation, e.g., $|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle$. Analogies are drawn between dot product notation and the inner product in Dirac notation, e.g., $\hat{\imath} \cdot \vec{F}$ and $\langle i|F\rangle$. Students are then guided to write the vector $|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ in a particular basis, e.g., $|F\rangle \doteq \begin{pmatrix} \langle i|F\rangle \\ \langle j|F\rangle \\ \langle k|F\rangle \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ and are helped to translate between different bases. The warm-up guides students to determine that in a given basis, ket states can be represented by column vectors (or column matrices), bra states can be represented by row vectors, inner products are numbers, and outer products are operators (or square matrices). Students also are guided to develop a functional understanding of the completeness relation in the familiar context of a three-dimensional vector space, e.g., in one part of the warm up, they are asked the following:

In the $\{|i\rangle, |j\rangle, |k\rangle\}$ *representation, the normalized basis vectors are chosen as* $|i\rangle \doteq \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|j\rangle \doteq \begin{pmatrix}0\\1\\0\end{pmatrix}$, *and* $|k\rangle \doteq \begin{pmatrix}0\\0\\1\end{pmatrix}$. *Compute the outer products* $|i\rangle\langle i|$, $|j\rangle\langle j|$, *and* $|k\rangle\langle k|$ *in matrix form. Add the matrices to find the operator* $\hat{I} = |i\rangle\langle i| + |j\rangle\langle j| + |k\rangle\langle k|$ *in this basis.*

Students also determine the identity operator in a different orthonormal basis and verify that the identity operator always has the same form as a unit matrix, regardless of the basis chosen.

The Dirac Notation QuILT-warm-up also helps students learn about projection operators in a given basis (i.e., using basis vectors $|i\rangle$, $|j\rangle$, and $|k\rangle$) and learn to differentiate them from the identity operator, e.g., through questions such as the following:

Consider the following conversation between Student A and Student B:

- *Student A: The projection operator acting on vector* $|F\rangle$ *is like the identity operator in that it returns the same vector* $|F\rangle$ *back along the direction of a basis vector.*
- *Student B: I disagree. The projection operator, e.g.,* $|i\rangle\langle i|$, *acting on vector* $|F\rangle$ *is not like the identity operator acting on vector* $|F\rangle$. *When the projection operator* $|i\rangle\langle i|$ *acts on* $|F\rangle$, *it does not return the same vector* $|F\rangle$. *Rather, it returns a basis vector* $|i\rangle$ *multiplied by the component of* $|F\rangle$ *along that basis vector* $|i\rangle$, *e.g.,* $\langle i|F\rangle$.

With whom do you agree? Explain your reasoning.

These types of conversations explicitly bring up common difficulties students have (i.e., confusing the identity operator with a projection operator). The student may undergo cognitive conflict

[45,46] and must decide which student he/she agrees with. The students are then given an opportunity to explain their reasoning, which will help them make sense of the concept.

The Dirac notation warm-up is a valuable stepping stone for students because it takes advantage of what they are familiar with from their previous physics courses (i.e., vector notation for three dimensional space) to help them learn about Dirac notation with which they are not familiar but must use extensively in quantum mechanics.

5.5.2 Dirac Notation QuILT-Part I (Basics)

The Dirac Notation QuILT-Part I includes the following topics: state of a quantum system, scalar products, Hilbert space, expansion of a state using a complete set of eigenstates, probability of measuring an eigenvalue of a Hermitian operator corresponding to an observable in a generic state, expectation value of an observable in a generic state, projection operator, and spectral decomposition of the identity operator (completeness relation). Each of the topics is discussed in different sections, and each section includes a summary of the main points. The sections include multiple-choice and open-ended questions. Many of the questions are paired—a student must first answer a multiple-choice or open-ended question, and then the subsequent question includes a conversation between two students discussing the answer to the previous question. Typically within the conversation, one of the students states a correct statement and the other states an incorrect statement based on common student difficulties. If the student had answered the multiple-choice question incorrectly and experiences cognitive conflict [45,46] while reading the conversation, the student has the opportunity to resolve his/her conflict and go back and change his/her answer to the multiple choice question. If the student does not recognize that he/she has answered incorrectly, a follow-up question or a summary of the section may explicitly state the answer. At this point, the student is given another opportunity to think further about the answer and fix his/her mistakes. An example of this sequence of questions (involving confusion between the identity operator and a projection operator) follows:

- *Act on a generic state $|\Psi\rangle$ with the operator $|q_n\rangle\langle q_n|$. That is, $|q_n\rangle\langle q_n|\Psi\rangle$. Which one of the following statements correctly describes what you obtain?*

(a) *You get back the same state $|\Psi\rangle$, because $|q_n\rangle\langle q_n|$ is the identity operator.*

(b) *You get the projection of $|\Psi\rangle$ along the direction of $|q_n\rangle$. $\langle q_n|\Psi\rangle$ is the component of $|\Psi\rangle$ along the direction of $|q_n\rangle$. The vector $|q_n\rangle$, which multiplies the coefficient $\langle q_n|\Psi\rangle$, gives the direction of the projected vector.*

(c) *You get the same state $|\Psi\rangle$ back, with the corresponding eigenvalue.*

(d) *It cannot be determined from the given information. The state $|\Psi\rangle$ has to be given explicitly in position representation for a given quantum system to be able to calculate the answer.*

- *Consider the following conversation between Student A and Student B.*
    - *Student A: I thought that $|q_n\rangle\langle q_n|$ was equal to the identity operator. Wasn't that what we had learned earlier in this tutorial? How is it that the same expression is the identity operator and the projection operator at the same time?*
    - *Student B: The expression that was equal to the identity operator was $\sum_{n=1}^{N}|q_n\rangle\langle q_n|$, where there is a sum over a complete set of basis vectors. Applying that on a state $|\Psi\rangle$ would give the same state back. An example of a projection operator is $|q_n\rangle\langle q_n|$. Acting with $|q_n\rangle\langle q_n|$ on a state $|\Psi\rangle$ gives the projection of that state along the direction of $|q_n\rangle$ as follows:*

$\lvert q_n\rangle$	$\langle q_n\lvert\Psi\rangle$
The vector multiplying the inner product	Inner product of $\lvert\Psi\rangle$ with $\lvert q_n\rangle$ equals the component of $\lvert\Psi\rangle$ along the direction of $\lvert q_n\rangle$

Do you agree with Student B's explanation?

After this sequence of questions, the projection operator is summarized as follows:

Summary of the projection operator:

- *The projection operator $\lvert q_n\rangle\langle q_n\rvert$ acting on a state $\lvert\Psi\rangle$ returns a vector in the direction of $\lvert q_n\rangle$ together with a number $\langle q_n\lvert\Psi\rangle$, which is the component of a state vector along the direction of the orthonormal basis vector $\lvert q_n\rangle$.*
- *Unlike the identity operator, the projection operator acting on a state vector need not return the same state vector back.*

The guided questions help students develop both content knowledge and problem-solving, reasoning, and metacognitive skills. For example, the expectation value is the average value of a large number of measurements performed on identically prepared systems. Students often use "plug and chug" approaches to determine an expectation value but fail to understand what it means conceptually. The following set of questions focuses students' attention on making the connection between the conceptual and quantitative approaches:

The **expectation value** *of an operator is the average value of the observable measured over many identical experiments performed on identically prepared systems in state $\lvert\Psi\rangle$. For a general quantum mechanical Hermitian operator $\hat{Q}$, the expectation value is represented by $\langle\Psi\lvert\hat{Q}\rvert\Psi\rangle$. If*

*$\hat{Q}$ has **discrete** eigenvalues q_n and eigenstates $|q_n\rangle$ where $n = 1,2, \ldots N$, let's write $\langle\Psi|\hat{Q}|\Psi\rangle$ in terms of the eigenstates $|q_n\rangle$ and eigenvalues q_n.*

- *Consider the following statement from Student A:*
  - *Student A: $|\langle q_n|\Psi\rangle|^2$ is the probability of measuring q_n when you measure observable Q in the state $|\Psi\rangle$. The expectation value is the average value of a large number of measurements performed on identically prepared systems. Since we know the probability of measuring each eigenvalue q_n of the operator $\hat{Q}$, the expectation value is $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n|\langle q_n|\Psi\rangle|^2$.*
  - *Student B: You cannot think about **expectation value** physically as an average of a large number of measurements on identically prepared systems. We must use our expansion $|\Psi\rangle = \sum_{n=1}^{N} a_n|q_n\rangle$, to calculate the expectation value $\langle\Psi|\hat{Q}|\Psi\rangle$.*

  With whom do you agree? Explain your reasoning.

- *Student A is correct. The expectation value is the average value of a large number of measurements on identically prepared systems, which can be represented mathematically by the equation $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n|\langle q_n|\Psi\rangle|^2$. But let's follow Student B's method using the expansion $|\Psi\rangle = \sum_{n=1}^{N} a_n|q_n\rangle$ to prove that the equation $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n|\langle q_n|\Psi\rangle|^2$, suggested by Student A, is correct. Act with $\hat{Q}$ on the state $|\Psi\rangle = \sum_{n=1}^{N} a_n|q_n\rangle$. What do you obtain?*
- *So far, we have $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} a_n q_n|q_n\rangle$. Insert what you obtained for a_n into $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} a_n q_n|q_n\rangle$.*

- *We now have* $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |q_n\rangle\langle q_n|\Psi\rangle$. *Now take the inner product of* $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |q_n\rangle\langle q_n|\Psi\rangle$ *with a "bra" state* $\langle\Psi|$ *to find the* ***expectation value*** $\langle\Psi|\hat{Q}|\Psi\rangle$. *Does your answer agree with Student A's statement from part (e)? If not, go back and check your work with a partner to obtain the equation for the expectation value of observable* $\hat{Q}$ *in terms of its complete set of eigenstates* $\{|q_n\rangle, n = 1,2, \ldots N\}$ *and eigenvalues* q_n, *i.e.,* $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$.
- *Repeat the calculation for the* ***expectation value*** $\langle\Psi|\hat{Q}|\Psi\rangle$ *of an operator* $\hat{Q}$ *with eigenstates* $|q\rangle$ *(which form a basis in an infinite-dimensional vector space) with* ***continuous*** *eigenvalues* q.

The Dirac notation QuILT strives to help students not only recall but also generate answers to questions in the context of Dirac notation. Students are often asked to find an expression and explain why their results make sense. If students have difficulty explaining their results in words, a follow-up question attempts to guide them to the correct understanding. For example, the following series of questions help students develop content knowledge along with problem-solving, reasoning, and metacognitive skills in the context of learning about the identity operator:

- *Act with the identity operator* $\hat{I}$, *written in terms of orthonormal eigenstates* $|q_n\rangle$ *of an operator* $\hat{Q}$ *with discrete eigenvalues* q_n, *on an arbitrary state vector* $|\Psi\rangle$. *What do you obtain?*
- *Explain your results from part (a) in a sentence.*
- *Consider the following statement made by a student:*

  "We can use the following analogy when reasoning about the identity operator:

$3\ hours = 3\ hours \times \left(\frac{60\ minutes}{1\ hours}\right) = 180\ minutes$. In this case, the identity operator is analogous to $\left(\frac{60\ minutes}{1\ hours}\right) = 1$. When you multiply $3\ hours$ by $\left(\frac{60\ minutes}{1\ hours}\right)$, you are causing a one-dimensional basis change from hours to minutes. Similarly, the identity operator helps us change basis in an N dimensional Hilbert space."

Do you agree with the student? Explain your reasoning.

- *So far we have $\hat{I}|\Psi\rangle = \sum_{n=1}^{N} |q_n\rangle\langle q_n|\Psi\rangle$. If $|\Psi\rangle = \sum_{n=1}^{N} a_n\,|q_n\rangle$, which one of the following is the correct expression for the coefficients a_n along the state $|q_n\rangle$ in the expansion of $|\Psi\rangle$?*
  - *a)* $a_n = \langle q_n|\Psi\rangle$
  - *b)* $a_n = \langle q_n|q_n\rangle$
  - *c)* $a_n = |\langle q_n|\Psi\rangle|^2$
  - *d)* $a_n = \langle \Psi|\Psi\rangle$

In sum, the Dirac notation tutorial guides students in learning content and developing problem-solving, reasoning, and metacognitive skills in the context of Dirac notation.

5.5.3 Dirac Notation QuILT-Part II (Position and Momentum Representations)

The Dirac Notation QuILT-Part II focuses on position and momentum representations. It includes the following topics: the relationship between a generic state vector and the wave function, position and momentum eigenstates, and position and momentum representations.

The Dirac Notation QuILT-Part II helps students build on what they learned about operators with a discrete eigenvalue spectrum to the continuous case, e.g., position and momentum operators. The focus of this part is on helping students connect state vectors and operators in Dirac notation with corresponding quantities in position or momentum representation (with or without using Dirac notation). Since students had difficulties with writing a generic state vector in position representation, the following sequence of questions help students connect a generic state vector $|\Psi\rangle$ to the wave function in position representation:

- *Consider a generic state vector* $|\Psi\rangle = \sum_{n=1}^{\infty} a_n |q_n\rangle$, *where* $a_n = \langle q_n|\Psi\rangle$. *Then, the state vector* $|\Psi\rangle$ *can be represented as a column vector like this:* $|\Psi\rangle \doteq \begin{pmatrix} \langle q_1|\Psi\rangle \\ \langle q_2|\Psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$, *where the* $\doteq$ *sign means that this is a representation of* $|\Psi\rangle$ *in the chosen basis, e.g.,* $\{|q_n\rangle, n = 1,2, \ldots \infty\}$. *Consider the following conversation between two students about the situation where basis vectors are chosen to be position eigenstates* $|x\rangle$ *or momentum eigenstates* $|p\rangle$, *each of which have a continuous eigenvalue spectrum.*
    - *Student 1: We cannot write state vector* $|\Psi\rangle$ *as a column vector if position eigenstates* $|x\rangle$ *are chosen as the basis vectors. State vector* $|\Psi\rangle$ *written as a linear superposition of position eigenstates* $|x\rangle$ *is* $|\Psi\rangle = \int_{-\infty}^{\infty} \Psi(x)|x\rangle dx$, *where* $\Psi(x) = \langle x|\Psi\rangle$. *But since this expansion of* $|\Psi\rangle$ *involves an integral instead of a summation, we cannot write* $|\Psi\rangle$ *as a column vector with respect to the basis vectors* $|x\rangle$.
    - *Student 2: I disagree. Even though the expansion of* $|\Psi\rangle$ *is an integral instead of a sum, we can still envision* $|\Psi\rangle$ *as a column vector with respect to the basis vectors* $|x\rangle$. *Like this:*

      $$|\Psi\rangle \doteq \begin{pmatrix} \langle x_1|\Psi\rangle \\ \langle x_2|\Psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \vdots \end{pmatrix} = \Psi(x).$$

- *Student 1: But why do the x's have indices? Don't position eigenstates $|x\rangle$ have a continuous eigenvalue spectrum x, not a discrete eigenvalue spectrum?*
- *Student 2: Yes, you are correct. Actually, you should think of $x_1 = \Delta x$, $x_2 = 2\Delta x$ … etc., and take the limit as $\Delta x \to 0$. I was simply making an analogy with the discrete eigenvalue spectrum case. However, the best way to write $|\Psi\rangle$ when position eigenstates $|x\rangle$ are chosen as the basis vectors is as $\Psi(x)$, which is also called the position space wave function. $\Psi(x)$ is a column vector with position eigenvalues x as a continuous index.*

Do you agree with Student 2? Explain your reasoning.

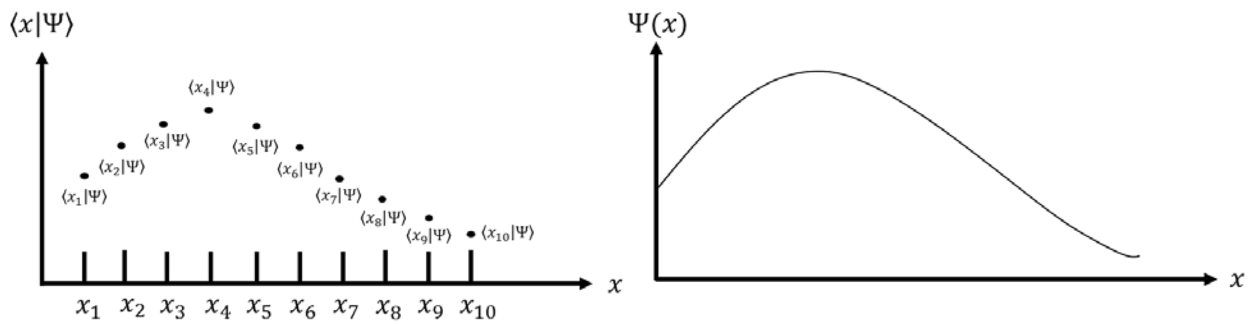


Figure 5-1. Figure in Dirac notation QuILT-Part II depicting the translation from a column vector representation of discrete points to a continuous set of numbers called the wave function

- *Consider the following graphs and statement made by Student A:*
  - *Student A: For a continuous variable like position, the column vector representation $|\Psi\rangle \doteq \begin{pmatrix} \langle x_1|\Psi\rangle \\ \langle x_2|\Psi\rangle \\ \vdots \end{pmatrix}$ is not convenient because we cannot write down an infinite number of components. We can translate from the column vector representation of discrete points (shown in the left figure 5-1 above) to a continuous set of numbers which is called the*

quantum mechanical wave function (shown in the right figure 5-2 above). The wave function is an infinite collection of numbers that represents the quantum state vector in terms of position eigenstates.

Explain why you agree or disagree with Student A's statement.

After learning about how to write a generic state in position and momentum representation, students are guided to learn how to write position and momentum eigenstates in position and momentum representation. Since students exhibited difficulties involving translating between different representations, the following sequence of questions helps students make connections between Dirac notation and wave functions in position and momentum representations (written with or without Dirac notation):

- *Which one of the following is the eigenstate of position* $|x'\rangle$ *with eigenvalue* x' *written in position representation, i.e.,* $\langle x|x'\rangle$*?*

  (a) $\langle x|x'\rangle = \Psi(x')$

  (b) $\langle x|x'\rangle = \delta(x - x')$

  (c) $\langle x|x'\rangle = \frac{e^{\frac{ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$

  (d) $\langle x|x'\rangle = \Psi(x)$

- *The position eigenstate written in position representation (when considered as a function of* x*) is called the:*

  (a) *Position eigenfunction in position representation.*

  (b) *Position eigenfunction in momentum representation.*

(c) *Position eigenfunction either in position or momentum representation since the expression for position eigenfunction is the same regardless of the representation.*

(d) *None of the above.*

- *Consider the following conversation between two students:*
    - *Student 1: The position eigenfunction should always be a delta function whether we write it in position or momentum representation.*
    - *Student 2: I disagree.* $\langle x|x'\rangle$ *cannot be the same as* $\langle p|x'\rangle$ *because when position eigenstate* $|x'\rangle$ *with eigenvalue* x' *is written by choosing position eigenstates* $|x\rangle$ *as basis vectors, we obtain* $\langle x|x'\rangle = \delta(x - x')$ *which is the position eigenfunction in the position representation. When the position eigenstate* $|x'\rangle$ *is written by choosing momentum eigenstates* $|p\rangle$ *as basis vectors, we obtain* $\langle p|x'\rangle$*, which is the position eigenfunction in the momentum representation. However,* $\langle p|x'\rangle$ *is not a delta function. The position eigenfunction is only a delta function in the position representation, but not in the momentum representation.*

With whom do you agree? Explain your reasoning.

Similar sequences of questions help students write position and momentum eigenstates in the momentum representation (with or without using the Dirac notation).

Students are also guided to generalize their answers involving position eigenstates or momentum eigenstates to a generic state, for example through the following guided sequence:

- *Consider the following conversation between two students:*

- *Student 1: The position operator $\hat{x}$ acting on a generic state $|\Psi\rangle$ written in Dirac notation without reference to a basis is $\hat{x}|\Psi\rangle$. Suppose we choose a basis in which the eigenstates of position, $|x\rangle$, are chosen as basis vectors. $\hat{x}|\Psi\rangle$ is represented in position representation by taking the scalar product of $\hat{x}|\Psi\rangle$ with $|x\rangle$, like this: $\langle x|\hat{x}|\Psi\rangle = x\Psi(x)$.*
- *Student 2: I don't see how that is correct. How did the state vector $|\Psi\rangle$ turn into the position space wave function $\Psi(x)$?*
- *Student 1: Earlier we learned that $\hat{x}|x'\rangle = x'|x'\rangle$ is the eigenvalue equation for the position operator $\hat{x}$ in Dirac notation without reference to a basis. In the position representation, we choose a basis in which the eigenstates of position, $|x\rangle$, are chosen as basis vectors. Then, $\hat{x}|x'\rangle$ is represented by taking the scalar product of $\hat{x}|x'\rangle$ with $|x\rangle$, like this: $\langle x|\hat{x}|x'\rangle = x'\langle x|x'\rangle = x'\delta(x - x')$, where $\langle x|x'\rangle = \delta(x - x')$ is a special type of position space wave function. We can generalize this logic to $\hat{x}|\Psi\rangle$, which is the position operator acting on any generic state $|\Psi\rangle$, as $\langle x|\hat{x}|\Psi\rangle = x\langle x|\Psi\rangle = x\Psi(x)$ in the position representation. Note than $\hat{x}$ can act on $\langle x|$ in $\langle x|\hat{x}|\Psi\rangle$ and give eigenvalue x because $\hat{x}$ is a Hermitian operator.*
- *Student 3: Or we can insert the identity operator written in terms of position eigenstates $\int_{-\infty}^{\infty}|x'\rangle\langle x'|dx'$ into the expression $\langle x|\hat{x}|\Psi\rangle$, like this:*

  $\int_{-\infty}^{\infty}\langle x|\hat{x}|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} x'\langle x|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} x'\delta(x - x')\Psi(x')dx' = x\Psi(x)$.
- *Student 2: I see. So the position operator $\hat{x}$ acting on a generic wave function $\Psi(x)$ in position representation just amounts to multiplication of $\Psi(x)$ by x.*

Do you agree with Student 1 and Student 3's explanations and Student 2's statement? Explain your reasoning.

In addition, students are guided to generalize their answers about position and momentum operators to a generic operator. For example, since students had difficulties with determining the representation of $\langle x|\hat{Q}|\Psi\rangle$ without using the Dirac notation, the following sequence of questions was implemented in the tutorial:

- *Suppose a generic operator $\hat{Q}$ depends only on position and momentum operators. How is $\hat{Q}$ acting on a generic state $|\Psi\rangle$, i.e., $\hat{Q}|\Psi\rangle$, represented in the position representation when basis vectors are chosen to be eigenstates of postion, $|x\rangle$?*

  (I) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)|\Psi\rangle$

  (II) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}(x, -i\hbar\frac{\partial}{\partial x})\langle x|\Psi\rangle$

  (III) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$

  (IV) $\langle x|\hat{Q}|\Psi\rangle = x\hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$

  (a) (I) and (IV) only

  (b) (II) and (III) only

  (c) (I), (II), and (III) only

  (d) All of the above.

- *Consider the following conversation between two students:*
  - *Student 1: The correct answer for the preceding is (b). It is just like $\langle x|\hat{p}|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$, except $\langle x|\hat{p}|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$ is a special case of $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$.*

- *Student 2: How is* $\langle x|\hat{p}|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$ *similar to* $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$*?*
- *Student 1: Well,* $\langle x|\hat{p}|p'\rangle$ *is like* $\langle x|\hat{Q}|\Psi\rangle$ *because the operator* $\hat{p}$ *corresponds to* $\hat{Q}$ *and state* $|p'\rangle$ *corresponds to state* $|\Psi\rangle$*. Both* $\hat{p}|p'\rangle$ *and* $\hat{Q}|\Psi\rangle$ *are operators acting on a state vector without reference to a basis. When basis vectors are chosen to be eigenstates of position,* $|x\rangle$*, and we take the scalar product of* $\hat{p}|p'\rangle$ *or* $\hat{Q}|\Psi\rangle$ *each with* $|x\rangle$*, we obtain the respective operators written in position representation acting on the respective position space wave function. The operators and state vectors in each case are represented in position representation by* $-i\hbar\frac{\partial}{\partial x}\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$ *and* $\hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$*. Also,* $\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}} = \langle x|p'\rangle$*, which is a momentum eigenfunction with eigenvalue* p'*, is a special type of position space wave function* $\Psi(x) = \langle x|\Psi\rangle$*.*

  Do you agree with Student 1's explanation? Explain your reasoning.

This type of sequence first asks students to commit to an answer in a multiple-choice question. The next question (a conversation between two students) assists students in recognizing the analogy between $\langle x|\hat{p}|p'\rangle$ and $\langle x|\hat{Q}|\Psi\rangle$. If students answered the multiple-choice question correctly, the next question confirms their answer. If students answered the multiple-choice question incorrectly, the next question may cause them to undergo cognitive conflict [45,45] and help them resolve the conflict by helping them understand conceptually that $\langle x|\hat{Q}|\Psi\rangle$ is $\hat{Q}|\Psi\rangle$ written in position representation.

Since the students exhibited difficulties when translating state vectors and operators between Dirac notation and position and momentum representation (with or without using the

Dirac notation), the QuILT also uses tables to help students make connections between the different representations, for example, see Table 5-16.

Table 5-16. Example of a table in the Dirac notation QuILT-Part II

	Position representation	Momentum representation
Position eigenstates $\|x'\rangle$		
Momentum eigenstates $\|p'\rangle$		
Position operator $\hat{x}$		
Momentum operator $\hat{p}$		
$\hat{Q}\|x'\rangle$		
$\hat{Q}\|p'\rangle$		
$\hat{Q}\|\Psi\rangle$		

As students work on the Dirac Notation QuILT-Part II, they are guided to fill in different parts of the table in different representations. At the end of each section, the correct parts of the table are shown so that students can check their work.

5.6 PRE/POST DATA

The Dirac Notation QuILT was administered to students in the first semester of an upper-level undergraduate quantum mechanics course ($N = 46$). The QuILT was also administered to graduate students who were enrolled in the first semester of a graduate level quantum mechanics course ($N = 45$). Students were given one week to work through the QuILT. The upper-level undergraduate students were given small credit for working through the QuILT and turning it in. The graduate students were required to work through the QuILT and turn it in, but it was not counted as part of a course grade (since their course grade in the TA training course in which they worked on this QuILT was scored as satisfactory or unsatisfactory).

We designed a pretest and posttest for the Dirac notation QuILT (Warm-up, Part I, and Part II) to assess the effectiveness of the QuILT. The pretests were administered in class immediately before students were given the Dirac notation QuILT and the posttests were administered in class immediately after the students turned in their completed Dirac notation QuILTs. We administered pretests for the Dirac notation QuILT warm-up to 27 upper-level undergraduate students and posttests for the Dirac notation QuILT warm-up to 41 upper-level undergraduate students. A pretest and posttest on the Dirac notation QuILT Parts I and II were administered to 46 upper-level undergraduate students and 45 graduate students. The undergraduate students were given small credit on the pretests if they completed them to the best of their ability, but they were not graded for correctness on the pretests. The undergraduate students were graded for correctness on the Dirac notation QuILT Part I and II posttests and the scores were part of their quiz grade. The graduate students were required to complete the pretests and posttests for the Dirac notation QuILT Part I and II, but they were not counted as part of their course grade.

We also compared the performance of the groups that learned from all parts of the Dirac Notation QuILT to students who did not work on the QuILT on questions related to Dirac notation on midterm exams and conceptual surveys. To determine whether the students who learned from the QuILT had good retention of concepts involving Dirac notation, we gave a retention quiz at the end of the semester to 24 upper-level students in the first semester of an upper-level undergraduate quantum mechanics course (a subset of the 46 upper-level undergraduate students who worked on the QuILT). The retention quiz was given approximately three months after the students worked on the Dirac notation QuILT.

The average pretest score for the Dirac Notation warm-up was 55% and the average posttest score was 91%. The average pretest score for the Dirac Notation Part I and II was 27% for undergraduate students and 74% for graduate students and the average posttest score was 80% for undergraduate students and 90% for graduate students. Average normalized gain [48] is commonly used to determine how much the students learned, taking into account their initial score on the pretest. It is defined as $\langle g \rangle = \frac{\%\langle S_f \rangle - \%\langle S_i \rangle}{100 - \%\langle S_i \rangle}$, in which $\langle S_f \rangle$ and $\langle S_i \rangle$ are the final (post) and initial (pre) class averages, respectively [48]. The average normalized gain on the Dirac notation Parts I and II pretest to post-test was 73% for undergraduate students and 61% for graduate students.

5.6.1 Pre/post data on student difficulties with Dirac notation in the context of a three-dimensional space

To determine the effectiveness of the Dirac notation warm-up on questions related to Dirac notation in the context of a three-dimensional space, students' scores on the Dirac notation QuILT warm-up pre/posttests were calculated. Table 5-17 shows the average pretest and posttest scores for questions related to Dirac notation in the context of a three-dimensional space. Table 5-17 shows that students' average scores were approximately 80% or higher on the post-test and many of the difficulties observed on the pre-test were reduced.

Table 5-17. Percentages of students correctly answering questions on the QuILT warm-up pre/posttest questions related to Dirac notation in the context of a three-dimensional space

Question	**Dirac notation warm-up Pre-test** ($N = 27$ UG)	**Dirac notation warm-up post-test** ($N = 41$ UG)
Assume that $\vert i\rangle, \vert j\rangle,$ and $\vert k\rangle$ form a complete set of orthonormal basis vectors. For vector $\vert\chi_1\rangle = a\vert i\rangle + b\vert j\rangle + c\vert k\rangle$ (a vector in a three-dimensional vector space), write the components a, b, and c in Dirac notation.	37%	90%
Assume that $\vert i\rangle, \vert j\rangle,$ and $\vert k\rangle$ form a complete set of orthonormal basis vectors. For vector $\vert\chi_1\rangle = a\vert i\rangle + b\vert j\rangle + c\vert k\rangle$ Represent $\vert\chi_1\rangle$ as a column vector in the given basis.	85%	93%
$\vert\chi_1\rangle = a\vert i\rangle + b\vert j\rangle + c\vert k\rangle$ and $\vert\chi_2\rangle = d\vert i\rangle + e\vert j\rangle + f\vert k\rangle$ are vectors in a three dimensional vector space. Write the outer product of "ket" vector $\vert\chi_1\rangle$ with "bra" vector $\langle\chi_2\vert$ in the given basis.	48%	76%
Is the outer product of a "ket" vector with a "bra" vector a scalar (number), a column vector, a row vector, or a 3×3 matrix in the given basis?	63%	93%
Write the identity operator in terms of $\vert i\rangle,\ \vert j\rangle,$ and $\vert k\rangle$, which form a complete set of orthonormal basis vectors for a three dimensional vector space.	48%	90%
For the vector $\vert\chi_1\rangle = a\vert i\rangle + b\vert j\rangle + c\vert k\rangle$, write down the projection operator that projects vector $\vert\chi_1\rangle$ along the direction of the unit vector $\vert i\rangle$.	18%	93%

5.6.2 Pre/post data on student difficulties involving quantum states

To determine the effectiveness of the Dirac notation QuILT on questions related to quantum states, students' scores on the pre/posttests for questions related to quantum states were calculated. Table 5-18 shows percentage of students answering questions related to quantum states correctly on the pretest and posttest. Responses to the question: "You are given a generic state $|\Psi\rangle$. How would you obtain the wave function in position representation from $|\Psi\rangle$" were considered correct if the student wrote $\langle x|\Psi\rangle$ or $\Psi(x)$. Responses to the questions such as "write a position eigenstate with eigenvalue x' in position representation" were considered correct if the student wrote it in Dirac notation (e.g., $\langle x|x'\rangle$) or without Dirac notation (e.g., $\delta(x-x')$). The student was not penalized if he/she did not write the normalization condition or wrote a negative sign in the wrong place.

Table 5-18 shows that students scored above 80% on all of the questions related to states in position or momentum representation written with or without Dirac notation (e.g., $\langle x|x'\rangle = ?$ and $\langle p|x'\rangle = ?$) on the posttest. Students' scores on generating expressions for states in position or momentum representation were slightly lower (but still above 70%). This significantly higher performance on posttest recall questions indicates that students have developed proficiency with recalling what the states look like in position and momentum representations with and without Dirac notation, but have more difficulty generating expressions for them.

Table 5-18. Comparison of the percentages of students who correctly answered questions related to quantum states on the Dirac notation QuILT pre/posttest. The number of students in the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

	Dirac notation Pretest		**Dirac notation Posttest**	
	UG (N=46)	G (N=45)	UG (N=43)	G (N=43)
Recall: $\langle x\|x'\rangle = ?$	35%	91%	81%	93%
Recall: $\langle p\|x'\rangle = ?$	20%	84%	81%	100%
Recall: $\langle x\|p'\rangle = ?$	20%	88%	81%	100%
Recall: $\langle p\|p'\rangle = ?$	35%	91%	88%	95%
Generate: You are given a generic state $\|\Psi\rangle$. How would you obtain the wave function in position representation from $\|\Psi\rangle$?	52%	87%	74%	91%
Generate: Write a momentum eigenstate with eigenvalue p' in position representation.	13%	58%	79%	88%
Generate: Write a momentum eigenstate with eigenvalue p' in momentum representation.	15%	49%	74%	70%

We also compared the performance of students who had learned from the Dirac notation QuILT vs. students who did not (see Table 5-19). On a conceptual, multiple-choice survey, students who had worked on the Dirac notation QuILT performed better than students who had traditional instruction in recognizing $\Psi(x) = \langle x|\Psi\rangle$, $\Phi(\mathrm{p}) = \langle \mathrm{p}|\Psi\rangle$, and the expansion of a generic state (see Table 5-19). Table 5-19 shows that students who learned from the QuILT were also less likely to be distracted by incorrect expressions for $\langle x|\Psi\rangle$, i.e., $\langle x|\Psi\rangle = \int x\Psi(x)dx$, which indicates that the QuILT helped students with the difficulty that the position (or momentum) operator is involved in determining the position (or momentum) space wave function.

We found that the QuILT group performance is significantly better on midterm questions related to writing position and momentum eigenstates in position and momentum representations (p-value, t-test <0.001), e.g., "write a momentum eigenstate with eigenvalue p' in position representation." Responses received full points if the student wrote his/her answer with or without Dirac notation in position representation. The scores on questions related to the physical significance of $\langle x|\Psi\rangle$ and $\langle p|\Psi\rangle$ were not significantly different from each other. Responses were considered correct if the student wrote that the physical significance of $\langle x|\Psi\rangle$ was $\Psi(x)$ or that it is the wave function in position representation or the position space wave function (similar scoring for $\langle p|\Psi\rangle$).

Table 5-19. Comparison of the performance of students who learned from the Dirac notation QuILT vs. students who did not do so on questions related to quantum states

Question	QuILT Group	Non-QuILT Group
Recognize: $\Psi(x) = \langle x\|\Psi\rangle$	96% ($N = 88$)	89% ($N = 184$)
Recognize: $\Phi(\mathrm{p}) = \langle \mathrm{p}\|\Psi\rangle$	93% ($N = 88$)	77% ($N = 184$)
Recognize:: $\|\Psi\rangle = \int \Psi(x)\|x\rangle dx$	84 % ($N = 88$)	63% ($N = 184$)
Recognize: $\|\Psi\rangle = \int \langle p\|\Psi\rangle \|p\rangle dp$	88% ($N = 88$)	78% ($N = 184$)
Recognize:$\langle x\|\Psi\rangle = \int \delta(x - x')\Psi(x')dx'$	80% ($N = 88$)	54% ($N = 184$)
Recognize that $\langle x\|\Psi\rangle = \int x\Psi(x)dx$ is an incorrect expression	79% ($N = 88$)	45% ($N = 184$)
Recall: What is the physical significance of $\langle x\|\Psi\rangle$?	91% ($N = 44$)	84% ($N = 82$)
Recall: What is the physical significance of $\langle p\|\Psi\rangle$?	91% ($N = 44$)	83% ($N = 82$)
Generate: write a position eigenstate with eigenvalue x' in position representation*	84% ($N = 44$ undergraduate students, midterm exam)	41% ($N = 82$ undergraduate students, midterm exam)
Generate: write a position eigenstate with eigenvalue x' in momentum representation*	89% ($N = 44$ undergraduate students, midterm exam)	34% ($N = 82$ undergraduate students, midterm exam)
Generate: write a momentum eigenstate with eigenvalue p' in position representation.*	79% ($N = 43$ undergraduate students) 89% ($N = 44$ undergraduate students, midterm exam) 88% ($N = 43$ graduate students)	44% ($N = 82$ undergraduate students, midterm exam)
Generate: write a momentum eigenstate with eigenvalue p' in momentum representation.*	74% ($N = 43$ undergraduate students) 81% ($N = 44$ undergraduate students, midterm exam) 70% ($N = 43$ graduate students)	32% ($N = 82$ undergraduate students, midterm exam)

*p-value on t-test<0.001 for students' responses on the midterm exam

We also investigated the extent to which students who learned from the QuILT retained information related to quantum states. Table 5-20 shows students' scores on questions related to quantum states directly after they had worked on the QuILT (the Dirac notation posttest) and the scores on a retention quiz given at the end of the semester. Students' scores remained approximately the same. The same scoring rubric was used in the Dirac notation posttest and retention quiz. On questions which involved recall (e.g., $\langle x|x'\rangle$), their scores increased. However, in questions asking students to generate expressions, students' scores stayed approximately the same or decreased slightly.

Table 5-20. Comparison of the percentages of students who correctly answered questions related to quantum states immediately after working on the Dirac notation QuILT (Dirac notation posttest) and at the end of the semester (Retention quiz)

Question	**Dirac notation Posttest** ($N = 43$ UG)	**Dirac notation Retention Quiz** ($N = 24$ UG)
Recall: $\langle x|x'\rangle = ?$	81%	96%
Recall: $\langle x|p'\rangle = ?$	81%	88%
Recall: $\langle p|p'\rangle = ?$	81%	96%
Generate: "Write a momentum eigenstate with eigenvalue p' in position representation."	79%	79%
Generate: "Write a momentum eigenstate with eigenvalue p' in momentum representation."	74%	67%

5.6.3 Pre/post data on student difficulties with obtaining the wave function in momentum representation from the wave function in position representation

To determine whether students learned that the wave function in momentum representation is the Fourier transform of the wave function in position representation, students' scores on the pre/posttests for questions related to this issue were computed. Table 5-21 shows that the percentages of students who generated a correct answer and were able to demonstrate that the wave function in momentum representation is the Fourier transform of the wave function in position representation increased.

Table 5-21. Percentages of undergraduate (UG) and graduate (G) students who correctly answered questions related to the fact that the wave function in momentum representation is the Fourier transform of the wave function in position representation on the Dirac notation pre/posttest

Question	**Dirac Notation Pretest**		**Dirac Notation Posttest**	
	UG ($N = 46$)	G ($N = 45$)	UG ($N = 43$)	G ($N = 43$)
Generate: Show that the wave function in position representation is the Fourier transform of the wave function in momentum representation.	17%	82%	67%	98%

We also compared the performance of students who had learned from the Dirac notation QuILT vs. students who did not on multiple-choice questions related to the relationship between $\Phi(p)$ and $\Psi(x)$. Table 5-22 shows that students who learned from the Dirac notation QuILT performed better on questions in which they were asked to recognize that the wave function in momentum representation is the Fourier transform of the wave function in the position representation. Table 5-22 also shows that students who learned from the QuILT performed better at recognizing incorrect statements about the relationship between $\Phi(p)$ and $\Psi(x)$.

Table 5-22. Percentages of students who correctly recognized answers to multiple-choice questions related to Fourier transforms.

Question	QuILT Group ($N = 88$)	Non-QuILT Group ($N = 184$)
Recognize: $\langle p\vert\Psi\rangle = \int\langle p\vert x\rangle\langle x\vert\Psi\rangle dx = \int e^{-ipx/\hbar}\Psi(x)dx$ (Ignore normalization issues.)	93%	69%
Recognize that "the wave function in momentum representation is $\Phi(p) = \int dx(-i\hbar\frac{\partial}{\partial x}\Psi(x))$" is an *incorrect* statement	73%	39%

5.6.4 Pre/post data on student difficulties involving quantum operators

We also examined the effectiveness of the Dirac notation QuILT in terms of students' performance on questions involving quantum operators. Table 5-23 shows students' average scores on questions related to quantum operators. For the question listed as $\hat{x}\delta(x-x')$ (or $x\delta(x-x')$ written in another form, responses were given full points if they were of the form $x\delta(x-x')$, $x'\delta(x-x')$, $x\langle x|x'\rangle$, $\langle x|x|x'\rangle$, $\langle x|\hat{x}|x'\rangle$. Half credit was given to responses that included $\langle x|x'\rangle$, but were otherwise incorrect. For the question listed as $\langle x|\hat{p}|p'\rangle$, students were given full credit if they wrote $\langle x|\hat{p}|p'\rangle = p'e^{ip'x/\hbar}$ (ignoring normalization issues). Students were not penalized if they put a negative sign in the exponent. Students were given half credit if they wrote $p'\langle x|p'\rangle$. For the question involving $\langle p|\hat{p}|p'\rangle$, students received full credit if they wrote $p'\delta(p-p')$ or $p\delta(p-p')$ and half credit if they wrote $p'\langle p|p'\rangle$ or $\delta(p-p')$. For the question involving $\langle x|\hat{Q}|\Psi\rangle$, students received full credit if they wrote both the operator and the generic state in position representation, i.e., $\langle \mathrm{x}|\hat{Q}|\Psi\rangle = Q(x, -i\hbar\frac{\partial}{\partial x})\Psi(\mathrm{x})$. Half credit was given if the student wrote $\langle x|\hat{Q}|\Psi\rangle = \Psi(x)$,

$\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\langle x|\Psi\rangle$, or $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\Psi(x)$. Except for the more general case $\langle x|\hat{Q}|\Psi\rangle$, over 75% of the students correctly answered questions related to quantum operators on the posttest.

Table 5-23. Comparison of the percentages of students correctly answering questions related to quantum operators on the Dirac notation QuILT pre/posttest. The number of students who took pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded

	Dirac notation Pretest		**Dirac notation Posttest**	
	UG ($N = 46$)	G ($N = 45$)	UG ($N = 43$)	G ($N = 43$)
Recall: $\hat{x}\delta(x - x')$ (or $x\delta(x - x') =$?	28%	60%	84%	91%
Recall:$\langle x|\hat{p}|p'\rangle =$?	20%	69%	77%	93%
Recall:$\langle p|\hat{p}|p'\rangle =$?	30%	82%	84%	95%
Recall:$\langle x|\hat{Q}|\Psi\rangle =$?	20%	46%	53%	58%

We compared the performance of students who learned from the Dirac notation QuILT vs. those who did not work on it on questions involving recognition of correct expressions for quantum operators. Table 5-24 shows the percentage of students in each group recognizing that the expressions are correct on a multiple-choice survey. It is interesting to note that students who worked on the Dirac notation QuILT did better in recognizing that the expression $\langle x|\hat{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$ is correct. This indicates that students who worked through the QuILT have a better understanding of the fact that there are two ways to think about $\langle x|\hat{p}|p'\rangle$: 1) act with $\hat{p}$ on p', pull out the p' from the inner product, and write $\langle x|p'\rangle$ in position representation; or 2) write $\hat{p}$ and $|p'\rangle$ in position representation first and then act with the operator $-i\hbar\frac{\partial}{\partial x}$ in position representation (without Dirac notation) on $e^{ip'x/\hbar}$ (momentum eigenstate with eigenvalue p' in position representation without Dirac notation).

Table 5-24. Comparison of the performance of students who learned from the Dirac notation QuILT vs. students who did not on questions related to quantum operators on a multiple-choice survey.

	QuILT group ($N = 88$)	**Non-QuILT Group** ($N = 184$)
Recognize: $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = p'e^{ip'x/\hbar}$	88%	67%
Recognize: $\langle x\|\hat{p}\|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x\|p'\rangle = -i\hbar\frac{\partial}{\partial x}e^{ip'x/\hbar}$	78%	52%
Recognize: $\langle p\|\hat{p}\|p'\rangle = p'\langle p\|p'\rangle = p'\delta(p-p')$	100%	85%
Recognize: $\langle x\|\hat{Q}\|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$	98%	87%

We also investigated the extent to which students who learned from the Dirac notation QuILT retained information related to quantum operators. Table 5-25 shows the percentage of students who correctly answered questions related to quantum operators directly after they had worked on the QuILT (the Dirac notation posttest) and the scores on the retention quiz given at the end of the semester. The same scoring rubric was used in the Dirac notation posttest and retention quiz. The percentages of students who correctly answered questions related to quantum operators remained approximately the same, with a slight decrease at the end of the semester.

Table 5-25. Comparison of percentages of students correctly answering questions about quantum operators directly after completing the Dirac notation QuILT (Dirac notation posttest) and at the end of the semester (Retention Quiz)

	Dirac Notation posttest ($N = 46$)	**Retention quiz** ($N = 24$)
$\langle x\|\hat{p}\|p'\rangle$	77%	71%
$\langle x\|\hat{Q}\|\Psi\rangle$	53%	46%

5.6.5 Pre-/post data on student difficulties involving expectation value

We examined the effectiveness of the Dirac notation QuILT in terms of helping students develop proficiency with finding expectation values. The following two open-ended question were administered to upper-level undergraduate students and graduate students on Dirac notation QuILT pretests and posttests.

