# INVERSE PROBLEM IN CLASSICAL STATISTICAL MECHANICS

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This thesis concentrates on the inverse problem in classical statistical mechanics and its applications. Let us consider a system of identical particles with the total energy $W + U$, where $W$ is a fixed scalar function, and $V$ is an additional internal or external potential in the form of a sum of $m$-particle interactions $u$. The inverse conjecture states that any positive, integrable function $\rho^{(m)}$ is the equilibrium $m$-particle density corresponding to some unique potential $u$. It has been proved for all $m \geq 1$ in the grand canonical ensemble by Chayes and Chayes [1]. Chapter 2 of this thesis contains the proof of the inverse conjecture for $m \geq 1$ in the canonical formulation. For $m = 1$, the inverse problem lies at the foundation of density functional theory for inhomogeneous fluids. More generally, existence and differentiability of the inverse map for $m \geq 1$ provides the basis for the variational principle on which generalizations to density functional theory can be formulated. Differentiability of the inverse map in the grand canonical ensemble for $m \geq 1$ is proved here in Section 3.2. In particular, this result leads to the existence of a hierarchy of generalized Ornstein-Zernike equations connecting the $2m$-,...,$m$-particle densities and generalized direct correlation functions. This hierarchy is constructed in Section 3.3.

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# 1.0 INTRODUCTION

## 1.1 PROBABILITY DENSITIES IN THE CANONICAL ENSEMBLE

Let us consider a system of $N$ identical particles, with coordinates $(x_1, ..., x_N)$, immersed in a thermal bath. The coordinates of each particle $x_i$ may be spatial, phase space, or discrete. In general, $x_i$ lie in some complete $\sigma$-finite measure space $(\Lambda, dx)$. The total energy of the system has the form $W+V$, where $W : \Lambda^N \to \mathbb{R}$ is a fixed measurable symmetric function (see Section 1.4 (iii) for the definition of "symmetric"), and $V$ is a sum of $m$-particle interactions $(1 \leq m \leq N)$, specifically $V = \hat{C}_{N,m}v$ for some a.e. finite and symmetric function $v$ on $\Lambda^m$. (The operator $\hat{C}_{N,m}$ is defined in 1.4.1. ) For example, when $m = 2$, $V$ is a sum of all possible pairwise interactions of $N$ identical particles. In the applications described bellow, $W$ is the internal energy of the system. The interpretation of $V$ depends on the problem at hand. When $m = 1$, it can be the external potential, when $m \geq 2$, it can be an additional interaction potential. In both cases $V$ can also play a role of a technical mean to derive equations for the system governed by energy $W$. This is the approach taken in Section 3.3.

The fundamental relation connecting statistical mechanics in the canonical formulation and thermodynamics is $-\ln Z(v) = F(v)$, where

$$Z(v) = \int_{\Lambda^N} e^{-W-V} d^N x \tag{1.1.1}$$

is the canonical partition function, and $F(v)$ is the Helmholtz potential (also called the Helmholtz free energy, because it is the maximal amount of energy available for the system to do work) [2].[1]

[1] The inverse temperature $\beta$ is set to 1.

If $e^{-W-V} \in L^1(\Lambda^N, d^N x)$, then

$$G_v := \frac{e^{-W-V}}{Z(v)}, \tag{1.1.2}$$

defines the canonical probability density. Moreover, for every $k \in \mathbb{N}$, the $k$-particle probability density, which is a $k$-variable reduction of $G_v$, is well defined by[3]:

$$\rho_v^{(k)} := \frac{N!}{(N-k)!} \int_{\Lambda^{N-k}} (G_v)(\cdot, x_{k+1}, ..., x_N) dx_{k+1} \cdots dx_N. \tag{1.1.3}$$

In particular, $\rho_v^{(k)} \in L^1(\Lambda^k, d^k x)$, and $\|\rho_v^{(k)}\|_{1(d^k x)} = \frac{N!}{(N-k)!}$.

## 1.2 PROBABILITY DENSITIES IN THE GRAND CANONICAL ENSEMBLE

Consider a system of identical particles, immersed in a thermal-particle reservoir. Accordingly, the system can be in different particle number states. As before, the coordinates of each particle $x_i$ lie in some complete $\sigma$-finite measure space $(\Lambda, dx)$. For each particle number $N$, the energy of the system has the form $W_N + V_N$, where $W_0 := 0$, $W_N : \Lambda^N \to (-\infty, \infty]$ is a fixed measurable symmetric function for $N \in \mathbb{N}$, and

$$V_N = \begin{cases} \hat{C}_{N,m} v & \text{if } N \geq m, \\ 0 & \text{if } 0 \leq N < m, \end{cases} \tag{1.2.1}$$

where $v$ is some measurable a.e. finite and symmetric function on $\Lambda^m$, and $\hat{C}_{N,m} v$ is defined in (1.4.1).

The fundamental relation in the grand canonical formulation is $-\ln \Xi(v) = \Omega(v)$, where

$$\Xi(v) := |||e^{-W-V}|||_{1(d\mu)} = 1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} d^N x \tag{1.2.2}$$

is the grand canonical partition function, and $\Omega(v)$ is the grand canonical potential, equal to the maximal amount of energy the system can convert into work [2].[2]

[2]The chemical potential $\mu$ is absorbed into $W$.

If $e^{-W-V} \in \mathbb{L}^1(d\mu) = \ell^1 \left[\bigoplus_{N=0}^{\infty} L^1\left(\Lambda^N, d^N x/N!\right)\right]$ (for the definition and properties of $\mathbb{L}^p$, see Appendix ), then it is possible to define a sequence of functions
$G_v := ((G_v)_N \mid N = 0, 1, 2, ...) \in \mathbb{L}^1(d\mu)$, where

$$(G_v)_N := \frac{e^{-W_N - V_N}}{\Xi(v)}, \tag{1.2.3}$$

is the grand canonical probability density. For any function $F \in \mathbb{L}^1(G_v d\mu)$, its equilibrium average is defined as $\langle F\rangle_v := (G_v)_0 F_0 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} (G_v)_N F_N d^N x$. Suppose that

$$n_k(v) := \left\langle \frac{N!}{(N-k)!} \right\rangle_v = \sum_{N=k}^{\infty} \frac{1}{(N-k)!} \int_{\Lambda^N} (G_v)_N d^N x < \infty \tag{1.2.4}$$

for some $k \in \mathbb{N}$. Then, $k$-particle probability density is a $k$-variable reduction of $G_v$ [3]:

$$\rho_v^{(k)} := (G_v)_k + \sum_{N=k+1}^{\infty} \frac{1}{(N-k)!} \int_{\Lambda^{N-k}} (G_v)_N(\cdot, x_{k+1}, ..., x_N) dx_{k+1} \cdots dx_N. \tag{1.2.5}$$

Note, that because $n_k(v) < \infty$, the Fubini-Tonelli theorem[4, Theorem 2.39] and monotone convergence[4, Theorem 2.14] imply that $\rho_v^{(k)} \in L^1(\Lambda^k, d^k x)$, and $||\rho_v^{(k)}||_{1(d^k x)} = n_k(v)$.

### 1.3 INTRODUCTION TO THE INVERSE PROBLEM

For fixed $W$, every potential $v$ produces an $m$-particle density $\rho_v^{(m)}$ according to (1.1.3) or (1.2.5). Roughly speaking, the inverse conjecture states the converse, namely that given a non-negative function $\rho^{(m)} \in L^1(\Lambda^m, d^m x)$, there exists a unique function $v$ such that $\rho^{(m)} = \rho_v^{(m)}$. (The function $v$ is customarily referred to as “the solution to the inverse problem.” )