1. *$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n. Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q_n\rangle$ and eigenvalues q_n. Show your work.*
2. *$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q\rangle$ and eigenvalues q. Show your work.*

For the discrete case, a student earned full credit if he/she correctly inserted the identity operator, used an expansion of the generic state $|\Psi\rangle = \sum c_n |q_n\rangle$, or conceptually reasoned that the expectation value is the sum of the eigenvalues of $\hat{Q}$ multiplied by the probability of obtaining the eigenvalue. A student earned 83% if he/she wrote the correct expression with no work or explanation provided or used the expansion $|\Psi\rangle = \sum c_n |q_n\rangle$ but did not define c_n. A student earned half credit if he/she inserted an identity operator or used an expansion of $|\Psi\rangle$ but did not arrive at the correct final result. All other answers were considered incorrect (no credit). The question involving an operator with continuous eigenvalues was graded using the same rubric for the discrete case, except that if a student inserted an identity operator involving a summation instead of an integral, he/she received 2/3 credit. Table 5-26 shows the percentages of students correctly answering questions related to expectation value on the pretest and posttest and their average scores.

We also investigated the extent to which the common difficulties in finding the expectation value were impacted after the students learned from the Dirac notation QuILT (see Table 5-27). The percentage of students answering correctly using the identity operator increased, and the difficulties involving inserting the identity operator, arbitrarily switching $|\Psi\rangle$ to $|q_n\rangle$, and writing the wrong expression for expectation value, were reduced.

Table 5-26. Comparison of the percentages of undergraduate students (UG) and graduate students (G) correctly answering questions related to expectation value on the Dirac notation QuILT pre/posttest and average scores. The number of students who took the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

	Dirac notation Pretest				**Dirac notation Posttest**			
	UG ($N = 46$)		G ($N = 45$)		UG ($N = 43$)		G ($N = 43$)	
	% correct	Average score	% correct	Average score	% correct	Average score	% correct	Average score
Generate: Find the expectation value of Q in the state $|\Psi\rangle$ in terms of eigenstates $|q_n\rangle$ and eigenvalues q_n (discrete case).	15%	31%	58%	71%	65%	83%	67%	86%
Generate: Find the expectation value of Q in the state $|\Psi\rangle$ in terms of eigenstates $|q\rangle$ and eigenvalues q (continuous case).	15%	21%	56%	67%	65%	77%	60%	81%

Table 5-27. Comparison of the common difficulties in finding expectation value for an operator with discrete eigenvalues on the Dirac notation pre-/posttest

	Dirac notation pretest		**Dirac notation posttest**	
	UG ($N = 46$)	G ($N = 45$)	UG ($N = 43$)	G ($N = 43$)
Correct, using identity operator	13	36	52	47
Correct, using expansion of $\|\Psi\rangle$	2	13	9	16
Correct, using conceptual reasoning	2	0	4	0
Correct, no work shown	11	2	4	7
Correct, but did not define c_n	4	13	7	5
Incorrect, using identity operator	7	2	2	0
Incorrect, using expansion of $\|\Psi\rangle$	7	2	0	7
Incorrect, arbitrarily switching $\|\Psi\rangle$ to $\|q_n\rangle$,	9	13	0	0
Incorrect, writing wrong expression for expectation value	11	2	2	2
Incorrect, writing expansion wrong, e.g., $\|\Psi\rangle = \sum q_n \|q_n\rangle$, $\|\Psi\rangle = q_n\|q_n\rangle$	0	4	2	2
Incorrect, writing $\hat{Q}\|\Psi\rangle = q_n\|q_n\rangle$, or $\hat{Q}\|\Psi\rangle = q_n\|\Psi\rangle$	0	0	0	5
Incorrect, inserting projection operator instead of identity operator	0	4	0	2
Other difficulties	13	4	5	4
Blank	26	2	5	0

To examine the long term effectiveness of the QuILT in helping students develop proficiency in finding expectation values, we compared the scores of students who had worked on the QuILT vs. those who did not do so on midterm and final exam questions. The midterm and final exam questions involving expectation value were exactly the same, i.e.,

$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n. Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q_n\rangle$ and eigenvalues q_n. Show your work.

Table 5-28 shows the average scores on the midterm and final exam questions. The midterm and final exam questions were graded using the same rubric as on the Dirac notation pre/posttest. On the midterm exams, the group of students who learned from the Dirac notation QuILT performed significantly better than those who did not work on the QuILT (p-value (t-test) <0.001). On the final exams, students who learned from the QuILT continued to perform significantly better than students who did not do so (p-value (t-test)<0.001).

Table 5-28. Comparison of the performance of students who learned from the Dirac notation QuILT vs. students who did not do so on questions related to the expectation value on midterm exams and final exams.

	Non-QuILT Group Years 1-4	**QuILT Group Years 5-6**
Average score (midterm exams)	50% ($N = 82$)	92% ($N = 42$)
Average score (Final exam)	67% ($N = 81$)	92% ($N = 42$)

We also investigated the extent to which students who learned from the Dirac notation QuILT can recognize the correct expression for the expectation value vs. students who did not work on the QuILT. Eighty-eight students who worked through the QuILT and 184 upper level students from 4 other universities were given that $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ forms a complete set of orthonormal eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with non-degenerate eigenvalues q_n and asked to evaluate the correctness of the statement $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$. Table 5-29 shows the percentage of students agreeing with the expression $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_n q_n |\langle q_n|\Psi\rangle|^2$, which is the correct expression for expectation value. The group of students who learned from the QuILT performed better in recognizing the correct expression for expectation value vs. students who had traditional instruction in relevant concepts.

Table 5-29. Comparison of the performance of students who learned from the Dirac notation QuILT vs. students who did not on a question related to expectation value.

	QuILT Group ($N = 88$)	**Non-QuILT group** ($N = 184$)
Recognize: The expectation value of an operator $\hat{Q}$ with a discrete eigenvalue spectrum q_n in state $\lvert\Psi\rangle$ is $\langle\Psi\lvert\hat{Q}\rvert\Psi\rangle = \sum_n q_n \lvert\langle q_n\lvert\Psi\rangle\rvert^2$	82	57

5.6.6 Pre/post data on student difficulties involving probabilities of measurements

To investigate the effectiveness of the QuILT in regards to helping students determine the probability distribution of measurement outcomes for an observable, the following question was asked on both the Dirac notation QuILT pretest and posttest:

$\lvert\Psi\rangle$ is a generic state of a quantum system and the states $\{\lvert q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q. What is the probability of measuring observable Q in the interval between q and $q + dq$ in the state $\lvert\Psi\rangle$?

Students were given full credit if they wrote $\lvert\langle q\lvert\Psi\rangle\rvert^2 dq$ and half credit if they wrote an answer of the form $\lvert\langle q\lvert\Psi\rangle\rvert^2$ or $\lvert\langle q_n\lvert\Psi\rangle\rvert^2$ (i.e., forgot to multiply by dq or treated it as a discrete case). Table 5-30 shows a comparison of the percentages of students correctly answering questions related to the probability distribution of measurement outcomes and their average scores on the pretests and posttests.

Table 5-30. Comparison of students' performance on the Dirac notation QuILT pre/posttest on questions related to probability of measurement outcomes. The number of students who took the pretest does not match the posttest because some students did not finish working the QuILT and their answers on the posttest were disregarded.

	Dirac notation Pretest				**Dirac notation Posttest**			
	UG ($N = 46$)		G ($N = 45$)		UG ($N = 43$)		G ($N = 43$)	
Generate: What is the probability of measuring observable Q in the interval between q and $q + dq$ in the state $\|\Psi\rangle$, given that $\|\Psi\rangle$ is a generic state of a quantum system and the states $\{\|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q?	% correct	Average score	% correct	Average score	% correct	Average score	% correct	Average score
	13	18	53	61	56	65	73	82

Writing down the probability distribution of measurement outcomes remained difficult for students after they had learned from the Dirac notation QuILT, possibly because of the strongly ingrained difficulties mentioned in the student difficulties section (i.e., assuming that the measurement process involves an operator acting on a generic state and assuming that the probability of measuring a particular outcome involves the corresponding operator in the expression).

Students who learned from the Dirac notation QuILT did perform better than students who did not do so on questions requiring them to recognize the probability distribution of measurement outcomes in Dirac notation. Eighty-eight students at the University of Pittsburgh who had worked on the Dirac notation QuILT ($N = 43$ undergraduate and $N = 45$ graduate students) and 184 upper-level students from 4 other universities were given that an operator $\hat{Q}$ corresponding to a physical observable Q has a continuous non-degenerate spectrum of eigenvalues, the states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with eigenvalues q, and at time $\mathrm{t} = 0$, the state of the system is $|\Psi\rangle$. They were asked to evaluate the correctness of the statement: If you measure Q at time $t = 0$, the probability of obtaining an outcome between q and $q + dq$ is $|\langle q|\Psi\rangle|^2 dq$. Table 5-31 shows the percentages of students who agreed with the expression. Students who had learned from the QuILT performed 49% better than those who did not.

We also asked these same students to evaluate the correctness of the statement: If you measure the position of the particle in the state $|\Psi\rangle$, the probability of finding the particle between x and $x + dx$ is $|\langle x|\Psi\rangle|^2 \mathrm{d}x$. Table 5-31 shows the percentages of students who correctly agreed with the statement. Students who had learned from the Dirac notation QuILT performed 18% better than those who did not.

Table 5-31. Comparison of the performance of students who learned from the Dirac notation QuILT vs. students who did not learn from it on questions related to the probability distribution of measurement outcomes in Dirac notation on a multiple-choice survey.

	QuILT Group $(N = 88)$	**Non-QuILT group** $(N = 132)$
Percentage of students selecting correct expression for probability $|\langle q|\Psi\rangle|^2 dq$	86	58
Percentage of students selecting correct expression for probability $|\langle x|\Psi\rangle|^2 dx$.	94	80

We also investigated the extent to which the Dirac notation QuILT helped students retain information about the probability distribution of measurement outcomes. The following open-ended question was administered at the end of the semester to 24 upper-level undergraduate students who had learned from the Dirac notation QuILT:

$|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n. What is the probability for measuring observable Q in the state $|\Psi\rangle$?

This question is analogous to the probability distribution of measurement outcomes question administered in the Dirac notation QuILT pre/posttest, except the operator has a discrete eigenvalue spectrum as opposed to a continuous eigenvalue spectrum. Students were given full credit if they wrote $|\langle q_n|\Psi\rangle|^2$ and half credit if they wrote an answer of the form $|\langle q|\Psi\rangle|^2 dq$ (i.e., multiplied by dq or treated this case as a continuous case). Table 5-32 shows the average scores on the pretests and posttests for the probability question. The averages stayed approximately the same, indicating that students retained most of the information from the Dirac notation QuILT about the probability distribution of measurement outcomes.

Table 5-32. Comparison of the percentages of students who answered questions about the probability distribution for measurement outcomes and their average scores directly after completing the Dirac notation QuILT (Dirac notation posttest) and at the end of the semester (retention quiz).

	Dirac notation posttest ($N = 46$)		**Retention quiz** ($N = 24$)	
Generate: *What is the probability distribution for measuring observable Q in the state $\vert\Psi\rangle$ given that $\vert\Psi\rangle$ is a generic state of a quantum system and the states $\{\vert q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n.*	% correct	Average score	% correct	Average score
	56	65	42	52

Since students struggle with the probability distribution of measurement outcomes even after they learned from the Dirac notation QuILT, the QuILT is being modified to address these difficulties in more depth.

5.7 SUMMARY AND CONCLUSION

Students have many common difficulties in learning Dirac notation. The Dirac notation QuILT is a research-based learning tool to improve students' understanding of Dirac notation. It makes use of a guided approach which keeps students actively engaged during the learning process and explicitly addresses many of the common difficulties that were discovered. The preliminary results indicate that the Dirac notation QuILT is effective at helping students connect quantitative procedures with qualitative concepts.

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APPENDIX B

DIRAC NOTATION QUILT

Pre-Test: Dirac Notation Warm-Up

For all of the following questions:

- Assume that $|i\rangle, |j\rangle$, and $|k\rangle$ form a complete set of orthonormal basis vectors.
- $|\chi_1\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ and $|\chi_2\rangle = d|i\rangle + e|j\rangle + f|k\rangle$ are vectors in a three dimensional vector space.

1. For vector $|\chi_1\rangle$:
   a. Write the components a, b, and c in Dirac notation.

   b. Represent $|\chi_1\rangle$ as a column vector in the given basis.

2. a. Write the outer product of "ket" vector $|\chi_1\rangle$ with "bra" vector $\langle\chi_2|$ in the given basis.

b. Is this outer product a scalar (number), a column vector, a row vector, or a 3×3 matrix in the given basis?

3. Write the identity operator in terms of $|i\rangle$, $|j\rangle$, and $|k\rangle$ which form a complete set of orthonormal basis vectors for a three dimensional vector space.

- $|i'\rangle$, $|j'\rangle$, and $|k'\rangle$ form another orthonormal basis for the same three dimensional vector space.

4. Consider the following statement:
   - The components of the vector $|\chi_1\rangle$ have fixed values even if we change the basis such that the orthonormal basis vectors are $|i'\rangle$, $|j'\rangle$, and $|k'\rangle$.

   Explain why you agree or disagree with this statement.

5. Choose all of the correct statements about the identity operator (assume three dimensional vector space):
   (I) In general, given an orthonormal basis set $|i\rangle, |j\rangle$, and $|k\rangle$, if we compute the outer product of each unit vector with itself and then add them up, we obtain the identity operator.
   (II) If we change the basis we have chosen to a different orthonormal basis set $|i'\rangle$, $|j'\rangle$, and $|k'\rangle$, compute the outer product of each new basis vector with itself and then add them up, we will still obtain the same identity operator.
   (III) The completeness relation or spectral decomposition of identity refers to writing the identity operator in terms of a complete set of basis vectors in a given vector space.

   a. (I) only
   b. (II) only
   c. (III) only
   d. (I) and (III) only
   e. All of the above

6. For the vector $|\chi_1\rangle$,
   a. Write down the projection operator that projects vector $|\chi_1\rangle$ along the direction of the unit vector $|i\rangle$.

   b. Using the projection operator from 6.a, show what happens to the vector $|\chi_1\rangle$ when the projection operator acts on it.

   c. Summarize your result in part 6.b in one sentence.

7. Consider the following statement made by Student A about vector $|\chi_1\rangle$:
   - Student A: $\langle k|\chi_1\rangle$ is a vector which points along the direction of $|k\rangle$.

   Do you agree with Student A? Explain your reasoning.

Dirac Notation Warm-Up: Getting Acquainted with Dirac Notation in a Familiar Context

The goals of the Dirac Notation Warm-Up are to help you use a familiar context to:

- Learn how to write a vector in a given vector space using Dirac notation.
- Learn how to write the scalar product (or inner product) using bra and ket notation and recognize that the scalar product is a number (it can have dimensions).
- Learn how to write the components of a vector along a complete set of orthonormal basis vectors using scalar products written in Dirac notation.
- Understand the difference between bra and ket vectors
    - Ket vectors can be represented as column vectors in a given basis.
    - Bra vectors can be represented as row matrices in a given basis.
- Understand the relationship between vector components in different orthonormal bases if the basis vectors are changed from one orthonormal basis to another.
- Learn how to write the outer product using bra and ket vectors and recognize that:
    - An outer product is a linear operator.
    - An outer product can be represented by an $N \times N$ square matrix in any given basis, where N is the dimension of the vector space.
- Compute the identity operator in an N dimensional vector space and recognize that:
    - The identity operator can be represented by a square matrix with 1's along the diagonal, regardless of which basis is chosen.
    - The identity operator acting on a vector does not change the vector.
    - The identity operator is found by taking the outer product of each normalized basis vector with itself then summing over them.
    - Completeness relation: for a given basis, summation over all the outer products of each orthonormal basis vector with itself is the identity operator.
    - The completeness relation can be used to decompose a vector into its components along the chosen orthonormal basis vectors.
- Understand that the projection operator formed from the outer product of a basis vector with itself acting on a generic vector returns the basis vector multiplied by the component of the generic vector along that basis vector.
- *Note*: The symbol "≐" used throughout this tutorial means "is represented in the given basis by…."

Dirac notation is used extensively in quantum mechanics in connection with state vector $|\Psi(t)\rangle$ which:

- Is an element of an abstract vector space (Hilbert space)
- Contains all possible information about the state of the quantum system at a given time t.

Here we familiarize you with Dirac notation in the context of a familiar vector, force $\vec{F}$, in a real physical three dimensional vector space. Just as force $\vec{F}$ can be represented as a vector (with a magnitude and direction) in the three dimensional real physical space we live in, the state vector $|\Psi\rangle$ can be represented as a vector in an abstract vector space.

In introductory physics, you learned that it is often convenient to choose an orthonormal coordinate system or "basis" and break up (or decompose) force into components along the directions of "basis vectors." In three dimensions, we typically name the three mutually orthogonal directions x, y, and z and the unit vectors (or normalized basis vectors) along those directions $\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$, respectively.

Then, we can write the force $\vec{F}$ as

$$\vec{F} = a\hat{\imath} + b\hat{\jmath} + c\hat{k} \tag{1}$$

where $a, b,$ and c are the components of the force $\vec{F}$ along $\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$, respectively.

In the familiar scalar (dot or inner) product notation:

$$a = \hat{\imath} \cdot \vec{F} \qquad\qquad b = \hat{\jmath} \cdot \vec{F} \qquad\qquad c = \hat{k} \cdot \vec{F} \tag{2}$$

Checkpoint 1:

Consider the following statements from Student A and Student B.

- Student A: $(a\hat{\imath} + b\hat{\jmath}) \cdot (c\hat{\imath} + d\hat{\jmath}) = ac + bd$, which is a number, or scalar.
- Student B: I disagree. $(a\hat{\imath} + b\hat{\jmath}) \cdot (c\hat{\imath} + d\hat{\jmath}) = ac\hat{\imath} + bd\hat{\jmath}$, which is a vector.

Explain why agree or disagree with each student.

Let's introduce the **Dirac notation** in which "ket" vectors are written as $|F\rangle$ and $|i\rangle$ rather than $\vec{F}$ and $\hat{\imath}$, respectively, and the scalar product is written as $\langle i|F\rangle$ rather than $\hat{\imath} \cdot \vec{F}$. $\langle F|$ and $\langle i|$ are called "bra" vectors, which lie in the "dual" space. The scalar product $\langle i|F\rangle$, which gives the component of a “ket” vector $|F\rangle$ along the direction of the “bra” vector $\langle i|$, is often called a “bracket.” Hence, in Dirac notation

$$|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle \tag{3}$$

$$a = \langle i|F\rangle \qquad b = \langle j|F\rangle \qquad c = \langle k|F\rangle \tag{4}$$

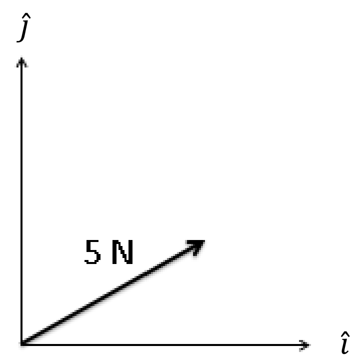


Figure 1

Checkpoint 2:

1. Consider the following statements from Student A and Student B.
   - Student A: $\langle i|F\rangle$ is a scalar which gives the magnitude of the force along the x direction.
   - Student B: I do not agree. $\langle i|F\rangle$ is a vector which points along the x direction.

Explain why you agree or disagree with each statement.

2. In Figure 1 (shown above), a force vector $|F\rangle$ with a magnitude of 5 N acts on an object in the plane of the paper (z-axis is perpendicular to the plane of the paper). The coordinate system, and therefore basis vectors (unit vectors along the the x, y, and z axes), is chosen such that the force $|F\rangle$ makes a 30° angle with the x axis. Find $\langle i|F\rangle$, $\langle j|F\rangle$, and $\langle k|F\rangle$.

Note that the choice of coordinate system or "basis" is up to us and it may be convenient to choose another orthononormal basis x', y', z' with unit vectors $\widehat{\imath'}$, $\widehat{\jmath'}$, and $\widehat{k'}$, respectively (e.g., in inclined plane problems, it may be convenient to choose basis vectors to be parallel and perpendicular to the incline rather than vertical and horizontal). In the new basis, force $\vec{F}$ can be written in the traditional notation and Dirac notation respectively as

$$\vec{F} = a'\hat{\imath}' + b'\hat{\jmath}' + c'\hat{k}' \tag{5}$$

$$|F\rangle = a'|i'\rangle + b'|j'\rangle + c'|k'\rangle \tag{6}$$

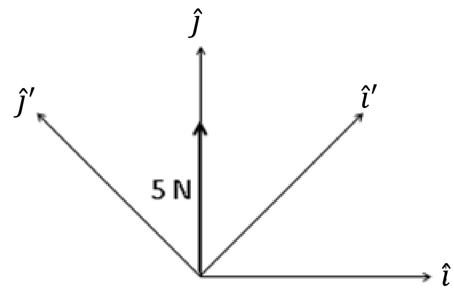


Figure 2

Checkpoint 3:

1. In Figure 2 (shown above), a force vector $|F\rangle$ with a magnitude of 5 N acts on an object in the plane of the paper. The coordinate system (and therefore basis vectors along the x, y, and z axes) are chosen such that the force $|F\rangle$ makes a 90° angle with the x axis (the identical coinciding z and z' axes are perpendicular to the plane of the paper). Find $\langle i|F\rangle$, $\langle j|F\rangle$, and $\langle k|F\rangle$.

2. In Figure 2, a force vector $|F\rangle$ with a magnitude of 5 N acts on an object in the plane of the paper. Basis vectors (unit vectors along the x', y', and z' axes) are chosen such that the force $|F\rangle$ makes a 45° angle with the x' axis (the identical coinciding z and z' axes are perpendicular to the plane of the paper). Find $\langle i'|F\rangle$, $\langle j'|F\rangle$, and $\langle k'|F\rangle$.

Using matrix representation once a basis (coordinate system) has been chosen

After we have chosen a set of basis vectors, it may be convenient to write the "ket" force vector in Eq. (3) as a column matrix $|F\rangle \doteq \begin{pmatrix} \langle i|F\rangle \\ \langle j|F\rangle \\ \langle k|F\rangle \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$. For the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation chosen, the normalized basis vectors (unit vectors along directions of orthonormal coordinate axes) are

$$|i\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |j\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |k\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{7}$$

Note that in $|F\rangle \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}$, $a, b,$ and c are components of vector $|F\rangle$ along the directions of basis vectors (unit vectors along the coordinate axes) and instead of an equality sign we choose the $\doteq$ sign to note that the equality is valid only with respect to a chosen basis. The "bra" vectors (used in the scalar product to find the component of $|F\rangle$ along the direction of the basis vectors, e.g., Eq. (4)) can be written as row matrices

$$\langle i| \doteq (1\ 0\ 0) \qquad \langle j| \doteq (0\ 1\ 0) \qquad \langle k| \doteq (0\ 0\ 1)$$

(Using traditional notation, column matrix form can be introduced as follows $\vec{F} \doteq \begin{pmatrix} \hat{\imath} \cdot \vec{F} \\ \hat{\jmath} \cdot \vec{F} \\ \hat{k} \cdot \vec{F} \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$.)

We can verify that scalar products work out as expected by multiplying the matrices:

$$a = \langle i|F\rangle = (1\ 0\ 0)\begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$b = \langle j|F\rangle = (0\ 1\ 0)\begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$c = \langle k|F\rangle = (0\ 0\ 1)\begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$1 = \langle i|i\rangle = (1\ 0\ 0)\begin{pmatrix}1\\0\\0\end{pmatrix}$$

$$0 = \langle i|j\rangle = (1\ 0\ 0)\begin{pmatrix}0\\1\\0\end{pmatrix}, \text{etc.}$$

We have shown that $a = \langle i|F\rangle$. But what is $\langle F|i\rangle$? Generally, $\langle F| = (a^* \quad b^* \quad c^*)$, where the asterisk denotes the complex conjugate of $a, b,$ and c. So $\langle F|i\rangle = (a^* \quad b^* \quad c^*)\begin{pmatrix}1\\0\\0\end{pmatrix} = a^*$. But in mechanics, the components $a, b,$ and c of the force vector $|F\rangle$ are real numbers, so $a^* = a$. In quantum mechanics, however, the components of state vector $|\Psi\rangle$ along the orthonormal basis vectors are in general complex numbers.

Checkpoint 4:

1. Consider the following statements from Student A and Student B.

- Student A: In $|F\rangle \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}$, a, b, and c have fixed values regardless of what basis we have chosen.
- Student B: That is not true. You can write the force vector as a column matrix only after you've chosen a basis or coordinate system. $a, b,$ and c give the components of force F along the directions of basis vectors $|i\rangle$, $|j\rangle$, and $|k\rangle$, respectively. If you choose a different basis, these components will be different.

Explain why you agree or disagree with Student A and Student B.

2. Do $\langle j|F\rangle$ and $\langle F|j\rangle$ differ from each other if $\langle j|F\rangle$ is a real number? Will they be different if $\langle j|F\rangle$ is a complex number?

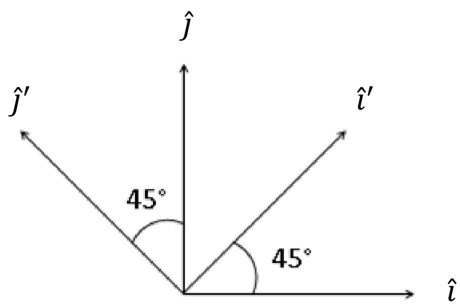


Figure 3

As noted previously, we can choose another orthonormal basis (coordinate axes) if that is convenient for solving a problem. For example, the normalized basis vectors $|i'\rangle$, $|j'\rangle$, and $|k'\rangle$ for the three dimensional vector space (unit vectors along directions of new orthogonal coordinate axes) are shown in Figure 3. (Note: The z and z' axes are perpendicular to the plane of the paper.)

In the {$|i\rangle$, $|j\rangle$, $|k\rangle$} representation, $|i'\rangle$, $|j'\rangle$, $|k'\rangle$ can be represented as follows:

$$|i'\rangle \doteq \begin{pmatrix} \langle i|i'\rangle \\ \langle j|i'\rangle \\ \langle k|i'\rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \qquad |j'\rangle \doteq \begin{pmatrix} \langle i|j'\rangle \\ \langle j|j'\rangle \\ \langle k|j'\rangle \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \qquad |k'\rangle \doteq \begin{pmatrix} \langle i|k'\rangle \\ \langle j|k'\rangle \\ \langle k|k'\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

(8)

These three equations can be combined into one equation involving a 3×3 rotation matrix that relates the basis vectors in the {$|i'\rangle$, $|j'\rangle$, $|k'\rangle$} representation to the basis vectors in the {$|i\rangle$, $|j\rangle$, $|k\rangle$} representation:

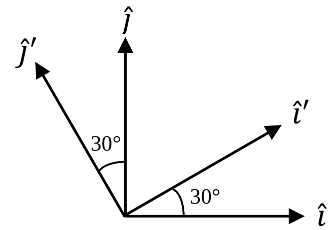
$$\begin{pmatrix} |i'\rangle \\ |j'\rangle \\ |k'\rangle \end{pmatrix} = \begin{pmatrix} \langle i|i'\rangle & \langle j|i'\rangle & \langle k|i'\rangle \\ \langle i|j'\rangle & \langle j|j'\rangle & \langle k|j'\rangle \\ \langle i|k'\rangle & \langle j|k'\rangle & \langle k|k'\rangle \end{pmatrix} \begin{pmatrix} |i\rangle \\ |j\rangle \\ |k\rangle \end{pmatrix}$$

On the other hand, **in the {$|i'\rangle$, $|j'\rangle$, $|k'\rangle$} representation**, $|i'\rangle$, $|j'\rangle$, $|k'\rangle$ can be represented as follows:

$$|i'\rangle \doteq \begin{pmatrix} \langle i'|i'\rangle \\ \langle j'|i'\rangle \\ \langle k'|i'\rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |j'\rangle \doteq \begin{pmatrix} \langle i'|j'\rangle \\ \langle j'|j'\rangle \\ \langle k'|j'\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |k'\rangle \doteq \begin{pmatrix} \langle i'|k'\rangle \\ \langle j'|k'\rangle \\ \langle k'|k'\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

(9)

Checkpoint 5:



1. In the figure shown above, what are the basis vectors $|i'\rangle$, $|j'\rangle$, $|k'\rangle$ in the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation?

2. In the figure shown above, write the rotation matrix which relates the basis vectors in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation to the basis vectors in the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation.

3. In the figure above, what are the basis vectors $|i'\rangle$, $|j'\rangle$, $|k'\rangle$ in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation?

4. Write a rotation matrix which relates the basis vectors in the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation to the basis vectors in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation in which the matrix elements are written in Dirac notation. Calculate the numerical values of each matrix element in the 3×3 rotation matrix for the case shown in the figure above.

5. If the force vector $|F\rangle$ written in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation is $|F\rangle \doteq \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix}$, what are a', b', and c' in Dirac notation?

Outer product of vectors and completeness relation

Linear operators act on vectors to give back another vector whose magnitude and direction may be different. The outer product of a "ket" vector $|F\rangle$ with a "bra" vector $\langle G|$ is written as $|F\rangle\langle G|$ and is an example of a linear operator. For example, the operator $|F\rangle\langle G|$ can act on the vector $|P\rangle$ and result in a vector $|F\rangle$ along with a complex number $C = \langle G|P\rangle$ which is the component of the vector $|P\rangle$ along the $|G\rangle$ direction:

$$(|F\rangle\langle G|)|P\rangle = |F\rangle(\langle G|P\rangle) = C|F\rangle. \tag{10}$$

We learned that after choosing a basis, we can write "bra" and "ket" vectors as row and column matrices. In the chosen basis (coordinates), the outer products become $N \times N$ square matrices where N is the dimensionality of the vector space. For example, in a 3 dimensional vector space, in a particular basis, if $|F\rangle \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ and $|G\rangle \doteq \begin{pmatrix} d \\ e \\ f \end{pmatrix}$, then $\langle G| \doteq \begin{pmatrix} d^* & e^* & f^* \end{pmatrix}$ and

$|F\rangle\langle G| \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}\begin{pmatrix} d^* & e^* & f^* \end{pmatrix} = \begin{pmatrix} ad^* & ae^* & af^* \\ bd^* & be^* & bf^* \\ cd^* & ce^* & cf^* \end{pmatrix}$, which is a 3×3 matrix.

Note that each matrix element of the outer product $|F\rangle\langle G|$ (such as ad^*, ae^*, etc.) is a number.

Checkpoint 6:

1. In the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation, the normalized basis vectors are chosen as $|i\rangle \doteq \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|j\rangle \doteq \begin{pmatrix}0\\1\\0\end{pmatrix}$, and $|k\rangle \doteq \begin{pmatrix}0\\0\\1\end{pmatrix}$. Compute the outer products $|i\rangle\langle i|$, $|j\rangle\langle j|$, and $|k\rangle\langle k|$ in matrix form. Add the matrices to find the operator $\hat{I} = |i\rangle\langle i| + |j\rangle\langle j| + |k\rangle\langle k|$ in this basis.

2. Use matrix multiplication to compute $\hat{I}|F\rangle$, where $|F\rangle \doteq \begin{pmatrix}a\\b\\c\end{pmatrix}$. $\hat{I}$ is called an identity operator. Describe the effect of operator $\hat{I}$ on $|F\rangle$ in a sentence.

3. In the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation, the normalized basis vectors $|i'\rangle$, $|j'\rangle$, and $|k'\rangle$ are represented as $|i'\rangle \doteq \begin{pmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\\0\end{pmatrix}$, $|j'\rangle \doteq \begin{pmatrix}-\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\\0\end{pmatrix}$, and $|k'\rangle \doteq \begin{pmatrix}0\\0\\1\end{pmatrix}$. Compute the outer products $|i'\rangle\langle i'|$, $|j'\rangle\langle j'|$, and $|k'\rangle\langle k'|$ in matrix form. Add the matrices to find the operator $\hat{I}' = |i'\rangle\langle i'| + |j'\rangle\langle j'| + |k'\rangle\langle k'|$ in this basis.

4. Is there any similarity between the matrices $\hat{I}$ and $\hat{I}'$ you found in parts (1) and (3) by computing the outer product of each unit vector in a given basis with itself and then adding all of them? Explain.

In general, given an orthonormal basis (coordinates), if we compute the outer product of each unit vector with itself and then add all of them, we obtain the identity operator. This relation is often called the **completeness relation**. Since the identity operator does not change a vector $|F\rangle$, the completeness relation is extremely useful for decomposing a vector $|F\rangle$ into its components along the chosen basis vectors, e.g., $|i\rangle, |j\rangle,$ and $|k\rangle$:

$$|F\rangle = \hat{I}|F\rangle = (|i\rangle\langle i| + |j\rangle\langle j| + |k\rangle\langle k|)|F\rangle = |i\rangle\langle i|F\rangle + |j\rangle\langle j|F\rangle + |k\rangle\langle k|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle \quad (11)$$

where $a, b,$ and c are the components of $|F\rangle$ along the basis vectors $|i\rangle, |j\rangle,$ and $|k\rangle$ as given by Eq. (4).

The identity operator can also be useful to find the relationship between components of a generic vector in different bases.

- Suppose the force vector is represented as $|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ in the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation. Thus, $a = \langle i|F\rangle$, $b = \langle j|F\rangle$, $c = \langle k|F\rangle$.
- We then choose a **new** basis $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ (shown in Figure 3) such that the force vector is represented as $|F\rangle = a'|i'\rangle + b'|j'\rangle + c'|k'\rangle$ in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation.

Then, $a' = \langle i'|F\rangle$, $b' = \langle j'|F\rangle$, $c' = \langle k'|F\rangle$.

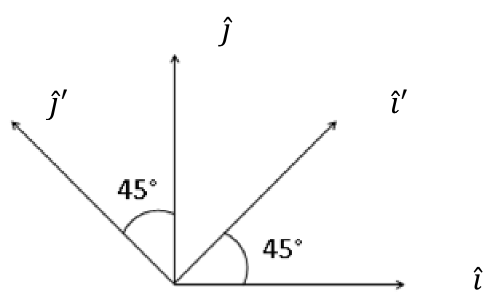


Figure 3

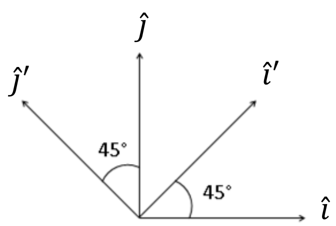
- How can we find a relationship between the components $a, b,$ and c and the components a', b', and c'?

One strategy, for example, to find a in terms of a', b', and c' is to insert the identity operator in terms of the basis vectors $|i'\rangle$, $|j'\rangle$ and $|k'\rangle$, e.g., $\hat{I}' = |i'\rangle\langle i'| + |j'\rangle\langle j'| + |k'\rangle\langle k'|$ as follows:

$$a = \langle i|F\rangle = \langle i|\hat{I}'|F\rangle = \langle i|\ \left(|i'\rangle\langle i'| + |j'\rangle\langle j'| + |k'\rangle\langle k'|\right)\ |F\rangle = \langle i|i'\rangle\langle i'|F\rangle + \langle i|j'\rangle\langle j'|F\rangle + \langle i|k'\rangle\langle k'|F\rangle$$

Using Eq. 8, $a = \langle i|i'\rangle\langle i'|F\rangle + \langle i|j'\rangle\langle j'|F\rangle + \langle i|k'\rangle\langle k'|F\rangle = \frac{1}{\sqrt{2}}(a' - b')$.

Checkpoint 7



1) Suppose in the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation, the force vector $|F\rangle \doteq \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = a'|i'\rangle + b'|j'\rangle + c'|k'\rangle$.

Are the components of $|F\rangle$ the same as the components $a, b,$ and c along the basis vectors in the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation? Explain. Find a relation between a' and $a, b,$ and c if the basis vectors in the two representations are related by the figure shown above.

2) In the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation, the force vector is $|F\rangle \doteq \begin{pmatrix} 3\ N \\ 7\ N \\ 2\ N \end{pmatrix} = 3N|i\rangle + 7N|j\rangle + 2N|k\rangle$.

Consider the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation in which the force is $|F\rangle = a'|i'\rangle + b'|j'\rangle + c'|k'\rangle$. What are the components a', b', and c' of force $|F\rangle$ if the basis vectors in the two representations are related by Figure 3?

3) Consider the following statements from Student A and Student B.
Student A: In a given basis, vector $|F\rangle$ can be written as a column matrix, an outer product $|F\rangle\langle G|$ as a square matrix, and a scalar product $\langle F|G\rangle$ as a number.
Student B: I only agree with the first part. I don't think that $|F\rangle\langle G|$ is different from $\langle F|G\rangle$. Both of these are operators.
Explain why you agree or disagree with Student A and Student B.

Projection Operator

Suppose we want to find the projection of a vector $|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ onto one of the orthonormal basis vectors, e.g., $|i\rangle$, $|j\rangle$, or $|k\rangle$. To project $|F\rangle$ onto one of the orthonormal basis vectors, we can act on the vector $|F\rangle$ with a projection operator corresponding to the basis vector. If we want to find the projection of $|F\rangle$ along the basis vector $|i\rangle$ (or x-coordinate), we can use the operator $|i\rangle\langle i|$ acting on vector $|F\rangle$ to obtain

$$|i\rangle\langle i|F\rangle = a|i\rangle\langle i|i\rangle + b|i\rangle\langle i|j\rangle + c|i\rangle\langle i|k\rangle = a|i\rangle.$$

We can check that the matrix representation of the projection operator $|i\rangle\langle i|$ acting on the vector $|F\rangle$ will also give us the same result for the projection of $|F\rangle$ along $|i\rangle$.

$$|i\rangle\langle i|F\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1 \quad 0 \quad 0) \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = a|i\rangle$$

The projection of $|F\rangle$ along a basis vector is also a vector.

Checkpoint 8:

1. Consider the following conversation between Student A and Student B:
   - Student A: The projection operator acting on vector $|F\rangle$ is like the identity operator in that it returns the same vector $|F\rangle$ back along the direction of a basis vector.
   - Student B: I disagree. The projection operator, e.g., $|i\rangle\langle i|$, acting on vector $|F\rangle$ is not like the identity operator acting on vector $|F\rangle$. When the projection operator $|i\rangle\langle i|$ acts on $|F\rangle$, it does not return the same vector $|F\rangle$. Rather, it returns a basis vector $|i\rangle$ multiplied by the component of $|F\rangle$ along that basis vector $|i\rangle$, e.g., $\langle i|F\rangle$.

With whom do you agree? Explain your reasoning.

2. Consider the conversation between Student A and Student B:
   - Student A: In the $\{|i'\rangle, |j'\rangle, |k'\rangle\}$ representation, the force vector $|F\rangle = a'|i'\rangle + b'|j'\rangle + c'|k'\rangle$. In the $\{|i\rangle, |j\rangle, |k\rangle\}$ representation, $|F\rangle = a|i\rangle + b|j\rangle + c|k\rangle$. Suppose the basis vectors in the two representations are related as in Figure 3. To determine if $|i\rangle\langle i|F\rangle = |i'\rangle\langle i'|F\rangle$, we must calculate the inner products $\langle i|F\rangle$ and $\langle i'|F\rangle$.
   - Student B: I disagree with you. If the basis vectors in the two representations are related as in Figure 3, it is not possible that $|i\rangle\langle i|F\rangle = |i'\rangle\langle i'|F\rangle$ because $|i\rangle$ and $|i'\rangle$ are basis vectors which point in different directions. Thus, there is no need to calculate the inner products $\langle i|F\rangle$ and $\langle i'|F\rangle$ to determine if $|i\rangle\langle i|F\rangle = |i'\rangle\langle i'|F\rangle$.

With whom do you agree? Explain your reasoning.

Dirac Notation Pretest/Posttest

Note: For all of the following questions,

- Ignore the normalization issues of the position and momentum eigenstates.
- Assume that a generic Hermitian operator $\hat{Q}$ corresponding to an observable Q only depends on position and momentum operators ($\hat{x}$ and $\hat{p}$, respectively).
- Assume that $|\Psi\rangle$ denotes a generic state of a system with Hamiltonian $\hat{H}$.
- Assume that the Hilbert space is infinite dimensional.
- Assume that the particle is confined in a one dimensional physical space.

1. a. Write a momentum eigenfunction with eigenvalue p' in the momentum representation.

   b. Write a momentum eigenfunction with eigenvalue p' in the position representation.

2. You are given a generic state vector $|\Psi\rangle$. How would you obtain the position space wave function from $|\Psi\rangle$?

3. $|x'\rangle$ is a position eigenstate with the eigenvalue x'. $|p'\rangle$ is a momentum eigenstate with the eigenvalue p'. Using the information given, fill the blanks on the right hand side in the following equations. If the left hand side shows an expression in Dirac notation, write it in

position or momentum representation on the right hand side and vice versa. There may be more than one correct answer for a given question. Your answer must be something different than what is shown on the left hand side to obtain credit for a given question.

a. $\langle x|x'\rangle =$ ________________

b. $\langle x|\hat{p}|p'\rangle =$ _______________

c. $\langle p|\hat{p}|p'\rangle =$ _______________

d. $x\delta(x - x') =$ ____________

e. $\langle x|p'\rangle =$ ________________

f. $\langle p|p'\rangle =$ ________________

g. $\langle p|x'\rangle =$ ________________

h. $\langle x|\hat{Q}|\Psi\rangle =$ ______________

4. Show that the wave function in the position representation is the Fourier transform of the momentum space wave function. Show all your work.

5. $|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q_n\rangle, n = 1,2,3 \ldots \infty\}$ are eigenstates of an operator $\hat{Q}$ corresponding to a physical observable with discrete eigenvalues q_n.

a) Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q_n\rangle$ and eigenvalues q_n. Show your work.

6. $|\Psi\rangle$ is a generic state of a quantum system. The states $\{|q\rangle\}$ are eigenstates of $\hat{Q}$ with continuous eigenvalues q.

a) What is the probability of measuring observable Q in the interval between q and $q + dq$ in the state $|\Psi\rangle$?

b) Find the expectation value of Q for state $|\Psi\rangle$ using a basis of eigenstates $|q\rangle$ and eigenvalues q. Show your work.

c) Write the spectral decomposition of the identity operator $\hat{I}$ (i.e., the completeness relation), using a complete set of eigenstates $|q\rangle$ of the operator $\hat{Q}$.

Dirac Notation Basics

- For all questions involving a generic operator $\hat{Q}$ corresponding to a physical observable Q, assume that it only depends on position $\hat{x}$ and momentum $\hat{p}$, i.e., $\hat{Q} = \hat{Q}(\hat{x}, \hat{p})$.
- For a Hermitian operator $\hat{Q}$, the notation $\langle\Psi|\hat{Q}|\Psi\rangle$ with $\hat{Q}$ between two vertical lines is the same as $\langle\Psi|\hat{Q}\Psi\rangle$, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi|\hat{Q}\Psi\rangle$ since a Hermitian operator can act forward or backwards on the state, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle = \langle\hat{Q}^\dagger\Psi|\Psi\rangle = \langle\hat{Q}\Psi|\Psi\rangle$. If an operator is not Hermitian (does not correspond to a physical observable), by convention the operator acts on the state after it (to the right of the operator), even if $\langle\Psi|\hat{Q}|\Psi\rangle$ notation is used.

The goals of this tutorial are to help you learn that:

- **The state of a quantum system $|\Psi\rangle$ is a vector**
  - that is an element of an N dimensional Hilbert space.
  - that contains all possible information about the quantum system.
- **Scalar products (or inner products) $\langle\phi|\psi\rangle$**
  - are defined as the component of one state $|\psi\rangle$ along another state $|\phi\rangle$.
  - are, in general, complex numbers (the number could have dimensions).
- **Hilbert Space**
  - A quantum state $|\Psi\rangle$ is a vector in the Hilbert space.
  - The dimensionality of the Hilbert space is given by the number of linearly independent vectors that span the Hilbert space.
  - The eigenstates of a non-degenerate Hermitian operator can be chosen as the basis vectors for the Hilbert space because they span the space.
- **Expansion of a state using a complete set of eigenstates**
  - A state $|\Psi\rangle$ can be written in terms of a linear superposition of a complete set of eigenstates $\{|q_n\rangle,\ n = 1, 2, 3 \dots N\}$ of any Hermitian operator $\hat{Q}$.
  - The coefficients in the expansion, $\langle q_n|\Psi\rangle$, are the components of the state $|\Psi\rangle$ along the direction of the eigenstates $|q_n\rangle$ of a Hermitian operator $\hat{Q}$.
- **Probability of measuring an eigenvalue of a Hermitian operator $\hat{Q}$ in a generic state $|\Psi\rangle$**
  - For orthonormal eigenstates $\{|q_n\rangle,\ n = 1, 2, 3 \dots N\}$ with **discrete** eigenvalues q_n, $|\langle q_n|\Psi\rangle|^2$ is the probability of measuring q_n for an observable Q
  - For orthonormal eigenstates $|q\rangle$ with **continuous** eigenvalues q, $|\langle q|\Psi\rangle|^2 dq$ is the probability of measuring the observable Q in a narrow range between q and $q + dq$.
- **Expectation value of an operator $\hat{Q}$ in a generic state $|\Psi\rangle$ in terms of eigenstates and eigenvalues of $\hat{Q}$**
  - The expectation value of a Hermitian operator $\hat{Q}$ with eigenstates $\{|q_n\rangle, n = 1,2, \dots N\}$ and **discrete** eigenvalues q_n in a generic state $|\Psi\rangle$ is $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$.
  - The expectation value of a Hermitian operator $\hat{Q}$ with eigenstates $|q\rangle$ and **continuous** eigenvalues q in a generic state $|\Psi\rangle$ is $\langle\Psi|\hat{Q}|\Psi\rangle = \int_{-\infty}^{\infty} q |\langle q|\Psi\rangle|^2\, dq$
- **Projection operator**
  - The projection operator $|q_n\rangle\langle q_n|$ acting on a state $|\Psi\rangle$ returns a vector in the direction of $|q_n\rangle$ together with a number $\langle q_n|\Psi\rangle$, which is the component of a state vector along the direction of the orthonormal basis vector $|q_n\rangle$.