For $m = 1$ this problem has its origin in the density functional theory (DFT) of inhomogeneous fluids derived in the grand canonical formulation[5, 6] which, in its turn, has been modeled on the DFT of many-electron systems [7, 8]. Both of these theories hinge on the existence and differentiability of the inverse map $\rho^{(1)} \mapsto v$ defined by $\rho^{(1)} = \rho_v^{(1)}$. The DFT for inhomogenius fluids, in particular, considers

$$\mathcal{F}[v(\rho^{(1)})] := \langle W + \ln G_v\rangle_v = -\ln \Xi(v) - \int_{\Lambda} \rho_v^{(1)} v \tag{1.3.1}$$

and

$$\Omega_u[v(\rho^{(1)})] := \langle W + U + \ln G_v \rangle_v = \mathcal{F}[v(\rho^{(1)})] + \int_\Lambda \rho^{(1)} u \tag{1.3.2}$$

as functionals of density $\rho^{(1)}$ for fixed internal energy $W$ and external potential $u$.[3] Moreover, the variational principle of DFT [5, 9]

$$0 = \frac{\delta \Omega_u}{\delta \rho^{(1)}} \Big|_{\rho^{(1)} = \rho_u^{(1)}} = \frac{\delta \mathcal{F}}{\delta \rho^{(1)}} \Big|_{\rho^{(1)} = \rho_u^{(1)}} + u, \tag{1.3.3}$$

implies differentiability of the map $\rho^{(1)} \mapsto v$. Equation (1.3.3) is the formal expression of the fact, proved by Jensen's inequality, that $\rho_u^{(1)}$ maximizes $\Omega_u$. Substituting $\rho_u^{(1)}$ into (1.3.2) and using (1.3.1), we also see that

$$\Omega_u(\rho_u^{(1)}) = \mathcal{F}(\rho_u^{(1)}) + \int_\Lambda \rho_u^{(1)} u = -\ln \Xi(u) = \Omega(u). \tag{1.3.4}$$

Therefore, the value of the maximum of $\Omega_u$ is the grand potential for the system with energy $W + U$.

Let $\mathcal{F} = \mathcal{F}_{id} + \mathcal{F}_{ex}$, where

$$\mathcal{F}_{id} := \int_\Lambda \rho^{(1)} (\ln \rho^{(1)} - 1) dx \tag{1.3.5}$$

is the intrinsic free energy of the ideal gas [3, Equation (3.1.22)]. The direct Ornstein-Zernike (OZ) correlation function is defined as [5, 3]

$$c^{(2)}(x_1, x_2) := -\frac{\delta^2 \mathcal{F}_{ex}}{\delta \rho^{(1)}(x_1) \delta \rho^{(1)}(x_2)}. \tag{1.3.6}$$

It is seen from (1.3.3) that

$$c^{(2)}(x_1, x_2) = \frac{\delta u(x_1)}{\delta \rho^{(1)}(x_2)} + \frac{1}{\rho^{(1)}(x_1)} \delta(x_1 - x_2). \tag{1.3.7}$$

On the other hand, by direct calculation, it can be shown that

$$\frac{\delta \rho^{(1)}(x_1)}{\delta u(x_2)} = -[\rho^{(1)}(x_1) \rho^{(1)}(x_2) h^{(2)}(x_1, x_2) + \rho^{(1)}(x_1) \delta(x_1 - x_2)], \tag{1.3.8}$$

where

$$h^{(2)}(x_1, x_2) := g^{(2)}(x_1, x_2) - 1 := \frac{\rho^{(2)}(x_1, x_2)}{\rho^{(1)}(x_1) \rho^{(1)}(x_2)} - 1. \tag{1.3.9}$$

[3] $\mathcal{F}[v(\rho^{(1)})]$ is called *intrinsic free energy functional* [3].

is the pair correlation function [3]. Substituting (1.3.7) and (1.3.8) into the identity

$$\int_\Lambda \frac{\delta v(x_1)}{\delta\rho^{(1)}(x_3)} \frac{\delta\rho^{(1)}(x_3)}{\delta v(x_2)} dx_3 = \delta(x_1 - x_2), \tag{1.3.10}$$

we obtain (formally) the OZ equation [10, 3]:

$$h^{(2)}(x_1, x_2) = c^{(2)}(x_1, x_2) + \int_\Lambda h^{(2)}(x_1, x_3)\rho^{(1)}(x_3)c^{(2)}(x_2, x_3)dx_3. \tag{1.3.11}$$

Equation (1.3.11) has a very neat physical interpretation as partitioning $h^{(2)}(x_1, x_2)$ into the direct contribution $c^{(2)}$ due to two particles situated at $(x_1, x_2)$ and indirect contribution due to all other particles.