- The projection operator $|q\rangle\langle q|$ acting on a state $|\Psi\rangle$ returns a vector in the direction of $|q\rangle$ together with a number $\langle q|\Psi\rangle$, which is the component of a state vector along the direction of the orthonormal basis vector $|q\rangle$.

- **Completeness relation**
  - The completeness relation can be written as $\sum_{n=1}^{N}|q_n\rangle\langle q_n| = \hat{I}$, where $\{|q_n\rangle, n = 1, 2, 3 \dots N\}$ form an orthonormal basis for an N dimensional vector space. $\hat{I}$ is the identity operator.
  - The completeness relation can be written as $\int_{-\infty}^{\infty}|q\rangle\langle q|dq = \hat{I}$, where $|q\rangle$ form an orthonormal basis for an infinite dimensional vector space.
  - The completeness relation is useful for decomposing a state vector into its components along each of the basis vectors.

State of the quantum mechanical system

1. Choose all of the following statements that are correct.

(I) In Dirac notation, eigenstates of a physical observable are generally labeled by the corresponding eigenvalue. For example, position eigenstates $|x\rangle$ are labeled by eigenvalues x, and momentum eigenstates $|p\rangle$ are labeled by eigenvalues p.

(II) The quantum state written in Dirac notation, $|\Psi\rangle$, lies in an abstract Hilbert space.

(III) The state $|\Psi\rangle$ contains all information one can obtain about the system at a given time.

(a) (I) and (II) only
(b) (II) and (III) only
(c) (I) and (III) only
(d) All of the above

2. Choose all of the following statements that are correct.

(I) The state vector in Dirac notation, $|\Psi\rangle$, is an abstract vector without reference to a coordinate system.

(II) When considered as a function of x, The infinite dimensional column vector $\langle x|\Psi\rangle = \Psi(x)$ is the wave function of the system at a given time. $\Psi(x) = \langle x|\Psi\rangle$ is obtained when $|\Psi\rangle$ is projected along the position eigenstates $|x\rangle$.

(III) The state vector $|\Psi\rangle$ and wave function $\Psi(x)$ have the same information, but $\Psi(x)$ is a vector with position eigenstates as the coordinate axes and $\Psi(x)$ for each x denotes the component of $|\Psi\rangle$ along the direction of $|x\rangle$.

(a) (I) and (II) only
(b) (I) and (III) only
(c) (II) and (III) only
(d) All of the above.

Summary of state vectors:

- The state of a quantum system is given by a vector $|\Psi\rangle$ in an abstract Hilbert space.
- The state $|\Psi\rangle$ contains all possible information about the quantum system at a given time.
- The state $|\Psi\rangle$ makes no reference to a particular basis until the basis vectors are chosen.
- The infinite dimensional column vector $\langle x|\Psi\rangle = \Psi(x)$ when considered as a function of x is the wave function of the system at a given time. $\Psi(x) = \langle x|\Psi\rangle$ is obtained when the position eigenstates $|x\rangle$ are chosen as the basis vectors to write state $|\Psi\rangle$.
- The State vector $|\Psi\rangle$ and wave function $\Psi(x)$ contain the same information, but $\Psi(x)$ is a vector with position eigenstates as the coordinate axes and $\Psi(x)$ for each x denotes the component of $|\Psi\rangle$ along the direction of $|x\rangle$.

Scalar product (Inner product)

3. The scalar product, or inner product, gives the component of a state, e.g., $|\Psi_2\rangle$, along another state, e.g., $|\Psi_1\rangle$. Choose all of the following notations that are correct for the scalar product that gives the component of state $|\Psi_2\rangle$ along state $|\Psi_1\rangle$?

(I) $\langle\Psi_1|\Psi_2\rangle$
(II) $|\Psi_1\rangle\langle\Psi_2|$
(III) $|\Psi_1\rangle|\Psi_2\rangle$

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only

4. Which one of the following equations is correct in general?
(a) $|\Psi_1\rangle\langle\Psi_2| = \langle\Psi_1|\Psi_2\rangle$
(b) $\langle\Psi_2|\Psi_1\rangle = \langle\Psi_1|\Psi_2\rangle$
(c) $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle^*$, where * denotes complex conjugate.
(d) $|\Psi_1\rangle\langle\Psi_2| = \langle\Psi_2|\Psi_1\rangle^*$, where * denotes complex conjugate.

5. Since the wave function is normalizable, the scalar product of a <u>normalized</u> state vector $|\Psi\rangle$ with itself gives
(a) $\langle\Psi|\Psi\rangle = 1$
(b) $\langle\Psi|\Psi\rangle = 0$
(c) $\langle\Psi|\Psi\rangle$ can be any finite number depending on the state.
(d) $\langle\Psi|\Psi\rangle = e^{i\varphi}$, where φ is a phase factor that depends on the state.

Summary of scalar products (inner products):

- A scalar product of state $|\Psi_2\rangle$ with $|\Psi_1\rangle$, $\langle\Psi_1|\Psi_2\rangle$, is defined as the component of state $|\Psi_2\rangle$ along state $|\Psi_1\rangle$.
- A scalar product is not a vector. In general, the scalar product is a complex number (may have units).
- Interchanging the "bra" and "ket" states in a scalar product produces its complex conjugate: $\langle\Psi_2|\Psi_1\rangle = \langle\Psi_1|\Psi_2\rangle^*$.
- The scalar product of a normalized state $|\Psi\rangle$ with itself gives 1, i.e., $\langle\Psi|\Psi\rangle = 1$.

Hilbert Space

6. Which one of the following statements is true about the Hilbert space corresponding to a spin ½ system?

(a) The Hilbert space is two dimensional and the spin operator corresponding to each of the spin components has two eigenstates that form a complete set of basis vectors.

(b) The Hilbert space is three dimensional because the physical laboratory space is three dimensional and Hilbert space is a mathematical representation of the real world.

(c) The Hilbert space is infinite dimensional, because a finite dimensional space cannot be the Hilbert space for any quantum mechanical system.

(d) None of the above.

7. Choose all of the following statements that are correct about the eigenstates of an operator in a Hilbert space.

(I) An operator in a finite-dimensional Hilbert space can have a finite number of discrete eigenvalues.

(II) An operator in an infinite-dimensional Hilbert space can have infinitely many discrete eigenvalues.

(III) An operator in an infinite-dimensional Hilbert space can have infinitely many continuous eigenvalues.

(a) (I) and (II) only

(b) (I) and (III) only

(c) (II) and (III) only

(d) All of the above.

8. Suppose Q is an observable for a given quantum system and its corresponding operator in the Hilbert space is $\hat{Q}$. Choose all of the following statements that are correct.

(I) $\hat{Q}$ must be a Hermitian operator.

(II) $\hat{Q} = \hat{Q}^\dagger$

(III) $\langle \phi | \hat{Q}\psi \rangle = \langle \hat{Q}\phi | \psi \rangle$ for all states $|\phi\rangle$ and $|\psi\rangle$ in the Hilbert space.

A. I only B. II only C. III only D. I and II only E. all of the above

9. "Any state vector in a Hilbert space can be expanded as a linear combination of a complete set of eigenstates of a Hermitian operator." Which one of the following is <u>necessarily implied</u> by this statement?

(a) All Hermitian operators commute with each other and have simultaneous eigenstates.

(b) Eigenstates of a Hermitian operator can be chosen to be the basis vectors in the Hilbert space.

(c) All Hermitian operators have real eigenvalues that correspond to results of measurements in physical space.

(d) The given statement is incorrect. The correct statement should read "Any vector in Hilbert space can <u>**only**</u> be expanded as a linear superposition of a complete set of <u>energy</u> eigenstates (eigenstates of the Hamiltonian operator)."

10. "Any state vector in the Hilbert space can be expanded as a linear superposition of a complete set of eigenstates of a Hermitian operator" is a correct statement. Choose all of the following that can be examples of the mathematical representation of this statement.

(I) $|\Psi\rangle = \sum_n C_n |\psi_n\rangle$, where $|\psi_n\rangle$ are energy eigenstates for a given quantum system and $C_n = \langle \psi_n | \Psi \rangle$ are appropriate expansion coefficients.

(II) $|\Psi\rangle = \int_{-\infty}^{\infty} \psi(x) |x\rangle dx$, where $|x\rangle$ are position eigenstates and $\psi(x) = \langle x | \Psi \rangle$ are appropriate expansion coefficients.

(III) $|\Psi\rangle = \sum_n C_n \langle \Psi | \psi_n \rangle$, where $|\psi_n\rangle$ are energy eigenstates and $C_n = \langle \psi_n | \Psi \rangle$ are appropriate expansion coefficients.

(a) (I) only

(b) (I) and (II) only

(c) (II) and (III) only

(d) All of the above.

Summary of Hilbert Space:

- Quantum state vectors are vectors in the Hilbert space.
- State vectors can be expanded as a linear superposition of a complete set of eigenstates of a Hermitian operator.
- The dimensionality of the Hilbert space is given by the number of linearly independent vectors in the space. The eigenstates of a Hermitian operator span the space which means that they form a complete set of basis vectors for the Hilbert space.
- When the measurement of an observable is performed in physical space, the values one measures are the eigenvalues of the corresponding Hermitian operator.

Checkpoint 1

Consider the following conversation between student A and student B:

- Student A: The Hilbert space for a particle interacting with a one-dimensional infinite square well is infinite-dimensional. Also, the position eigenstates form a complete set of basis vectors for the space and the position of the particle has infinitely many values within the width of the square well.
- Student B: I disagree. The Hilbert space for a particle interacting with a one-dimensional infinite square well is one-dimensional, because the well is one-dimensional and the particle is confined in one dimension.

Which student, if either, do you agree with and why?

Expansion of a state vector in terms of a complete set of eigenstates

11. Earlier you learned that any vector in the Hilbert space can be expanded as a linear superposition of a complete set of eigenstates of a Hermitian operator $\hat{Q}$. For an operator $\hat{Q}$ with eigenstates $\{|q_n\rangle,\ n = 1,2,3 \ldots N\}$ (which form an orthonormal basis for an N dimensional vector space) and **discrete** eigenvalues q_n, choose all of the following statements that are correct about the coefficients C_n in the expansion

$|\Psi\rangle = \sum_n C_n |q_n\rangle$.

(I) To find C_n, we take the scalar product with an eigenstate $|q_n\rangle$. Then,

$$\langle q_n|\Psi\rangle = \sum_m C_m \langle q_n|q_m\rangle = \sum_m C_m \delta_{nm} = C_n.$$

(II) To find C_n, we take the scalar product with an eigenstate $|q_n\rangle$. Then,

$$\langle q_n|\Psi\rangle = \sum_n C_n \langle q_n|q_n\rangle = \sum_n C_n.$$

(III) The coefficient C_n for a particular eigenstate $|q_n\rangle$ in the expansion $|\Psi\rangle = \sum_n C_n |q_n\rangle$ is related to the probability of measuring the corresponding eigenvalue q_n when a measurement of observable Q is made in the state $|\Psi\rangle$.

(a) (I) and (II) only
(b) (I) and (III) only
(c) (II) and (III) only
(d) All of the above.

12. Consider the following conversation between Student A and Student B.

- Student A: In the preceding question, statement (II) seems to make more sense than statement (I), because we are using the expansion $|\Psi\rangle = \sum_n C_n|q_n\rangle$ as opposed to $|\Psi\rangle = \sum_m C_m|q_m\rangle$.
- Student B: But *m* and *n* are just "dummy" indices. They both can range from 1 to *N*, where *N* is the dimension of the Hilbert space.
- Student A: What is the point of changing the label from n to m in the expansion of $|\Psi\rangle$ ($|\Psi\rangle = \sum_n C_n|q_n\rangle \to |\Psi\rangle = \sum_m C_m|q_m\rangle$) in statement (I)?
- Student B: If you take the scalar product of $|\Psi\rangle = \sum_n C_n|q_n\rangle$ with an eigenstate $\langle q_n|$ with the same index n, like in statement (II), you obtain $\langle q_n|\Psi\rangle = \sum_n C_n\langle q_n|q_n\rangle = \sum_n C_n$. You end up with a sum over all C_n's. This is incorrect. You must take the inner product with a different "dummy" indexed state $|\Psi\rangle = \sum_m C_m|q_m\rangle$, so that you get $\langle q_n|\Psi\rangle = \sum_m C_m\langle q_n|q_m\rangle = \sum_m C_m\delta_{nm} = C_n$. Instead of $\langle q_n|q_n\rangle = 1$, you obtain $\langle q_n|q_m\rangle = \delta_{nm}$ which gets rid of the summation. This is the correct answer, which is just a single coefficient C_n, not a sum $\sum_n C_n$.
- Student A: I see. If we choose a different dummy index for state $|\Psi\rangle = \sum_m C_m|q_m\rangle$ when taking the inner product, we get $\langle q_n|q_m\rangle = \delta_{nm}$, which gets rid of the sum over n.

Do you agree with Student B's explanation? Explain why or why not.

13. Consider the following conversation between Student A and Student B.

- Student A: For an operator with a discrete eigenvalue spectrum, such as energy, we can talk about measuring each of the eigenvalues. We can calculate the probabilities for measuring each of them individually.
- Student B: I agree. But we cannot talk about the probability of measuring a particular position because position is a continuous variable which has infinitely many possibilities. So the probability of each position is zero. For an operator that has a continuous eigenvalue spectrum, like position or momentum, we should talk about measuring a value in a narrow range. For example, the probability of measuring position between x and $x + dx$ is $|\Psi(x)|^2 dx$.

Do you agree with Student A and/or Student B? Explain your reasoning.

14. For an arbitrary physical observable Q with **discrete** eigenvalues q_n and eigenstates $|q_n\rangle$, where

$n = 1,2, \dots N$, write the **probability** of measuring eigenvalue q_n as a result of a measurement of Q performed when the system is in the state $|\Psi\rangle$.

15. A) Earlier you learned that any vector in the Hilbert space can be expanded as a linear superposition of a complete set of eigenstates of a Hermitian operator $\hat{Q}$. In the case of an operator $\hat{Q}$ with **continuous** eigenvalues q and eigenstates $|q\rangle$ (which form an orthonormal basis for an infinite-dimensional vector space), choose all of the following statements that are correct about the coefficients $C(q)$ in the expansion

$|\Psi\rangle = \int_{-\infty}^{\infty} C(q)|q\rangle dq$? *(Hint: This is similar to question 11, except the eigenvalues are continuous).*

(I) To find $C(q)$, we take the scalar product with an eigenstate $|q\rangle$. Then, $\langle q|\Psi\rangle = \int_{-\infty}^{\infty} C(q')\langle q|q'\rangle dq' = \int_{-\infty}^{\infty} C(q')\delta(q - q')dq' = C(q)$.

(II) Physically, the coefficient $C(q)$ is the component of the state $|\Psi\rangle$ along the direction of the eigenvector $|q\rangle$ (with eigenvalue q).

(III) The coefficient $C(q) = \langle q|\Psi\rangle$ in the expansion $|\Psi\rangle = \int_{-\infty}^{\infty} C(q)|q\rangle dq$ is related to the probability of measuring the eigenvalue q between q and $q + dq$ when observable Q is measured in the state $|\Psi\rangle$.

(a) (I) and (II) only
(b) (I) and (III) only.
(c) (II) and (III) only
(d) All of the above.

15. B) Consider the following statement made by a student about the preceding question:

"Just like in the discrete case, we must use different "dummy" indices when finding the coefficients $C(q)$ in the expansion of $|\Psi\rangle = \int_{-\infty}^{\infty} C(q)|q\rangle dq$. If we used the same "dummy" index, we would end up with an integration over all $C(q)$, like this: $\langle q|\Psi\rangle = \int_{-\infty}^{\infty} C(q)\langle q|q\rangle dq = \int_{-\infty}^{\infty} C(q)dq$. This is incorrect. You must take the inner product with a different "dummy" indexed state $\langle q|\Psi\rangle = \int_{-\infty}^{\infty} C(q')\langle q|q'\rangle dq' = \int_{-\infty}^{\infty} C(q')\delta(q - q')dq' = C(q)$, so that you get $\langle q|\Psi\rangle = C(q)$.

Do you agree with the student? Explain your reasoning.

16. Earlier, you learned that for an operator $\hat{Q}$ corresponding to a physical observable Q with eigenstates $\{|q_n\rangle,\ n = 1,2, \dots N\}$ with **discrete** eigenvalues q_n

(I) $\langle q_n|\Psi\rangle$ is the **probability amplitude** for measuring q_n if we measure observable Q

(II) $|\langle q_n|\Psi\rangle|^2$ is the **probability** for measuring q_n if we measure observable Q.

Before Dirac notation was introduced, physicist Max Born interpreted the probabilistic nature of quantum mechanics and proposed the following statements for the continuous case for observable x which has a continuous eigenvalue spectrum:

(I) $\Psi(x)$ is the **probability density amplitude** for measuring position.

(II) $|\Psi(x)|^2$ is the **probability density** for measuring position.

(III) $|\Psi(x)|^2 dx$ is the **probability** of finding the particle in the narrow range between x and $x + dx$ when position of the particle is measured.

Write each of these expressions (probability density amplitude, probability density, and probability of measuring position in a narrow range between x and $x + dx$) in Dirac notation.

(a) $\Psi(x) =$

(b) $|\Psi(x)|^2 =$

(c) $|\Psi(x)|^2 dx =$

17. Dirac extended Born's interpretation to apply to measurements of not only position but **any** physical observable.

(a) Keeping in mind your answers to the two preceding questions, for an arbitrary physical observable Q with eigenstates $|q\rangle$ with **continuous** eigenvalues q, write the **probability** of measuring observable Q between q and $q + dq$ as a result of a measurement performed when the system is in the state $|\Psi\rangle$.

(b) Consider the following statement from a student:

- Student B: You cannot think about **expectation value** physically as an average of a large number of measurements on identically prepared systems. We must use our expansion $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$, to calculate the expectation value $\langle\Psi|\hat{Q}|\Psi\rangle$.

  Do you agree with Student B? Explain your reasoning.

18. The **expectation value** of an operator is the average value of the observable measured over many identical experiments performed on identically prepared systems in state $|\Psi\rangle$. For a general quantum mechanical Hermitian operator $\hat{Q}$, the expectation value is represented by $\langle\Psi|\hat{Q}|\Psi\rangle$. If $\hat{Q}$ has **discrete** eigenvalues q_n and eigenstates $|q_n\rangle$ where $n = 1,2, \dots N$, let's write $\langle\Psi|\hat{Q}|\Psi\rangle$ in terms of the eigenstates $|q_n\rangle$ and eigenvalues q_n.

(a) Write $|\Psi\rangle$ as a linear superposition of the eigenstates of $\hat{Q}$.

(b) Consider the following conversation between two students:

- Student A: If we write $|\Psi\rangle$ as a linear superposition of the eigenstates of $\hat{Q}$, we obtain
  $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$, where a_n is a complex coefficient.
- Student B: I agree with you. But we know that the expansion coefficients, a_n, are the eigenvalues q_n of the operator $\hat{Q}$. So we can write $|\Psi\rangle$ as a linear superposition of the eigenstates of $\hat{Q}$ like this: $|\Psi\rangle = \sum_{n=1}^{N} q_n |q_n\rangle$.

With whom do you agree? Explain your reasoning.

(c) The linear superposition of $|\Psi\rangle$ in terms of the eigenstates of $\hat{Q}$ can be written as $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$, where a_n is the expansion coefficient and gives the component of the state $|\Psi\rangle$ along the direction of the nth eigenstate $|q_n\rangle$. Write a_n explicitly in terms of $|\Psi\rangle$ and $|q_n\rangle$.

(d) What is the probability of measuring q_n when you measure observable Q in the state $|\Psi\rangle$?

(e) Consider the following statement from Student A:

- Student A: $|\langle q_n|\Psi\rangle|^2$ is the probability of measuring q_n when you measure observable Q in the state $|\Psi\rangle$. The expectation value is the average value of a large number of measurements performed on identically prepared systems.

Since we know the probability of measuring each eigenvalue q_n of the operator $\hat{Q}$, the expectation value is $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$.

Do you agree with Student A's statement? Explain your reasoning.

(f) Student A is correct. The expectation value is the average value of a large number of measurements on identically prepared systems, which can be represented mathematically by the equation $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$. But let's follow Student B's method from question 17 (b) using the expansion $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$ to prove that the equation $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$, suggested by Student A, is correct. Act with $\hat{Q}$ on the state $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$. What do you obtain?

(g) So far, we have $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} a_n q_n |q_n\rangle$. Using your answer from part (c), insert what you obtained for a_n into $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} a_n q_n |q_n\rangle$.

(h) We now have $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |q_n\rangle\langle q_n|\Psi\rangle$. Now take the inner product of $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |q_n\rangle\langle q_n|\Psi\rangle$ with a "bra" state $\langle\Psi|$ to find the **expectation value** $\langle\Psi|\hat{Q}|\Psi\rangle$. Does your answer agree with Student A's statement from part (e)? If not, go back and check your work with a partner to obtain the equation for the expectation value of observable $\hat{Q}$ in terms of its complete set of eigenstates $\{|q_n\rangle, n = 1,2, \ldots N\}$ and eigenvalues q_n, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$.

(i) Repeat the calculation for the **expectation value** $\langle\Psi|\hat{Q}|\Psi\rangle$ of an operator $\hat{Q}$ with eigenstates $|q\rangle$ (which form a basis in an infinite-dimensional vector space) with **continuous** eigenvalues q.

19. Suppose an operator $\hat{Q}$ corresponding to a physical observable Q has eigenstates $\{|q_n\rangle, n = 1,2, \dots N\}$ with discrete eigenvalues q_n. Which of the following are correct about the expression $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2$?

(I) $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2 = 1$

(II) $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2$ is equal to a real number.

(III) $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2$ is equal to a complex number that does have an imaginary part.

(a) (II) only
(b) (III) only
(c) (I) and (II) only
(d) None of the above.

20. Consider the following conversation between two students about the preceding question:

- Student A: I don't see how $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2 = 1$.
- Student B: Let me show you.

1. We can start with $\langle\Psi|\Psi\rangle = 1$, since any state vector can be normalized to 1.
2. Insert the identity operator, written in terms of the eigenstates $\{|q_n\rangle, n = 1,2, \dots N\}$ of the operator $\hat{Q}$, like this: $1 = \langle\Psi|\Psi\rangle = \sum_{n=1}^{N} \langle\Psi|q_n\rangle\langle q_n|\Psi\rangle$.
3. Using the fact that $\langle\Psi|q_n\rangle^* = \langle q_n|\Psi\rangle$, we can write
$1 = \langle\Psi|\Psi\rangle = \sum_{n=1}^{N} \langle\Psi|q_n\rangle\langle q_n|\Psi\rangle = \sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2$.

- Student A: I see. Is there any physical significance to $\langle q_n|\Psi\rangle$?
- Student B: Yes. $\langle q_n|\Psi\rangle$ is the probability amplitude and $|\langle q_n|\Psi\rangle|^2$ is the probability for measuring q_n if we measure observable Q.
- Student A: So based on the mathematical expression $\sum_{n=1}^{N} |\langle q_n|\Psi\rangle|^2 = 1$, the probabilities of measuring different eigenvalues q_n when we measure the observable Q must add up to 1.

Do you agree with Student A and Student B? Explain your reasoning.

Summary of the expansion of a state vector in terms of a complete set of eigenstates:

- We can write the state vector in terms of a linear superposition of the energy eigenstates, position eigenstates, or eigenstates of any other Hermitian operator since each of them spans the space.
  - If $\hat{Q}$ has eigenstates $|q_n\rangle$ ($n = 1,2, \ldots N$) with **discrete** eigenvalues q_n, then $|\Psi\rangle = \sum_{n=1}^{N} a_n |q_n\rangle$, in which a_n is the component of the state $|\Psi\rangle$ along $|q_n\rangle$, i.e., $a_n = \langle q_n|\Psi\rangle$.
  - If $\hat{Q}$ has eigenstates $|q\rangle$ with **continuous** eigenvalues q, then $|\Psi\rangle = \int_{-\infty}^{\infty} a_q |q\rangle\, dq$, in which a_q is the component of the state $|\Psi\rangle$ along the eigenstate $|q\rangle$, i.e., $a_q = \langle q|\Psi\rangle$.
  - If a Hermitian operator $\hat{Q}$ has a discrete eigenvalue spectrum, the expansion of a state vector $|\Psi\rangle$ in terms of the eigenstates $|q_n\rangle$ of the Hermitian operator is a sum. If a Hermitian operator $\hat{Q}$ has a continuous eigenvalue spectrum, the expansion of a state vector vector $|\Psi\rangle$ in terms of the eigenstates $|q\rangle$ of the Hermitian operator is an integral.
  - For **discrete** eigenvalues q_n, $\left|\langle q_n|\Psi\rangle\right|^2$ is the **probability** of measuring q_n for an observable Q when the system is in the state $|\Psi\rangle$.
  - For **continuous** eigenvalues q, $|\langle q|\Psi\rangle|^2 dq$ is the **probability** of measuring an observable Q in a narrow range between q and $q + dq$ when the system is in the state $|\Psi\rangle$.
- The **expectation value** of a Hermitian operator $\hat{Q}$ in a generic state $|\Psi\rangle$ is the average value of the observable Q measured over many identical experiments performed on identically prepared systems in state $|\Psi\rangle$.
  - In a generic state $|\Psi\rangle$, the expectation value for an operator $\hat{Q}$ with eigenstates $|q_n\rangle$ $(n = 1, 2, \ldots N)$ with **discrete** eigenvalues q_n is $\langle\Psi|\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} q_n |\langle q_n|\Psi\rangle|^2$
  - In a generic state $|\Psi\rangle$, the expectation value for an operator $\hat{Q}$ with eigenstates $|q\rangle$ with **continuous** eigenvalues q is $\langle\Psi|\hat{Q}|\Psi\rangle = \int_{-\infty}^{\infty} q |\langle q|\Psi\rangle|^2\, dq$

Checkpoint 2

Choose all of the following statements which are correct for a given quantum system about an operator $\hat{Q}$ that corresponds to a physical observable Q with discrete eigenvalues q_n and eigenstates $|q_n\rangle$:

(I) $|\Psi\rangle = \sum_n C_n |q_n\rangle$, where $C_n = \langle q_n|\Psi\rangle$ are expansion coefficients.
(II) $\langle q_n|\Psi\rangle$ is the probability of measuring q_n in a generic state $|\Psi\rangle$.
(III) $|C_n|^2 = |\langle q_n|\Psi\rangle|^2$ is the probability of measuring q_n in a generic state $|\Psi\rangle$.

(a) (I) only
(b) (II) only
(c) (I) and (II) only
(d) (I) and (III) only
(e) None of the above.

Projection Operator

22. In the Hilbert space in which $|q_n\rangle$ is a vector, which one of the following statements is correct about the expression $|q_n\rangle\langle q_n|$, where $\{|q_n\rangle, n = 1,2,3, \ldots N\}$ form an orthonormal basis for an N dimensional vector space?
(a) $|q_n\rangle\langle q_n|$ is equal to the number 1.
(b) $|q_n\rangle\langle q_n|$ is a scalar, but one cannot determine what number it is equal to without knowing what $|q_n\rangle$ is explicitly.
(c) $|q_n\rangle\langle q_n|$ is an outer product, so it is an operator.
(d) $|q_n\rangle\langle q_n|$ is a vector.

23. Act on a generic state $|\Psi\rangle$ with the operator $|q_n\rangle\langle q_n|$. That is, $|q_n\rangle\langle q_n|\Psi\rangle$. Which one of the following statements correctly describes what you obtain?
(a) You get back the same state $|\Psi\rangle$, because $|q_n\rangle\langle q_n|$ is the identity operator.
(b) You get the projection of $|\Psi\rangle$ along the direction of $|q_n\rangle$. $\langle q_n|\Psi\rangle$ is the component of $|\Psi\rangle$ along the direction of $|q_n\rangle$. The vector $|q_n\rangle$, which multiplies the coefficient $\langle q_n|\Psi\rangle$, gives the direction of the projected vector.
(c) You get the same state $|\Psi\rangle$ back, with the corresponding eigenvalue.
(d) It cannot be determined from the given information. The state $|\Psi\rangle$ has to be given explicitly in position representation for a given quantum system to be able to calculate the answer.

24. Consider the following conversation between Student A and Student B.
- Student A: I thought that $|q_n\rangle\langle q_n|$ was equal to the identity operator. Wasn't that what we had learned earlier in this tutorial? How is it that the same expression is the identity operator and the projection operator at the same time?
- Student B: The expression that was equal to the identity operator was $\sum_{n=1}^{N}|q_n\rangle\langle q_n|$, where there is a sum over a complete set of basis vectors. Applying that on a state $|\Psi\rangle$ would give

the same state back. An example of a projection operator is $|q_n\rangle\langle q_n|$. Acting with $|q_n\rangle\langle q_n|$ on a state $|\Psi\rangle$ gives the projection of that state along the direction of $|q_n\rangle$ as follows:

$$|q_n\rangle \qquad \langle q_n|\Psi\rangle$$

The vector multiplying the inner product	Inner product of $|\Psi\rangle$ with $|q_n\rangle$ equals the component of $|\Psi\rangle$ along the direction of $|q_n\rangle$

Do you agree with Student B's explanation? Explain why or why not.

Summary of the projection operator:

- The projection operator $|q_n\rangle\langle q_n|$ acting on a state $|\Psi\rangle$ returns a vector in the direction of $|q_n\rangle$ together with a number $\langle q_n|\Psi\rangle$, which is the component of a state vector along the direction of the orthonormal basis vector $|q_n\rangle$.
- Unlike the identity operator, the projection operator acting on a state vector need not return the same state vector back.
- The projection operator formed with orthonormal eigenstates of a Hermitian operator $\hat{Q}$ with discrete or continuous eigenvalues has a similar affect on a generic state $|\Psi\rangle$ as follows:
    - $|q_n\rangle\langle q_n|$ is a projection operator, e.g., written in terms of orthonormal eigenstates $|q_n\rangle$ with **discrete** eigenvalues q_n of an operator $\hat{Q}$. The projection operator $|q_n\rangle\langle q_n|$ projects a generic state $|\Psi\rangle$ along the direction of vector $|q_n\rangle$.
    - $|q\rangle\langle q|$ is a projection operator, e.g., written in terms of orthonormal eigenstates $|q\rangle$ with **continuous** eigenvalues q of an operator $\hat{Q}$. The projection operator $|q\rangle\langle q|$ projects a generic state $|\Psi\rangle$ along the direction of vector $|q\rangle$.

Completeness Relation

The completeness relation can be written in terms of orthonormal eigenstates $|q_n\rangle$ of an operator $\hat{Q}$ with discrete eigenvalues q_n. Mathematically, the completeness relation is $\sum_{n=1}^{N}|q_n\rangle\langle q_n| = \hat{I}$, where $\{|q_n\rangle,\ n = 1, 2, 3 \ldots N\}$ is an orthonormal basis for an N dimensional Hilbert space and $\hat{I}$ is the identity operator which can be represented by an $N \times N$ identity matrix. Completeness (of a set of basis vectors, e.g., eigenstates of an operator corresponding to a physical observable) means that an arbitrary state vector $|\Psi\rangle$ can be written in terms of the complete set of basis vectors.

24. a) Act with the identity operator $\hat{I}$, written in terms of orthonormal eigenstates $|q_n\rangle$ of an operator $\hat{Q}$ with discrete eigenvalues q_n, on an arbitrary state vector $|\Psi\rangle$. What do you obtain?

b) Explain your results from part (a) in a sentence.

c) Consider the following statement made by a student:
"We can use the following analogy when reasoning about the identity operator: $3\ hours = 3\ hours \times \left(\frac{60\ minutes}{1\ hours}\right) = 180\ minutes$. In this case, the identity operator is analogous to $\left(\frac{60\ minutes}{1\ hours}\right) = 1$. When you multiply $3\ hours$ by $\left(\frac{60\ minutes}{1\ hours}\right)$, you are causing a one-dimensional basis change from hours to minutes. Similarly, the identity operator helps us change basis in an N dimensional Hilbert space."
Do you agree with the student? Explain your reasoning.

25. So far we have $\hat{I}|\Psi\rangle = \sum_{n=1}^{N}|q_n\rangle\langle q_n|\Psi\rangle$. If $|\Psi\rangle = \sum_{n=1}^{N} a_n\,|q_n\rangle$, which one of the following is the correct expression for the coefficients a_n along the state $|q_n\rangle$ in the expansion of $|\Psi\rangle$?

(a) $a_n = \langle q_n|\Psi\rangle$
(b) $a_n = \langle q_n|q_n\rangle$
(c) $a_n = |\langle q_n|\Psi\rangle|^2$
(d) $a_n = \langle\Psi|\Psi\rangle$

The identity operator acting on an arbitrary state $|\Psi\rangle$ is $\hat{I}|\Psi\rangle = \sum_{n=1}^{N}|q_n\rangle\langle q_n|\Psi\rangle = \sum_{n=1}^{N} a_n|q_n\rangle$. This shows that a generic state $|\Psi\rangle$ can be written in terms of a complete set of eigenstates which span the Hilbert space. We often use the completeness relation to decompose a generic state $|\Psi\rangle$ into its components along each of the basis vectors (eigenstates of a Hermitian operator can be chosen to be the basis vectors in the Hilbert space).

23. Re-calculate expectation value of $\hat{Q}$ in state $|\Psi\rangle$, $\langle\Psi|\hat{Q}|\Psi\rangle$, by using the completeness relation $\sum_{n=1}^{N}|q_n\rangle\langle q_n| = \hat{I}$ inserted into the expression $\langle\Psi|\hat{Q}|\Psi\rangle$ and compare to your answer for question 18 part (h).

24. The completeness relation can also be written in terms of the eigenstates of an operator $\hat{Q}$ with a **continuous** eigenvalue spectrum. The completeness relation corresponding to a Hermitian operator $\hat{Q}$ with eigenstates $|q\rangle$ with continuous eigenvalues q is $\int_{-\infty}^{\infty}|q\rangle\langle q|dq = \hat{I}$, where $\hat{I}$ is an infinite-dimensional identity matrix.

(a) What is the result of $\hat{I}$ (completeness relation written in terms of a complete set of eigenstates $|q\rangle$) acting on $|\Psi\rangle$?

(b) So far we have $|\Psi\rangle = \hat{I}|\Psi\rangle = \int_{-\infty}^{\infty}|q\rangle\langle q|\Psi\rangle dq$. Explain whether $\langle q|\Psi\rangle$ is a number, operator, or vector for a given value of q.

(c) Consider the following conversation between Student A and Student B:

- Student A: The component of $|\Psi\rangle$ along the basis vector $|q\rangle$ is $a_q = \langle q|\Psi\rangle$, which is a number for a given value of q. So we are free to move $\langle q|\Psi\rangle$ in the integral $|\Psi\rangle = \hat{I}|\Psi\rangle = \int_{-\infty}^{\infty}|q\rangle\langle q|\Psi\rangle dq = \int_{-\infty}^{\infty}\langle q|\Psi\rangle|q\rangle dq$. So $|\Psi\rangle = \int_{-\infty}^{\infty} a_q|q\rangle dq$.

- Student B: I disagree with you. We cannot simply move $\langle q|\Psi\rangle$ around inside the integral, like this $\int_{-\infty}^{\infty}|q\rangle\langle q|\Psi\rangle dq \neq \int_{-\infty}^{\infty}\langle q|\Psi\rangle|q\rangle dq$.

With whom, if either, do you agree? Explain your reasoning.

(d) Using your answers to the preceding parts (a-c), what is the expression for an arbitrary state $|\Psi\rangle$ written in terms of continuous eigenstates $|q\rangle$ of a Hermitian operator $\hat{Q}$ and numbers $a_q = \langle q|\Psi\rangle$?

(e) Use your answers to the preceding parts (a-d) to calculate the expectation value $\langle\Psi|\hat{Q}|\Psi\rangle$ in terms of eigenstates $|q\rangle$ with continuous eigenvalues q of a Hermitian operator $\hat{Q}$.

25. Which one of the following relations is correct about an operator $\hat{Q}$ with eigenstates $\{|q_n\rangle$, $n = 1,2,3 \ldots N\}$ (which form an orthonormal basis for an N dimensional vector space) and **discrete** eigenvalues q_n?

(a) $\hat{Q} = \sum_{n=1}^{N} q_n|q_n\rangle$

(b) $\hat{Q} = \sum_{n=1}^{N} q_n\langle q_n|q_n\rangle$

(c) $\hat{Q} = \sum_{n=1}^{N} q_n|q_n\rangle\langle q_n|$

(d) $\hat{Q} = q_n|q_n\rangle$

26. To check your answer to the preceding question, you must show that the operator $\hat{Q}$ acting on any generic state gives the same result as the right hand side of the expression in the preceding question.

(a) Act with the operator $\hat{Q}$ on a generic state $|\Psi\rangle$, like this: $\hat{Q}|\Psi\rangle$. Now insert the identity operator, written in terms of the orthonormal eigenstates $\{|q_n\rangle,\ n = 1,2,3 \ldots N\}$ of the operator $\hat{Q}$, between the operator $\hat{Q}$ and generic state $|\Psi\rangle$.

(b) Consider the following statement from a student:

- Student 1: We have $\hat{Q}|\Psi\rangle = \sum_{n=1}^{N} \hat{Q}\,|q_n\rangle\langle q_n|\Psi\rangle = \sum_{n=1}^{N} q_n\,|q_n\rangle\langle q_n|\Psi\rangle$. We can think of $\hat{Q}|\Psi\rangle$ like this:$\hat{Q}|\Psi\rangle = [\sum_{n=1}^{N} \hat{Q}\,|q_n\rangle\langle q_n|]|\Psi\rangle = [\sum_{n=1}^{N} q_n\,|q_n\rangle\langle q_n|]|\Psi\rangle$, such that the terms in the brackets must be equal. So the operator $\hat{Q} = \sum_{n=1}^{N} q_n|q_n\rangle\langle q_n|$.

Do you agree with student 1? Explain your reasoning.

(d) Using your answers to the preceding parts, determine the expression for a Hermitian operator $\hat{Q}$ with eigenstates $|q\rangle$ with **continuous** eigenvalues q in terms of the eigenstates $|q\rangle$ and eigenvalues q.

Summary of the completeness relation:

- A complete set of orthonormal eigenstates of a Hermitian operator $\hat{Q}$ with discrete or continuous eigenvalues can be used to write the completeness relation.
- The completeness relation is useful for decomposing a state vector into its components along each of the basis vectors.
  - The completeness relation for basis vectors with a **discrete** eigenvalue spectrum is $\sum_{n=1}^{N}|q_n\rangle\langle q_n| = \hat{I}$, where $\{|q_n\rangle,\ n = 1, 2, 3 \dots N\}$ is an orthonormal basis for an N dimensional vector space (e.g., formed with a complete set of eigenstates $|q_n\rangle$ with eigenvalues q_n of an operator $\hat{Q}$ corresponding to an observable Q).
  - The completeness relation for basis vectors with a **continuous** eigenvalue spectrum is $\int_{-\infty}^{\infty}|q\rangle\langle q|dq = \hat{I}$, where $|q\rangle$ is an orthonormal basis for an infinite-dimensional vector space (e.g., formed with a complete set of eigenstates $|q\rangle$ with eigenvalues q of an operator $\hat{Q}$ corresponding to an observable Q).
- The identity operator doesn't change the vector it acts on.
- An operator $\hat{Q}$ with a complete set of orthonormal eigenstates $\{|q_n\rangle,\ n = 1,2,3 \dots N\}$ with **discrete** eigenvalues q_n can be written as $\hat{Q} = \sum_{n=1}^{N} q_n|q_n\rangle\langle q_n|$.
- An operator $\hat{Q}$ with a complete set of orthonormal eigenstates $|q\rangle$ with **continuous** eigenvalues q can be written as $\hat{Q} = \int_{-\infty}^{\infty} q|q\rangle\langle q|dq$.

Checkpoint 3

Assume we have a generic vector $|G\rangle = a|i\rangle + b|j\rangle + c|k\rangle$ in a three dimensional Hilbert space where $a, b,$ and c are complex numbers and $|i\rangle, |j\rangle$ and $|k\rangle$ form an orthonormal basis.

a. Write the projection operator that projects any vector along the basis vector $|i\rangle$.

b. Use the projection operator you constructed to find the components of state $|G\rangle$ along the direction $|i\rangle$.

c. Act with the identity operator, written in terms of the basis vectors $|i\rangle$, $|j\rangle$, and $|k\rangle$ on the vector $|G\rangle$.

d. Write down, in your own words, the difference between a projection operator and the identity operator based upon your answers to the preceding parts.

Answers to Checkpoints

Checkpoint 1: Student A. There are an infinite number of values of position in a one-dimensional infinite square well.

Checkpoint 2: (d)

Checkpoint 3:

a. $|i\rangle\langle i|$

b. $|i\rangle\langle i|G\rangle = a|i\rangle$

c. $|i\rangle\langle i|G\rangle + |j\rangle\langle j|G\rangle + |k\rangle\langle k|G\rangle = a|i\rangle + b|j\rangle + c|k\rangle = |G\rangle$

d. The identity operator acting on a state gives the same state back. A projection operator acting on a state gives a component of the state along a basis vector times a basis vector.

Dirac Notation: Focus on Position and Momentum Representation

- Throughout this homework, the normalization issues for the position and momentum eigenstates are ignored.
- In all of the questions below, $|\Psi\rangle$ denotes a generic state of a quantum system with Hamiltonian $\hat{H}$.
- Assume that the Hilbert space is infinite dimensional.
- For all questions involving a generic operator $\hat{Q}$, assume that it only depends on position $\hat{x}$ and momentum $\hat{p}$ and has no explicit time dependence.
- Assume the particle is confined in a one dimensional physical "laboratory" space.
- Assume $\sum_n$ refers to a summation over a complete set of states ($n = 1,2,3 \ldots \infty$).

The goals of this homework are to help you learn about:

➢ **Connecting Dirac notation with function space (position and momentum representation)**

- **Relationship between state vector $|\boldsymbol{\Psi}\rangle$ and the wave function $\boldsymbol{\Psi(x)}$**
  - In the position representation, $\langle x|\Psi\rangle = \Psi(x)$ is the projection of state vector $|\Psi\rangle$ along the eigenstate of position $|x\rangle$ (position eigenstates $\{|x\rangle\}$ form a complete set of basis vectors). The column vector $\Psi(x)$ (considered as a function of x) is called the *position space wave function*.
  - In the momentum representation, $\langle p|\Psi\rangle = \Phi(p)$ is the projection of state vector $|\Psi\rangle$ along the eigenstate of momentum $|p\rangle$ (momentum eigenstates $\{|p\rangle\}$ form a complete set of basis vectors). The column vector $\Phi(p)$ (considered as a function of p) is called the *momentum space wave function*.
  - The position space wave function $\Psi(x)$ and momentum space wave function $\Phi(p)$ can be considered as infinite-dimensional column vectors.
  - The momentum space wave function $\Phi(p) = \langle p|\Psi\rangle$ and position space wave function $\Psi(x) = \langle x|\Psi\rangle$ are a Fourier transform and inverse Fourier transform of each other, respectively.
- **Position and momentum eigenstates**
  - The position eigenstate with eigenvalue x' can be written as:
    - $|x'\rangle$ in Dirac notation.
    - $\langle x|x'\rangle = \delta(x - x')$ in the position representation. $\delta(x - x')$ is also called the *position eigenfunction in position representation* and a form of the orthogonality relation.
    - $\langle p|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ in the momentum representation. $\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ is also called the *position eigenfunction* in momentum representation.
  - The momentum eigenstate with eigenvalue p' can be written as:
    - $|p'\rangle$ in Dirac notation
    - $\langle x|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ in the position representation. $\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ is also called the *momentum eigenfunction in position representation*.
    - $\langle p|p'\rangle = \delta(p - p')$ in the momentum representation. $\delta(p - p')$ is also called the *momentum eigenfunction in momentum representation* and a form of the orthogonality relation.
- **Position and momentum representation**
  - For a generic state $|\Psi\rangle$ and a generic operator $\hat{Q}$ (which depends only on operators $\hat{x}$ and $\hat{p}$):
    - In the **position** representation, $\hat{Q}|\Psi\rangle$ is represented by $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$

- In the **momentum** representation, $\hat{Q}|\Psi\rangle$ is represented by $\langle p|\hat{Q}|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\Phi(p)$

➢ **For a given quantum system, the Hamiltonian operator $\hat{H}$ and its eigenstates (energy eigenstates)**
  - $|E_n\rangle = |\Psi_{E_n}\rangle = |\Psi_n\rangle$ for $n = 1,2, \ldots\infty$, represent a complete set of energy eigenstates with eigenvalue E_n.
  - The eigenvalue equation for the Hamiltonian operator is $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$.
  - The expectation value of energy in state $|\Psi\rangle$ is $\langle\Psi|\hat{H}|\Psi\rangle = \sum_n E_n|\langle\psi_n|\Psi\rangle|^2$.

Connecting Dirac notation with function space (position and momentum representation)

❖ **By the end of this tutorial, you will be able to determine the functions in the following table:**

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)		
Momentum eigenstates (or momentum eigenfunctions)		
Position operator $\hat{x}$		
Momentum operator $\hat{p}$		
$\hat{Q}|x'\rangle$		
$\hat{Q}|p'\rangle$		
$\hat{Q}|\Psi\rangle$		

❖ **Relationship between state vector $|\Psi\rangle$ and the wave function for a given quantum system**

1. Choose all of the following statements that are correct about the generic state vector $|\Psi\rangle$

   (I) $\Psi(x) = \langle x|\Psi\rangle$ is a representation of the state vector $|\Psi\rangle$ in the position representation and is called the position space wave function.

   (II) $\Phi(p) = \langle p|\Psi\rangle$ is a representation of the state vector $|\Psi\rangle$ in the momentum representation and is called the momentum space wave function.

   (III) The state vector $|\Psi\rangle$ can be written as a column vector once a basis has been chosen.

   (a) (I) only

(b) (I) and (II) only
(c) (I) and (III) only
(d) (II) and (III) only
(e) All of the above.

2. Consider the following conversation between two students:
   - Student A: In the preceding question, we can also write $\Psi(x)$ as $|\Psi\rangle = \Psi(x)$.
   - Student B: I disagree. $|\Psi\rangle \doteq \Psi(x)$, where the $\doteq$ sign means that the equality is valid only with respect to a chosen basis. $\Psi(x)$ is a representation of $|\Psi\rangle$ in position representation when we choose a complete set of position eigenstates, $|x\rangle$, as our basis vectors, so we can write $\Psi(x) = \langle x|\Psi\rangle$.

With whom do you agree? Explain your reasoning.

3. Earlier you learned that in a three dimensional space, a generic state $|G\rangle$ can be written as $|G\rangle = a|i\rangle + b|j\rangle + c|k\rangle$, where $|i\rangle$, $|j\rangle$, and $|k\rangle$ form an orthonormal basis and a, b, and c are complex numbers. Thus, a generic state $|G\rangle$ can be written as a column vector once a basis is chosen, i.e.,

$$|G\rangle \doteq \begin{pmatrix} \langle i|G\rangle \\ \langle j|G\rangle \\ \langle k|G\rangle \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

where the $\doteq$ sign means that the equality is valid only with respect to a chosen basis.

In quantum mechanics, the generic state vector $|\Psi\rangle$ is a vector in the Hilbert space, which is infinite dimensional. The generic state $|\Psi\rangle$ can be written in terms of a linear superposition of a complete set of eigenstates of any Hermitian operator $\hat{Q}$.

(a) Suppose a Hermitian operator $\hat{Q}$ has a complete set of eigenstates $\{|q_n\rangle, n = 1,2, \ldots \infty\}$ with discrete eigenvalues q_n. Write $|\Psi\rangle$ in terms of a linear superposition of a complete set of eigenstates $\{|q_n\rangle,\ n = 1, 2, 3 \ldots \infty\}$.

(b) Keeping in mind how the generic state $|G\rangle$ is written as a column vector, write $|\Psi\rangle$ as an infinite dimensional column vector with respect to the orthonormal basis $|q_n\rangle$.

4. Consider a generic state vector $|\Psi\rangle = \sum_{n=1}^{\infty} a_n|q_n\rangle$, where $a_n = \langle q_n|\Psi\rangle$. Then, the state vector $|\Psi\rangle$ can be represented as a column vector like this: $|\Psi\rangle \doteq \begin{pmatrix} \langle q_1|\Psi\rangle \\ \langle q_2|\Psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$, where the $\doteq$ sign means that this is a representation of $|\Psi\rangle$ in the chosen basis, e.g., $\{|q_n\rangle, n = 1,2, \ldots \infty\}$. Consider the following conversation between two students about the situation where basis vectors are chosen to be position eigenstates $|x\rangle$ or momentum eigenstates $|p\rangle$, each of which have a continuous eigenvalue spectrum.
   - Student 1: We cannot write state vector $|\Psi\rangle$ as a column vector if position eigenstates $|x\rangle$ are chosen as the basis vectors. State vector $|\Psi\rangle$ written as a linear superposition of position

eigenstates $|x\rangle$ is $|\Psi\rangle = \int_{-\infty}^{\infty} \Psi(x)|x\rangle dx$, where $\Psi(x) = \langle x|\Psi\rangle$. But since this expansion of $|\Psi\rangle$ involves an integral instead of a summation, we cannot write $|\Psi\rangle$ as a column vector with respect to the basis vectors $|x\rangle$.

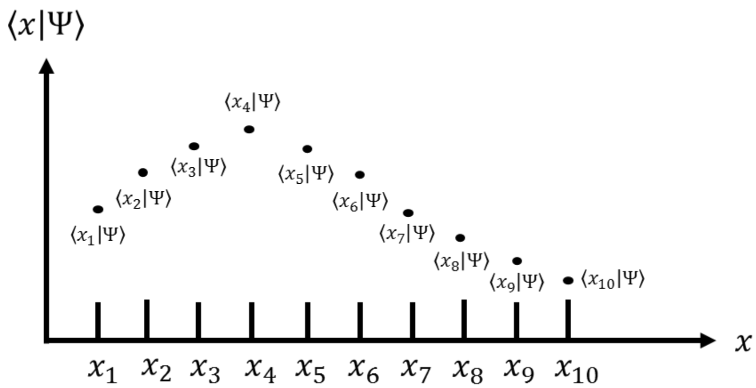
- Student 2: I disagree. Even though the expansion of $|\Psi\rangle$ is an integral instead of a sum, we can still envision $|\Psi\rangle$ as a column vector with respect to the basis vectors $|x\rangle$. Like this:

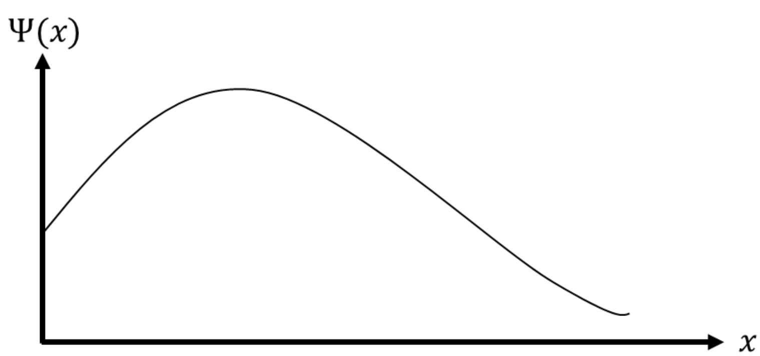
$$|\Psi\rangle \doteq \begin{pmatrix} \langle x_1|\Psi\rangle \\ \langle x_2|\Psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \vdots \end{pmatrix} = \Psi(x).$$

- Student 1: But why do the x's have indices? Don't position eigenstates $|x\rangle$ have a continuous eigenvalue spectrum x, not a discrete eigenvalue spectrum?
- Student 2: Yes, you are correct. Actually, you should think of $x_1 = \Delta x$, $x_2 = 2\Delta x$ … etc., and take the limit as $\Delta x \to 0$. I was simply making an analogy with the discrete eigenvalue spectrum case. However, the best way to write $|\Psi\rangle$ when position eigenstates $|x\rangle$ are chosen as the basis vectors is as $\Psi(x)$, which is also called the position space wave function. $\Psi(x)$ is a column vector with position eigenvalues x as a continuous index.

Do you agree with Student 2? Explain your reasoning.

5. Consider the following graphs and statement made by Student A:





- Student A: For a continuous variable like position, the column vector representation $|\Psi\rangle \doteq \begin{pmatrix} \langle x_1|\Psi\rangle \\ \langle x_2|\Psi\rangle \\ \vdots \end{pmatrix}$ is not convenient because we cannot write down an infinite number of components. We can translate from the column vector representation of discrete points (shown in the top figure above) to a continuous set of numbers which is called the quantum mechanical wave function (shown in the bottom figure above). The wave function is an infinite collection of numbers that represents the quantum state vector in terms of position eigenstates.

Explain why you agree or disagree with Student A's statement.

6. Consider the following conversation between three students:
   - Student A: How does the expansion of $|\Psi\rangle$ in terms of a complete set of position eigenstates $|x\rangle$, $|\Psi\rangle = \int_{-\infty}^{\infty} \Psi(x)|x\rangle dx$, help you in questions involving the measurement of the position of the particle?
   - Student B: $|\Psi(x_0)|^2 dx = |\langle x_0|\Psi\rangle|^2 dx$ gives us the probability of finding the particle in a narrow range between x_0 and $x_0 + dx$ when we measure the position of the particle.
   - Student C: But I thought that the probability of finding the particle in a narrow range between x_0 and $x_0 + dx$ was $\int_{x_0}^{x_o+dx} x|\Psi(x)|^2 dx$.
   - Student A: So is the probability of finding the particle in a narrow range between x_0 and $x_0 + dx$ represented mathematically as $\int_{x_0}^{x_o+dx} x|\Psi(x)|^2 dx = x_0|\Psi(x_0)|^2 dx$?
   - Student B: No. It is just $|\Psi(x_0)|^2 dx$ not $x_0|\Psi(x_0)|^2 dx$. $|\Psi(x_0)|^2$ is the probability density at position x_0. We multiply $|\Psi(x_0)|^2$ by a width dx to obtain the probability of finding the particle in a narrow range between x_0 and $x_0 + dx$.

Do you agree with Student B's explanation? Explain your reasoning.

7. Write the generic state vector $|\Psi\rangle$ as a column vector in the momentum representation when momentum eigenstates $|p\rangle$ are chosen as basis vectors.

8. Write the probability of finding the particle with a momentum between p_0 and $p_0 + dp$ when we measure the momentum of the particle.

Position and Momentum Eigenstates

❖ **Position eigenstates**

- The following questions about position eigenstates in position and momentum representation and the position operator in position representation will help you determine the functions in the shaded boxes in the table below:

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)		
Momentum eigenstates (or momentum eigenfunctions)		
Position operator $\hat{x}$		
Momentum operator $\hat{p}$		
$\hat{Q}\|x'\rangle$		
$\hat{Q}\|p'\rangle$		
$\hat{Q}\|\Psi\rangle$		

9. Choose all of the following equations that are correct for the position eigenstate $|x'\rangle$ with eigenvalue x'.

(I) $\hat{x}|x'\rangle = x'|x'\rangle$

(II) $\langle x|\hat{x}|x'\rangle = x'\langle x|x'\rangle = x'\delta(x - x')$

(III) $\langle x|\hat{x}|x'\rangle = x\delta(x - x') = x'\delta(x - x')$

(a) (I) and (II) only

(b) (I) and (III) only

(c) (II) and (III) only

(d) All of the above.

10. Consider the following conversation between Student A and Student B.

- Student B**:** I don't understand how $\hat{x}|x'\rangle = x'|x'\rangle$ and $\langle x|\hat{x}|x'\rangle = x\delta(x-x') = x'\delta(x-x')$ can both be correct. They are two different eigenvalue equations for the same operator $\hat{x}$, so shouldn't one of them be incorrect?
- Student A**:** Actually, $\hat{x}|x'\rangle = x'|x'\rangle$ and $x\delta(x-x') = x'\delta(x-x')$ convey the same information. The former is the eigenvalue equation for the position operator $\hat{x}$ in Dirac notation, and the latter is the eigenvalue equation for the position operator in the position representation. In the position representation, $\hat{x}$ is equivalent to a multiplication by x. We can also write $\langle x|\hat{x}|x'\rangle = x\delta(x-x') = x'\delta(x-x')$ since $\langle x|x'\rangle = \delta(x-x')$, which is zero for all position eigenvalues except when $x = x'$.

With whom do you agree? Explain.

11. Which one of the following is the eigenstate of position $|x'\rangle$ with eigenvalue x' written in position representation, i.e., $\langle x|x'\rangle$?

    (e) $\langle x|x'\rangle = \Psi(x')$
    (f) $\langle x|x'\rangle = \delta(x-x')$
    (g) $\langle x|x'\rangle = \frac{e^{\frac{ipx\prime}{\hbar}}}{\sqrt{2\pi\hbar}}$
    (h) $\langle x|x'\rangle = \Psi(x)$

    B) The position eigenstate written in position representation (when considered as a function of x) is called the:
    (e) Position eigenfunction in position representation.
    (f) Position eigenfunction in momentum representation.
    (g) Position eigenfunction either in position or momentum representation since the expression for position eigenfunction is the same regardless of the representation.
    (h) None of the above.

12. Consider the following conversation between two students:
    - Student 1: The position eigenfunction should always be a delta function whether we write it in position or momentum representation.
    - Student 2: I disagree. $\langle x|x'\rangle$ cannot be the same as $\langle p|x'\rangle$ because when position eigenstate $|x'\rangle$ with eigenvalue x' is written by choosing position eigenstates $|x\rangle$ as basis vectors, we obtain $\langle x|x'\rangle = \delta(x-x')$ which is the position eigenfunction in the position representation. When the position eigenstate $|x'\rangle$ is written by choosing momentum eigenstates $|p\rangle$ as basis vectors, we obtain $\langle p|x'\rangle$, which is the position eigenfunction in the momentum representation. However, $\langle p|x'\rangle$ is not a delta function. The position eigenfunction is only a delta function in the position representation, but not in the momentum representation.

With whom do you agree? Explain your reasoning.

13. Which one of the following is the eigenstate of position $|x\rangle$ with eigenvalue x written in momentum representation, i.e., $\langle p|x\rangle$ (position eigenfunction in momentum representation)?

(a) $\langle p|x\rangle = \Psi_x(p) = \frac{e^{\frac{-ipx}{\hbar}}}{\sqrt{2\pi\hbar}}$

(b) $\langle p|x\rangle = \Psi_x(p) = \delta(p - x)$

(c) $\langle p|x\rangle = \Psi_x(p) = \delta(p - p')$

(d) $\langle p|x\rangle = \Psi_x(p) = \delta(x - x')$

❖ **Momentum eigenstates**

- So far, you have learned about position eigenstates in position and momentum representation and the position operator in position representation.
- The following questions about momentum eigenstates in position and momentum representation and the momentum operator in position and momentum representation will help you determine the functions in the shaded boxes of the table below:

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)	$\langle x\|x'\rangle = \delta(x - x')$	$\langle p\|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
Momentum eigenstates (or momentum eigenfunctions)		
Position operator $\hat{x}$	x	
Momentum operator $\hat{p}$		
$\hat{Q}\|x'\rangle$		
$\hat{Q}\|p'\rangle$		
$\hat{Q}\|\Psi\rangle$		

14. Which one of the following is the eigenstate of momentum $|p'\rangle$ with eigenvalue p' in momentum representation, i.e., $\langle p|p'\rangle$ (momentum eigenfunction in momentum representation)?

(a) $\langle p|p'\rangle = \Phi(p')$

(b) $\langle p|p'\rangle = \delta(p - p')$

(c) $\langle p|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$

(d) $\langle p|p'\rangle = \frac{e^{\frac{-ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$

15. Choose all of the following equations that are correct for the momentum eigenstate $|p'\rangle$ with eigenvalue p'.

(I) $\hat{p}|p'\rangle = p'|p'\rangle$

(II) $\langle p|\hat{p}|p'\rangle = p'\langle p|p'\rangle = p'\delta(p-p')$

(III) $\langle p|\hat{p}|p'\rangle = p\delta(p-p') = p'\delta(p-p')$

(a) (I) and (II) only
(b) (I) and (III) only
(c) (II) and (III) only
(d) All of the above.

16. Which one of the following is the eigenstate of momentum in position representation, i.e., $\langle x|p\rangle$ (momentum eigenfunction in position representation)?

(a) $\langle x|p\rangle = \Psi_p(x) = \delta(x-x')$
(b) $\langle x|p\rangle = \Psi_p(x) = \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}$
(c) $\langle x|p\rangle = \Psi_p(x) = \delta(p-p')$
(d) $\langle x|p\rangle = \Psi_p(x) = \delta(x-p)$

17. Substitute the expression you chose for the momentum eigenfunction in the position representation in the preceding question and the expression for the momentum operator (one dimensional) in position representation, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, in the eigenvalue equation for momentum, $\hat{p}\Psi_{p'}(x) = p'\Psi_{p'}(x)$, where $\Psi_{p'}(x)$ is the eigenstate of momentum with eigenvalue p' in position representation Check whether the eigenvalue equation is satisfied. If not, correct your answer to the preceding question. Show **all** your work in the space provided below.

18. The eigenstates of a Hermitian operator with different eigenvalues are orthonormal[1] to each other. Position and momentum operators ($\hat{x}$ and $\hat{p}$) each have a continuous eigenvalue spectrum. Assume that the Hamiltonian operator ($\hat{H}$) for a given quantum system has a non-degenerate discrete eigenvalue spectrum. Choose all of the following that are correct about the scalar product of two eigenstates of an operator.

(I) $\langle x|x'\rangle = \delta(x-x')$

(II) $\langle p|p'\rangle = \delta(p-p')$

(III) $\langle E|E'\rangle = \delta_{EE'}$, where E denotes energy.

Note: In more common notation $\langle E|E'\rangle = \delta_{EE'}$ *can be written as* $\langle \Psi_{E_1}|\Psi_{E_2}\rangle = \langle \Psi_1|\Psi_2\rangle = \delta_{12}$, *where* $|E_1\rangle = |\Psi_{E_1}\rangle = |\Psi_1\rangle$.

(a) (III) only
(b) (I) and (II) only
(c) (I) and (III) only
(d) All of the above.

19. Consider the following conversation between two students about a position eigenfunction and a momentum eigenfunction in the position representation:

- Student 1: A position eigenstate is represented in position representation as $\langle x|x'\rangle = \delta(x-x')$ such that

$\delta(x-x')$ is a special type of position space wave function $\Psi(x) = \langle x|\Psi\rangle$ in which position has a definite value of x'.

- Student 2: I agree with you. In addition, a momentum eigenstate is represented in position representation as $\langle x|p'\rangle = \Psi_{p'}(x) = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$. $\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ is another special type of position space wave function $\Psi(x) = \langle x|\Psi\rangle$ where momentum has a definite value p'. Instead of being sharply peaked like a delta function, a momentum eigenfunction in the position representation is spread out as $\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ (which is a linear combination of sine and cosine functions over all position with a definite momentum p' and wave number $k' = \frac{p'}{\hbar}$) and the probability density is uniform.

Do you agree with Student 1, Student 2, both, or neither? Explain your reasoning.

[1] $|x'\rangle$ and $|x\rangle$ or $|p'\rangle$ and $|p\rangle$ are not actually normalized because the inner products are $\langle x|x'\rangle = \delta(x-x')$ and $\langle p|p'\rangle = \delta(p-p')$. $\delta(x-x')$ and $\delta(p-p')$ are not normalized because they diverge when $x = x'$ or $p = p'$, respectively. It is actually the integral over all space of a Dirac delta function that equals 1, e.g., $\int_{-\infty}^{\infty}\delta(x-x')dx = 1$. However, we will ignore these normalization issues for position and momentum eigenstates.

20. Consider the following conversation between two students:
    - Student 1: $\langle p|p'\rangle = \delta(p-p')$ is a special type of momentum space wave function $\Phi(p) = \langle p|\Psi\rangle$, in which momentum has a definite value p'. A momentum eigenfunction in the momentum representation, $\delta(p-p')$, is a very sharply peaked wave function about $p = p'$ in momentum representation.
    - Student 2: I agree with you. In addition, a position eigenstate $|x'\rangle$ with eigenvalue x' represented in momentum representation is $\langle p|x'\rangle = \Phi_{x'}(p) = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$. $\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ is also a special type of momentum space wave function $\Phi(p) = \langle p|\Psi\rangle$ in which position has a definite value x' (x' is fixed in $\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$, which is a function of p).

Do you agree with Student 1, Student 2, neither, or both? Explain your reasoning.

21. Is the position eigenstate (or position eigenfunction) in the momentum representation in the preceding question localized or an extended function of momentum p (consider the real and imaginary parts)? Explain your reasoning.

❖ Position and Momentum Operators

Up to this point, you have learned about

- The position eigenstate in position and momentum representation.
- The position operator in position representation.
- The momentum eigenstate in position and momentum representation.
- The momentum operator in position and momentum representation.
- The following questions will help you determine the position operator $\hat{x}$ in momentum representation (shaded box below).

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)	$\langle x\|x'\rangle = \delta(x-x')$	$\langle p\|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
Momentum eigenstates (or momentum eigenfunctions)	$\langle x\|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|p'\rangle = \delta(p-p')$
Position operator $\hat{x}$	x	
Momentum operator $\hat{p}$	$-i\hbar\frac{\partial}{\partial x}$	p
$\hat{Q}\|x'\rangle$		
$\hat{Q}\|p'\rangle$		
$\hat{Q}\|\Psi\rangle$		

22. You have not yet learned about the position operator in momentum representation. Which one of the following equations would help you identify the position operator $\hat{x}$ in momentum representation?
    (a) $\hat{x}\Psi(x) = x\Psi(x)$, where $\Psi(x) = \langle x|\Psi\rangle$ is a generic state $|\Psi\rangle$ written in position representation.
    (b) $\hat{x}\Phi_{x'}(p) = x'\Phi_{x'}(p)$, where $\Phi_{x'}(p) = \langle p|x'\rangle$ is the position eigenfunction with eigenvalue x' in momentum representation.
    (c) $\hat{x}\Phi(p) = x\Phi(p)$, where $\Phi(p) = \langle p|\Psi\rangle$ is a generic state $|\Psi\rangle$ written in momentum representation.
    (d) $\hat{x}\Psi_{p'}(x) = x'\Psi_{p'}(x)$, where $\Psi_{p'}(x) = \langle x|p'\rangle$ is the momentum eigenfunction with eigenvalue p' in position representation.

23. The correct answer to the preceding question is (b). Consider the eigenvalue equation for the position operator in momentum representation, $\hat{x}\Phi_{x'}(p) = x'\Phi_{x'}(p)$, in which $\Phi_{x'}(p) = \langle p|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ is the position eigenfunction with eigenvalue x' in momentum representation. Which one of the

following must be the position operator in momentum representation to satisfy the eigenvalue equation $\hat{x}\Phi_{x'}(p) = x'\Phi_{x'}(p)$?

(a) x

(b) $i\hbar\frac{\partial}{\partial x}$

(c) $i\hbar\frac{\partial}{\partial p}$

(d) p

24. Substitute in the answer you selected in the preceding question (for the position operator in momentum representation) into the eigenvalue equation for the position operator in momentum representation, $\hat{x}\Phi_{x'}(p) = x'\Phi_{x'}(p)$, in which $\Phi_{x'}(p) = \langle p|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ is the position eigenfunction with eigenvalue x' in momentum representation. Check whether the eigenvalue equation is satisfied. If not, correct your answer to the preceding question. Show **all** your work in the space provided below.

❖ So far, you have been able to fill in the following boxes with the appropriate functional representations. If you did not calculate the correct functions as shown below, go back and check your work.
   - The following questions will help you generalize what you learned about position and momentum operator in position and momentum representation to a generic operator $\hat{Q}$ acting on a position eigenstate $|x'\rangle$, momentum eigenstate $|p'\rangle$, and generic state $|\Psi\rangle$.

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)	$\langle x\|x'\rangle = \delta(x - x')$	$\langle p\|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
Momentum eigenstates (or momentum eigenfunctions)	$\langle x\|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|p'\rangle = \delta(p - p')$
Position operator $\hat{x}$	x	$i\hbar\frac{\partial}{\partial p}$
Momentum operator $\hat{p}$	$-i\hbar\frac{\partial}{\partial x}$	p
$\hat{Q}\|x'\rangle$		
$\hat{Q}\|p'\rangle$		
$\hat{Q}\|\Psi\rangle$		

25. Consider the following conversation between two students:

- Student 1: The position operator $\hat{x}$ acting on a generic state $|\Psi\rangle$ written in Dirac notation without reference to a basis is $\hat{x}|\Psi\rangle$. Suppose we choose a basis in which the eigenstates of position, $|x\rangle$, are chosen as basis vectors. $\hat{x}|\Psi\rangle$ is represented in position representation by taking the scalar product of $\hat{x}|\Psi\rangle$ with $|x\rangle$, like this: $\langle x|\hat{x}|\Psi\rangle = x\Psi(x)$.
- Student 2: I don't see how that is correct. How did the state vector $|\Psi\rangle$ turn into the position space wave function $\Psi(x)$?
- Student 1: Earlier we learned that $\hat{x}|x'\rangle = x'|x'\rangle$ is the eigenvalue equation for the position operator $\hat{x}$ in Dirac notation without reference to a basis. In the position representation, we choose a basis in which the eigenstates of position, $|x\rangle$, are chosen as basis vectors. Then, $\hat{x}|x'\rangle$ is represented by taking the scalar product of $\hat{x}|x'\rangle$ with $|x\rangle$, like this: $\langle x|\hat{x}|x'\rangle = x'\langle x|x'\rangle = x'\delta(x-x')$, where $\langle x|x'\rangle = \delta(x-x')$ is a special type of position space wave function. We can generalize this logic to $\hat{x}|\Psi\rangle$, which is the position operator acting on any generic state $|\Psi\rangle$, as $\langle x|\hat{x}|\Psi\rangle = x\langle x|\Psi\rangle = x\Psi(x)$ in the position representation. Note than $\hat{x}$ can act on $\langle x|$ in $\langle x|\hat{x}|\Psi\rangle$ and give eigenvalue x because $\hat{x}$ is a Hermitian operator.
- Student 3: Or we can insert the identity operator written in terms of position eigenstates $\int_{-\infty}^{\infty}|x'\rangle\langle x'|dx'$ into the expression $\langle x|\hat{x}|\Psi\rangle$, like this: $\int_{-\infty}^{\infty}\langle x|\hat{x}|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} x'\langle x|x'\rangle\langle x'|\Psi\rangle dx' = \int_{-\infty}^{\infty} x'\delta(x-x')\Psi(x')dx' = x\Psi(x)$.
- Student 2: I see. So the position operator $\hat{x}$ acting on a generic wave function $\Psi(x)$ in position representation just amounts to multiplication of $\Psi(x)$ by x.

Do you agree with Student 1 and Student 3's explanations and Student 2's statement? Explain your reasoning.

26. Choose all of the following that correctly describe the momentum operator $\hat{p}$ in position representation acting on a generic position space wave function $\Psi(x)$, i.e., $\hat{p}(x, -i\hbar\frac{\partial}{\partial x})\Psi(x)$.

(I) $\hat{p}\Psi(x) = \hat{p}\langle p|\Psi\rangle$

(II) $\hat{p}\Psi(x) = -i\hbar\frac{\partial}{\partial x}\Psi(x)$

(III) $\hat{p}\Psi(x) = \langle x|\hat{p}|\Psi\rangle$

(IV) $\hat{p}\Psi(x) = \langle p|\hat{p}|\Psi\rangle$

(a) (I) only

(b) (II) only

(c) (I) and (IV) only

(d) (II) and (III) only

27. Consider the following conversation between Student A and Student B:

- Student A: The eigenvalue equation for momentum, $\hat{p}|p'\rangle = p'|p'\rangle$, in position representation when the basis vectors are chosen to be the eigenstates of position, $|x\rangle$, is given by the expression $\langle x|\hat{p}|p'\rangle = p'\langle x|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$. This is because $\langle x|\hat{p}|p'\rangle = \langle x|p'|p'\rangle$, and since p' sandwiched in the middle is a number, we are left with $p'\langle x|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$.
- Student B: I agree with you. But we can also think about it as $\langle x|\hat{p}|p'\rangle = \hat{p}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p'\rangle = -i\hbar\frac{\partial}{\partial x}\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right) = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$, where $\hat{p}\left(x, -i\hbar\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial x}$ is the momentum operator in position representation. Here, $\langle x|p'\rangle = \Psi_{p'}(x) = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ is a momentum eigenfunction with eigenvalue p' in position representation (which is a special type of position space wave function $\Psi(x) = \langle x|\Psi\rangle$, where $|\Psi\rangle = |p'\rangle$, a momentum eigenstate).

Do you agree with Student A and Student B? Explain why or why not.

Note: For a Hermitian operator $\hat{Q}$, the notation $\langle\Psi|\hat{Q}|\Psi\rangle$ with $\hat{Q}$ between two vertical lines is the same as $\langle\Psi|\hat{Q}\Psi\rangle$, i.e., $\langle\Psi|\hat{Q}|\Psi\rangle = \langle\Psi|\hat{Q}\Psi\rangle$ since a Hermitian operator can act forward or backwards on the state. If an operator is not Hermitian (does not correspond to a physical observable), one should assume that the operator acts on the state after it (to the right of the operator) even if the notation $\langle\Psi|\hat{Q}|\Psi\rangle$ is used.

28. Suppose a generic operator $\hat{Q}$ depends only on position and momentum operators. How is $\hat{Q}$ acting on a generic state $|\Psi\rangle$, i.e., $\hat{Q}|\Psi\rangle$, represented in the position representation when basis vectors are chosen to be eigenstates of postion, $|x\rangle$?

(V) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)|\Psi\rangle$

(VI) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}(x, -i\hbar\frac{\partial}{\partial x})\langle x|\Psi\rangle$

(VII) $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$

(VIII) $\langle x|\hat{Q}|\Psi\rangle = x\hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$

(e) (I) and (IV) only
(f) (II) and (III) only
(g) (I), (II), and (III) only
(h) All of the above.

29. Consider the following conversation between two students:

- Student 1: The correct answer for question 28 is (b). It is just like question 27, except question 27 is a special case of question 28.
- Student 2: How is $\langle x|\hat{p}|p'\rangle = p'\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$ similar to $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$?
- Student 1: Well, in question 26, $\langle x|\hat{p}|p'\rangle$ is like $\langle x|\hat{Q}|\Psi\rangle$ because the operator $\hat{p}$ corresponds to $\hat{Q}$ and state $|p'\rangle$ corresponds to state $|\Psi\rangle$. Both $\hat{p}|p'\rangle$ and $\hat{Q}|\Psi\rangle$ are operators acting on a state vector without reference to a basis. When basis vectors are chosen to be eigenstates of position, $|x\rangle$, and we take the scalar product of $\hat{p}|p'\rangle$ or $\hat{Q}|\Psi\rangle$ each with $|x\rangle$, we obtain the respective operators written in position representation acting on the respective position space wave function. The operators and state vectors in each case are represented in position representation by $-i\hbar\frac{\partial}{\partial x}\left(\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}\right)$ and $\hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$. Also, $\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}} = \langle x|p'\rangle$, which is a momentum eigenfunction with eigenvalue p', is a special type of position space wave function $\Psi(x) = \langle x|\Psi\rangle$.

Do you agree with Student 1's explanation? Explain your reasoning.

30. Suppose a generic operator $\hat{Q}$ only depends on the position and momentum operators. How is $\hat{Q}$ acting on a generic state $|\Psi\rangle$, i.e., $\hat{Q}|\Psi\rangle$, representated in the momentum representation when basis vectors are chosen to be eigenstates of momentum, $|p\rangle$?

(I) $\langle p|\hat{Q}|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)|\Psi\rangle$

(II) $\langle p|\hat{Q}|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\langle p|\Psi\rangle$

(III) $\langle p|\hat{Q}|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\Phi(p)$

(IV) $\langle p|\hat{Q}|\Psi\rangle = p\hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\Phi(p)$

(a) (I) and (II) only
(b) (II) and (III) only
(c) (II), (III), and (IV) only
(d) All of the above

31. Consider the following conversation between Student A and Student B:

- Student A: Is $\hat{Q}(x, -i\hbar\frac{\partial}{\partial x})$ the operator $\hat{Q}$ in the position representation, where $\hat{Q}$ is a function of position and momentum operators written in position representation, i.e., x and $-i\hbar\frac{\partial}{\partial x}$, respectively?
- Student B: Yes. Suppose $\hat{Q}$ is the kinetic energy operator. In position representation, $\hat{Q}$ will be $\frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}$, if the particle is confined in one spatial dimension.
- Student A: And if $\hat{Q}$ is the kinetic energy operator in momentum representation, $\hat{Q}$ will be $\frac{\hat{p}^2}{2m} = \frac{p^2}{2m}$, since the momentum operator $\hat{p} = p$ in the momentum representation. In other words, in the momentum representation, momentum operator $\hat{p}$ acting on a state $\Phi(p)$ simply amounts to multiplication of $\Phi(p)$ by p to yield $p\Phi(p)$, i.e., $\hat{p}\Phi(p) = p\,\Phi(p)$.

Do you agree with Student A, Student B, both, or neither? Explain your reasoning.

❖ So far, you have learned about
  - The position eigenstates in position and momentum representation.
  - The momentum eigenstates in position and momentum representation.
  - The position operator $\hat{x}$ in position and momentum representation.
  - The momentum operator $\hat{p}$ in position and momentum representation.
  - A generic operator $\hat{Q}$ in position and momentum representation.
  - If you did not calculate the correct functions as shown in the table below, go back and check your work.

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)	$\langle x\|x'\rangle = \delta(x - x')$	$\langle p\|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
Momentum eigenstates (or momentum eigenfunctions)	$\langle x\|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|p'\rangle = \delta(p - p')$
Position operator $\hat{x}$	x	$i\hbar\frac{\partial}{\partial p}$
Momentum operator $\hat{p}$	$-i\hbar\frac{\partial}{\partial x}$	p
$\hat{Q}\|x'\rangle$	$\langle x\|\hat{Q}\|x'\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\langle x\|x'\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\delta(x - x')$	$\langle p\|\hat{Q}\|x'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\langle p\|x'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
$\hat{Q}\|p'\rangle$	$\langle x\|\hat{Q}\|p'\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\langle x\|p'\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|\hat{Q}\|p'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\langle p\|p'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\delta(p - p')$
$\hat{Q}\|\Psi\rangle$	$\langle x\|\hat{Q}\|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\langle x\|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$	$\langle p\|\hat{Q}\|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\langle p\|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\Phi(p)$

❖ **For a generic state $|\Psi\rangle$, momentum space wave function $\Phi(p)$ and position space wave function $\Psi(x)$ are a Fourier transform and inverse Fourier transform of each other, respectively.**

Problem: Show that the momentum space wave function $\Phi(p)$ is the Fourier transform of the position space wave function $\Psi(x)$. The Fourier transform of a general function $f(x)$ is $g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)dx$.

The problem has been broken down into several multiple choice questions to guide your solution.

32. Which one of the following is the correct expression for $\Phi(p)$?

    (a) $\langle x|p\rangle$
    (b) $\langle p|\Psi\rangle$
    (c) $\langle p|x\rangle$
    (d) $\langle \Psi|p\rangle$

33. Using the completeness relation, insert a complete set of **position eigenstates** into the momentum space wave function, $\langle p|\Psi\rangle$. What do you obtain?

    (a) $\int_{-\infty}^{\infty} dx\langle p|p\rangle\langle p|\Psi\rangle$
    (b) $\int_{-\infty}^{\infty} dx\langle p|x\rangle\langle x|\Psi\rangle$
    (c) $\int_{-\infty}^{\infty} dp\langle p|x\rangle\langle x|\Psi\rangle$
    (d) $\int_{-\infty}^{\infty} dp\langle p|p\rangle\langle p|\Psi\rangle$

34. The expression after you insert the complete set $\hat{I} = \int_{-\infty}^{\infty} |x\rangle\langle x|dx$ should be $\int_{-\infty}^{\infty} dx\langle p|x\rangle\langle x|\Psi\rangle$. What is $\langle p|x\rangle$? You can go back to question **11** for help.

35. Rewrite the expression $\int_{-\infty}^{\infty} dx\langle p|x\rangle\langle x|\Psi\rangle$, using your answer to the preceding question in place of $\langle p|x\rangle$.

36. Rewrite your answer to the preceding question replacing $\langle x|\Psi\rangle$ with $\Psi(x)$, since $\Psi(x) = \langle x|\Psi\rangle$ is the most common notation for the wave function in position representation.

37. The Fourier transform of a general function $f(x)$ is $g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)dx$. Compare this with your answer to the preceding question. The two expressions are analogous. *(Hint: Using the de Broglie relation, one can show that $p = \hbar k$, where p is the momentum and k is the wave number.)*

Summary: Connecting Dirac notation with function space (position and momentum representation)

- **Relationship between state vector $|\Psi\rangle$ and the wave function**
  - $\Psi(x) = \langle x|\Psi\rangle$ is the representation of the state vector $|\Psi\rangle$ in the position representation (when a complete set of eigenstates of position $|x\rangle$ are chosen as basis vectors, i.e., $|\Psi\rangle = \int_{-\infty}^{\infty} \Psi(x)|x\rangle dx$) and is called the *position space wave function*.
  - $\Phi(p) = \langle p|\Psi\rangle$ is the representation of the state vector $|\Psi\rangle$ in the momentum representation (when a complete set of eigenstates of momentum $|p\rangle$ are chosen as basis vectors, i.e., $|\Psi\rangle = \int_{-\infty}^{\infty} \Phi(p)|p\rangle dp$) and is called the *momentum space wave function*.
  - The position space wave function $\Psi(x)$ and momentum space wave function $\Phi(p)$ can be represented as infinite dimensional column vectors in the position and momentum representation, respectively.
  - The momentum space wave function $\Phi(p) = \langle p|\Psi\rangle$ and position space wave function $\Psi(x) = \langle x|\Psi\rangle$ are a Fourier transform and inverse Fourier transform of each other, respectively.
- **Position and momentum eigenstates**
  - The position eigenstates with eigenvalue x' can be written as:
    - $|x'\rangle$ in Dirac notation without reference to a basis.
    - $\langle x|x'\rangle = \delta(x - x')$ in position representation.
    - $\langle p|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ in momentum representation.
  - The momentum eigenstates with eigenvalue p' can be written as:
    - $|p'\rangle$ in Dirac notation without reference to a basis.
    - $\langle x|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$ in the position representation.
    - $\langle p|p'\rangle = \delta(p - p')$ in the momentum representation.
- **$\hat{Q}|\Psi\rangle$ in position and momentum representations**
  - For a generic state $|\Psi\rangle$ and generic operator $\hat{Q}$ which depends only on $\hat{x}$ and $\hat{p}$:
    - $\hat{Q}|\Psi\rangle$ is represented by $\langle x|\hat{Q}|\Psi\rangle$ in the **position** representation, which is by definition $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$, where $\Psi(x) = \langle x|\Psi\rangle$.
    - $\hat{Q}|\Psi\rangle$ is represented by $\langle p|\hat{Q}|\Psi\rangle$ in the **momentum** representation, which is by definition $\langle p|\hat{Q}|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p}, p\right)\Phi(p)$, where $\Phi(p) = \langle p|\Psi\rangle$.
  - Special cases of $\hat{Q}$ in position and momentum representations:
    - $\hat{Q} = \hat{x}$
      - Position representation: $\langle x|\hat{x}|\Psi\rangle = \hat{x}(x, -i\hbar\frac{\partial}{\partial x})\langle x|\Psi\rangle = x\Psi(x)$
      - Momentum representation: $\langle p|\hat{x}|\Psi\rangle = \hat{x}(i\hbar\frac{\partial}{\partial p}, p)\langle p|\Psi\rangle = i\hbar\frac{\partial}{\partial p}\Phi(p)$
    - $\hat{Q} = \hat{p}$
      - Position representation: $\langle x|\hat{p}|\Psi\rangle = \hat{p}(x, -i\hbar\frac{\partial}{\partial x})\langle x|\Psi\rangle = -i\hbar\frac{\partial}{\partial x}\Psi(x)$
      - Momentum representation: $\langle p|\hat{p}|\Psi\rangle = \hat{p}(i\hbar\frac{\partial}{\partial p}, p)\langle p|\Psi\rangle = p\Phi(p)$

	Position representation	Momentum representation
Position eigenstates (or position eigenfunctions)	$\langle x\|x'\rangle = \delta(x-x')$	$\langle p\|x'\rangle = \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
Momentum eigenstates (or momentum eigenfunctions)	$\langle x\|p'\rangle = \frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|p'\rangle = \delta(p-p')$
Position operator $\hat{x}$	x	$i\hbar\frac{\partial}{\partial p}$
Momentum operator $\hat{p}$	$-i\hbar\frac{\partial}{\partial x}$	p
$\hat{Q}\|x'\rangle$	$\langle x\|\hat{Q}\|x'\rangle = \hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\langle x\|x'\rangle =$ $\hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\delta(x-x')$	$\langle p\|\hat{Q}\|x'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\langle p\|x'\rangle =$ $\hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$
$\hat{Q}\|p'\rangle$	$\langle x\|\hat{Q}\|p'\rangle = \hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\langle x\|p'\rangle =$ $\hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|\hat{Q}\|p'\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\langle p\|p'\rangle =$ $\hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\delta(p-p')$
$\hat{Q}\|\Psi\rangle$	$\langle x\|\hat{Q}\|\Psi\rangle = \hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\langle x\|\Psi\rangle =$ $\hat{Q}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$	$\langle p\|\hat{Q}\|\Psi\rangle = \hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\langle p\|\Psi\rangle =$ $\hat{Q}\left(i\hbar\frac{\partial}{\partial p},p\right)\Phi(p)$

	Position representation	Momentum representation
Special Case: $\hat{Q} = \hat{x}$		
$\hat{x}\|x'\rangle$	$\langle x\|\hat{x}\|x'\rangle = x'\langle x\|x'\rangle = x'\delta(x-x') = x\delta(x-x')$	$\langle p\|\hat{x}\|x'\rangle = i\hbar\frac{\partial}{\partial p}\langle p\|x'\rangle = i\hbar\frac{\partial}{\partial p}\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}} = x'\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ •
$\hat{x}\|p'\rangle$	• $\langle x\|\hat{x}\|p'\rangle = x\langle x\|p'\rangle = x\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|\hat{x}\|p'\rangle = i\hbar\frac{\partial}{\partial p}\langle p\|p'\rangle = i\hbar\frac{\partial}{\partial p}\delta(p-p')$ •
$\hat{x}\|\Psi\rangle$	• $\langle x\|\hat{x}\|\Psi\rangle = x\langle x\|\Psi\rangle = x\Psi(x)$	• $\langle p\|\hat{x}\|\Psi\rangle = i\hbar\frac{\partial}{\partial p}\langle p\|\Psi\rangle = i\hbar\frac{\partial}{\partial p}\Phi(p)$
Special Case: $\hat{Q} = \hat{p}$	•	•
$\hat{p}\|x'\rangle$	$\langle x\|\hat{p}\|x'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x\|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x')$	• $\langle p\|\hat{p}\|x'\rangle = p\langle p\|x'\rangle = p\frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$ •
$\hat{p}\|p'\rangle$	• $\langle x\|\hat{p}\|p'\rangle = p'\langle x\|p'\rangle = p'\frac{e^{\frac{ip'x}{\hbar}}}{\sqrt{2\pi\hbar}}$	$\langle p\|\hat{p}\|p'\rangle = p'\langle p\|p'\rangle = p'\delta(p-p') = p\delta(p-p')$ •
$\hat{p}\|\Psi\rangle$	$\langle x\|\hat{p}\|\Psi\rangle = -i\hbar\frac{\partial}{\partial x}\langle x\|\Psi\rangle = -i\hbar\frac{\partial}{\partial x}\Psi(x)$	$\langle p\|\hat{p}\|\Psi\rangle = p\langle p\|\Psi\rangle = p\Phi(p)$

Hamiltonian operator for a given quantum system and its eigenstates (energy eigenstates)

38. For a given quantum system, what is $\hat{H}$ acting on an energy eigenstate $|\psi_n\rangle$ (also represented by $|E_n\rangle$ or $|\Psi_{E_n}\rangle$) equal to?

    (a) $\hat{H}|\psi_n\rangle = E|\psi_n\rangle$, where E is the average of all possible energies of the system.
    (b) $\hat{H}|\psi_n\rangle = \sum_n E_n |\psi_n\rangle$, where E_n is the energy of the n^{th} state.
    (c) $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, , where E_n is the energy of the n^{th} state.
    (d) None of the above. The Hamiltonian of a system must be known explicitly to determine the answer.

39. Consider the following conversation between Student A and Student B about the preceding question (the symbols have the same meaning as in the preceding question):

    - Student A**:** The answer should be choice (d) for the previous question. The Hamiltonian $\hat{H}$ describes the system, and we cannot determine what will happen without knowing $\hat{H}$ explicitly.
    - Student B**:** I agree. But this time we are given that $|\psi_n\rangle$ are the energy eigenstates. Energy eigenstates $|\psi_n\rangle$ are the eigenstates of the Hamiltonian $\hat{H}$. Any operator acting on one of its eigenstates will give the same state back with the corresponding eigenvalue.
    - Student A: Right. So we do need to know the Hamiltonian $\hat{H}$ of a system to calculate the energy eigenstates $|\psi_n\rangle$ and eigenvalues E_n.
    - Student B: Yes. We would need the Hamiltonian $\hat{H}$ for a given quantum system to calculate the energy eigenstates $|\psi_n\rangle$ and eigenvalues E_n explicitly, but we are asked to select an expression for the eigenvalue equation for $\hat{H}$. The expression in choice (c) is correct, even though we don't know what the explicit $|\psi_n\rangle$'s and E_n's are without knowing the Hamiltonian $\hat{H}$.