The existence of the inverse map for $m = 1$ has been proved by Chayes, Chayes, and Lieb [11, 1] for both the canonical and grand canonical ensembles. Moreover, the same authors [11] has shown that the inverse map $\rho^{(1)} \mapsto v$ is differentiable in the grand canonical formulation, thus verifying the cornerstone assumption of classical DFT.

**Remark 1.3.1.** It is proper to note here that reference [11] also contains a proof of the differentiability of $\rho^{(1)} \to v$ in the canonical formulation. However, it has been known in physics for quite a long time that such a derivative does not exist [12], and that is precisely the reason why DFT can only be formulated rigorously in the grand canonical formulation [13, 14, 15]. (See also Remark 3.2.1 bellow.) An oversight in the proof in [11] is that the restriction $\|\rho^{(1)}\|_{1(dx)} = N$ has not been imposed.

The existence (but not differentiability) of the inverse map for $m \geq 1$ has been proved by Chayes and Chayes for the *grand canonical* ensemble back in eighties [1]. Assuming $\rho^{(m)} \mapsto v$ is also differentiable, equations (1.3.1-1.3.4) readily generalize to

$$\mathcal{F}[v(\rho^{(m)})] = -\ln \Xi(v) - \frac{1}{m!} \int_\Lambda \rho_v^{(m)} v, \tag{1.3.12}$$

$$\Omega_u[v(\rho^{(1)})] = \mathcal{F}[v(\rho^{(m)})] + \frac{1}{m!} \int_\Lambda \rho^{(m)} u, \tag{1.3.13}$$

$$0 = \frac{\delta\Omega_u}{\delta\rho^{(m)}} \Big|_{\rho^{(m)} = \rho_u^{(m)}} = \frac{\delta\mathcal{F}}{\delta\rho^{(m)}} \Big|_{\rho^{(m)} = \rho_u^{(m)}} + u, \tag{1.3.14}$$

and

$$\Omega_u(\rho_u^{(m)}) = \mathcal{F}(\rho_u^{(m)}) + \frac{1}{m!}\int_\Lambda \rho_u^{(m)} u = -\ln \Xi(u) = \Omega(u). \tag{1.3.15}$$

The variational principle (1.3.14) provides the basis on which generalizations to DFT and its numerous implications can be constructed. Such generalizations have already been developed for many-electron systems, where kinetic energy is considered to be a functional of the two-particle density [16, 17], and some effort in this direction has also been made for classical fluids [18].

The inverse conjecture for $m \geq 2$ has another important application in coarse-grained (CG) numerical simulations. Typically, a CG system is created by mapping groups of atoms onto CG sites with the effect of considerable reduction in the number of degrees of freedom. The effective interaction potentials for CG sites are then constructed by matching thermodynamic properties, force fields, or structure of the original (atomistic) and CG models [19]. The common methods in the third category are Iterative Boltzmann Inversion (IBI) [20, 21] and Inverse Monte Carlo (IMC) [22]. In these techniques, the structural data calculated numerically for CG model are “inverted” to obtain effective CG interaction potentials. The input functions are usually 2-, 3-, and 4-particle densities, and so the inversion procedure is precisely the numerical solution of the inverse problem, that is the problem of finding (unique) $v$ such that $\rho_v^{(m)} = \rho^{(m)}$ for given $\rho^{(m)}$. In uniform fluids the 2-,...,4-particle densities are functions of only few parameters (bond lengths, bending angles, and dihedral angles), and can easily be discretized.