With whom do you agree? Explain.

40. Consider the following conversation between Student A and Student B:
    - Student A: The eigenvalue equation for a Hamiltonian $\hat{H}$ without choosing a basis (e.g., position or momentum representation) is $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$. $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ can be written in position representation as $\hat{H}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi_n(x) = E_n\Psi_n(x)$. We can see this by taking the inner product of $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ with $\langle x|$, like this: $\langle x|\hat{H}|\Psi_n\rangle = \langle x|E_n|\Psi_n\rangle$. Using the fact that $\langle x|\hat{Q}|\Psi\rangle = \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\langle x|\Psi\rangle = \hat{Q}(x, -i\hbar\frac{\partial}{\partial x})\Psi(x)$ for any generic operator $\hat{Q}$ and state $|\Psi\rangle$, $\langle x|\hat{H}|\Psi_n\rangle = \langle x|E_n|\Psi_n\rangle$ can be written as $\hat{H}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi_n(x) = E_n\Psi_n(x)$.
    - Student B: I disagree with you. We can't write the eigenvalue equation for the Hamiltonian $\hat{H}$ as $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ because we don't know the Hamiltonian explicitly. Also, we can't write the Hamiltonian in terms of $\hat{x}$ and $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ as $\hat{H}(x, -i\hbar\frac{\partial}{\partial x})$ if we don't know the Hamiltonian explicitly.

With whom do you agree? Explain your reasoning below.

Problem: Show that the expectation value of energy in a generic state $|\Psi\rangle$ of the system is

$\langle\Psi|\hat{H}|\Psi\rangle = \sum_n |C_n|^2 E_n$, where C_n ($n = 1,2,3 \ldots \infty$) are the coefficients in the expansion $|\Psi\rangle = \sum_{n=1}^{\infty} C_n |\Psi_n\rangle$. E_n is the eigenvalue for the n^{th} energy eigenstate $|\Psi_n\rangle$.

The problem has been broken down into several multiple choice questions to guide your solution.

41. Student A uses the completeness relation and inserts a complete set of energy eigenstates $|\Psi_n\rangle$, where $n = 1,2,3 \ldots \infty$, into the expression for the expectation value $\langle\Psi|\hat{H}|\Psi\rangle$, so that it becomes $\sum_n \langle\Psi|\hat{H}|\psi_n\rangle\langle\psi_n|\Psi\rangle$. Choose all of the following statements that are correct about the new expression $\sum_n \langle\Psi|\hat{H}|\psi_n\rangle\langle\psi_n|\Psi\rangle$.

    (I) It is the same as the expression $\langle\Psi|\hat{H}|\Psi\rangle$, because $\sum_n |\psi_n\rangle\langle\psi_n|$ is equal to the identity operator.

    (II) One can use $\langle\Psi|\hat{H}|\Psi\rangle$ and $\sum_n \langle\Psi|\hat{H}|\psi_n\rangle\langle\psi_n|\Psi\rangle$ interchangeably based upon convenience because they are equal.

    (III) $\sum_n |\psi_n\rangle\langle\psi_n|$ is an operator, so it changes the expression when you insert it in the middle in $\langle\Psi|\hat{H}|\Psi\rangle$. Thus, the new expression is not the same as the old expression.

    (a) (I) only
    (b) (II) only
    (c) (III) only
    (d) (I) and (II) only

42. Choose all of the following statements that are correct.

    (I) $\sum_n \langle\Psi|\hat{H}|\psi_n\rangle\langle\psi_n|\Psi\rangle = \sum_n E_n \langle\Psi|\psi_n\rangle\langle\psi_n|\Psi\rangle$, because $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ and E_n is a number that can be pulled out of the inner product.

    (II) $\langle\Psi|\psi_n\rangle = \langle\psi_n|\Psi\rangle^*$.

    (III) $C_n = \langle\psi_n|\Psi\rangle$ (where $|\Psi\rangle = \sum_{n=1}^{\infty} C_n|\Psi_n\rangle$).

    (a) (I) and (II) only
    (b) (I) and (III) only
    (c) (II) and (III) only
    (d) All of the above.

43. Use your answers to the four preceding questions to show that $\langle\Psi|\hat{H}|\Psi\rangle = \sum_n |\langle\psi_n|\Psi\rangle|^2 E_n = \sum_n |C_n|^2 E_n$.

Summary of the Hamiltonian operator for a given quantum system with a non-degenerate, discrete eigenvalue spectrum:

- The result of the Hamiltonian operator $\hat{H}$ for a given system acting on an energy eigenstate state is given by the eigenvalue equation $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$. In position representation, the eigenvalue equation for the Hamiltonian operator can be written as $\hat{H}\left(x, -i\hbar\frac{\partial}{\partial x}\right)\Psi_n(x) = E_n\Psi_n(x)$.
- The expectation value of energy in a generic state $|\Psi\rangle$ is $\langle\Psi|\hat{H}|\Psi\rangle = \sum_n |C_n|^2 E_n$, where $C_n = \langle\Psi_n|\Psi\rangle$ is the coefficient in the expansion $|\Psi\rangle = \sum_{n=1}^{\infty} C_n|\Psi_n\rangle$ and E_n is the eigenvalue of the n^{th} energy eigenstate $|\Psi_n\rangle$.

Checkpoint

Consider the following statement about a particle in a one dimensional infinite square well:

a) If the state of the system at time $t = 0$ is $|\Psi\rangle = \frac{1}{\sqrt{2}}[|\Psi_1\rangle + |\Psi_2\rangle]$, in which $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are the lowest two energy eigenstates (ground state and first excited state with energy eigenvalues E_1 and E_2, respectively), $|\Psi\rangle$ satisfies the eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$.

Explain why you agree or disagree with this statement.

b) Work out $\hat{H}|\Psi\rangle$ for $|\Psi\rangle = \frac{1}{\sqrt{2}}[|\Psi_1\rangle + |\Psi_2\rangle]$ to check whether it satisfies the energy eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$.

Answer to Checkpoints

a. Disagree. It is not an eigenstate of the Hamiltonian (not a stationary state).

b. $\hat{H}|\Psi\rangle = \hat{H}(\frac{1}{\sqrt{2}}[|\Psi_1\rangle + |\Psi_2\rangle]) = \frac{1}{\sqrt{2}}[E_1|\Psi_1\rangle + E_2|\Psi_2\rangle] \neq E\hat{H}(\frac{1}{\sqrt{2}}[|\Psi_1\rangle + |\Psi_2\rangle]) \neq E|\Psi\rangle$

6.0 DEVELOPING AND EVALUATING AN INTERACTIVE TUTORIAL ON MACH-ZEHNDER INTERFEROMETER WITH SINGLE PHOTONS

6.1 INTRODUCTION

Quantum mechanics can be a challenging subject for students partly because it is unintuitive and abstract [1-6]. An experiment which has been conducted in undergraduate laboratories to illustrate fundamental principles of quantum mechanics involves the Mach-Zehnder Interferometer (MZI) with single photons [7]. We are developing and evaluating a quantum interactive learning tutorial (QuILT) using gedanken (thought) experiments and simulations involving a MZI with single photons. The QuILT focuses on helping students learn topics such as the wave-particle duality, interference of a single photon with itself, probabilistic nature of quantum measurements, and the collapse of a quantum state upon measurement. Students also learn how photo-detectors and optical elements such as beam splitters in the path of the MZI with single photons affect the measurement outcomes.

Figure 6-1 shows the MZI setup. For simplicity, the following assumptions are made: 1) all optical elements are ideal; 2) the non-polarizing beam splitters (BS1 and BS2) are infinitesimally thin such that there is no phase shift when a single photon propagates through them; 3) the monochromatic +45º polarized single photons travel the same distance in vacuum in the upper path (U) and lower path (L) of the MZI; and 4) the initial MZI without the phase shifter is set up such that there is completely constructive interference at detector 1 (D1) and destructive interference at detector 2 (D2).

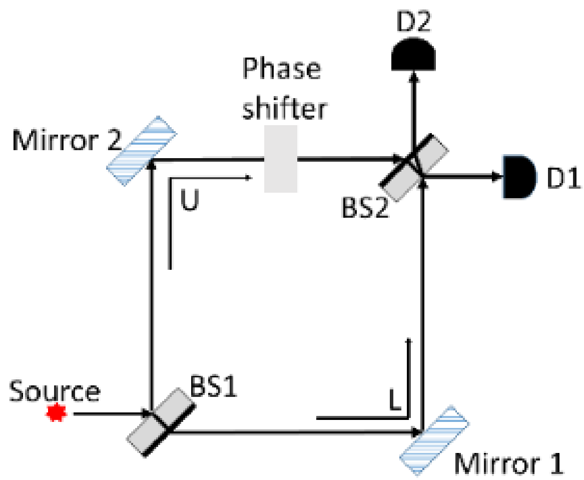


Figure 6-1. MZI setup with a phase shifter in the U path

If a single photon is emitted from the source in Figure 6-1, BS1 causes the photon to be in a superposition of the path states U and L. The photon path states reflect off the mirrors and recombine in BS2. BS2 mixes the photon path states such that both components of the photon path state can be projected into D1 and D2. The projection of both components leads to interference at the detectors. Depending on the thickness of the phase shifter, interference observed at detectors D1 and D2 can be constructive, destructive, or intermediate. Observing interference of a single photon with itself at D1 and D2 can be interpreted in terms of not having "which-path" information (WPI) about the single photon [7]. WPI is a common terminology associated with these types of experiments popularized by Wheeler [8]. WPI is unknown (as in the setup shown in Fig. 6-1) if both components of the photon path state can be projected into D1 and D2 and the projection of both components at each detector leads to interference. When WPI is unknown and a large number of single photons are sent through the setup, if a phase shifter is inserted in one of the paths of the MZI (as in the U path in Fig. 6-1) and its thickness is varied, the probability of photons arriving at

D1 and D2 will change with the thickness of the phase shifter due to interference of the components of the single photon state from the U and L paths.

On the other hand, if the components of the photon path state are not recombined, there is no possibility for interference of the photon path states to occur at the detectors. In this case, WPI is known about a photon. WPI is "known" about a photon if only one component of the photon path state can be projected into D1 and D2. For example, if BS2 is removed from the setup (see Fig. 6-2), WPI is known for all single photons arriving at the detectors because only the component of a photon state along the U path can be projected in D1 and only the component of a photon state along the L path can be projected in D2. When WPI is known, each detector (D1 and D2) has an equal probability of clicking. A detector clicks when a photon is detected by it and is absorbed (the state of the single photon collapses, i.e., the single photon state is no longer in a superposition of the U and L path states). However, when WPI is known, there is no way to know a priori which detector will click when a photon is sent until the photon state collapses either at D1 or at D2 with equal likelihood. When WPI is known, changing the thickness of a phase shifter in one of the paths does not affect the probability of each detector clicking when photons are registered (equal probability for all thicknesses of phase shifter) [7].

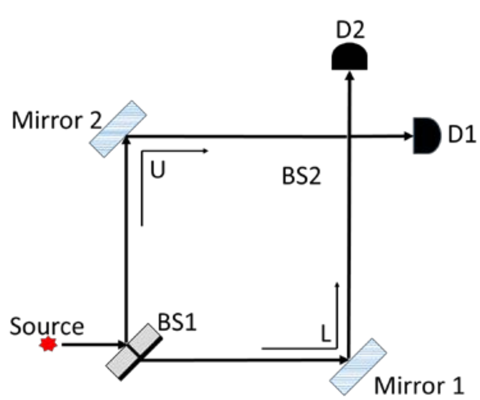


Figure 6-2. MZI setup with beam-splitter 2 (BS2) removed

6.2 METHODOLOGY FOR THE INVESTIGATION OF STUDENT DIFFICULTIES

Student difficulties with the MZI with single photons were investigated by administering open-ended questions to upper-level undergraduate and graduate students and conducting individual interviews with 15 students in quantum mechanics courses after traditional instruction in relevant concepts. The open-ended questions were graded using rubrics which were developed by two of the investigators together. A subset of the open-ended questions were graded separately by the investigators. After comparing the grading of the open-ended questions, the investigators had an inter-rater reliability of 70%. The investigators discussed any disagreements in grading and resolved them. The final inter-rater reliability is better than 90%.

The individual interviews used a think-aloud protocol to better understand the rationale for student responses before, during, and after the development of different versions of the MZI tutorial and the corresponding pre-test and post-test. During the semi-structured interviews, students were asked to verbalize their thoughts while they answered questions. During the interviews, we provided students with a pen and paper and asked them to “think aloud” [9] while answering the questions. Students first read the questions on their own and answered them without interruptions except that we prompted them 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, we asked them to further clarify and elaborate issues that they had not clearly addressed earlier.

6.3 STUDENT DIFFICULTIES

During the preliminary development of the QuILT, we investigated the difficulties students have with the relevant concepts including the wave-particle duality of a photon, interference of a single photon with itself, probabilistic nature of quantum measurements, and the collapse of a quantum state upon measurement in order to effectively address them. As noted, we conducted 15 individual semi-structured, think-aloud interviews with upper-level undergraduate and graduate students using different versions of an open-ended survey or earlier versions of the QuILT in which students were first asked to think aloud as they answered the questions related to the setup (including those with and without the beam splitter BS2) to the best of their ability without being disturbed. Later, we probed students further and asked them for clarification of points they had not made clear. Since both undergraduate and graduate students exhibited the same difficulties, we will not differentiate between the two groups further. Some of the common difficulties found in the interviews included students struggling with the interference of a classical beam of light through the MZI, ignoring the wave nature of single photons, claiming that a photon is split into two photons after BS1 (see Fig. 6-1), and how BS2 affects measurement outcomes.

Difficulty with the interference of light waves at detectors after passing through the MZI: Interviews suggest that many students did not take into account the interference phenomenon of a classical beam of light. For example, regarding a beam of light with intensity I propagating through the setup shown in Fig. 6-1, one student stated: “There will be billions of photon[s] in one beam so… approximately half go through U and half go through L. When going through BS2 they also have equal chance to reach D1 [and] D2. So the [intensity] on each [detector] will be $I/2$.” Further probing indicates that students with these types of responses had some idea that a beam of light can be treated as a stream of photons but they often failed to invoke the wave nature of light which would lead, e.g., to constructive interference at D1 and destructive interference at D2 for the setup without a phase shifter.

In addition to difficulties involving the intensity of a light beam through the MZI, students also had difficulty reasoning about a large number of single photons emitted from the source and how the single photons would propagate through the MZI. Students were asked to explain why they agreed or disagreed with the statement for the setup shown in Fig. 6-1: "If the source emits N photons one at a time, the number of photons reaching detectors D1 and D2 will be $N/2$ each." Many students agreed with this statement. For example, one student stated, "I agree because the photon has equal probability of reflecting or transmitting when it hits the beam splitter." Students with this type of response had difficulty reasoning about how the beam splitter causes a photon to be in a superposition of the U and L path states. They also did not take into account the phase shifts of each photon path component and how the phase difference between the U and L paths causes constructive and destructive interference at the detectors.

Difficulties due to a single photon as a point particle model: Students struggled with the concept of the wave/particle duality of a single photon and the fact that interference can be observed at the detectors due to a single photon state from the two paths (e.g., in Fig. 6-1, the photon state is in a superposition of the U and L path states after BS1 which can interfere at the detectors D1 and D2). Students often treated a single photon as a point particle, ignoring the wave-like nature of a single photon through the MZI. Some students claimed that a single photon can be split into two parts and it is the two photons that interfere at the detectors (instead of the fact that interference is due to the wave nature of single photons). For example, one student said "it seems like [each photon with half of the energy of the incoming photon traveling along the U and L paths of the MZI is] the only way for a photon to interfere with itself and have some probability of going through either path until getting measured." Other students claimed that neither the photon nor its energy will be split in half after BS1, but that each photon is localized in either the U or L path. These types of reasoning difficulties indicate that students struggled with the fact that a single photon can behave as a wave passing through the MZI and be in a superposition of U and L path states until a measurement is performed, e.g., at the detectors D1 and D2, and the state collapses.

Difficulty with the role of BS2: Several students claimed that either removing or inserting BS2 will not change the probability of the single photons arriving at each detector. For example, one student supplemented his claim as follows: "I don't see how BS2 affects/causes any asymmetry to make probabilities D1≠D2 or how BS2 causes a loss of photons." Another student who made similar claims about what happens at the detectors with and without BS2 stated, "I say still 50% each since it's symmetric." Students who treated a single photon as a point particle and ignored its wave nature did not take into account the phase shifts affecting the components of the photon state along the U and L paths due to BS1 and BS2 (e.g., in Fig. 6-1) which influence the interference of the single photons at the detectors D1 and D2.

Difficulty with how a detector collapses the single photon state: Students often asserted that inserting an additional detector in the U or L path of the MZI would not affect the interference at the detectors D1 and D2 at the end. They had difficulty with the fact that an additional detector, e.g., in the L path of the MZI in Figure 6-1, would collapse the state of the photon to the U or L path state so that D1 or D2 click with equal probability and the interference is destroyed. Instead, many students claimed that the photon state would remain delocalized in a superposition of the U and L path states (as in Fig. 6-1) and interference would be observed at D1 and D2. Some students correctly stated that a detector placed in the L path would absorb some photons but incorrectly inferred that there would still be interference displayed by the photons that reach D1 and/or D2. For example, one student said "Now path L is blocked [by a detector in the L path], so only ½ as many photons should hit the [detector D1 or D2 at the end]. I don't see how there can be any but constructive interference since path lengths are the same." Further probing of students with these types of responses suggests that they struggled with how placing a detector in the U or L path amounts to a measurement and destroys the delocalized single photon state which was in a superposition of the U and L path states before the measurement.

6.4 QUILT DEVELOPMENT (WARM-UP AND CONCEPTUAL TUTORIAL)

The difficulties discussed above indicate that even after traditional instruction, upper-level undergraduate and graduate students would benefit from a tutorial-based approach to better learn the concepts involving a single photon propagating through a MZI. Given the common difficulties exhibited, we developed a Quantum Interactive Learning Tutorial (QuILT) on the MZI with single photons. The QuILT includes a warm-up and a tutorial which helps students learn these concepts. It makes use of a computer simulation in which students can manipulate the MZI setup to predict and observe what happens at the detectors for different setups. The QuILT can be used in class to give students an opportunity to work together and check their answers with a partner.

The MZI with single photons QuILT builds on students' prior knowledge and was developed by taking into account the difficulties discussed above. The development of the QuILT was a cyclical, iterative process which included the following stages: 1) development of a preliminary version of the QuILT based on the research on student difficulties; 2) implementation and evaluation of the QuILT by administering it to individual students and measuring its effectiveness via pre-/post-tests; and 3) refinement and modifications based upon the feedback from the implementation and evaluation. The QuILT was also iterated with four faculty members and two graduate students to ensure that the content and wording of the questions are appropriate. We administered the QuILT to several graduate students and upper-level undergraduate students to ensure that the guided approach is effective and the questions were unambiguously interpreted. Modifications were made based upon the feedback. When the QuILT proved to be effective in individual administration and students' pre-/post-test performance showed significant improvement, it was administered to students in two upper-level undergraduate quantum mechanics courses ($N = 44$) and graduate students who were enrolled in the first semester of a graduate level quantum mechanics course ($N = 45$).

To evaluate the effectiveness of the QuILT, a pretest was administered to 44 upper-level undergraduate students in junior/senior level quantum mechanics courses and 45 graduate students enrolled in the first semester of a graduate level quantum mechanics course. After the students completed the pretest, they were given one week to work through the QuILT and were then given a posttest. Any students who did not work through the QuILT for any reason were omitted from the posttest data. The graduate students were enrolled in a teaching assistant training class, during which they learned about instructional strategies for teaching introductory physics courses. They were asked to work through the MZI conceptual tutorial to learn about the effectiveness of tutorials. They were given credit for completing the pretest, conceptual tutorial, and posttest. However, their performance on the posttest was not part of the final grade for the teaching assistant training class.

6.4.1 MZI with Single Photons-Warm-up

The MZI with single photons warm-up helps students review the interference at the detectors due to the superposition of light from two paths of the MZI in a classical situation. It uses the analogy of a wave pulse on a rope which is either reflected or transmitted, depending on the physical properties of the rope. Students are then guided to reason about the reflection, transmission, and propagation of electromagnetic waves through different media.

For example, one of the questions helps students to reason about the reflection of a wave pulse at a fixed end:

A rope has a fixed end because it is tied to a pillar at that end. You hold the other end and give the rope a sudden jerk to produce a pulse. The pulse travels towards the fixed end and reflects back. Which of the following is true for the reflected pulse due to reflection at the fixed end?

(a) *It is inverted.*
(b) *It is upright (not inverted).*
(c) *There is no reflected pulse.*
(d) *None of the above.*

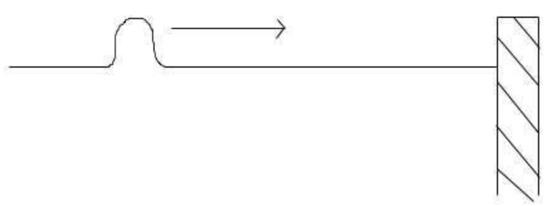


Figure 6-3. Reflection of a wave pulse on a rope

Other questions help students reason about the phase shifts of a wave propagating through a medium as in the following example:

You give the rope a sudden jerk to produce a pulse in the lower density rope. The pulse travels towards your friend and partly gets transmitted to the higher density rope. Which one of the following phase shifts is introduced in the transmitted pulse at the interface? (Hint: Think about whether there can be any discontinuity in the wave profile as it gets transmitted at the interface.)

a) zero
b) π/2
c) π
d) None of the above.

Figure 6-4. Transmission of a wave pulse through ropes of different densities. $\boldsymbol{\rho_L}$ denotes the density of lower density rope and $\boldsymbol{\rho_H}$ denotes the density in the higher density rope.

Students are also given checkpoints which help them think about the correct answer. For example, after the question shown above, students are given the following checkpoint:

The transmitted pulse is upright (not inverted) and in terms of sinusoidal waves this corresponds to a phase shift of zero.

Students are then guided to reason about the parallels between the wave pulse on the rope and an electromagnetic wave propagating through different media. For example, the following part of the QuILT warm-up helps students learn about the phase shift when an electromagnetic wave is incident on a medium of higher refractive index:

We can see a parallel between the mass density of a rope and the refractive index of a medium. Lower mass density is analogous to lower refractive index and higher mass density is analogous to higher refractive index. We can use this analogy to calculate the phase shift (change in phase) of light introduced by reflection or transmission at the interface between two media. We will also discuss the propagation of light through a refractive medium.

Light (plane harmonic electromagnetic wave) is incident from air onto a glass surface. The light gets partially reflected back into the air after striking the air-glass interface. Which one of the following phase shifts is introduced in the reflected light due to the reflection at the interface? Always assume that the angle of incidence is smaller than the Brewster's angle.

(a) zero
(b) $\pi/2$
(c) π
(d) None of the above.

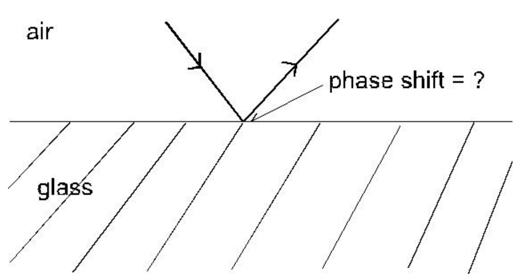


Figure 6-5. Reflection of light at an air-glass interface

Light initially traveling in a medium with a lower refractive index (e.g., air) undergoes a phase shift of π at the interface when it gets reflected from an interface with a medium having a higher refractive index.

After working on the warm-up, students should be able to determine the phase shifts of an electromagnetic wave propagating through the MZI and the type of interference (constructive or destructive) observed at each detector.

6.4.2 MZI with single photons-conceptual part of the QuILT

The conceptual part of the QuILT helps students reason about how a single photon exhibits both the properties of a wave and a particle in different parts of the same experiment, has a non-zero probability of being found in two locations (state is a superposition of path states) simultaneously, and interferes with itself due to the two possible paths through the MZI. Students also are guided to think about how adding or removing optical elements such as beam-splitter 2 or detectors can give "which-path" information about the photon arriving at the detectors D1 and D2 and affect whether interference is observed at the detectors. Checkpoints are also included to help students check their answers and verify that they are reasoning correctly up to a certain point. For example, the following series of questions are designed to help students reason about the role of beam-splitter 1 and how the photon can be localized or delocalized depending on the situation:

Consider the following conversation between three students:

- *Student A: BS1 divides the photon state into two halves. That means that a photon has been divided into two photons with the energy of each photon in the two paths being half of the* *energy of the photon that entered BS1. If the path difference in the U and L paths of the MZI were set up such that there was an intermediate interference at each detector D1 and D2 (neither fully constructive nor fully destructive), there would be a possibility of both detectors registering a photon at the same time with half the energy of the incoming photon.*

- *Student B: I disagree. Beam-splitter 1 causes the incoming photon state to become a superposition of the two path states U and L, but neither the photon nor its energy is split in half. If the energy was split in half, this would mean that the wavelength of the photon was doubled, which is not the case. Beam-splitter 1 simply makes the single photon state delocalized.*
- *Student C: I agree with Student B's statement. For a single photon, if the MZI was set up such that there was intermediate interference at detectors D1 and D2, only one detector will register a photon, not both. Registering a photon corresponds to a measurement which collapses the state of the photon at the point of detection and localizes it (the photon gets absorbed). We observe interference at the detectors because a single photon interferes with itself.*

With whom do you agree? You can agree with more than one student.

(a) Student A

(b) Student B

(c) Student C

Discuss your preceding answer with a partner and explain your reasoning.

Consider the following conversation between three students:

- *Student A: How can a single photon be in both the U and L paths of the MZI simultaneously if only one detector D1 or D2 clicks and registers a photon? It must go through only one path if only one detector clicks.*
- *Student B: Registering of a photon at the detector corresponds to a measurement of the photon's position via its interaction with the atoms in the detector. The photon is absorbed by the detector during the detection process.*
- *Student C: I agree with Student B's statement. A single photon can be delocalized or localized depending on the situation. For example, the single photon state is delocalized while going through the U and L paths but becomes localized upon detection because measurement collapses the state. Then, the photon gets absorbed by the material in the detector.*

With whom do you agree?

Discuss your preceding answer with a partner and explain your reasoning.

Consider the following conversation between Student A and Student B about the MZI with point detectors as shown in Fig. 6-1:

- *Student A: I don't understand. Since a single photon is delocalized and can be in both the upper and lower paths of the MZI simultaneously, there should be a finite probability that detectors D1 and D2 will both click at the same time and each would register the photon when a single photon is sent through the MZI.*
- *Student B: I disagree. For a given photon, only one of the detectors will click because there is only a single photon and the photon state collapses upon measurement and becomes localized upon detection of the photon. Then, the photon gets absorbed by the material in the detector.*

- *Student C: Yes. The clicking events due to registering of a photon at either of the detectors are complementary (only one of the detectors will click and detect a photon). Thus, it is not necessary to have both detectors D1 and D2 in the experiments we have discussed so far. A single detector can yield the same information. If the detectors are symmetrically situated as in the figure above, the interference observed at one detector will be correlated with the other. In our present case, chosen to be the same set up as in the warm-up (see Fig. 6-1), detector D1 is set up to show completely constructive interference and will always register the photon and detector D2 will show completely destructive interference and will never register the photon.*

With whom do you agree? You may agree with more than one student.

(a) Student A

(b) Student B

(c) Student C

(d) None of the above

Discuss your preceding answer with a partner and explain your reasoning.

- *Checkpoint:*
  - *When a detector clicks, the detector registers a photon and localizes it (the photon gets absorbed).*
  - *For a given photon, only one of the detectors in the MZI will click or register a photon because measurement collapses the state of the photon.*
  - *The registering events of a photon at either of the detectors are complementary (only one of them will click for a given photon) because the state of the photon becomes localized upon detection at a detector.*

In the conceptual part of the QuILT, the delayed choice experiment is discussed to help students reason that causality is not violated in this type of an experiment. The delayed choice experiment involves inserting or removing beam-splitter 2 after the photon has already passed through beam-splitter 1. Because the photon is in a superposition state after passing through beam-splitter 1, adding or removing beam-splitter 2 after the photon has already passed through beam-splitter 1 does not cause the photon to "choose" one path or the other; rather, beam-splitter 2 allows both components of the photon path state to be projected in both detectors so that interference is displayed at the detectors. If beam-splitter 2 is removed, the photon is still in a superposition of the path states, but only one component of the photon path state can be projected in each detector and interference is not observed.

For example, the following series of questions helps students reason about how the interference is affected when beam-splitter 2 is removed or inserted after the photon propagates through beam-splitter 1.

Consider the single photon experiment with the MZI setup, but with a removable second beam-splitter (BS2).

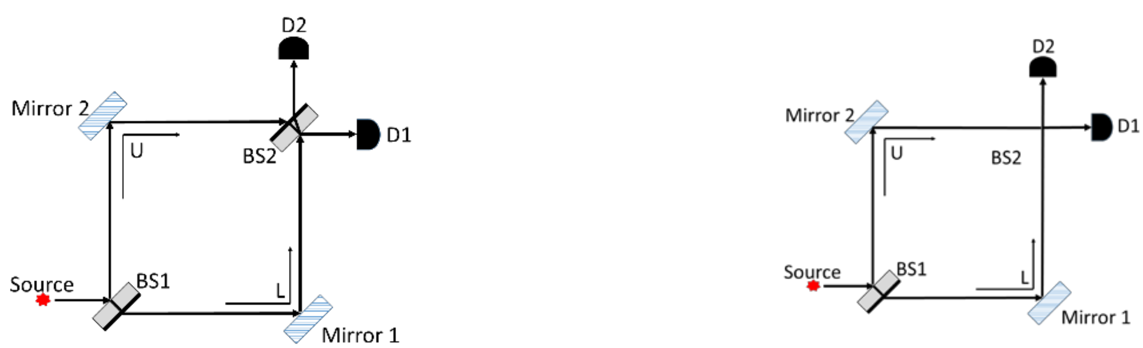


Figure 6-6. MZI setup with a removable beam-splitter 2 (BS2)

If the second beam-splitter BS2 is removed before the photon passes through BS1 (see the figure 6-6 to the right above), which one of the following is true about a single photon propagating through the MZI (after BS1) before it reaches detector D1 or D2?

(a) It is delocalized, which means it is in a superposition state of the U and L path states.

(b) It will either propagate along the U path or along the L path, not along both paths at the same time.

(c) It must take the U path because the state of the photon has collapsed to the upper path state before the photon reaches the detector.

(d) It must take either the U or L path, but the probability is higher for it to take the U path.

What would have happened to the photon state if BS2 was removed after the photon had already propagated through BS1?

If the second beam-splitter BS2 is removed, choose all of the following statements that are true:

(I) We have WPI about the photon when a detector D1 or D2 registers a photon.

(II) Placing the detector D1 anywhere in the U path is equivalent to placing it at the end of the path.

(III) Placing the detector D2 anywhere in the L path is equivalent to placing it at the end of the path.

(a) and (II) only

(b) and (III) only

(c) and (III) only

(d) All of the above.

Choose all of the following statements that are true about the case in which the second beam-splitter BS2 is removed:

(I) The point detectors D1 and D2 can only project the superposition state of the photon along the U path state or L path state, respectively.

(II) No interference is observed at either detector and each detector has a 50% probability of registering a photon, regardless of the phase difference between the U and L paths.

(III) It is useless to calculate the phase difference between the photon state due to the U and L paths for information about interference because we have WPI about each photon that arrives at detectors D1 or D2 (because detector D1 can only project the component along the U path and detector D2 can only project the component along the L path).

(a) and (II) only

(b) (I) and (III) only

(c) (II) and (III) only

(d) All of the above.

Students are also guided to think about how placing additional detectors in the paths of the MZI can destroy the interference observed at the detectors. If an additional detector is placed in one path of the MZI, the photon path state collapses to either one path state or the other. After the photon state collapses to either one path state or the other, there is no possibility for interference to occur at the detectors at the end after BS2 because interference is only observed when both path states of the photon can be projected in a detector after beam-splitter 2. The following series of questions helps students reason about the role of an additional detector placed in one of the paths of the MZI:

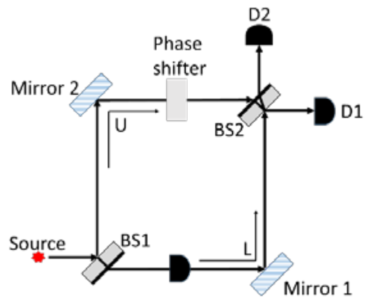


Figure 6-7. Schematic of MZI with additional photo-detector in L path

Now we will explore how inserting additional photo detectors in the U and/or L paths can yield information about which path the single photon went through (WPI) and destroy the interference at the detectors placed after BS2. A photo-detector absorbs the photons that it detects.

Choose all of the following statements that are correct if you insert an additional detector into the lower path (see figure 6-7 above) and the source emits a large number (N) of single photons.

(I) The interference is unchanged (without the phase shifter, N photons reach D1 and no photons reach D2).

(II) The interference vanishes.

(III) Changing the thickness of the phase shifter will not affect the number of photons reaching detectors D1 and D2.

a) (I) only

b) (II) only

c) (II) and (III) only

d) None of the above.

Explain your reasoning for the preceding question.

In figure 6-7, why will changing the thickness of the phase shifter not affect the number of photons arriving at the detectors? Explain your reasoning below.

Consider the following conversation between three students:

- *Student A: A photon can transmit through detector L, and thus the photon can remain in a superposition state of both paths (simultaneously in the U and L paths). Thus, we could observe interference even if detector L is present.*
- *Student B: I disagree with you. If detector L clicks, the photon is absorbed by detector L and that photon never arrives at either detector after BS2. If detector L doesn't click, the state of the photon collapses such that the photon is no longer in the superposition of the U and L paths. The photon is now only in the U path. Thus, we have WPI about all of the photons that arrive at the detectors and we will not observe interference.*
- *Student C: I agree with student B. If detector L doesn't click, the detectors D1 and D2 have equal probability of clicking (25%).*

With whom do you agree? Explain.

Students also are given the opportunity to check their answers to questions about the effect of placing an additional detector into one of the paths of the MZI on the interference after BS2 using a computer simulation [10]. In the computer simulation, a screen is used in place of point detector D1 and the photon has a transverse Gaussian width as opposed to being a collimated beam having an infinitesimally small transverse width. Students are told that the advantage of the screen (as opposed to point detectors D1 and D2) is that an interference pattern is observed without placing a phase shifter in one of the paths and changing the path length difference between the two paths. For the case with point detectors D1 and D2, the thickness of the phase shifter must be changed in order to observe interference (if interference is displayed in a particular case). In the computer simulation, the photon with a transverse Gaussian width is used to understand the pattern on the screen in the simulation. Students are guided to think about how the transverse Gaussian profile of the photon may yield constructive or destructive interference at different points on the screen, creating an interference pattern on the screen (in situations in which it should be observed).

Figure 6-8 shows a screen shot of the simulation in which an additional detector was placed in one of the paths of the MZI. The screen in the simulation is used in place of detector D1 and shows that there are no interference fringes when an additional detector is placed in one of the paths of the MZI.

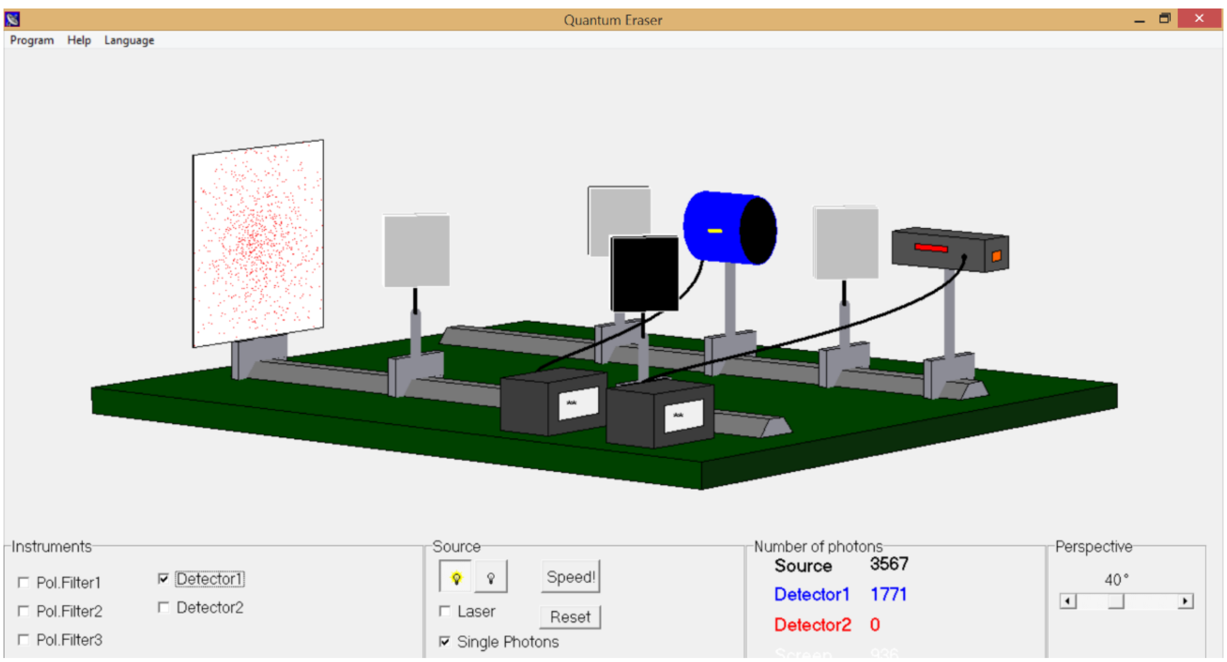


Figure 6-8. Screen shot of the computer simulation [10] in which an additional detector (blue device) is placed in one of the paths of the MZI.

“Interaction-free” measurement is also discussed in the conceptual tutorial. Interaction-free measurement occurs, e.g., when the presence of a bomb can be detected without light ever reaching it and detonating it. The following series of questions guide students to reason about interaction-free measurement:

Consider the situation in which a photo-detecting bomb is placed in the L path, as shown below. If the bomb registers a photon, it detonates. The MZI is set up such that there is completely constructive interference at detector D1 if there was no bomb.

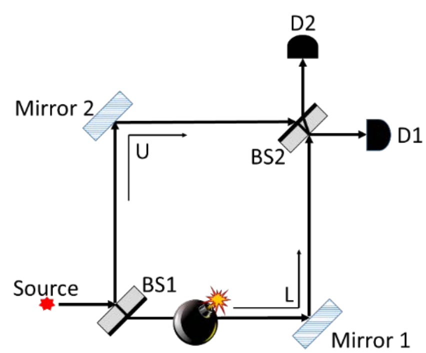


Figure 6-9. MZI with a photo-detecting bomb placed in the L path

If we send single photons from the source, what is the probability that the bomb will detonate?

If we send single photons from the source, what is the probability that the final detector D1 will register a photon (see figure 6-9)?

If we send single photons from the source, what is the probability that the final detector D2 will register a photon (see figure 6-9)?

What is the probability that you detect a bomb placed in the L path without the bomb detonating?

After working on the conceptual part of the QuILT, students should be able to qualitatively reason about how a single photon can exhibit the properties of both a wave and a particle. They should also be able to describe how a photon can be delocalized or localized and that measurement of a photon's position at the detector collapses the photon path state. Students should also be able to explain the roles of BS1, BS2, and additional detectors placed in the MZI and how these affect the interference at the detector. Students should also be able to reason about whether a particular MZI setup gives WPI about a single photon and whether inserting a phase shifter will change the number of photons arriving at detectors D1 and D2.

6.5 PRELIMINARY EVALUATION

Once we determined that the QuILT was effective in individual administration, it was administered to 44 upper-level undergraduate students in a first semester junior/senior quantum mechanics course and 45 graduate students in a first semester graduate level quantum mechanics course. Students were first administered the pretest. They then worked through the QuILT in class in small groups and then were asked to work on whatever they could not finish in class as homework. The completed QuILT was collected as a homework and counted for a small portion of the homework grade for that week. Next, students were given a posttest, which had the same questions as the pretest. Table 6-1 shows the common difficulties and percentages of students displaying them on the pre/posttest questions and Table 6-2 displays the average percentage scores on pretest and posttest questions. Average normalized gain [11] is commonly used to determine how much the students learned, taking into account their initial scores on the pretest. It is defined as $\langle g \rangle = \frac{\%\langle S_f \rangle - \%\langle S_i \rangle}{100 - \%\langle S_i \rangle}$, in which $\langle S_f \rangle$ and $\langle S_i \rangle$ are the final (post) and initial (pre) class averages, respectively [11]. The average normalized gain from pretest to posttest on questions related to difficulties involving interference of light, the wave/particle duality of a single photon, the role of BS2, and the role of additional detectors placed in one of the paths of the MZI was 0.72.

Question 1 on the pre/posttest assessed student understanding of the classical interference of light in a situation in which a beam of light (instead of single photons) is sent through the MZI. In the first year of administration, 36 students were asked to explain why they agreed or disagreed with the following statement for the basic MZI setup (Fig. 6-1): "If the source produces light with intensity I, the intensity of light at each point detector D1 and D2 will be $I/2$ each." In the second year of administration, this question was tweaked and 53 students were asked to explain why they agreed or disagreed with the following statements for the basic MZI setup (Fig. 6-1): "If the source emits N photons one at a time, the number of photons reaching detectors D1 and D2 will be $N/2$ each." Both statements are incorrect because the MZI setup is such that there is completely constructive interference at D1 and destructive interference at D2. Therefore, the light (or single photons) from the U and L paths arrives completely in phase at detector D1 with intensity I (N photons arrive there) and arrives out of phase at D2 and no light (or photon) arrives there. However, Table 6-1 shows that 66% of the students incorrectly agreed with this statement in the pretest, indicating that they did not take into account the interference phenomenon taking place at the detectors. After working on the QuILT, this difficulty was reduced. Students were given full credit for this question if they stated that they disagreed with the statement and explained that there would be constructive interference at detector D1 and destructive interference at D2.

Table 6-1. Common difficulties and percentages of undergraduate students (UG) and graduate students (G) displaying them on the MZI pre/posttest questions involving single photons. The number of students who took the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

Common Difficulty	**Pretest UG** $(N = 44)$	**Pretest G** $(N = 45)$	**Posttest UG** $(N = 38)$	**Posttest G** $(N = 45)$
Q1 Ignoring interference phenomena	66	56	21	36
Q2 BS1 causes the photon to split into two parts and halves the photon energy	32	24	11	20
Q2 Photon must take either U or L path	43	36	11	16
Q3 and Q4 Removing or inserting BS2 does not affect the probability of the detectors D1 and D2 registering photons	41	47	16	9
Q5 A photo-detector placed in the U or L path may absorb photons but does not affect whether interference is observed if photons arrive at detectors D1 and D2	41	40	0	7

Table 6-2. Average percentage scores on the MZI pre/posttest for undergraduate students (UG) and graduate students (G). The number of students who took the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

		Q1	**Q2**	**Q3**	**Q4**	**Q5**
UG ($N = 44$)	**Pretest**	8	31	18	11	61
UG ($N = 38$)	**Posttest**	72	86	87	70	97
G ($N = 45$)	**Pretest**	21	41	22	13	50
G ($N = 45$)	**Posttest**	66	76	86	72	87

Question 2 on the pre/posttest assessed students' understanding of the wave nature of a photon. Students were asked to consider the following conversation between two students and explain why they agreed or disagreed with the statements:

Student 1: *"BS1 causes the photon to split in two parts and the energy of the incoming photon is also split in half. Each photon with half the energy travels along the U and L paths of the MZI and produces interference at the detectors."*

Student 2: *"If we send one photon at a time through the MZI, there is no way to observe interference at the detectors. Interference is due to the superposition of waves from the U and L paths. A single photon must choose either the U or L path."*

Neither student is correct because a photon does not split into two parts with half the energy of the incoming photon but a single photon can be in a superposition of the U and L path states. 32% of the undergraduate students and 24% of the graduate students incorrectly agreed with Student 1 in the pretest. After working on the QuILT, Table 6-1 shows that this difficulty involving the splitting of photons was reduced. Furthermore, 43% of the undergraduate students and 36% of the graduate students incorrectly agreed with Student 2 in Question 2 on the pretest claiming that a photon must take either the U or L path. In the posttest, students performed better. Students who stated that they disagreed with both students and stated correct reasons were given full credit. Some students who agreed with Student 1 (i.e., that the photon is split with half the energy) wrote statements that were partially correct, e.g., "I agree with student 1 because the photon goes into a superposition state and interferes with itself." Students who wrote these types of statements received half credit since at least the photon going into a superposition of path states after BS1 is correct. Students who agreed with Student 2 (i.e., that the photon must choose either the U or L path) were given a score of zero.

Questions 3 and 4 on the pre/posttests assessed student understanding of the role of BS2. If BS2 is present, it evolves the state of the photon such that both the U and L path components of the photon state can be projected into each detector and the photon interferes with itself at the detectors D1 and D2. In the setup students were given, without the phase shifter in Fig. 6-1 (when BS2 is present), constructive interference occurs at D1 (the single photons always arrive at D1) and destructive interference occurs at D2 (no photon reaches D2). If BS2 is not present, the photon is still in a superposition of U and L path states after BS1 but only the U path component can be projected in detector D1 and only the L path component can be projected in detector D2. Thus, the photons do not display interference and each detector registers the photons with 50% probability. In the pretest, 41% of the undergraduate students and 47% of the graduate students incorrectly claimed that removing or inserting BS2 will not change the probability of the photon arriving at D1 and D2. This high percentage is consistent with the fact that these students did not acknowledge the wave nature and interference effects of single photons in response to other questions as well. Students often explicitly claimed that the photon behaves as a point particle and it would not matter whether BS2 was present or not—each detector would register the photon with 50% probability. In the QuILT, students learned that if BS2 is present, it evolves the state of the photon such that the photon state from both paths can be projected into each detector and interference is displayed at D1 and D2. Table 6-1 shows that in the posttest, students performed better. Students were given full credit on these questions if they stated that 1) when BS2 is present, D1 registers all photons and D2 registers zero photons, and 2) when BS2 is removed, D1 registers 50% of the photons and D2 registers 50% of the photons. Students were given half credit if they stated that the probabilities would change depending on whether BS2 was present or missing, but wrote the wrong probabilities. Students were given zero credit if they stated that the probabilities do not change whether BS2 is present or missing.

In Question 5 on the pre/posttests, students were shown a MZI with an additional detector placed in the L path between BS1 and BS2. They were then asked to describe how this situation compares to the situation in Fig. 6-1 in which no detector is present in the L path. In the new situation, if the detector does not absorb the photon, the photon path state must collapse to the U path. WPI is known and interference not displayed. Table 6-1 shows that in the pretest, 41% of the undergraduate students and 40% of the graduate students incorrectly claimed that adding a detector in the L path would not change anything or would only affect the fact that less photons arrive at detectors D1 and D2 because some photons are absorbed. These students struggled with the fact that the detector in the L path acts as a measurement device and will collapse the photon state of the photons not absorbed by it to the U path state. After working on the QuILT, the difficulty with the effect of an additional detector placed in the L path of the MZI was eliminated (see Table 6-1). Students were given full credit if they stated either that there would be no interference or that there would be $N/4$ photons that reach each of the detectors (as opposed to N photons reaching detector D1 and 0 photons reaching D2) when an additional detector is placed in one of the paths of the MZI.

As shown in Table 6-2, many students still had difficulty with Questions 1 and 4 on the posttest. Question 1 relates to the interference phenomenon in the context of a beam of light that students were supposed to have learned about in the QuILT warmup at home (ungraded) before the actual QuILT in class. In the future, the warmup should be administered as a graded homework to ensure that students complete it before working on the QuILT in class. Regarding the difficulty with Question 4 focusing on the role of BS2 on measurement outcomes, students who had difficulty on the posttest were often partially correct. In particular, many correctly claimed that inserting BS2 would remove WPI but incorrectly claimed that the probabilities of detection of the photons at D1 and D2 would not change. For example, one student stated "the probabilities do not change, but we no longer have 'which-path' information about each incident photon." Some students displayed another difficulty and claimed that D1 would register a photon 50% of the time and D2 would never register a photon because although the photon arrives there, it "gets killed." We have taken into account these findings from in-class administration in the next version of the QuILT. In addition, we are also developing an additional QuILT which strives to help students connect conceptual aspects of the MZI with single photons with mathematical formalism using a simple two state system involving photon path states.

Table 6-2 shows that the performance of graduate students was approximately equal to or slightly higher than undergraduate students on the pretest. In contrast, on the posttest, undergraduate students performed slightly better than graduate students. This may be due, in part, to the fact that graduate students' performance on the posttest was not part of their final grade for the teaching assistant training class. Graduate students may not have worked through the tutorial in an engaged manner, i.e., contemplating their difficulties and repairing their knowledge structure, and this could have resulted in the persistence of difficulties and a smaller increase in their scores from the pretest to posttest. These results demonstrate the importance of students being actively engaged and motivated while learning. In particular, if students are aware that they are not going to be graded on their performance on a posttest, they may not be motivated to engage with the material in the tutorial (especially if they are working on the tutorial on their own as a homework assignment).

6.6 SUMMARY

The MZI QuILT focuses on helping students comprehend the wave-particle duality of a single photon, interference of a single photon with itself, and how measurement collapses the delocalized superposition state of a single photon. In fact, many students in the class discussed in the preceding section stated that it was one of their favorite QuILTs. For example one student stated “The [MZI QuILT] was pretty cool because I had no idea what the concept of which path information was before.” The preliminary evaluations are encouraging.

6.7 ACKNOWLEDGEMENTS

We thank the National Science Foundation for awards PHY-0968891 and PHY-1202909. We thank Albert Huber for developing the simulation that we adapted in the QuILT and for allowing us to us to reference the computer simulation throughout the MZI conceptual tutorial. We also are thankful to various members of the department of physics and astronomy at the University of Pittsburgh for helpful conversations and suggestions during the development of the tutorial. We are especially grateful to R.P. Devaty for reading through the tutorial and giving feedback during various stages of its development.

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7.0 DEVELOPING AND EVALUATING A QUANTUM INTERACTIVE LEARNING TUTORIAL ON A QUANTUM ERASER

7.1 INTRODUCTION

Quantum mechanics can be a challenging subject for students partly because it is unintuitive and abstract [1-6]. An experiment which has been conducted in undergraduate laboratories to illustrate fundamental principles of quantum mechanics involves the Mach-Zehnder Interferometer (MZI) with single photons [7]. We are developing and evaluating a quantum interactive learning tutorial (QuILT) on a quantum eraser using gedanken (thought) experiments and simulations involving a MZI with single photons. The QuILT focuses on helping students learn topics such as the wave-particle duality of a photon, interference of a single photon with itself, probabilistic nature of quantum measurements, and collapse of a quantum state upon measurement. Students also learn how photo-detectors and optical elements such as beam splitters and polarizers in the paths of the MZI affect the measurement outcomes. In particular, they learn to reason systematically about a quantum eraser setup in which placing a polarizer with specific orientations in a particular location in the MZI setup can result in interference of a single photon with itself due to erasure of "which-path" information (WPI) [7].

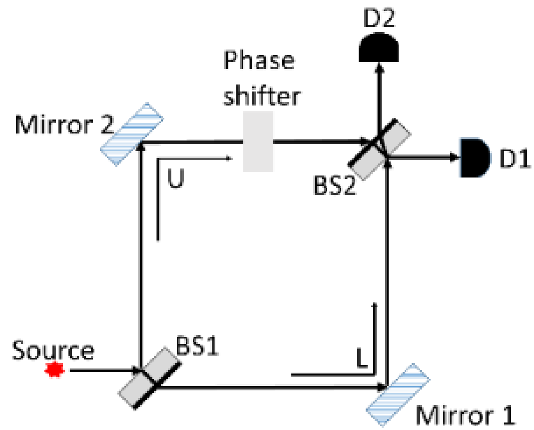


Figure 7-1. MZI setup with a phase shifter in the U path

Figure 7-1 shows the MZI setup. For simplicity, the following assumptions are made: 1) the source emits either +45° polarized single photons or unpolarized photons (in which half of the photons emitted are vertically polarized and half of the photons emitted are horizontally polarized) one at a time; 2) all optical elements are ideal; 3) the non-polarizing beam splitters (BS1 and BS2) are infinitesimally thin such that there is no phase shift when a single photon propagates through them; 4) the monochromatic single photons travel the same distance in vacuum in the upper path (U) and lower path (L) of the MZI; and 5) the initial MZI without the phase shifter is set up such that there is completely constructive interference at detector 1 (D1) and destructive interference at detector 2 (D2).

If a single photon is emitted from the source in Figure 7-1, BS1 causes the photon to be in a superposition of the path states U and L. The photon path states reflect off the mirrors and recombine in BS2. BS2 mixes the photon path states such that both components of the photon path state can be projected into both detectors D1 and D2. The projection of both components leads to interference at the detectors. Depending on the thickness of the phase shifter, interference observed at detectors D1 and D2 can be constructive, destructive, or intermediate. Observing interference of a single photon with itself at D1 and D2 can be interpreted in terms of not having "which-path" information (WPI) about the single photon [7]. WPI is a common terminology associated with these types of experiments popularized by Wheeler [8]. WPI is unknown (as in the setup shown in Fig. 7-1) if both components of the photon state can be projected in each of the detectors D1 and D2 and the projection of both components at each detector leads to interference. When WPI is unknown and a large number of single photons are sent through the setup, if a phase shifter is inserted in one of the paths of the MZI (as in the U path in Fig. 7-1) and its thickness is varied, the probability of each photon arriving at D1 and D2 will change with the thickness of the phase shifter due to interference of the components of the single photon state from the U and L paths.

On the other hand, if both components of the photon path state cannot be projected at each of the detectors, there is no possibility for interference of the photon path states to occur at the detectors. In this case, WPI is known about a photon at the detectors D1 and D2. Thus, WPI is "known" about a photon if only one component of the photon path state can be projected in detector D1 and the other component is projected in detector D2. For example, if BS2 is removed from the setup (see Fig. 7-2), WPI is known for all single photons arriving at the detectors because only the component of a photon state along the U path can be projected in D1 and only the component of a photon state along the L path can be projected in D2. When WPI is known, each detector (D1 and D2) has an equal probability of clicking. A detector clicks when a photon is detected by it and is absorbed (the state of the single photon collapses at the detector, i.e., the single photon state is no longer in a superposition of the U and L path states). However, when WPI is known, there is no way to know a priori which detector will click when a photon is sent until the photon state collapses either at D1 or at D2 with equal likelihood. When WPI is known, changing the thickness of a phase shifter in one of the paths does not affect the probability of each detector clicking when photons are registered (equal probability for all thicknesses of phase shifter) [7].

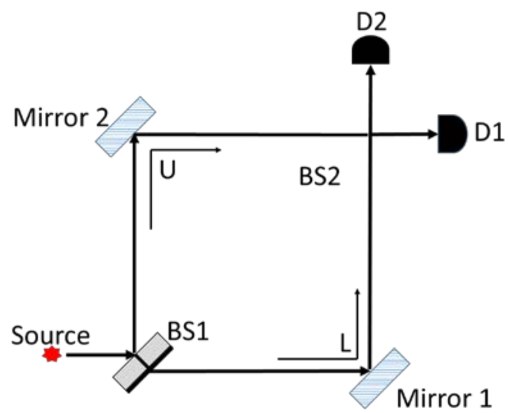


Figure 7-2. MZI setup with beam-splitter 2 (BS2) removed

When polarizers are added to the MZI setup, they can affect (and even eliminate) the interference of a single photon with itself at the detectors. For example, in Figure 7-3, two orthogonal polarizers are placed in the U and L paths of the MZI. If the source emits a large number (N) of +45° polarized single photons, $N/2$ photons are absorbed by the polarizers. In all the MZI setups discussed, it is assumed that the detectors are polarization sensitive. If a detector measures a vertically polarized photon, since it can only project one component of the photon path state (i.e., the U path state), WPI is known. If a detector measures a horizontally polarized photon, since it can only project one component of the photon path state (i.e., the L path state), WPI is known. WPI is known for all photons arriving at the detectors, and there is an equal probability of each detector registering a photon ($N/4$ photons arrive at each detector). There is no interference observed at the detectors. Inserting a phase shifter and changing its thickness gradually will not affect the number of photons arriving at the detectors.

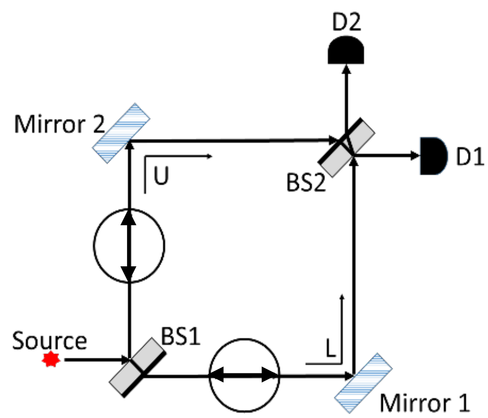


Figure 7-3. MZI setup with a polarizer with a vertical transmission axis placed in the U path and a polarizer with a horizontal transmission axis placed in the L path.

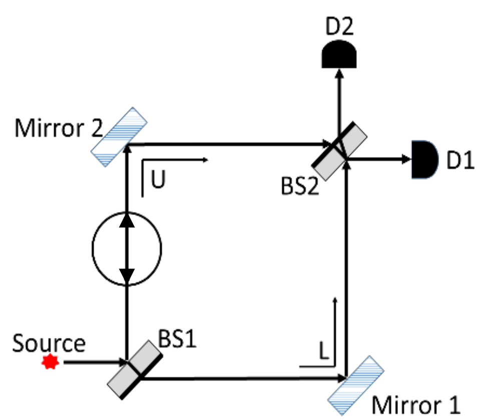


Figure 7-4. MZI setup with a polarizer with a vertical transmission axis placed in the U path

Inserting one polarizer also affects the interference observed at the detectors. If a polarizer with a vertical transmission axis is placed in the U path (see Fig. 7-4), WPI is known for some photons (but not all). If a detector measures horizontally polarized photons, it can only be projected into the detector from the L path state and WPI is known. Thus, no interference is observed at the detectors for horizontally polarized photons. However, if a detector measures vertically polarized photons, both the U and L path components of the photon state must have been projected into the detector. Thus, WPI is unknown for vertically polarized photons. Inserting a phase shifter and gradually changing its thickness will affect the number of vertically polarized photons arriving at the detectors (but not the number of horizontally polarized photons since WPI is known for those photons for the setup in Figure 7-4).

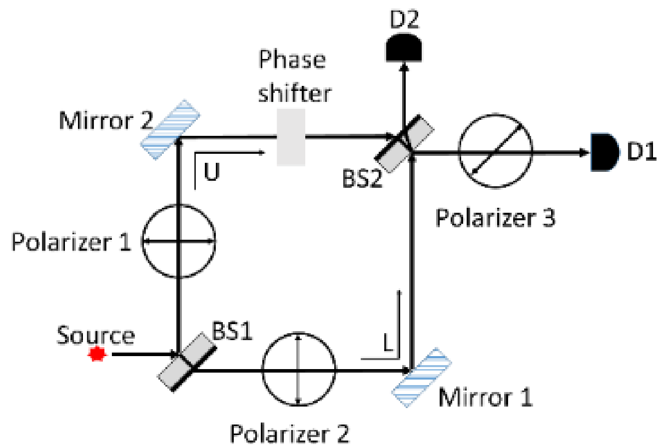


Figure 7-5. Quantum eraser setup

Figure 7-5 shows a quantum eraser setup in which two orthogonal polarizers are placed in the two paths of the MZI and a third polarizer is placed between BS2 and D1. The third polarizer has a transmission axis which is different from the two orthogonal polarizers. Without polarizer 3, WPI is known for all photons arriving at the detectors (as in Figure 7-3) and interference is not observed at the detectors. However, when polarizer 3 is inserted between BS2 and D1, it causes both the U and L path states to be projected into D1 and WPI is unknown for all photons. For example, due to the effect of polarizer 3, if D1 measures vertically polarized photons, both the U and L path states contribute to it and WPI is unknown. Similarly, if D1 measures horizontally polarized photons, both the U and L path states contribute to it and WPI is unknown. Interference is observed at detector D1. If a phase shifter is inserted into one of the paths of the MZI, changing its thickness gradually will change the number of photons arriving at D1. Because polarizer 3 eliminates WPI at the detector D1, this MZI setup is called a quantum eraser. However, WPI is known at D2 and no interference is observed there. Inserting a phase shifter into one of the paths of the MZI and changing its thickness gradually will not affect the number of photons that arrive at D2.

The quantum eraser setup also distinguishes between unpolarized photons and a stream of photons which have been polarized at +45°. If the source emits unpolarized photons, one can consider half of the photons emitted to be vertically polarized and half of the photons emitted to be horizontally polarized. For the MZI setups in Figures 7-3 and 7-4, polarized and unpolarized single photons behave similarly in terms of the fraction of photons that display interference (i.e., fraction of photons for which there is WPI). In the quantum eraser setup, if we use unpolarized photons and consider them to be a mixture of half vertically polarized and half horizontally polarized photons at random, approximately $N/4$ vertically polarized photons are absorbed by the horizontal polarizer and the other $N/4$ vertically polarized photons go through the L path. Therefore, even if these photons go through polarizer 3, WPI is known for them and they will not show interference. Inserting a phase shifter and changing its thickness gradually will not affect the number of photons arriving at the detectors. However, if the source emits a stream of +45° polarized single photons, it is not emitting a mixture but rather each photon is in a superposition state of vertical and horizontal polarization states, $|+45°\rangle = \frac{|H\rangle+|V\rangle}{\sqrt{2}}$. The +45° polarized photon has a probability of remaining in a superposition of the L and U path states after passing through the vertical and horizontal polarizers in the two paths (the path and polarization states both become important). Thus, the photons exiting BS2 and propagating through polarizer 3 are in a superposition state of U and L paths and both components of the photon path state can be projected into detector D1. WPI is unknown and interference is observed at D1. Inserting a phase shifter and changing its thickness gradually will affect the number of photons arriving at D1.

7.2 METHODOLOGY OF THE INVESTIGATION OF STUDENT DIFFICULTIES

Student difficulties with the MZI with polarizers were investigated by administering open-ended questions to upper-level undergraduate and graduate students and conducting individual interviews with 15 students in quantum mechanics courses after traditional instruction in relevant concepts. The traditional instruction in the first semester undergraduate quantum mechanics course included a discussion of the analogy between polarization states and spin ½ states. An overview of the MZI setup was given and students learned about phase differences, reflection off of mirrors, propagation of light through the beam splitters, and the meaning of what happens when the detectors “click.” Students were instructed about the concept of how the path and polarization states are connected and that this is important while reasoning about an MZI with polarizers in the two paths. The open-ended questions were graded using rubrics which were developed by two of the investigators together. A subset of the open-ended questions were graded separately by the investigators. After comparing the grading of the open-ended questions, the investigators had an initial inter-rater reliability of 70%. The investigators discussed any disagreements in grading and resolved them. The final inter-rater reliability is better than 90%.

The individual interviews used a think-aloud protocol to better understand the rationale for student responses before, during, and after the development of different versions of the quantum eraser QuILT and the corresponding pre-test and post-test. During the semi-structured interviews, students were asked to verbalize their thoughts while they answered questions. During the interviews, we provided students with a pen and paper and asked them to "think aloud" [8] while answering the questions. Students first read the questions on their own and answered them without interruptions except that we prompted them 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, we asked them to further clarify and elaborate issues that they had not clearly addressed earlier.

7.3 STUDENT DIFFICULTIES

During the preliminary development of the QuILT, we investigated the difficulties students have with relevant concepts including how placing polarizers in the paths of the MZI affect the interference observed at the detectors. We conducted 15 individual semi-structured think-aloud interviews with upper-level undergraduate and graduate students using different versions of an open-ended survey or earlier versions of the QuILT in which students were first asked to think aloud [9] as they answered the questions related to the setup including those with polarizers at various locations (some of the configurations being the quantum eraser) to the best of their ability without being disturbed. Later, we probed students further and asked them for clarification of points they had not made clear. Since both undergraduate and graduate students exhibited the same difficulties, we will not distinguish between the two groups further. Some of the difficulties include how a single photon can interfere with itself, how polarizers can act as partial measurement devices and alter the state of a photon, and how WPI can be erased, e.g., by introducing polarizer 3 in Fig. 7-5.

Difficulty with how a single polarizer in the U or L path of the MZI may or may not collapse the state of a single photon so WPI may or may not be known: Interviews suggest that many students had difficulty with how the interference at D1 and D2 is affected by placing a single polarizer, e.g., with a vertical polarization axis in the U path of the MZI (see Fig. 7-4). In this situation, if the source emits unpolarized single photons, there are three possible measurement outcomes due to the polarizer: 1) the photon is absorbed by the polarizer and it does not reach the detectors D1 or D2 (25% probability); 2) the photon is not absorbed by the vertical polarizer but both the photon path state and polarization state collapse, i.e., the photon is now in the L path with a horizontal polarization (25% probability); and 3) the photon is not absorbed by the vertical polarizer and the polarization state of the photon collapses but not the path state, i.e., the vertical polarizer collapses the photon polarization state to vertical polarization state but the photon remains in a superposition of the U and L path states (50% probability). WPI is known if the photon collapses to the horizontal polarization state. However, WPI is unknown if the photon has a vertical polarization state since the vertical polarizer does not collapse the path state of those photons. Photons with a vertical polarization state display constructive interference at D1 and destructive interference at D2 in the given setup without the phase shifter. Thus, D1 will register all single photons with a vertical polarization (50% of photons emitted from the source) and 12.5% of the single photons emitted from the source which collapsed to the horizontal polarization state due to the vertical polarizer in the L path. D2 will register only photons with a horizontal polarization (12.5% of the photons emitted from the source). Many students struggled with the fact that a single polarizer collapses the path state for some of the photons and thus there are some photons that show interference and others that do not show interference. Some students correctly stated that if one polarizer with a vertical polarization axis is placed in the L path, fewer photons would reach the detectors D1 and D2 but they incorrectly claimed that all of them that reach there would display interference. For example, one student said “some of the photons won’t make it to the [detectors]. 75% [of the photons display interference] because only half of the photons in path [L] will go through.” Another student stated that “all of [the photons display interference] since … every photon splits between both paths.” In addition, discussions with students suggest that they often had difficulty with the fact that the interference is due to a photon interfering with itself (the wave nature of a photon), not a photon splitting into two and the two photons interfering with each other.

Difficulty with how two orthogonal polarizers placed in the U and L paths of the MZI collapse both the path and polarization states for ALL photons: Students often incorrectly claimed that the effect of placing two orthogonal polarizers in the two paths of the MZI (see Fig.7-3) is not different from the effect of a single polarizer in one path (see Fig. 7-4) except that fewer photons would reach the detectors. In particular, the two orthogonal polarizers collapse the photon path state to either the U or L path state. WPI is known about all the photons in Fig. 7-3, interference is destroyed, and the detectors register photons with equal probability. Many students stated that “less photons would reach the [detectors]” but that interference would still be displayed. For example, one student stated that “50% [of the photons emitted by the source display interference because] we don’t measure anything until the photons hit the [detector] so their state vector doesn’t collapse until then.” These students struggled with the fact that two orthogonal polarizers placed in the two paths of the MZI correspond to a measurement of photon polarization such that either the photon gets absorbed by the polarizer or the photon with a vertical polarization that reaches D1 or D2 came only from the MZI path in which the vertical polarizer is and the photon with a horizontal polarization came only from the path in which the horizontal polarizer is. Thus, WPI is known about all photons that reach D1 and D2 and no interference is observed. Students had difficulty with the fact that once a photon reaches the polarizers, the measurement of polarization collapses the state of the photon such that if a detector registers a photon with a horizontal polarization, it must have come from the U path and if a detector registers a photon with a vertical polarization, it must have come from the L path.

Difficulty with how a quantum eraser setup in Fig. 7-5 erases WPI and restores interference of single photons at detector D1: In contrast to the MZI setup with two orthogonal polarizers in which WPI is known about all photons regardless of whether they are initially polarized or unpolarized, the addition of the third polarizer (see Fig. 7-5) causes both components of the photon path state to be projected into D1, erasing WPI about the +45° polarized single photons arriving at D1 as discussed earlier (but not of unpolarized single photons). If a phase shifter is inserted in one of the paths of the MZI and its thickness is gradually changed, the interference displayed at D1 will change. Some students incorrectly claimed that the quantum eraser setup (see Fig. 7-5) is not different from the setup in which two orthogonal polarizers are placed in the U and L paths (see Fig. 7-3) except fewer photons would reach D1 because some will be absorbed by polarizer 3. Moreover, many students could not articulate why the quantum eraser setup shows interference effects at D1 and the setup with two orthogonal polarizers placed in the paths of the MZI does not show interference. For example, one student said “not as many photons will go through. 25% [of the photons will display interference] because only half of the photons going through BS2 will make it through” but he had difficulty with the fact that the quantum eraser setup would show interference and that the setup with two orthogonal polarizers would not. Some students stated that none of the photons would display interference, e.g., “0% [of photons display interference], they are all independent photons." These types of responses indicate that some students who may understand that two orthogonal polarizers in U and L paths collapse the state of the photon have difficulty with the role of the third polarizer in Fig. 7-5.

7.4 QUILT DEVELOPMENT

The difficulties discussed above indicate that even after traditional instruction in these topics, students had many difficulties. Given the common difficulties exhibited, upper-level undergraduate and graduate students would benefit from a research-based approach, e.g., a tutorial-based approach to become familiar with the concepts involving a single photon propagating through the MZI with different polarizer setups. We developed a Quantum Interactive Learning Tutorial (QuILT) on a MZI with polarizers which culminates in helping students learn about the quantum eraser setup. The QuILT helps students reason about how polarizers placed in the paths of the MZI can affect the interference observed at the detectors after BS2. The QuILT also makes use of a computer simulation [10] in which students can insert one (or more) polarizers with their transmission axes aligned at different angles and observe what happens at the detectors for different setups. The QuILT can be used in class to give students an opportunity to work together in small groups and discuss their responses with peers.

The MZI with polarizers QuILT builds on students' prior knowledge and was developed by taking into account the difficulties discussed above. The development of the QuILT was a cyclical, iterative process which includes the following stages: 1) development of a preliminary version of the QuILT based on the research on student difficulties; 2) implementation and evaluation of the QuILT by administering it to individual students and measuring the effectiveness of it via pre-/post-tests; and 3) refinement and modifications based upon the feedback from the implementation and evaluation. The QuILT was also iterated with four faculty members and two graduate students to ensure that the content and wording of the questions were appropriate. We administered the QuILT to several graduate students and upper-level undergraduate students one-on-one to ensure that the guided approach was effective and the questions were unambiguously interpreted. Modifications were made based upon the feedback. When we found that the QuILT was effective in individual administration and students' pre-/post-test performance showed significant improvement, the QuILT was administered to students in two upper-level undergraduate quantum mechanics courses ($N = 44$) and graduate students enrolled in the first semester of a graduate level quantum mechanics course ($N = 45$).

To assess the effectiveness of the QuILT, a pretest was administered to 44 upper-level undergraduate students in a junior/senior level quantum mechanics course and 45 graduate students enrolled in the first semester of a graduate level quantum mechanics course. After the students completed the pretest and worked on part of the QuILT in class, they were given one week to work through the entire QuILT as part of a homework assignment and were then given a posttest. Any students who did not work through the QuILT were omitted from the posttest data (the student work on the QuILT was collected and graded for a small portion of the homework grade for that week).

The graduate students were enrolled in a teaching assistant training class, during which they learned about instructional strategies for teaching introductory physics courses. They were asked to work through the MZI conceptual tutorial to learn about the effectiveness of tutorials.

They were given credit for completing the pretest, conceptual tutorial, and posttest. However, their performance on the posttest was not part of the final grade for the teaching assistant training class.

7.4.1 MZI with one polarizer

The QuILT strives to help students reason about how one polarizer would affect the interference and number of photons arriving at the detectors. For example, the following series of questions help students reason about how +45° polarized photons emitted from the source propagate through a MZI with a horizontal polarizer in the U path and whether there is any difference between a stream of unpolarized photons (i.e., an equal mixture of horizontally and vertically polarized single photons) and a stream of +45° polarized single photons:

N photons emitted with polarization $|{+45°}\rangle = \frac{|H\rangle + |V\rangle}{\sqrt{2}}$

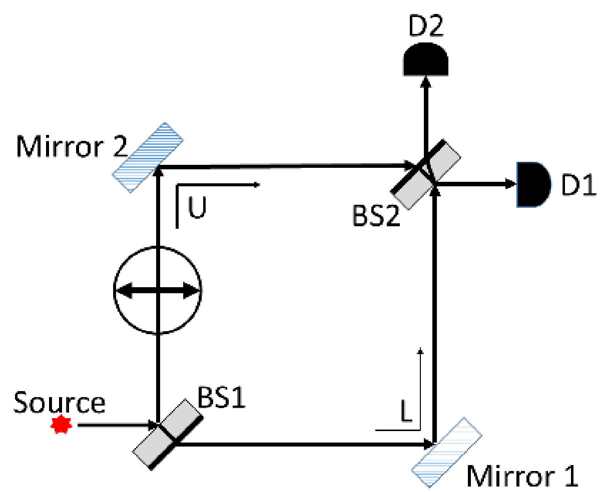


Figure 7-6. MZI setup with a polarizer with a horizontal transmission axis in the U path

Choose all of the following statements that are true about what happens when you insert a *polarizer with a horizontal polarization axis in the U path and turn on the +45° polarized single photon source (see figure 7-6 above) and a large number of photons (N) are sent one at a time. Assume that the polarization at the detectors D1 and D2 is being measured in the horizontal and vertical polarization basis.*

(I) Approximately $N/4$ photons will get absorbed by the horizontal polarizer in the U path.

(II) Out of the photons that propagate through BS2, $N/4$ photons do not show interference and have equal probability of arriving at either detector 1 or detector 2.

(III) The photons with a horizontal polarization component will interfere because we do not have WPI for those photons.

(IV) Fewer photons arrive at detector D1 compared to the case without polarizer 1.

(a) (I) and (II) only

(b) (I) and (III) only

(c) (I), (II) and (III) only

(d) All of the above.

Explain your reasoning for the preceding question.

Consider the following conversation between two students. Assume that the polarization at the detectors D1 and D2 is being measured in the horizontal and vertical polarization basis.

- *Student 1: How is the case in which the source emits +45° polarized single photons* ***different*** *from the case in which the source emits unpolarized photons? Will the interference be different for the figure 7-6 if the source emits +45° polarized single photons instead of unpolarized photons?*

- *Student 2: We can think of a +45° polarized photon as a* ***superposition of horizontal and vertical polarizations****, e.g.,* $|+45°\rangle = \frac{|H\rangle+|V\rangle}{\sqrt{2}}$*. The source emitting a superposition is, in general, NOT equivalent to a source emitting an equal mixture of horizontally and vertically polarized photons, as in the case for unpolarized photons emitted by the source. If the source emits +45° polarized photons:*

1) *The photon state after exiting the horizontal polarizer in the U path in figure 7-6 must only have a horizontal polarization component in the U path.*
2) *The photon state in the L path in figure 7-6 is +45° (a superposition of both vertical and horizontal polarization components,* $|+45°\rangle = \frac{|H\rangle+|V\rangle}{\sqrt{2}}$*).*
3) *We have WPI about a photon with a vertical polarization component arriving at the detectors because we know it could <u>not</u> have come from the upper path. Vertically polarized photons do not display interference and have equal probability of arriving at detectors D1 and D2. We <u>don't</u> have "which path" information about a photon with a horizontal polarization component because it could have come from either the U or L path.*
4) *At detector D1, the horizontal polarization component of the photon state arrives in phase from the U and L paths. Thus, the horizontal component of the photon state leads to constructive interference at detector D1.*
5) *At detector D2, the horizontal polarization component of the photon arrives out of phase from the U and L paths and the horizontal components of the photon state display destructive interference, so no horizontally polarized photons arrive there and no vertically polarized photons would reach detector D2.*

Do you agree with Student 2's explanation? Explain.

These types of questions help students reason about whether one has WPI for photons when there is one polarizer in one of the paths of the MZI and the fraction of photons that display interference. Students are also guided to compare the behavior of a stream of unpolarized and polarized photons. After students work through these guided problems, they are given checkpoints so that they can verify their responses.

Students can also use the computer simulation to observe that there will be some photons that display interference and others that do not for the case in which one polarizer is present in the MZI (see Fig. 7-7). In the computer simulation, a screen is used in place of point detector D1 and each photon has a transverse Gaussian width as opposed to being a collimated beam having an infinitesimally small transverse width. Students are told that the advantage of the screen is that an interference pattern is observed without placing a phase shifter in one of the paths and changing the path length difference between the two paths. For the case with point detectors D1 and D2, the thickness of the phase shifter must be changed in order to observe interference (if it is displayed in a particular case). In the computer simulation, a photon with a transverse Gaussian width is used to understand the pattern on the screen in the simulation. Students are guided to think about how the transverse Gaussian profile of the photon may result in different phase differences at different points on the screen if the photon state collapses there (which may yield constructive or destructive interference at different points on the screen), creating an interference pattern on the screen.

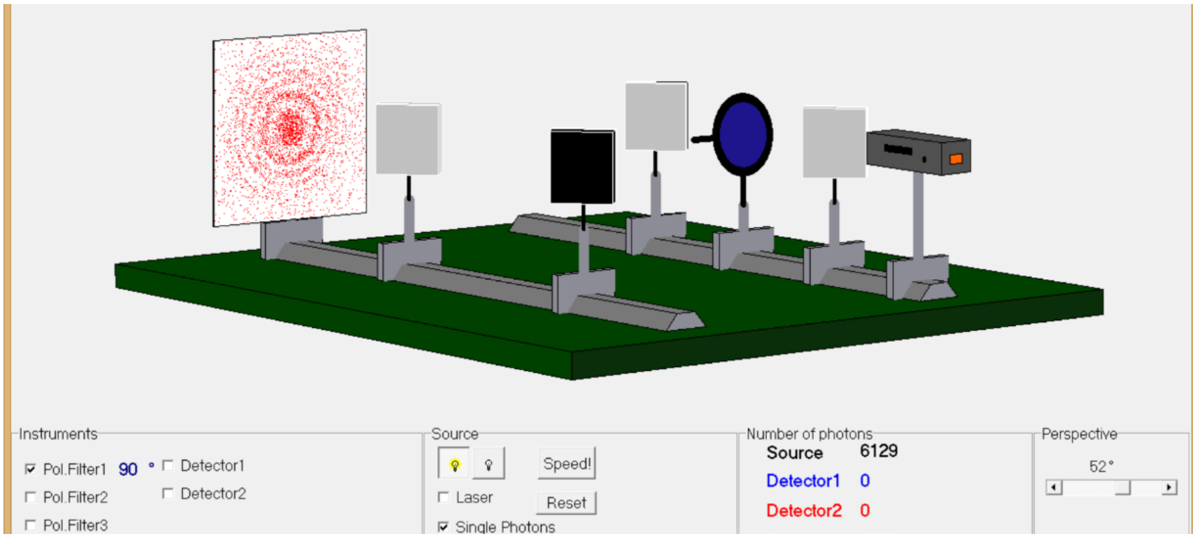


Figure 7-7. Computer simulation showing a polarizer (blue object) with a horizontal polarization axis placed in one path of the MZI. The handle on the polarizer indicates polarization axis. An interference pattern overlaid by a Gaussian profile indicates that there are some photons that display interference and others that do not.

7.4.2 MZI with two orthogonal polarizers

Since students had difficulty reasoning about how two orthogonal polarizers would eliminate the interference at the detectors, the QuILT strives to help students with this concept. For example, the following question helps students think about the number of photons arriving at the detectors and whether they display interference for the MZI setup with two orthogonal polarizers placed in the two paths of the MZI when the source emits +45° single photons:

If you place two polarizers with orthogonal polarization axes in the MZI setup (see figure 7-3) and turn on the +45° polarized single photon source, choose all of the following statements that are correct about what you expect to observe at the detectors after a very large number of photons (N) have been emitted from the source.

(I) *Interference is displayed and it is identical to that observed with only one of the polarizers present.*

(II) *No interference is displayed.*

(III) $N/4$ *photons reach detector D1.*

(IV) *Placing a phase shifter in one of the paths and changing its thickness gradually WILL NOT change how many photons arrive at the detectors.*

(a) *(I) only.*

(b) *(I) and (III) only.*

(c) *(II) and (III) only.*

(d) *(II), (III), and (IV) only.*

B) Explain your reasoning for the preceding question.

After students work through these types of guided questions, they are given checkpoints to verify their responses. Students can also use the computer simulation to verify that when two orthogonal polarizers are placed in the two paths of the MZI, there is no interference displayed (see Fig. 7-8).

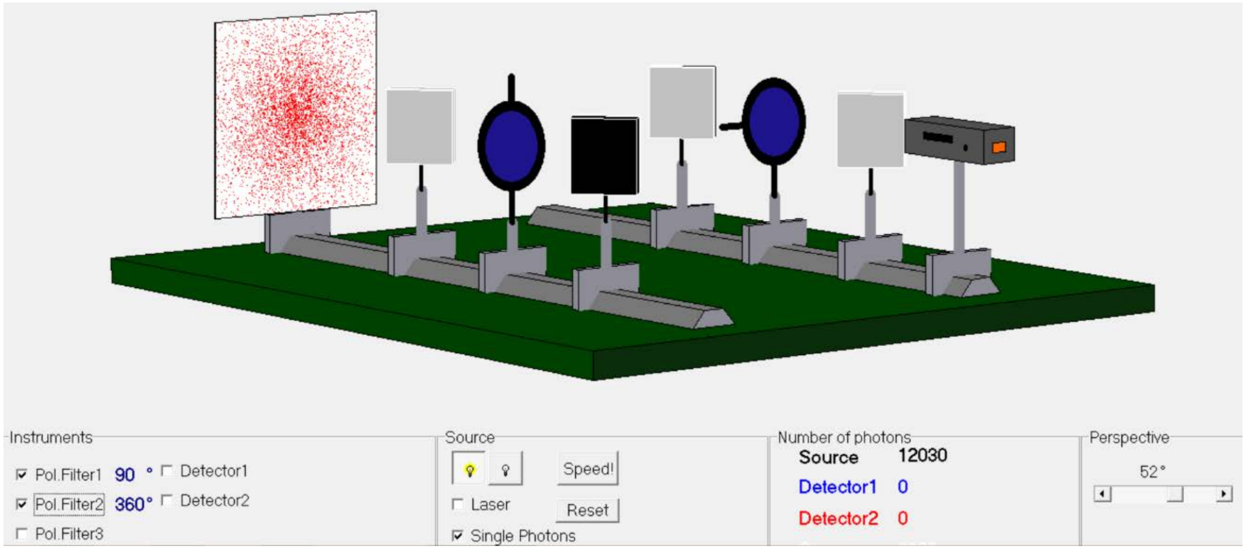


Figure 7-8. Computer simulation with polarizers (blue objects) with orthogonal polarization axes placed in the two paths of the MZI. No interference pattern is observed at the screen.

7.4.3 MZI Setup-Quantum Eraser

Many students had difficulty reasoning about the difference between the case in which two orthogonal polarizers are placed in the two paths of the MZI (see Fig. 7-3) vs. the quantum eraser setup (i.e., the case in which two orthogonal polarizers are placed in the two paths of the MZI and a third polarizer is placed between BS2 and D1, see Fig. 7-5). The following series of questions was included in the QuILT to help them reason about the number of photons reaching detectors D1 and D2 and whether interference would be observed with +45° polarized single photons emitted from the source:

You insert a polarizer with a horizontal polarization axis in the U path and a polarizer with a vertical polarization axis in the L path. You also insert a third polarizer with a +45° polarization *axis before detector D1. When you turn on the +45° polarized single photon source, what do you expect to observe at the detectors?*

(I) No interference is observed at the detectors.

(II) Interference is displayed at detector D1.

(III) $N/4$ photons reach detector D1.

(IV) Placing a phase shifter in one of the paths and changing its thickness gradually WILL NOT change the number of photons reaching detector D1.

(a) (II) only

(b) (I) and (III) only

(c) (II) and (III) only

(d) (I), (III), and (IV) only

Explain your reasoning for the preceding question.

Consider the following conversation between three students:

- *Student A: How can you tell that approximately 1/4th of the +45° polarized photons emitted from the source arrive at detector D1 shown in the figure 7-9 and show interference?*
- *Student B: Let me show you a qualitative description of the approximate numbers in a diagram (see Figure. 7-9).*

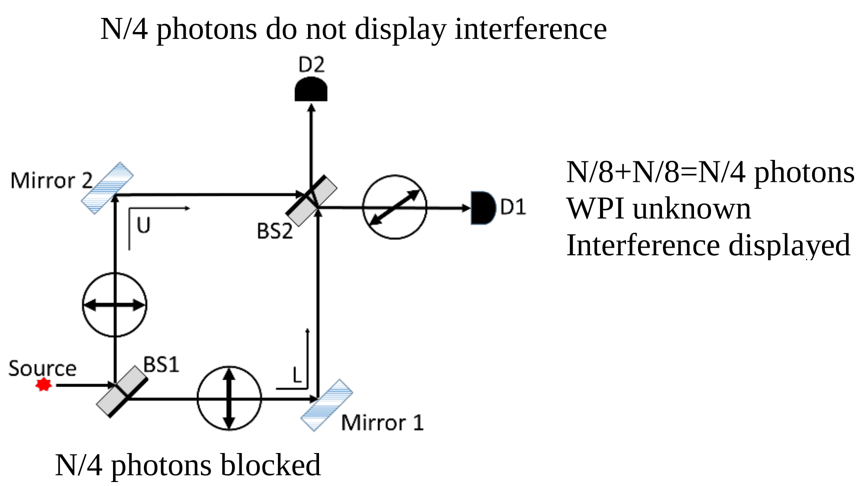


Figure 7-9. Qualitative description of the number of photons reaching the detectors in a quantum eraser setup.

There is interference displayed at detector D1 because the +45° polarizer "erases" the WPI for the photons passing through it. The +45° polarizer shown in Fig. 7-9 causes both the U and L components of the photon state to have polarization components along the +45° axis, and thus they are no longer orthogonally polarized and can interfere. The phase difference between the two paths in the setup is such that the vertically and horizontally polarized components arrive in phase between BS2 and detector D1, recombining to form a photon with a +45° polarization component. Thus, no photon is absorbed by the +45° polarizer.

- *Student A: Why don't the photons arriving at detector D2 display interference?*
- *Student B: Orthogonally polarized beams of light do not interfere, regardless of the phase difference between them. The +45° polarized photon can be in a superposition of both the U and L path states and horizontal and vertical polarization states.*
- *Student C: However, the two orthogonally polarized components of the photon state arriving from the two paths between BS2 and D2 cannot interfere. We have WPI for those photons*

arriving at detector D2 since there is no +45° polarizer between BS2 and detector D2 and thus there will be no interference displayed in the given case when we have two orthogonal polarizers in the U and L paths.

Do you agree with Student B and Student C? Explain.

Students can use the computer simulation to verify that the quantum eraser setup gives rise to interference (see Figure 7-10) in this case.

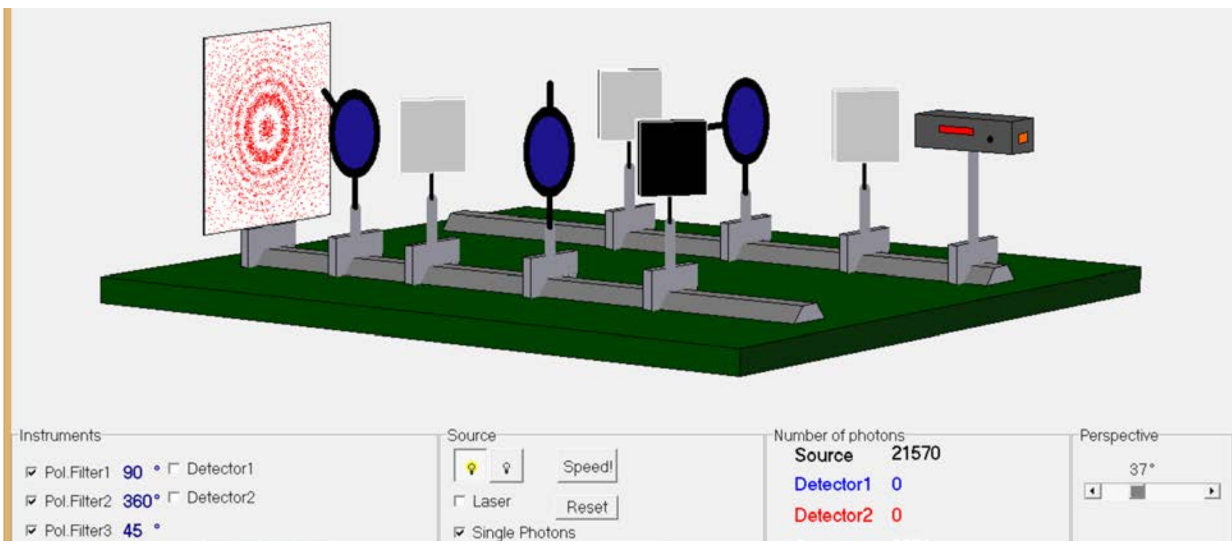


Figure 7-10. Computer simulation showing the quantum eraser MZI setup. Interference is observed at the screen.

Students are also guided to think about how the quantum eraser case distinguishes a stream of unpolarized photons (e.g., a mixture of horizontally and vertically polarized photons) from a stream of +45° photons:

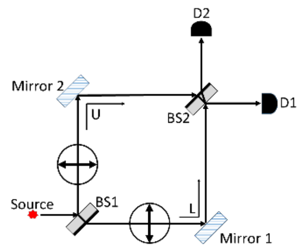
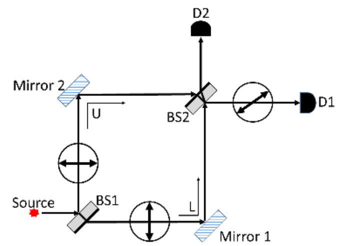
Consider the following conversation between two students:

- *Student 3: In figure 7-5, even if the source emits unpolarized photons, the polarizer with a +45° axis will erase the WPI.*
- *Student 4: I disagree. If the source emits unpolarized photons, we can consider half of the photons emitted to be vertically polarized and half of the photons emitted to be horizontally polarized. Approximately $N/4$ vertically polarized photons are absorbed by the horizontal polarizer and the other $N/4$ vertically polarized photons go through the L path. Therefore, even if these photons go through polarizer 3, we have WPI for them and they will not show interference.*
- *Student 3: I see. In the same manner, $N/4$ horizontally polarized photons are absorbed by the vertical polarizer and the other $N/4$ horizontally polarized photons go through the U path. Therefore, we have WPI for each photon, even if it goes through polarizer 3.*
- *Student 4: Even if a phase shifter is placed in one of the paths of the MZI and its thickness is gradually changed, this will not affect the number of photons arriving at the detectors. The addition of the third polarizer between BS2 and D1 simply blocks half of the photons but it does not cause the single photon to have interfering polarization components along the eraser direction.*

Do you agree with the students? Explain your reasoning.

Students are also given a table (see Table 7-1) as a summary to help them compare the differences between the case in which two orthogonal polarizers are placed in the two paths of the MZI (see Fig. 7-3) vs. the quantum eraser setup (see Fig. 7-5) and the differences between a source emitting a stream of unpolarized photons vs. a stream of +45° photons.

Table 7-1. Comparison of the MZI setup with two orthogonal polarizers placed in the paths of the MZI vs. the Quantum Eraser setup

MZI setup: Two orthogonal polarizers		MZI setup: Quantum eraser	
			
Unpolarized photons	+45° Polarized photons	Unpolarized photons	+45° Polarized photons
MZI setup is NOT a quantum eraser. If a phase shifter is inserted and its thickness is gradually changed, the number of photons arriving at the detectors does not change. No interference displayed at D1 or D2.	MZI setup is NOT a quantum eraser. If a phase shifter is inserted and its thickness is gradually changed, the number of photons arriving at the detectors does not change. No interference displayed at D1 or D2.	MZI setup is NOT a quantum eraser. If a phase shifter is inserted and its thickness is gradually changed, the number of photons arriving at the detectors does not change. No interference is displayed at D1 or D2.	MZI setup is a quantum eraser. If a phase shifter is inserted and its thickness is gradually changed, the number of photons arriving at the detectors changes. Interference is observed at D1 which changes based upon the phase difference introduced by the phase shifter. No interference at D2.

After working on the QuILT, students should be able to qualitatively reason about how adding polarizers can affect (or eliminate) the interference observed at the detectors. They should also be able to determine whether WPI is known for some (or all photons) and whether inserting a phase shifter and changing its thickness gradually would affect the number of photons arriving at the detectors in the different cases in which polarizers are inserted into the paths of the MZI.

7.5 PRELIMINARY EVALUATION

Once we determined that the QuILT was effective in individual administration, it was given to 44 upper-level undergraduates in a first semester quantum mechanics course and 45 first-year graduate students. To evaluate the effectiveness of the QuILT, a pretest was administered to 44 upper-level undergraduate students in junior/senior level quantum mechanics courses and 45 graduate students enrolled in the first semester of a graduate level quantum mechanics course. After the students completed the pretest, they were given one week to work through the QuILT and were then given a posttest, which had analogous questions as the pretest except that the orientations of the polarizers differed (e.g., instead of vertical and horizontal polarizers in the two paths and source emitting $+45^0$ polarized single photons, the posttest had $+45^{\circ}$ and -45° polarizers in the two paths and a source emitting vertically polarized single photons). Any students who did not work through the QuILT for any reason were omitted from the posttest data.

The graduate students were enrolled in a teaching assistant training class, during which they learned about instructional strategies for teaching introductory physics courses. They were asked to work through the QuILT to learn about the effectiveness of tutorials. They were given credit for completing the pretest, conceptual tutorial, and posttest. However, their performance on the posttest was not part of the final grade for the teaching assistant training class.

Table 7-2 shows the common student difficulties and percentages of students exhibiting those difficulties on the pretest and posttest. Table 7-3 shows the average percentage score on questions on the pre/posttest. Part (a) of each question asks students to compare two different MZI setups with polarizers and describe how they are different, e.g., “You insert a polarizer with a vertical polarization axis in the U path of the MZI. Describe what you would observe at D1 and D2 and how this situation will differ from the case in which there is no polarizer in path U." Part (b) asks for the percentage of photons that display interference. Average normalized gain [11] is commonly used to determine how much the students learned, taking into account their initial score on the pretest. It is defined as $\langle g \rangle = \frac{\%\langle S_f \rangle - \%\langle S_i \rangle}{100 - \%\langle S_i \rangle}$, in which $\langle S_f \rangle$ and $\langle S_i \rangle$ are the final (post) and initial (pre) class averages, respectively [11]. The average normalized gain from pre-/posttest using the rubric on questions related to MZI with polarizers was 0.7.

Table 7-2. Common difficulties and percentages of undergraduate students (UG) and graduate students (G) displaying them on the pre/posttest questions involving a MZI with polarizers. The number of students who took the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

Difficulty	**Pretest UG ($N = 44$)**	**Pretest G ($N = 45$)**	**Posttest UG ($N = 39$)**	**Pretest G ($N = 45$)**
Q1 One polarizer in the path of the MZI will not change the interference	34	36	10	13
Q2 An MZI setup with two orthogonal polarizers placed in the two paths (one in each path) is not different from the setup with one polarizer except fewer photons reach the detector and interference is displayed regardless of the polarizer setup	39	47	8	27
Q3 The quantum eraser setup is not different from placing two orthogonal polarizers in the two paths of the MZI except fewer photons reach the detectors	41	47	5	29

Table 7-3. Average percentage scores of undergraduate (UG) and graduate (G) students on the pretest and posttest questions involving a MZI with polarizers. The number of students who took the pretest does not match the posttest because some students did not finish working through the QuILT and their answers on the posttest were disregarded.

		Q1a	Q1b	Q2a	Q2b	Q3a	Q3b
UG ($N = 44$)	**Pretest**	10	16	17	20	11	14
UG ($N = 38$)	**Posttest**	86	81	85	85	86	85
G ($N = 45$)	**Pretest**	21	26	36	40	29	31
G ($N = 45$)	**Posttest**	69	71	67	73	67	76

Question 1 on the pre/posttest assessed student understanding of the effect of one polarizer placed in one of the paths of the MZI (see Fig. 7-4). Students were asked to explain how inserting a polarizer with a vertical polarization axis in the U path of the MZI would affect what happens at the detectors compared to the original MZI setup in which there is no polarizer (part a) and they were asked to write down the percentage of photons displaying interference at the detectors (part b). In the pretest, 34% of the undergraduate students and 36% of the graduate students correctly noted that the single polarizer would absorb some of the photons and thus fewer photons would reach the detectors, but they incorrectly claimed that all of the photons reaching the detector would display interference. After working on the QuILT, the difficulty with how one polarizer will affect the interference was reduced (see Table 7-2).

Question 2 on the pre/posttest assessed student understanding of the effect of placing two orthogonal polarizers in the two paths of the MZI (see Fig. 7-3). Students were asked to describe how this situation is different from the case in which there was only one polarizer present and what percentage of photons would display interference. After working through the QuILT, the difficulty with how two orthogonal polarizers affect the interference at the detectors was reduced (see Table 7-2).

Question 3 on the pre/posttest assessed student understanding of a quantum eraser (see Fig. 7-5). The addition of the third polarizer causes both components of the photon path state to be projected in the detector D1, erasing WPI about the photons arriving at D1. As the thickness of the phase shifter is varied, the interference displayed at D1 will change (unlike the setup without polarizer 3). In the pretest, 41% of undergraduate students and 47% of graduate students incorrectly claimed that the quantum eraser setup is not different from the setup with two orthogonal polarizers in the paths of the MZI or that fewer photons would reach D1 and/or D2 but otherwise they are the same. After working through the QuILT, this difficulty was reduced (see Table 7-2).

Even after working through the QuILT, some students continued to have difficulty with the situation in which only one polarizer is placed in one of the paths of the MZI on the posttest (Q1a and Q1b, see Table 7-3). For example, one student incorrectly claimed that "75% of the photons [display interference] because 50% of the initial photons take path L and make it to the [detector] and 50% of the 50% taking path U make it so 50% + 25% = 75%." These types of responses indicate that students may reason that any photon passing through the polarizers and arriving at the detector must interfere with itself regardless of the setup. Some of these students had difficulty with the concept of how a single polarizer placed in one of the paths of the MZI involves a measurement of the photon state that may provide WPI for some photons but not others.

We are developing a related QuILT which will help students connect the qualitative understanding of a quantum eraser with mathematical formalism using a product space of a two state system for both the photon path and polarization states. This QuILT strives to also help students develop a quantitative understanding of how polarizers affect measurement outcomes and how quantum erasers work.

The performance of graduate students was higher than undergraduate students on the pretest (see Table 7-3). In contrast, on the posttest, undergraduate students performed slightly better than graduate students. This may be due, in part, to the fact that graduate students' performance on the posttest was not part of their final grade for the teaching assistant training class. Graduate students may not have worked through the tutorial in an engaged manner, i.e., contemplating their difficulties and repairing their knowledge structure, and this could have resulted in the persistence of difficulties and a smaller increase in their scores from the pretest to posttest. These results demonstrate the importance of students being actively engaged and motivated while learning. In particular, if students are aware that they are not going to be graded on their performance on a posttest, they may not be motivated to engage with the material in the tutorial (especially if they are working on the tutorial on their own as a homework assignment).

7.6 SUMMARY

The QuILT uses a MZI experiment with single photons to help students learn how polarizers affect the interference of a single photon with itself in an exciting context. By taking into account students' prior knowledge and difficulties, the QuILT helps students learn how interference at the detectors in the MZI setup can be reinstated by introducing a third polarizer with a certain orientation between BS2 and a detector. Many students stated that it was one of their favorite QuILTs, e.g., "I had no idea what the concept of [WPI] was…. The concept of a quantum eraser was…pretty mind-blowing at first."

7.7 ACKNOWLEDGEMENTS

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8.0 FROM INSTRUCTIONAL GOALS TO GRADING PRACTICES: THE CASE OF GRADUATE TEACHING ASSISTANTS

8.1 INTRODUCTION

Grading is considered as a means to shape student behavior and learning by communicating (both implicitly and explicitly) the instructors' goals to their students [1-5]. However, teachers' instructional decisions are shaped in the midst of classroom events by a constellation of occasionally conflicting beliefs, goals, knowledge, and action plans triggered by various aspects of the immediate context (e.g., students disagreeing about their grades, expectations of peers and administrators, workload, etc.) [6]. Thus, it is reasonable to expect that instructors' grading decisions would serve only some of their goals and possibly not align well with some of their stated goals.

The likelihood of such inconsistencies increases in the setting of introductory physics courses, where graduate TAs are frequently those responsible for grading students' work. Graduate TAs are newcomers to the scientific community, taking their first steps in their new roles as researchers and instructors and striving to meet the expectations of senior scientists, research advisors, and course instructors. The resources accessible to them are commonly their own experiences as novice students as well as the requirements of the departments and/or lecturers they assist. TAs usually have a narrow window in time to develop their personal approach towards instruction in general, and in particular, to design grading methods that transmit adequately their instructional values and beliefs. Moreover, many of the TAs in physics departments in the U.S.

(the context of this study) have differing international backgrounds. They need to adapt their prior experiences, which reflect different educational systems, to a new educational setting in a short time period. Professional development programs, which TAs can be required to participate in, might serve to resolve such possible mismatches between their goals and practice, providing an opportunity for them to distill their goals and direct their actions to achieve their goals.

Prominent teacher educators [7] recommend that professional development programs should attend in an explicit manner to existing beliefs and knowledge that teachers hold about the learners, the “material,” learning, and instruction and will provide time and support for teachers’ reflections on their goals, classroom experiences, and beliefs [8-10]. In a review of research on professional development programs for practicing teachers, Borko [11] suggests that for teachers’ reflections to foster learning they should take place in “strong professional communities” (p.6) and make use of “records of practices” (p.7). However, the time constraints within which TA training programs typically take place provide few opportunities for the experiences suggested by teacher educators. Moreover, while it is recommended that such programs would attend to existing beliefs, physics TAs’ knowledge and beliefs have only recently attracted researchers attention [12-22].

In this study, we investigate TAs’ perceptions in an area for which graduate TAs are often responsible: grading students’ work in an introductory physics course. The TAs worked in groups, serving as ad-hoc professional communities, in which they examined a set of student solutions for a problem designed to provide an opportunity for a spectrum of more or less expert-like problem-solving practices. The TAs were guided to reflect on their grading decisions and explain what they valued and disregarded in students’ solutions and why. This activity served to gauge their goals and considerations in grading as well as stir a discussion examining their instructional decisions in light of their goals. The findings of this first component of the study can inform providers of professional development regarding physics TAs' prior knowledge. We also examined the evolution of the TAs' perceptions after this short professional development intervention at the end of the semester, when they would have had the opportunity to connect their professional development experience with their day-to-day teaching. The findings of this second component of the study can inform providers of professional development for physics TAs on the possible worth, if at all, of short professional development interventions. The choice to examine TAs' beliefs at the end of the semester considers a situative perspective on teachers' learning, realizing that teachers' learning take place both in formal professional development programs as well as in their day-to-day teaching practice. In particular, the knowledge that TAs have constructed in a professional development program can later evolve or dissolve within their teaching practice.

We studied the grading decisions and considerations of 43 graduate TAs participating in a TA training program at a large research university. In particular, we studied TAs' considerations related to product-oriented learning goals (i.e., to develop students' understanding of disciplinary concepts and principles) and to process-oriented learning goals (i.e., to help students become more expert-like in their approach to problem solving and to make better use of problem solving as a tool for learning). These goals were found to be common for instructors of introductory physics courses [23]. We examined TAs' grading decisions in light of research-based instructional strategies targeting these goals (i.e., developing expert-like problem-solving practices [24-29] or enhancing learning disciplinary concepts and principles through problem solving [30-32]). In particular, we focused on the recommendation to require students to explicate their reasoning and to follow a prescribed problem-solving strategy as means to develop expert-like practice [26]. Within an instructional approach based on formative assessment [33], grading could promote these practices by rewarding them. Accordingly, we examined the extent to which TAs' grading decisions (i.e., scoring of student solutions) and considerations (i.e., solution features noticed/graded on and reasons for grading) promote prescriptive problem-solving strategies and articulation of reasoning.

8.2 BACKGROUND AND LITERATURE REVIEW

Our study is based on two lines of research: 1) research-based instructional strategies aimed to promote expert-like problem-solving approaches as well as learning through problem solving and their implications in grading, and 2) research on TAs' beliefs and practices related to learning and teaching in general and, in particular, problem solving.

8.2.1 Promoting desired problem solving practices via grading

Significant research [24-29,34] has documented differences between experts and novices when approaching problems. Both use heuristics to guide their search process, identifying the gap between the problem goal and the state of the solution and taking action to bridge this gap. However, novices approach problems in a haphazard manner, while experts devote time and effort to describe qualitatively the problem situation, identify theoretical models that may be useful in the analysis of the problem, and retrieve effective representations based on their well-organized domain knowledge. In addition, experts devote time to plan a strategy for constructing a solution by devising, frequently in a backward manner, a useful set of intermediate goals and means to achieve them. Experts also engage more than novices in self-monitoring their progress towards a solution by evaluating former steps and revising their choices. [26]. Instruction can help students develop expert-like problem-solving approaches and learn from problem solving by encouraging students to follow a prescribed, systematic problem-solving process where they explicate, for example [24-29, 35]:

1) how they translate the problem situation to describe it in physics terms;
2) their plan for the solution and in particular, the sub-problems used in the construction of a solution; and
3) how they evaluate the reasonability of the results.

Grading can encourage students to follow such a systematic problem-solving process if instructors assess students on the use of problem-solving strategies such as drawing a diagram, listing known and unknown quantities, clarifying their considerations in setting up sub-problems, and evaluating the answer.

Furthermore, better performing students utilize problem solving as a learning opportunity more effectively by providing more self-explanations (i.e., content-relevant articulations formulated after reading a line of a worked-out example which state something beyond what the sentence explicitly said [36]), even though their self-explanations might be fragmented and sometimes incorrect [36, 37]. Students learn by articulating their understanding of how relevant concepts and principles are used to solve a problem by identifying and attempting to resolve conflicts between their own mental models and the scientific model conveyed by peers' solutions or worked-out examples [38]. It is reasonable to expect that student solutions articulating the solver's reasoning provide him/her with an artifact to reflect on to determine whether he/she invoked appropriate physics principles and applied those principles adequately. Thus, to encourage students to learn from problem solving, grading should encourage students to explain their reasoning.

In summary, student behavior in a course is more likely to be affected by grading practices than by instructor statements or other actions [3,4]. Students often adjust their behavior in a manner that will help them achieve better grades on homework, quizzes, and exams [39,40]. In particular, in the spirit of formative assessment [33], grading can provide feedback that moves learning forward, communicating to learners what practices are useful in learning a particular discipline [41] and opening the possibility for students to help one another and to use test results as feedback for what to focus on in future learning activities [41-47]. In particular, grading practices could be designed to promote behaviors such as prescribed problem-solving strategies and the articulation of reasoning underlying a solution.

8.2.2 TAs' instructional beliefs and practices about learning and teaching as related to problem solving

Misalignments between TAs' instructional beliefs about teaching and their teaching practices have been identified in several studies [14-22]. TAs' beliefs about their role as an instructor vary significantly—from transmitter of knowledge at one end of the spectrum to facilitator of knowledge construction at the other [18, 20]. TAs display discrepancies between their stated beliefs and their actual practice in the classroom regarding active participation in the learning process (e.g., endorsing the goal of engaging students in sense-making while devoting much of their time to transmitting knowledge or valuing example solutions which reflect an expert-like problem-solving approach but creating brief example solutions which do not reflect an expert approach) [12, 19, 22].

Teachers' perceptions of teaching and learning in general, and TAs' perceptions in particular, are shaped by their past experiences and their current teaching situation [48,49]. TAs' past experiences as students shape their intuitive perceptions about learning and teaching, and these views are often deeply rooted and highly resistant to change [13, 48]. For example, in the laboratory context, TAs believe that students learn similarly to them and implement instructional strategies that were effective for them (but not necessary beneficial for students) [13]. TAs acknowledge instructional strategies from educational research, but disregard them for their own views of appropriate instruction, e.g., that the material should be made clear by the TA and that students need direct instruction and extensive practice to learn the required concepts [13].

According to the above, TAs' own practices in problem solving can serve as indicators of their beliefs regarding learning and teaching problem solving. Mason and Singh demonstrated that while nearly 90% of graduate students reported that they explicitly think about the underlying concepts when solving introductory physics problems, approximately 30% of them stated that solving introductory physics problems merely requires a "plug and chug" strategy [50]. They explain their findings in that when graduate students solve introductory problems, these are essentially exercises as opposed to problems. Thus, TAs can immediately recognize the principles required to solve the problem and they perceive problem solving as not requiring much thought or reflection. Many of the graduate students stated that reflection after problem solving is unnecessary because the problem was so obvious [50]. Thus, TAs who teach recitations or laboratory sections may not model, coach, or assess explication of reasoning or reflection because they believe it is not required.

Lin et al. [12] studied TAs' beliefs about the learning and teaching of problem solving using example problem solutions. This study revealed a discrepancy between TAs' stated goals and practice. For example, when TAs were asked to evaluate three different versions of example solutions, many valued solutions comprising of features described in research literature as supportive of helping students develop an expert-like problem-solving approach. Most TAs expressed process-oriented learning goals (i.e., to help students become more expert-like in their problem solving approaches and to make better use of problem solving as a tool for learning [51]) when contemplating the use of example solutions in introductory physics. This finding seems to contradict the expectation based on their problem solving practices when solving introductory physics problems, as stated above. However, their own designed example solutions did not include features supportive of helping students' development of an expert-like approach. When TAs were unaware of the conflict between their stated goals and practice, they tended to prefer product-oriented solutions (i.e. solutions in which the rationale is not included [51]). It is reasonable to assume that a similar discrepancy may arise in the context of grading, i.e., TAs may have productive beliefs about the role of grading in the learning process, but employ grading practices which do not align with those beliefs.

TAs' current teaching situations also contribute to their perceptions of teaching and learning. Since limited training and feedback is offered to new TAs, many rely on "on the job" experiences in the classroom to learn how to teach [52]. As mentioned above, graduate TAs have recently experienced the culture of introductory physics classrooms as students, and are now advised as new instructors by the physics faculty teaching the course. Thus, one might expect graduate TAs' beliefs regarding learning and teaching problem solving to be influenced by those of physics faculty. A recent study by Hora et al. [53] investigated the beliefs of 56 math and science instructors at undergraduate universities. They described instructors' beliefs about student learning in general, and in particular, in the context of solving problems. Faculty stated that students learn by practice and perseverance, hands-on application, articulation of their own ideas and problem-solving processes to others, active construction, connection to experience, repetition, and memorization. In this study, faculty members indicated that they believe students learn best when they study and practice problem solving diligently on their own. Many instructors stated that learning occurs over time through sustained engagement with the material. Approximately one-third of the interviewed faculty members stated that learning varies from person to person and no single type of instruction is adequate for all students. Many physics instructors believe that a central goal of physics instruction is to improve students' problem-solving approaches. Furthermore, they reject the view that expert problem solving is an accumulation of knowledge built from solving a large set of physics problems [23]. Many instructors state that they believe students can learn to solve problems by watching experts solve problems or reading example solutions, extracting the strategies underlying these solutions, and reflectively attempting to work problems [23]. In regards to grading problem solutions, a study by Henderson et al. [54] demonstrated that most instructors know that there are advantages for students to show their reasoning in problem solutions because it 1) helps students rehearse and improve their problem-solving skills and understanding of physics concepts; and 2) it allows the instructor to observe and diagnose student difficulties. However, less than half of the instructors interviewed gave students an incentive in their grading for explaining their reasoning. Many instructors placed the "burden of proof" of student understanding on themselves when assigning a score to a student solution. TAs' beliefs with regard to learning from example solutions [23] were found to echo those of faculty, suggesting that TAs' ideas reflect the instructional culture in an introductory physics course set by the faculty.

8.2.3 Changing TAs' instructional beliefs and practice

Teachers' decision-making is described in the educational literature as an implicit process, drawing upon tangled and occasionally conflicting conceptions [55-59]. Schoenfeld [6] describes teachers' decisions as shaped by a constellation of highly activated beliefs, goals, knowledge, and action plans. Occurrences in the immediate context spur teachers to activate different beliefs, goals, knowledge, and action plans, and teachers' reactions to these occurrences are interpreted in light of their former experiences. Much of an experienced teacher's decision making is automated and the teacher is no longer aware of the reasons that led to the development of the routine [60-65]. Since instructors' interpretations of classroom events are shaped by former experiences and beliefs, a major challenge for professional development is that even when instructors believe in an instructional goal and attempt to direct their instruction to achieve it, their prior beliefs may conflict with and distort the attempt [58,66-68]. As a result, teacher educators recommend that a long-term professional development intervention is needed and should be contextualized in teachers' everyday practices. This would allow them to reflect on their goals, actions, and achievements in order for fundamental changes in teacher practice to take place [9,11,69-72].

According to Thompson and Zeuli [73], transformative learning experiences for teachers are characterized by:

1) creating a high level of cognitive dissonance to upset the balance between teachers' beliefs and practices;

2) providing sufficient time, structure, and support for teachers to think through the dissonance they experience (i.e., providing opportunities for discussion and reflection with peers);
3) embedding dissonance-creating and dissonance-resolving activities in teachers' own classroom situations and their own practices of teaching and learning;
4) enabling teachers to develop a new repertoire of practice that fits with their new understanding (i.e., moving from a new understanding to a change in practice); and
5) engaging teachers in a continuous, iterative process of improvement, promoting collaboration, awareness, and reflection on teaching practice via case discussions and examination of students' work [9].

There is no reason to believe that TAs' decision making is different than faculty. Accordingly, the principles of professional development discussed above, which have been shown to be successful in professional development of physics teachers [69, 70], can guide professional development programs to assist TAs in transforming their perceptions regarding teaching and learning while taking into account both their prior experiences, beliefs about ideal teaching, as well as their present teaching situations. Thus, TAs may undergo transformative learning experiences if they are given opportunities to undergo cognitive dissonance, i.e., by contemplating potential conflicts between alternative instructional approaches they attempt to use in their classrooms, their own goals, and research-based teaching strategies.

Indeed, physics TAs have expressed that while it is important to learn about theories of learning, putting the theory into practice in the classroom setting was crucial in helping them personally accept that a particular instructional strategy is effective [74]. TAs' development of pedagogical content knowledge [75,76] was shown to follow three phases: 1) accepting; 2) actualizing; and 3) internalizing [74]. In the accepting phase, TAs learned about the various components of pedagogical content knowledge, including knowledge of students' understanding of science, instructional strategies for teaching science, and knowledge of assessment in science. In the actualizing phase, TAs connected their acquired pedagogical content knowledge to the classroom. TAs' perceived that their pedagogical content knowledge generally improved as a result of their classroom experiences. Lastly, TAs internalized pedagogical content knowledge when they could rationalize about its usefulness in the classroom [74].

In a similar manner, professional development programs focused on TAs' ideas about grading should extend further than exposing the TAs to grading approaches recommended in educational literature. It should also allow them to relate the educational literature to their own classroom practice, engage them in peer collaboration to continuously examine their experience, and better align their practice and their goals.

However, TAs are commonly encouraged to focus more on research than teaching and the TA's supervising instructor may be unwilling to assist the TA because of time constraints [48,52]. Furthermore, TAs' coursework responsibilities, research responsibilities, adjustment to a new lifestyle, and other stresses in their lives may limit the time they can invest into changing their teaching practices. Thus, one may wonder whether professional development programs can be designed to, on one hand, follow the recommendation for contextualizing TAs' learning in reflecting on their experiences, while, on the other hand, meet their time constraints. In particular, can short-term professional development experiences that follow these guidelines assist TAs in transforming their perceptions regarding teaching and learning? As part of this study we will examine to what extent, if at all, a short-term intervention designed along the aforementioned lines achieve these goals.

8.3 METHODOLOGY AND DATA COLLECTION

The study involved graduate TAs at a research university in the U.S. and probed their perceptions at two points in time: 1) when they entered their teaching career; and 2) after a semester of teaching experience and a semester-long TA training course. Three consecutive weekly sessions at the outset of the training course revolved around a group administered interactive questionnaire (GAIQ), encouraging reflection on the various facets of teaching problem solving. The GAIQ consisted of a three-part questionnaire designed to encourage reflection on 1) the design of sample solutions; 2) grading decisions; and 3) the design of problems. The questionnaire required TAs to make judgments regarding artifacts designed to simulate those they likely encounter in their teaching environment as well as artifacts designed to explicate their attitudes towards research-based instructional practices intended to promote expert-like problem solving approaches [77]. After the TAs completed each part of the questionnaire individually, they discussed their decisions and considerations in groups of three. A whole-class discussion took place immediately in which the TAs shared the ideas their group agreed upon as well as unresolved conflicts. Thus, the discussions in groups and in the whole-class forum were expected to externalize conflicting viewpoints and help TAs realize implicit conflicts and discuss how to remedy them. These activities were meant to help TAs align their instructional decisions with their stated goals. At the end of each session, the TAs individually completed a questionnaire in which they were asked to summarize their ideas following the discussion.

The GAIQ activities served not only as means for professional development but also as a data collection tool in order to study TAs' grading decisions and considerations in this simulated environment. In particular, we examined their individual answers in session 2 that focused on grading. After a semester of teaching experience, the TAs were again asked to work through the individual component of the GAIQ questionnaire. In this context, we investigated TAs' grading decisions and considerations when grading student solutions designed to elicit conflicting grading approaches. We also examined whether TAs' stated goals for grading were consistent with their grading decisions and the extent to which TAs' grading decisions and considerations changed after a short professional development intervention and one semester of teaching experience.

In particular, we examined the following four research questions:

8.3.1 Research questions

Research question 1 (RQ1): What were TAs' grading decisions at the beginning of their teaching appointment?

Research question 2 (RQ2): What were TAs' considerations underlying their grading decisions at the beginning of their teaching appointment?

RQ1 and RQ2 were examined in the context of a task asking TAs to grade a set of specially designed student solutions. To answer RQ1, we examined TAs' scores on the student solutions. To answer RQ2, we identified the solution features that TAs mentioned and graded on and the reasons they provided for assigning a particular score. In both questions we distinguished between TAs' perceptions in a quiz or homework context (by asking whether they would score the same student solution differently in these two contexts and why). We did so because these two contexts may trigger different grading considerations for TAs. For example, TAs may either be more lenient in grading the quiz due to the time constraints on students or they may grade more harshly because they believe students should have mastered the material before taking the quiz. TAs may also require more reasoning in a homework context because students have more time to create detailed, systematic solutions. Indeed, an examination of how the beliefs and values of physics faculty influence their choice of physics problems for their students in an introductory physics course found that many instructors do not grade on problem features that they see as beneficial for students' learning because they are concerned that these features will result in student stress, especially on exams [78].

Research questions 1 and 2 focus on TAs' prior perceptions about grading. Specifically, we hope the answers to these questions would inform providers of professional development about the extent to which TAs' perceptions are aligned with the recommendations in the literature. Thus, we will discuss our findings in light of grading practices suggested in the literature as means to promote expert-like problem solving.

Research question 3 (RQ3): To what extent are the grading decisions of TAs aligned with their general beliefs about the purposes of grading?

RQ3 aims to examine the findings for questions 1 and 2 in a critical manner. As mentioned earlier, different beliefs, goals, and knowledge related to grading may be triggered in different contexts, possibly conflicting with each other. To identify possible conflicts, we studied the differences between manifested goals when TAs are asked to state their goals in a general context and TAs' decisions when grading concrete solutions. Along with the literature [73] suggesting to anchor conceptual change in a cognitive conflict, we believe that identifying such conflicts can serve teacher educators to initiate a conceptual change process for TAs.

Finally, research question 4 examines the potential of a short professional development experience to change TAs perceptions:

Research question 4 (RQ4): How do TAs' grading decisions and considerations change after a short professional development intervention and a semester of teaching experience?

As described in the literature review, an intervention might inspire transformative learning experiences if it is embedded in practice and provides opportunities for cognitive dissonance. Furthermore, instructional approaches can become more ingrained as well as fade away as TAs gain teaching experience. Thus, we investigated how TAs' perceptions regarding grading evolve when TAs are exposed to a short intervention regarding grading as well as after they have developed their own instructional approaches while teaching.

8.3.2 Participants

We collected grading data from two different semesters of a professional development program led by one of the authors (C.S.). A total of 43 TAs were enrolled in the program, which was designed to prepare the TAs for their teaching appointments. The participants' national backgrounds were varied; in total, there were 14 graduate students from the U.S., 17 graduate students from China, and 12 students from other countries. Most of the TAs were concurrently teaching a recitation or laboratory section. A majority of the TAs were also tutors in a physics exploration center where introductory students are assisted with their physics homework and labs.

8.3.3 Data Collection

TAs' perceptions about grading were inferred from their responses to the GAIQ [77], which was designed to elicit TAs' stated beliefs about grading in general as well as reveal their grading decisions and considerations in a simulated grading context. The GAIQ served as part of a professional development program that was designed to encourage reflection on the various facets of teaching problem solving. The GAIQ methodology attempts to replicate the features of a semi-structured interview within a written questionnaire in order to yield more rich and comprehensive data resembling data acquired in an interview while reducing the time required for data collection and analysis. Additionally, the GAIQ allows for some exchange and clarification to take place in a standardized manner that minimizes the danger of specific interviewer interventions reducing reliability and validity. We followed the GAIQ sequence shown in Table 8-1.

The questionnaire included both general questions and concrete questions asking the respondent to compare and make judgments about a set of artifacts that differ in features [77]. The artifacts consisted of a set of student solutions to a core problem [Fig. 8-1].

Homework Problem
You are whirling a stone tied to the end of a string around in a vertical circle having a radius of 65 cm. You wish to whirl the stone fast enough so that when it is released at the point where the stone is moving directly upward it will rise to a maximum height of 23 meters above the lowest point in the circle. In order to do this, what force will you have to exert on the string when the stone passes through its lowest point one-quarter turn before release? Assume that by the time you have gotten the stone going and it makes its final turn around the circle, you are holding the end of the string at a fixed position. Assume also that air resistance can be neglected. The stone weighs 18 N.

The correct answer is 1292 N.

Figure 8-1. Core problem

Physics faculty at several institutions examined the problem and verified that the problem was appropriate though difficult for a student in an introductory physics course. The problem included several features of a context-rich problem [79] (i.e. it was not broken into parts, did not include diagram, was set in a realistic context, etc.). The features of the problem were chosen to require an average student to engage in a search process as opposed to an algorithmic procedure, thus it allowed for a spectrum of more or less expert-like problem solving practices. The solutions were taken from a pool of student solutions to the problem that was given on a final exam. They were chosen to reflect differences between expert and novice problem solving from the research literature such as existence of a diagram describing the problem, explication of sub-problems, justification of solution steps, evaluation of final answer, etc. [79]. Most features were triangulated in at least two artifacts.

Data was collected at the beginning and end of the fall semester in the context of a TA training course. At the beginning of the semester (i.e., the pre-lesson stage), the TAs wrote an essay responding to the following general questions:

1) What, in your view, is the purpose of grading students' work?
2) What would you like students to do with the graded solutions returned to them?
3) What do you think most of them actually do?
4) In your opinion, are there other situations besides the final exam and quizzes in which students should be graded?
5) Does grading serve the same purposes for these situations?

In the pre-lesson stage of the GAIQ, the TAs also filled out a worksheet asking them to make decisions about the set of student solutions and encouraging their introspection regarding their instructional choices. Here we focus on two solutions (see Fig. 8-2). These two solutions were chosen because they trigger conflicting instructional considerations in assigning a grade. We suggest that the reader examine the student solutions (see Fig. 8-2) and think about how to grade them. Please note that clearly incorrect aspects of the solutions are indicated by boxed notes. In comparing student solution D (SSD) to student solution E (SSE) (see Fig. 8-2), note that both include the correct answer. However, only SSD includes a diagram, articulation of the principles used to find intermediate variables, and clear justification for the final result. In contrast, SSE is brief with no explication of reasoning. However, the elaborated reasoning in SSD reveals two canceling incorrect calculations, involving misreading of the problem situation as well as misuse of energy conservation to imply circular motion with constant speed. In contrast, SSE, being very brief, does not give away any evidence for mistaken ideas. However, the three lines of work in SSE are also present in SSD, suggesting that Student E might be guided by a similar thought process as Student D. Thus, TAs' grading of SSE and SSD could reveal to what extent they encourage the use of a prescribed problem-solving strategy and showing reasoning explicitly.

Table 8-1. GAIQ sequence of grading activities

<table>
<tr><th colspan="2">Time</th><th>Activity</th></tr>
<tr><td rowspan="3">Beginning of semester</td><td>Pre-lesson</td><td>Individually, TAs wrote an essay regarding the purpose of grading. They then completed a worksheet which asked them to grade student solutions (see Fig. 8-2) in homework (HW) and quiz contexts, list features of each solution, and explain why they weighed the features to arrive at a final score (see Fig. 8-3).</td></tr>
<tr><td>In-lesson</td><td>In groups of 3, TAs graded the student solutions using a group worksheet and then participated in a whole-class discussion in which the groups shared their grading approaches.</td></tr>
<tr><td>Post-lesson</td><td>Individually, TAs were given a list of 20 solution features and asked to rate how much they liked each feature. They were then asked to re-grade the student solutions, keeping in mind the in-class discussions and 20 features they rated.</td></tr>
<tr><td rowspan="2">End of semester</td><td>Pre-lesson</td><td>Individually, TAs wrote an essay regarding the purpose of grading. They then completed a worksheet which asked them to grade the student solutions (see Fig. 8-2) in HW and quiz contexts, list features of each solution, and explain why they weighed the features to arrive at a final score (see Fig. 8-3).</td></tr>
<tr><td>Reflection</td><td>TAs were given copies of their pre-lesson activities from the beginning of the semester and were asked to make comparisons between their responses on the beginning of the semester pre-lesson activities and the end of semester grading activities.</td></tr>
</table>

TAs were asked to grade the student solutions for both homework and quiz contexts, list characteristic solution features, and explain why they weighed the different features to obtain a final score. The TAs were told to assume that they were the instructors of the class and had the authority to make grading decisions. An example response (transcribed) is shown in Figure 8-3.

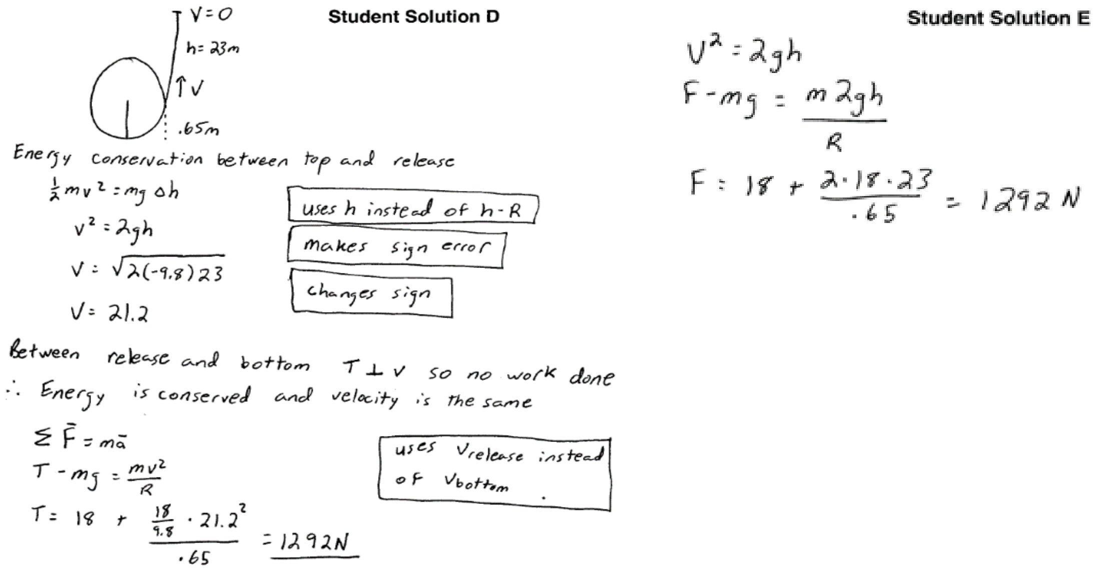

Figure 8-2. Student solution D (SSD) and student solution E (SSE)

Features: Solution E	**Score**		**Reasons: explain your reasoning for weighing the different features to result with the score you arrived at.**
	Q	HW	
No word explanation *No figure* *No error* *Precise and concise*	***10***	***9***	*There are no explanations in this solution, which means I could not know whether the student really knows the process or he/she just misdid like solution D. This is why I put 1 point off from this solution if this was HW. However, in the quiz time is limited, I will give a full grade to this solution*

Figure 8-3. One component of a sample TAs' worksheet (transcribed) related to SSE which was part of the pre-grading activity

During the in-lesson stage of the GAIQ, the TAs worked in groups of three in which they were asked to grade the student solutions again. After they had graded the solutions, a representative from each group shared their grading approaches with the entire class. Two of the authors (C. S. and E.M.) were present in the class, and E.M. focused on observing and documenting the TAs' comments during the group and whole-class discussions.

The post-lesson stage of the GAIQ was completed after the in-lesson stage to give TAs the opportunity to reflect on the group and class discussions and refine their perceptions about grading. Keeping in mind the group and class discussions, the TAs completed an individual worksheet in which they rated twenty solution features according to how much they liked each feature. Using their ratings for each feature, they re-graded the student solutions in the simulated grading context.

The pre-lesson, in-lesson, and post-lesson components of the GAIQ sequence of grading activities were completed by two cohorts of TAs within the first month of the TA training course when the TAs had very little teaching experience. The end of semester task was administered to 18 TAs (who were enrolled in the 2nd cohort) in the last class of the TA training course. It included the same essay and grading activity as in the pre-lesson stage.

8.4 DATA ANALYSIS AND FINDINGS

8.4.1 RQ1: What were TAs' grading decisions at the beginning of their teaching appointment?

Analysis. TAs' grading decisions (i.e., their scoring of student solutions) for SSD and SSE were represented on a graph of SSE vs. SSD scores, both in a quiz as well as in a homework context (see Fig. 8-4).

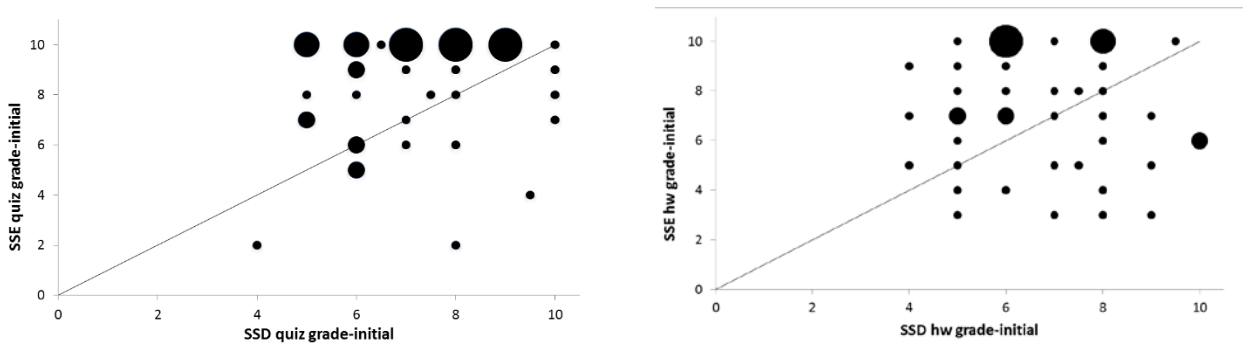

Figure 8-4. Distribution of 43 TA grades on SSD and SSE at the beginning of the semester (initial), quiz and HW. The size of the bubble represents the number of TAs at that particular point.

Findings. We found that in a quiz context, TAs graded a solution which includes the correct answer, lacks reasoning, and possibly obscures physics mistakes (SSE) higher than a solution which includes the correct answer, shows detailed reasoning, and includes canceling physics mistakes (SSD). In the quiz context, many more TAs graded SSE higher than SSD ($N = 28$, 65%) compared to those who graded SSE lower than SSD ($N = 10$, 23%), transmitting a message that is counterproductive to promoting the use of prescribed problem-solving strategies and providing explication of reasoning. We found a similar gap in the HW context, although the gap is somewhat softened: 58% of TAs ($N = 25$) graded SSE higher than SSD while 35% ($N = 15$) graded SSE lower than SSD. In a quiz context, TAs graded SSE significantly higher than SSD (SSE_{avg}=8.3 compared to SSD_{avg}=7.1, p-value (t-test)=0.010). In a homework, the averages are comparable (SSE_{avg}=7.1 and SSD_{avg}=6.7, p-value (t-test)=0.41).

8.4.2 RQ2: What were TAs' considerations underlying their grading decisions at the beginning of their teaching appointment?

We determined TAs' considerations in grading by analyzing: 1) the solution features they mentioned and graded on; and 2) the reasons they state for assigning a final score. We will discuss our methods and analysis of these two components in the following sections.

8.4.2.1 Solution features mentioned/graded on

Analysis. The pre-lesson stage of the GAIQ sequence asked TAs to grade student solutions SSD and SSE, list solution features, and explain their reasons for why they weighed the different features to arrive at a final score (see Fig. 8-3). Data analysis involved coding the features listed by TAs in the worksheets into a combination of theory-driven and emergent categories. We identified 21 solution features. We made a distinction between features that were merely mentioned or weighed in grading. For example, the sample TA listed "no figure" as a feature in SSE (solution feature "figure" was considered "mentioned"), but when assigning a grade, s/he did not refer to this feature when explaining how s/he obtained a score (solution feature "figure" was not included in grading) (see Fig. 8-3). Thus, the sample TA would be counted as mentioning solution feature "figure" but not counted as grading on it. A TA who graded on a solution feature was counted as both mentioning and grading on it. For example, if the sample TA had not written "no word explanation" in the Feature column, the feature "explanation" would have still been considered to be mentioned because this TA wrote "There are no explanations in this solution" as a reason for the final score he/she would assign to this solution (of course, the feature would also be considered to be graded on). The coding was done by two of the researchers (E.M. and A.M.) individually. Initially, their coding matched in 70% of the cases. In cases where disagreement occurred, this was usually due to vagueness in the wording of TAs' written statements. After comparing codes, the researchers discussed any disagreements with two other researchers (E.Y. and C.H.) until full agreement was reached. The researchers made use of the TAs' answers in the post-lesson stage (see Table 8-1) to clarify vague statements made by TAs. Finally, to ease representation and sense making, the features were grouped into 5 clusters, as shown in Table 8-2.

Data analysis also involved evaluation of the solution features with regard to the literature recommendations. Thus, we assigned each feature a +, - , or 0 to signify whether grading based on the presence/absence of the feature is productive (+), counterproductive (-), or neutral (0) in terms of encouraging students to follow a prescribed problem-solving approach and/or explain their reasoning (see Table 8-2). Accordingly, we also judged the clusters. Cluster 1 (C1) includes both features related to initial problem analysis as well as evaluation of the final result, and cluster C2 involves features related to explication of reasoning (i.e., articulation and justification of principles). We consider that TAs who grade on solution features included in C1 and C2 are encouraging students to follow prescribed problem-solving strategies [24-30, 36-38]. Thus, we assigned these clusters as (+) for being productive in encouraging expert-like approaches to problem solving. Cluster 3 (C3) includes domain-specific features, such as invoking relevant physics principles and applying them properly. C3 was determined to be productive in encouraging expert-like problem-solving approaches because students should learn domain knowledge through problem solving. Cluster 4 (C4) includes features related to elaboration which emerged during the coding process. These features were not assigned to the "explication" category because they were imprecise (e.g., "written statements" could be interpreted to mean articulation of principles or simply a written statement, e.g., "conservation of energy"). Features in C4 could be productive, counterproductive, or neutral in encouraging expert-like problem-solving approaches (assigned +, -, 0 respectively). For example, grading for conciseness could transmit a message to the students that physics problems should be solved with little detail (assigned as (-) for being counterproductive), while grading for written statements could transmit a message that explication of the thought process is important for learning from problem solving (assigned (+) for being productive). The feature of organization was assigned to be neutral (0) because it has a vague meaning. If a TA says that a solution is "organized" he/she could mean that the solution is neatly written, or that it is systematic. Showing algebraic steps, while helpful in solving problems, is not necessarily part of an expert-like approach, and it too was assigned to be neutral (0). Finally, cluster 5 (C5) focuses on correctness of algebra and final answer. TAs who weigh these features heavily in grading may transmit a message to the student that a correct final result is acceptable without justification. Since grading on this cluster discourages students from following a prescribed problem-solving approach, this cluster was assigned to be counterproductive (-) with regards to encouraging the use of prescribed problem-solving strategies.

Table 8-2. Sample features sorted into clusters and sample citations

<table>
<tr><td>C1 (+)
Problem description
& evaluation</td><td colspan="2">Visual representation (e.g., "diagram"); articulating the target variables and known quantities (e.g., "knowns/unknowns"); evaluation of the reasonability of the final answer (e.g., "check")</td></tr>
<tr><td>C2 (+)
Explication of problem-solving approach</td><td colspan="2">Explicit sub-problems (e.g., "solution in steps"); articulation of principles (e.g., "labels energy conservation use"; justifying principles (e.g., "explained the reason he used the formulas")</td></tr>
<tr><td>C3 (+)
Domain knowledge</td><td colspan="2">Essential principle invoked (e.g., "sums forces, energy conservation") ; essential principle is applied adequately</td></tr>
<tr><td rowspan="3">C4
Elaboration</td><td>(+)</td><td>Explanation; written statements (e.g., "verbal explanations)</td></tr>
<tr><td>(0)</td><td>Organization (e.g., "good presentation"); showing algebraic steps (e.g., "solution in steps")</td></tr>
<tr><td>(-)</td><td>Conciseness (e.g., "short and concise")</td></tr>
<tr><td>C5 (-) Correctness</td><td colspan="2">Algebraic errors (e.g., "makes sign error"); correct final answer (e.g., "final result right")</td></tr>
</table>

In order to quantitatively represent the features weighed by groups of TAs who have differing grading decisions, we display the distribution of features mentioned and graded on by TAs who graded SSE higher than SSD and the TAs who graded SSE lower than SSD. While TAs' grading decisions differ in quiz and HW context, we found little difference in the solution clusters they considered in these contexts. Thus, we present findings related to grading considerations merely for the quiz context (see Appendix C for the percentages of TAs mentioning and grading on features in the HW and quiz contexts, Figs. C-1 through C-5).

Findings. We found a significant gap between the percentage of TAs who mentioned features from clusters which promote prescribed problem-solving strategies (i.e. clusters C1, C2, and C4(+), see Figs. 8-5 through 8-7) and the percentage of TAs who stated that they grade on these features. This gap was more evident in the group that scored SSE greater than SSD, in the quiz as well as in the HW context. Thus, many TAs were aware of features related to explication and prescribed problem-solving strategies, but few graded on these same features.

For example, regarding features from the problem description and evaluation cluster (C1), while many TAs (40-80%) mentioned features from this cluster, few (20% or fewer) considered these features in grading, regardless of whether they are present (as in SSD) or missing (as in SSE) (see Fig. 8-5). TAs who graded SSD higher than SSE were more likely to grade on C1 than TAs who graded SSE higher than SSD. We conclude that even though TAs were aware of features related to problem description and evaluation (C1), they were not committed to grade on features in this cluster.

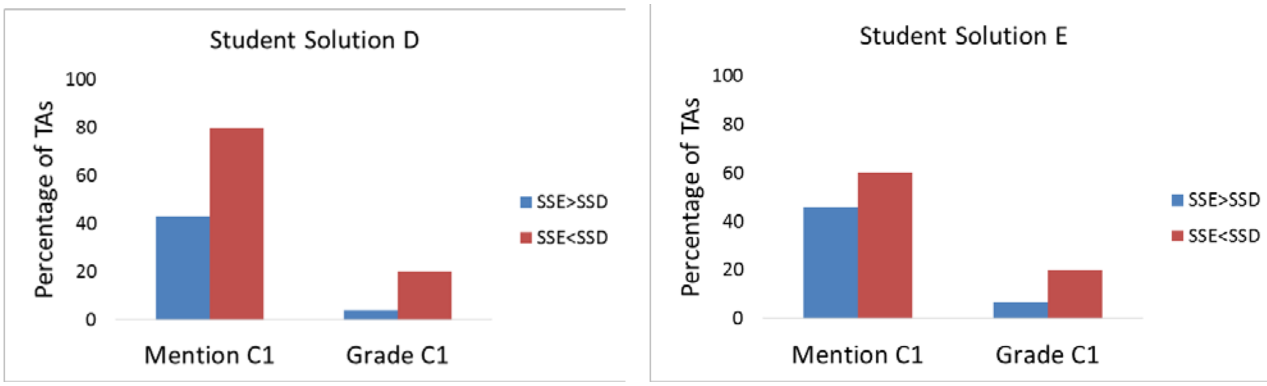

Figure 8-5. Percentage of TAs mentioning and grade on features from C1 (problem description and evaluation) on SSD and SSE in a quiz context ($N_{SSE>SSD\ Quiz}$=28 TAs, $N_{SSE<SSD\ Quiz}$=10 TAs).

Regarding explication of reasoning (C2), more TAs mentioned features from this cluster even though they did not consider them in their grading. This behavior was similar between the SSE<SSD and the SSE>SSD groups (see Fig. 8-6). In contrast to the description and evaluation cluster, that was treated similarly whether it was present (SSD) or missing (SSE), a larger portion of TAs took the explication cluster into account when they graded SSD (where explication was present) than when they graded SSE (where it was missing).

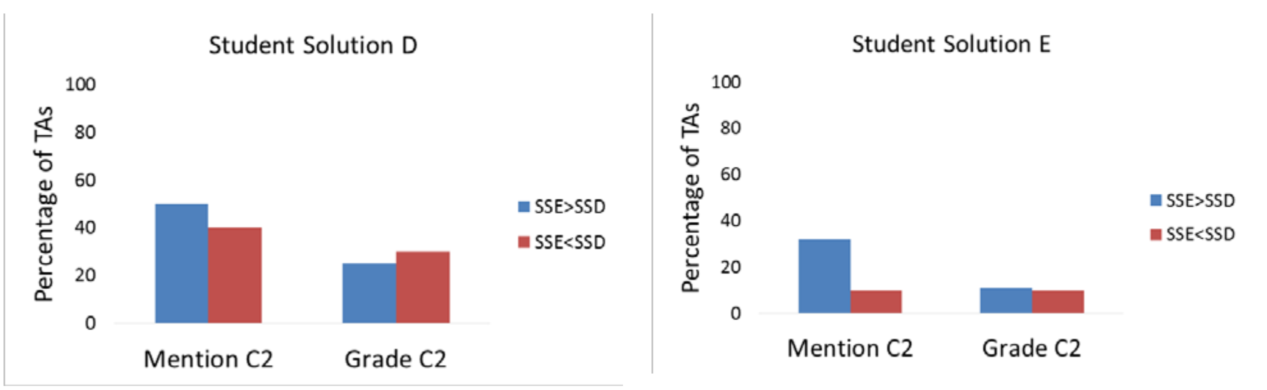

Figure 8-6. Percentage of TAs mentioning and grading on features from C2 (explication of problem-solving approach) on SSD and SSE in a quiz context ($N_{SSE>SSD\ Quiz}$=28 TAs, $N_{SSE<SSD\ Quiz}$=10 TAs).

Cluster C4(+) (i.e., explanation, written statements) also relates to explication, however, in an ill-defined manner. Similar to TAs' considerations involving C1 and C2, more TAs noticed features from C4(+) than graded on these features (see Fig. 8-7). Here, the difference between the SSE<SSD and the SSE>SSD groups became more prominent, especially for SSE (in which written statements were missing). Many more TAs in the SSE<SSD group graded on features from C4(+) cluster than in the SSE>SSD group. However, it is worthwhile noting that few TAs graded on explanation and written statements in SSD, a solution which includes many written statements.

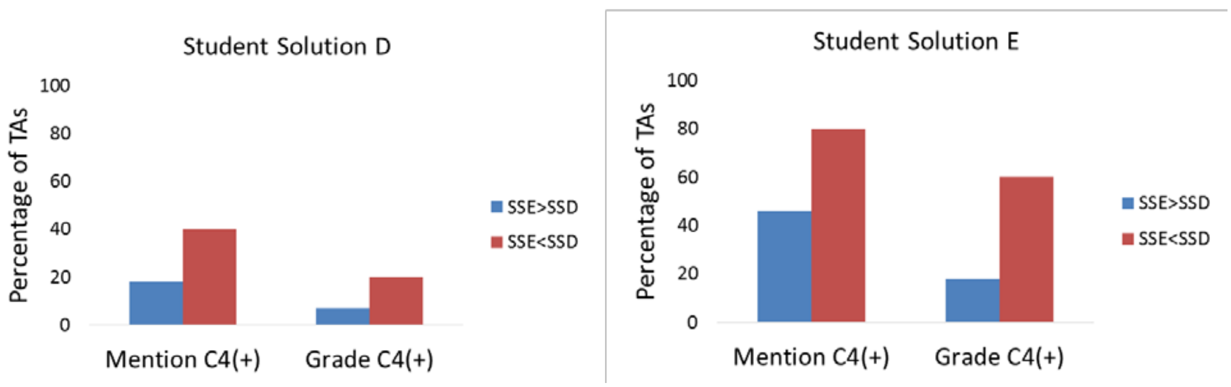

Figure 8-7. Percentage of TAs mentioning and grading on features from C4(+) (explanation; written statements) on SSD and SSE in a quiz context ($N_{SSE>SSD\ Quiz}$=28 TAs, $N_{SSE<SSD\ Quiz}$=10 TAs).

This last result can be interpreted to indicate that TAs use a subtractive grading scheme, taking points off from SSE for missing explanations (C4(+)), but not weighing this cluster in grading SSD, where it is present. Use of a subtractive grading scheme is also evident from analyzing other clusters that are most prominent in TAs' grading: domain knowledge (C3) and correctness (C5(-)) (see Appendix C, Figs. C-3 and C-5). Over 70% of all TAs graded on features related to physics knowledge in SSD, where physics concepts and principles are inadequately applied. However, 40% or fewer TAs said that they grade on domain knowledge in SSE, where no apparent mistakes were evident, though the physics knowledge was not explicated. Additionally, approximately 50% of all TAs graded on correctness (errors) in SSD because it has explicit algebraic mistakes. Only a few TAs (less than 20%) explicitly said that they grade on correctness (no apparent algebraic mistakes) in SSE.

Our findings indicate that TAs mention solution features related to explication and using prescribed problem-solving strategies, but do not necessarily grade on these features. Many TAs mentioned features related to initial problem analysis and evaluation (cluster C1), however, 20% or fewer of the TAs stated that they graded on these features. Similarly, TAs often mentioned features from cluster C2 (explication), especially in regards to SSD where C2 is adequately demonstrated, but few of them indeed grade on features from this cluster in either SSE or SSD.

8.4.2.2 Reasons and stated purposes for grading

Analysis. In the pre-lesson stage of the GAIQ sequence, TAs were asked to explain their reasons for why they weighed the different solution features to arrive at a final score. We found that, in addition to grading on specific solution features, TAs mentioned other alternative reasons unrelated to specific solution features. We focus on SSE because few TAs mentioned reasons for the grade on SSD and the ones who did mention reasons mostly focused on physics and mathematical mistakes. We also investigated TAs' stated purposes for grading using the essay they wrote in the pre-lesson stage of the GAIQ sequence. TAs' reasons for grading and beliefs about the purpose of grading were coded using a bottom-up approach (i.e., coding categories were determined after surveying the data). The coding of reasons and purposes for grading was completed by two of the researchers (E.M. and A.M.) together. Any disagreements were resolved with the help of two other researchers (E.Y. and C.H.) until full agreement was reached.

In order to quantitatively represent the reasons for grading mentioned by groups of TAs who are likely to have differing considerations in grading, we display the distribution of reasons of TAs who graded SSE higher than SSD and TAs who graded SSE lower than SSD.

Findings. In their grading of SSE, many TAs were reluctant to deduct points for the lack of reasoning, possibly since it did not contain any apparent mistakes. However, they gave alternative reasons for the grade on SSE such as adequate evidence, time/stress, and aesthetics (see Table 8-3). In the quiz context, eight TAs took the burden of proof of the student's understanding on themselves, stating: "SSE is brief, but I can still understand what was done" and "the student obviously knew what he was doing." In contrast, eight TAs mentioned that SSE contained inadequate evidence in the quiz context, stating that "we cannot determine if he has fully understood the points of the problem" and "it doesn't show if he/she is actually thinking correctly." A larger number of TAs ($N = 16$) noted that SSE contains inadequate evidence of understanding in the homework context. Five TAs noted that they would be lenient in grading on the quiz because of the time limitations in a quiz context. Additionally, five TAs mentioned aesthetics as a reason for the grade on SSE in the quiz context, stating that they liked the conciseness of SSE. Table 8-3 shows the percentages of TAs who consider the different reasons (evidence of students' thought processes, time limitations, or their preference for aesthetics) in their grading of SSE in the quiz vs. homework contexts. We found that the difference between HW and quiz grading may stem from TAs' consideration of evidence of students' thought processes and consideration of time limitations in a quiz. Of the TAs who scored SSE higher than SSD, more of them mention adequate evidence and time/stress in the quiz context and the number of TAs who mention inadequate evidence increases in the homework context. Conversely, of the TAs who score SSE lower than SSD, none of them mention adequate evidence as a reason for the grade on SSE and over 50% of them mention inadequate evidence as a reason for the grade on SSE in both the homework and quiz contexts.

Table 8-3. Reasons for SSE grade in the quiz and homework (HW) context before teaching experience and professional development. Each TA could provide more than one reason**.**

Reasons for SSE grade		SSE>SSD		SSE<SSD	
		Quiz (N=28)	HW (N=25)	Quiz (N=10)	HW (N=15)
Adequate evidence	The TA can understand the student's thought process, e.g., "SSE is brief, but I can still understand what was done."	8 (28%)	3 (12%)	0 (0%)	0 (0%)
Inadequate evidence	The TA cannot understand the student's thought process, e.g., "He didn't prove that he understood the problem or accidentally [got it]."	2 (7%)	6 (24%)	6 (60%)	10 (67%)
Time/stress	There is limited time on a quiz, so lenient grading is warranted, e.g., "In the quiz in which time is limited, I will give a full grade to this solution."	5 (18%)	0 (0%)	0(0%)	0 (0%)
Aesthetics	Physics problems should be solved in a brief, condensed way, e.g., "The student had the right idea of how to approach the problem in the simplest way. This approach is more preferable in quizzes because of its conciseness."	5 (18%)	4 (16%)	0 (0%)	0 (0%)

TAs' general goals about the purposes of grading (i.e., their answers to the question asked in the pre-lesson stage of the GAIQ, "What, in your view, is the purpose of grading students' work?") fell into four categories—to provide a learning opportunity for the student, to provide instructors with feedback on common difficulties of their students, to provide institutions with grades, and to motivate students (e.g., to turn in their homework or to study harder). There was little difference in the purposes for grading mentioned by the two groups of TAs who scored SSE>SSD and SSD<SSD. Thus, we show the combined data for all the TAs (see Fig. 8-8).

Almost all of the TAs state that grading serves as a learning opportunity for the student—to reflect on their mistakes and learn from them. Approximately half of the TAs state that it is for the benefit of the instructor to understand student difficulties (see Fig. 8-8). Our findings indicate that most TAs have goals that are aligned with formative assessment goals (i.e., for the purpose of giving feedback to both the student and instructor) as opposed to summative assessment goals (i.e., for the purpose of ranking students or assigning a final grade).

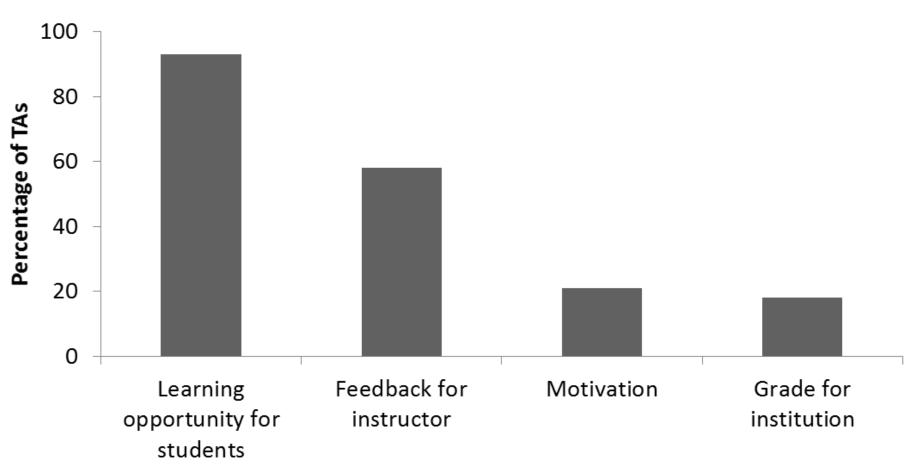

Figure 8-8. Responses to the purpose of grading before teaching experience and professional development.

8.4.3 RQ3: To what extent are the grading decisions of TAs aligned with their general beliefs about the purposes of grading?

Given the findings of RQ1 and RQ2, an inconsistency surfaces between TAs' stated beliefs about grading and their grading decisions. Our data suggest that many TAs' stated goals for grading are aligned with formative assessment goals. However, their grading decisions are not aligned with these stated goals. The majority of TAs grade SSE greater than SSD, implicitly transmitting a message that discourages explication of reasoning and use of expert-like problem-solving strategies (e.g., draw a diagram, list knowns/unknowns, etc.). TAs' grading decisions do not encourage students to provide evidence about their thinking – evidence that would enable students to reflect and learn from their mistakes. Similarly, TAs' grading considerations and accepting of inadequate evidence are also in conflict with their stated purposes for grading as a means of determining common student difficulties. Furthermore, even though many TAs state that they grade in order to provide feedback to students about their problem-solving process, they do not necessarily grade on features related to problem description, evaluation, and explication. To summarize: there are inconsistencies between TAs' stated beliefs about the purposes of grading and their grading decisions. This result is consistent with the results involving TAs' consideration of solution features—many TAs are aware of solution features related to prescribed problem-solving strategies, but they do not grade on them.

8.4.4 RQ4: How do TAs' grading decisions, considerations, and beliefs change within a short professional development intervention and after a semester of teaching experience?

Data Collection and analysis. To examine how TAs' grading decisions and beliefs changed within the brief professional development intervention, one of the researchers (E.M.) observed and took notes during group and whole-class discussions (i.e., the in-lesson stage of the GAIQ, see Table 8-1), which was intended to elicit conflicting viewpoints about grading. To investigate how TAs' grading perceptions change after one semester of teaching experience that followed this intervention, 18 TAs (a subset of the 43 TAs – one of the two cohorts) were asked to complete a final grading activity at the end of the semester. The final grading activity included the same components as the pre-lesson activity of the GAIQ at the beginning of the semester (i.e., TAs were asked to write an essay regarding grading and grade the same student solutions SSD and SSE). In addition, the TAs were provided with the worksheets they completed in the pre-lesson stage at the beginning of the semester (see Table 8-1). The same data analysis as in the pre-lesson activity was completed on the final grading activity. We discuss below the findings in the change in TAs': 1) grading decisions; and 2) grading considerations and beliefs about the purpose of grading after a semester of teaching experience and a brief professional development intervention.

8.4.4.1 Observation of group and in-class discussions within the professional development intervention

Findings. During the group and in-class discussions, many TAs were not aware that there was a conflict between their stated goals for grading as a formative assessment of students' problem-solving and their grading decisions, especially in regards to SSE. Some TAs were aware of the conflict, but made little effort to resolve it.

In the group discussions, many of the groups continued to score SSE highly, with a score of 9 or 10. It was often the case that all three of the TAs in one group had previously given SSE a score of 10 on their individual worksheet in the pre-lesson stage of the GAIQ. As a result, in the group grading activity, all three TAs agreed on a final score of 10 for SSE and remained unaware of the conflict between their grading practice and stated purposes for grading. Other groups stated that there was disagreement in their group about the grading of SSE, and they could not come to a consensus. Furthermore, they were unable to suggest ways to resolve this conflict when reporting their group grading to the entire class. During the in-class discussions, none of the TAs explicitly stated that their essay regarding the purpose of grading had an impact on their group grading of the student solutions.

8.4.4.2 Change in TAs' grading decisions after one semester of teaching experience

Findings. We find that TAs' grading decisions (i.e., their scoring of SSE and SSD) do not change significantly after a brief professional development experience and one semester of teaching experience. Similar to the beginning of the semester, at the end of the semester, the majority of TAs grade SSE significantly higher than SSD (see Fig. 8-9): SSE_{avg}=8.3 and SSD_{avg}=6.6, p-value (t-test)=0.01). The average quiz grade of SSE and SSD of the subgroup of 18 TAs does not change significantly over the course of the semester (the average SSE score remains 8.3) and the average SSD score changes from 7.1 to 6.6 from the beginning to the end of the semester). Even after a semester of experience and professional development, TAs graded a solution which provides minimal reasoning, lacks effective problem-solving strategies, and possibly obscures physics mistakes higher than a solution which includes detailed reasoning, productive problem-solving strategies, and canceling physics mistakes. If anything, their grading shifted further from being aligned with their stated beliefs about the purpose of grading (there continued to be a significant difference between their scores on SSE and SSD in the final activity).

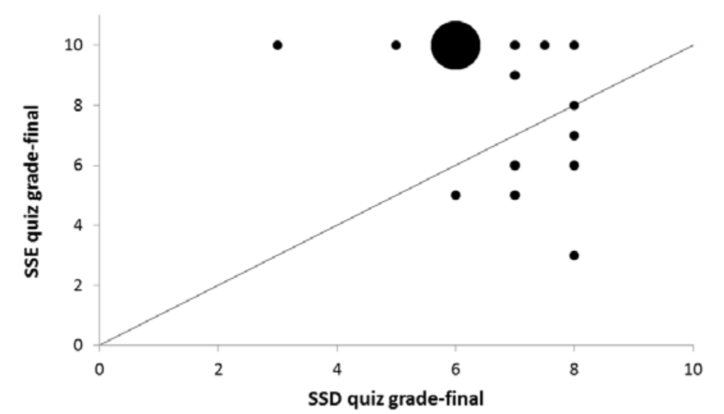

Figure 8-9. Distribution of 18 TA quiz grades (SSE vs. SSD) and at the end of the semester (final). The size of the bubble represents the number of TAs at that particular point.

8.4.4.3 Change in TAs' grading considerations and beliefs about the purpose of grading

Regarding the solution features, there was little change in the distribution of solution features mentioned and graded on by TAs. We also investigated the change in TAs' reasons for assigning a specific grade. For the end of semester data, we focus only on SSE because few TAs mentioned reasons for the grade on SSD and they mostly focused on physics and mathematical mistakes. The most common reasons for grading SSE were coded in four categories (see Table 8-4).

Generally, TAs' stated reasons for the final grade on SSE remained approximately the same. Tables 8-3 and 8-4 show that in the group of TAs who score SSD>SSE, there was a small increase in the percentage of TAs who stated that SSE does not give evidence of understanding (from approximately 65% to 94%) after teaching experience and the professional development program. However, regarding the group of TAs who scored SSE>SSD, the percentage of TAs stating that SSE includes adequate evidence remained approximately the same.

Table 8-4. Reasons for the final grade on SSE in the Quiz and homework (HW) contexts after (final) teaching experience and PD. TAs could state more than one reason.

Reasons for SSE Grade	Final			
	SSE>SSD		SSD>SSE	
	Quiz ($N = 11$)	HW ($N = 8$)	Quiz ($N = 6$)	HW ($N = 8$)
Adequate evidence	4 (36%)	1 (13%)	0 (0%)	0 (0%)
Inadequate evidence	2 (18%)	0 (0%)	6 (100%)	7 (88%)
Time/stress	0	0 (0%)	0 (0%)	0 (0%)
aesthetics	2 (18%)	0 (0%)	0 (0%)	0 (0%)

Similar to the lack of change in TAs' grading decisions and considerations, TAs' general beliefs about the purpose of grading did not change significantly. Most TAs continued to state productive purposes, i.e., that grading is a means for students to learn from their mistakes. However, the percentage of TAs stating that grading can serve as a formative assessment tool for the instructor decreased by approximately 20%. The number of TAs who state that grading is a means to give a final grade (i.e., summative assessment tool) increased by approximately 20%. It is possible that their teaching experiences partly resulted in this change: while TAs may initially believe that student solutions provide feedback to the instructor as to what difficulties are common among students, the TAs' grading experiences may have instilled in some TAs the belief that surveying student solutions to determine common difficulties is impractical given the amount of grading that needs to be done. They may then believe that the purpose of grading is primarily to provide a learning opportunity for students and a means to assign students' grades for the institution. In summary, TAs' grading practices, considerations, and stated purposes for grading did not change significantly after a brief professional development intervention and one semester of teaching experience. In fact, TAs' grading decisions and considerations continued to be in conflict with their stated purposes for grading.

8.5 STUDY LIMITATIONS

The findings of this study can be examined in the context of the larger university system. Since the TAs graded designed student solutions, this does not fully reflect TAs' actual grading approaches (although it mimics the "real" grading situation as closely as possible). In actual practice, TAs' grading approaches may become even more focused on correctness as opposed to encouraging prescribed problem-solving approaches due to external factors, such as large grading workload and a lack of control and involvement in the design of courses, in particular, homework, quizzes, and exams. Further research on TAs' grading of actual student solutions from classes they are teaching is needed to validate the results of our study.

Furthermore, TAs' prior educational experiences can impact their grading practices. Prior research has shown that American, Chinese, and other international TAs perform similarly in identifying common student difficulties [80]. When examining how the grading practices and considerations of international TAs compared to those of American TAs, we did not find differences, though it is not possible to determine whether differences are significant between the groups due to the small numbers of each group.

We note that, due to the low number of TAs in this study, it is difficult to draw definite conclusions about TAs' grading practices in general. Additional studies are needed to corroborate the results and draw more robust conclusions about TAs' grading approaches. In addition, the grading activity discussed in this study was only one component of the professional development program, and additional activities may provide further insights or refinement of the results. Investigations of more intensive professional development programs will determine the extent to which additional scaffolding helps TAs align their learning goals to their grading practice.

8.6 DISCUSSION

The educational literature suggests to encourage students to employ systematic approaches to problem solving (i.e., initial qualitative analysis, planning, and evaluation) and to explicate their reasoning. Grading communicates the instructors' expectations [1-5], and can thus serve to encourage students to employ systematic approaches and explicate their reasoning during problem solving.

We examined TAs' grading decisions and considerations when entering their teaching appointment. We found that most of the TAs indeed realized the existence of solution features reflecting a systematic and explicated problem-solving approach when describing students' solutions. Also, most TAs perceived the goal of assessment as formative, serving the process of learning by helping ingrain in students expert-like approaches to problem solving. Thus, one might expect their grading to encourage systematic problem solving.

However, when asked to list the features they grade on, TAs commonly did not state that they grade for the solution features representing expert problem solving, whether in a quiz or homework context. Indeed, we found that most of the TAs graded a solution which provides minimal reasoning while possibly obscuring physics mistakes higher than a solution that shows detailed reasoning and includes canceling physics mistakes. This tendency was most evident in a quiz context and somewhat softened in a homework context. Thus, TAs gave up weighing these "process-oriented" features that they were aware of in favor of "product-oriented" features such as the correctness of the final answer. Accordingly, their main reason for weighing specific features and ignoring others was the extent to which the solution provided *evidence* that would allow instructors to diagnose students' work (this requirement softened in light of time limitations in a quiz or aesthetics, i.e. the expectation that physics problems should be solved in a brief, condensed way). To summarize, TAs' grading decisions are often in conflict with their general beliefs about the purpose of grading.

Our findings regarding TAs' grading decisions and considerations are aligned with prior research on physics faculty grading practices [54] in which the instructors often faced internal conflicts when assigning a score. Most instructors resolved these conflicts by placing the burden of proof on themselves rather than on the student (i.e., they were willing to believe that a student understood the physics, even in cases where evidence of understanding was ambiguous) [54]. The results of our study also echo the findings of Lin et al. [12], who found that the goal of helping students develop an expert-like problem solving approach underlies many TAs' considerations for the use of example solutions, however, TAs do not use many features described in the research literature as supportive of this goal when designing example solutions. Our results indicate that TAs are using a subtractive scheme, removing points for explicit physics and mathematical errors. While many TAs are aware of productive solution features, very few TAs explicitly wrote down a rubric including these features and consistently used it to grade in the homework and quiz contexts.

A possible explanation for TAs' grading preferences is their prior experiences as students. Faculty often do not give incentives for showing reasoning [54]. Since TAs are recent undergraduate students, it is reasonable to expect their grading approaches would reflect the manner they were graded as undergraduates. Yet another explanation for our findings is that introductory physics problems are essentially exercises for TAs, thus, they do not feel the need to explain their reasoning or reflect on their problem-solving process [50] and do not think it appropriate to require their students to do something that they do not find valuable to do themselves. Furthermore, TAs, being physics graduate students, are likely to be intrinsically motivated to learn from their mistakes (even if their own graded work includes only marks based on errors) and might expect their students to do the same. Unfortunately, introductory students often do not have the intrinsic motivation to examine their graded work thoroughly and learn from their mistakes [43].

This study involved also a brief professional development experience providing opportunities for reflection on the teaching of problem solving, and in particular on grading. These opportunities included small group discussions and class discussions about how to model, coach, and assess students' problem-solving skills.

We examined whether TAs' grading decisions, considerations, and beliefs change after a short professional development intervention and a semester of teaching experience. We found that there was little change in TAs' grading practices, considerations, and beliefs after the brief professional development intervention regarding grading. TAs maintained their general goals for grading – to provide a learning opportunity for the student as well as to provide instructors with feedback on common difficulties of their students. However, TAs' grading decisions and the features they grade on did not change significantly after a semester of teaching experience. In particular, they still did not reward explication and the use of prescribed problem-solving strategies at the end of the semester. There was little change in the TAs' reasons for grading, and many TAs still mentioned that SSE contained adequate evidence of understanding. TAs remained unaware of the implicit conflict between their stated purposes for grading and their grading approaches. If TAs were made aware of the implicit conflict during the group discussions, they were unable to resolve the conflict and report their resolution to the entire class.

We conclude that the short professional development intervention which was meant to trigger in TAs a conflict between various goals and practice and provide tools for aligning their grading practices to better match their goals did not achieve its goals because: 1) apparently it did not serve to make TAs realize that there was an implicit conflict between their stated purposes for grading and their grading approaches; and 2) if the conflict was externalized and TAs realized that there was an implicit conflict, they did not have the tools to remedy the conflict. These findings are aligned with prior research showing that it is difficult for teachers to alter their views on student learning and that professional development should be long term, allowing them to bring evidence from the class and reflect on their practices in light of their goals to allow a meaningful change process [73, 81].

We conclude that in order for professional development programs to help TAs improve their grading decisions and considerations, more explicit scaffolding may be needed to ensure that all TAs undergo cognitive dissonance and resolve their conflicts in a manner that will benefit their students. Furthermore, since TAs were often unable to remedy the conflict within the group discussions about grading, TAs should be given additional opportunities to both generate solutions to this conflict and share these solutions with the whole class. For example, TAs can collaborate with each other in developing grading rubrics or analyze experts' solutions and contrast them with students' solutions. These types of tasks may help TAs contemplate how grading is an instructional tool that can help students learn from problem solving. As a result, TAs may be able to reconcile their instructional goals with their grading practices.

8.7 ACKNOWLEDGEMENTS

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APPENDIX C

PERCENTAGES OF TAS MENTIONING AND GRADING ON FEATURES ON CLUSTERS C1-C5 IN HOMEWORK AND QUIZ CONTEXTS

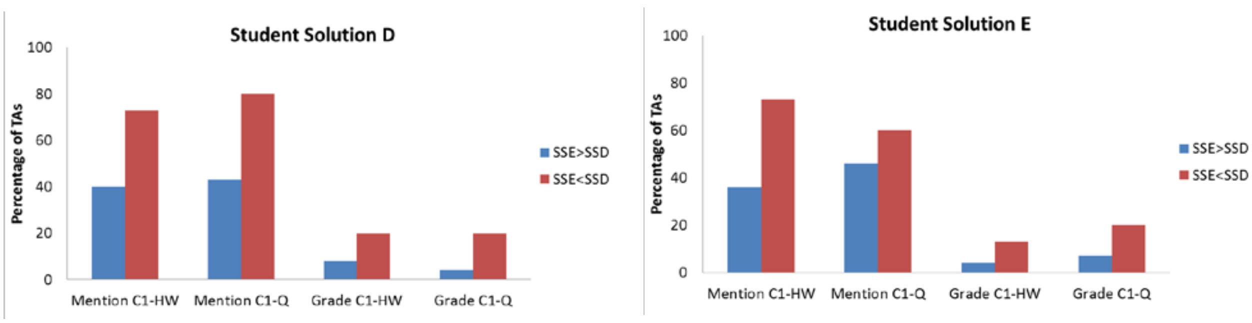

Figure C-1. Percentage of TAs mentioning and grading on features from C1 (problem description and evaluation) on SSD and SSE in a homework (HW) and quiz (Q) context ($N_{SSE>SSD\ Q}$=28 TAs, $N_{SSE>SSD\ HW}$=25 TAs, $N_{SSE<SSD\ Q}$=10 TAs, $N_{SSE<SSD\ HW}$=15 TAs).

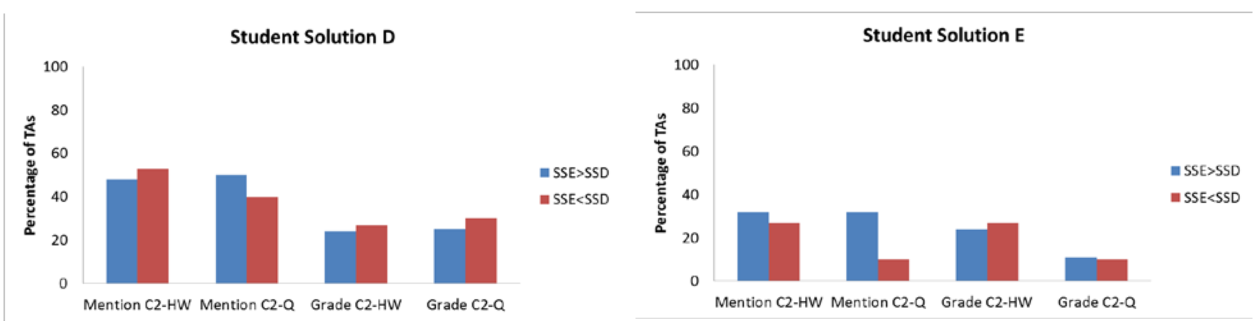

Figure C-2. Percentage of TAs mentioning and grading on features from C2 (explication of problem-solving approach) on SSD and SSE in a homework (HW) and quiz (Q) context ($N_{SSE>SSD\ Q}$=28 TAs, $N_{SSE>SSD\ HW}$=25 TAs, $N_{SSE<SSD\ Q}$=10 TAs, $N_{SSE<SSD\ HW}$=15 TAs).

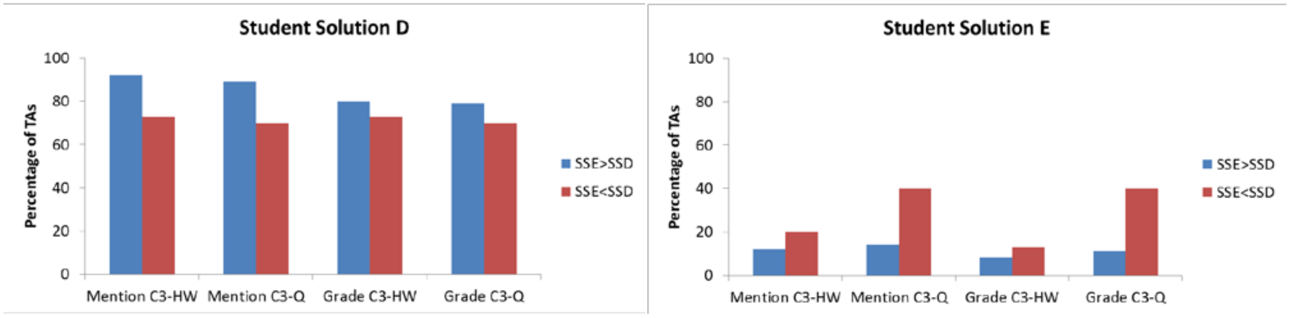

Figure C-3. Percentage of TAs mentioning and grading on features from C3 (domain knowledge) on SSD and SSE in a homework (HW) and quiz (Q) context ($N_{SSE>SSD\ Q}$=28 TAs, $N_{SSE>SSD\ HW}$=25 TAs, $N_{SSE<SSD\ Q}$=10 TAs, $N_{SSE<SSD\ HW}$=15 TAs).

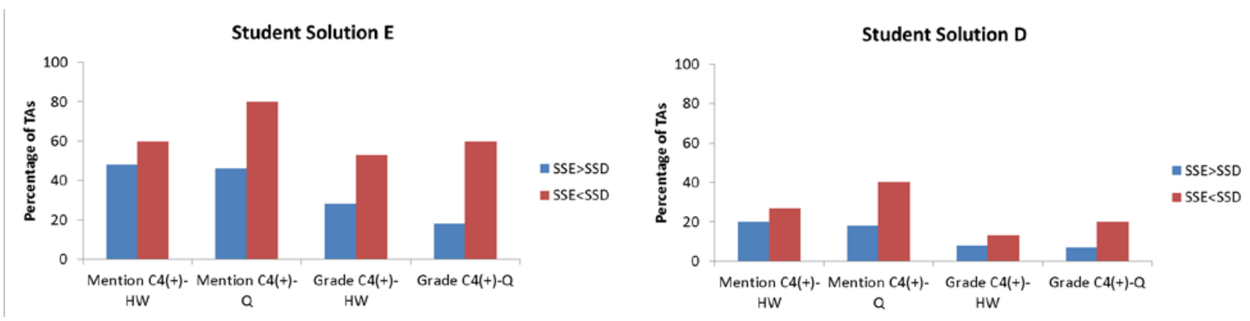

Figure C-4. Percentage of TAs mentioning and grading on features from C4(+) (explanation; written statements) on SSD and SSE in a homework (HW) and quiz (Q) context ($N_{SSE>SSD\ Q}$=28 TAs, $N_{SSE>SSD\ HW}$=25 TAs, $N_{SSE<SSD\ Q}$=10 TAs, $N_{SSE<SSD\ HW}$=15 TAs).

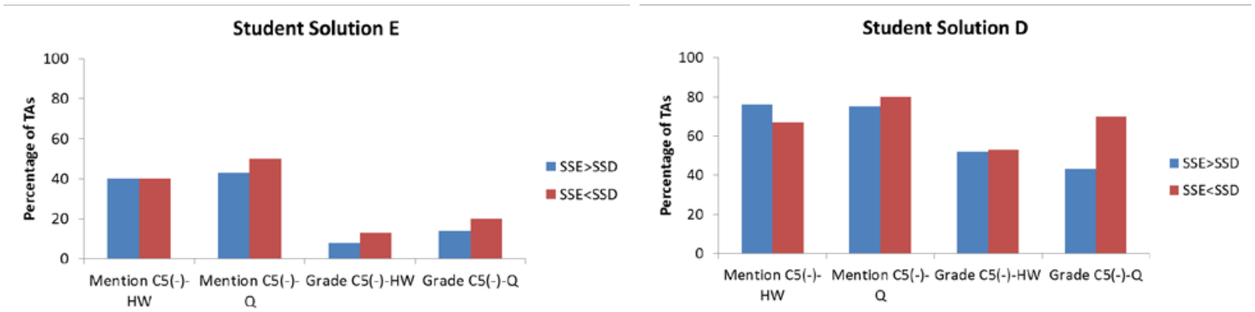

Figure C-5. Percentage of TAs mentioning and grading on features from C5(-) (correctness) on SSD and SSE in a homework (HW) and quiz (Q) context ($N_{SSE>SSD\ Q}$=28 TAs, $N_{SSE>SSD\ HW}$=25 TAs, $N_{SSE<SSD\ Q}$=10 TAs, $N_{SSE<SSD\ HW}$=15 TAs).

9.0 FUTURE OUTLOOK

The studies presented in this thesis can be extended in several different ways. The studies discussed in chapters 1 and 2 can be extended by further investigations of analogous patterns of difficulties in quantum mechanics and introductory classical mechanics. In this way, the framework can be refined. Furthermore, as discussed in chapter 2, upper-level undergraduate and graduate students displayed difficulties associated with unproductive epistemological views of learning quantum mechanics. Since quantum mechanics is an abstract subject, epistemological views can play an important role in either enhancing or undermining student learning. The study can be expanded upon by investigating how instructors can guide students in developing productive epistemological views of quantum mechanics. In particular, how does instructors' use of terminology and framing, e.g., of "doing" vs. understanding the "origins" of quantum mechanics affect students' performance? In addition, can student discussions clarify the terminology and help them make distinctions between "doing" quantum mechanics, understanding quantum interpretations, and the underlying reasons for why the postulates of quantum mechanics correctly predict physical phenomena?

The studies in chapters 3 and 4 can be expanded upon by investigating the benefits of teaching Dirac notation to students before they begin to learn about quantum measurement and the probability distribution of measurement outcomes in position or momentum representation. In the first semester of a junior/senior level quantum mechanics course, the concepts of measurement and probability distribution for measurement outcomes for observables are often first taught in the position (or momentum) representation. However, Dirac notation is a simple yet elegant way to represent quantum states, probability distribution of measurement outcomes, and expectation values. My research showed that students often used Dirac notation as a tool to help them determine probability distributions of measurement outcomes in position representation. It would be interesting to investigate the effects of teaching students Dirac notation first before discussing the concepts of the probability distribution for measurement outcomes for observables, expectation values, and time development of quantum states in the position or momentum representation. Do students perform better if they are facile in using Dirac notation when learning about the aforementioned concepts?

Chapters 4, 5, and 6 discussed the development of Quantum Interactive Learning Tutorials (QuILTs) for upper-level quantum mechanics courses. These QuILTs discuss a variety of quantum mechanics concepts, and it may be beneficial for students if the QuILTs were broken up into smaller sections. The conceptual part of the MZI tutorial could be broken into sections entitled, e.g., “the role of beam splitter 1,” “the role of an additional detector placed in one of the paths of the MZI,” and “how does one polarizer affect the interference observed at the detectors?” Further research can investigate whether students benefit from learning about these topics in smaller “chunks” and whether they are able to internalize and retain the information for a longer period of time.

The conceptual part of the MZI QuILT made use of a computer simulation in which a single photon had a transverse Gaussian profile. A screen was used in place of a point detector to display an interference pattern. It may also be beneficial for the conceptual part of the MZI QuILT to use a computer simulation in which the path of the photon through the MZI is highly collimated as opposed to a photon with a transverse Gaussian profile. Students can compare the two cases in the computer simulations (photons with a transverse Gaussian profile vs. a highly collimated stream of single photons) and check their results for a highly collimated stream of single photons via the related MZI tutorial, which focuses on using mathematical formalism using a product space of two state system for both the photon path and polarization states.

The study on teaching assistants' (TAs') grading goals and practices can be extended by investigating how TAs themselves prefer to be graded or receive feedback. In groups, TAs can discuss situations in which they felt they received good/poor feedback from their instructors via grading. In turn, they may be more inclined to grade in a manner which sends a productive message to introductory students, i.e., problems should be solved using effective problem solving heuristics in order to develop robust problem-solving strategies and learn physics. In addition, further investigations can shed light on how TAs develop rubrics for grading. In particular, what types of solution features do TAs weigh in their grading by including them in their rubric and which features do they weigh the most? Do TAs grade consistently with their rubric? Are the requirements in their rubrics aligned with suggested physics education research grading practices? In addition, since many TAs have time constraints and often rush through the task of grading, it may be beneficial to assist TAs in developing multiple-choice questions that assess a physics concept in the same manner as an open ended question but have the benefits of being objective and quick to grade.