Formally, solutions to the inverse problem are maximizers of the following functional of potential $v$ for given density $\rho^{(m)}$:

$$\mathcal{A}_{\rho^{(m)}}(v) := -\ln \Xi(v) - \frac{1}{m!}\int_\Lambda \rho^{(m)} v. \tag{1.3.16}$$

Indeed, if $\rho^{(m)} = \rho_u^{(m)}$ for some $u$, then it can be shown by Jensen’s inequality that $\mathcal{A}_{\rho^{(m)}}(u) \geq \mathcal{A}_{\rho^{(m)}}(v)$ for all $v$. On the other hand, if $u$ maximizes $\mathcal{A}_{\rho^{(m)}}$, then

$$0 = \frac{\delta \mathcal{A}_{\rho^{(m)}}}{\delta v}\,|_{v=u} = \frac{1}{m!}[\rho^{(m)} - \rho_u^{(m)}], \tag{1.3.17}$$

which suggests that minimizers of $\mathcal{A}_{\rho^{(m)}}$ are solutions to the inverse problem. Substituting $u$ in (1.3.16), we obtain.

$$\mathcal{A}_{\rho^{(m)}}(u) = -\ln \Xi(u) - \frac{1}{m!}\int_{\Lambda^m} \rho_u^{(m)} u = \mathcal{F}(\rho^{(m)}). \tag{1.3.18}$$

Thus, the value of the maximum of $\mathcal{A}_{\rho^{(m)}}$ is the intrinsic free energy for the system with energy $W + U$. Equations (1.3.16-1.3.18) are also valid in canonical formulation, with $\Xi(v)$ replaced by $Z(v)$.

As was pointed out by Caillol in his lucid analysis [9], equations (1.3.16), (1.3.17), and (1.3.18) are dual to (1.3.13), (1.3.14), and (1.3.15) respectively. The author also comments that while the variational principle in (1.3.13-1.3.15) serves as the foundation for DFT (when $m = 1$), the one in (1.3.16-1.3.18) has been overlooked. Curiously though, this principle is precisely the basis of the solution to the inverse problem and it has been used in numerical simulations for decades.

Strangely enough, the inverse conjecture has never been proved for the canonical ensemble when $m \geq 2$, even though numerical simulations are often performed in this setting. As was mentioned earlier, the multi-particle inverse problem for the grand canonical distribution, was solved by Chayes and Chayes [1]. However, the conclusions derived in [1] can not be transferred to the canonical distribution without a proof. This is because the setting of the grand canonical ensemble allows to essentially uncouple interactions, which is not possible when the number of particles is fixed.

The proof of the inverse conjecture in the canonical ensemble for $m \geq 1$ is contained in Chapter 2 of this treaties, and it can also be read in [23]. The variational part of the argument consists in proving the existence of the unique maximizer of $\mathcal{A}$, followed by verifying that every maximizer is a solution, and finally showing that the solution is unique. The issues specific for the canonical ensemble are formulated as measure-theoretic properties of U-statistics that apparently can not be found elsewhere, and are addressed in Section 2.3 here. As such, the results in Section 2.3 (which can also be found in [24] ) have value of their own, quite independent of the inverse problem.

The inverse problem in the grand canonical formulation is discussed in Chapter 3. Section 3.1 contains the detailed proof of the inverse conjuncture in the grand canonical ensemble for $m \geq 1$. The proof is based on the outline in [1, Section 4], and many of the arguments are variations of the methods found in [11, 1]. However, unlike in [1, Section 4], we do not require that the measure $|\Lambda|$ is finite, or that the ensemble is truncated (i.e. $W_N = \infty$ for all $N > \tilde{N}$). Differentiability of the inverse map for $m \geq 1$ is addressed in Section 3.2. The results for $m \geq 2$ are new, however, even for the case of $m = 1$ our approach is different then in [11]. There, the derivative of $\rho^{(1)} \to u = v + \ln(\rho^{(1)})$ is considered, where $u$ is in $L^\infty(\Lambda, dx)$, but $v$ and $\ln(\rho^{(1)})$ are not. Therefore, the derivative of $\rho^{(1)} \to v$ is not clearly defined. We state the problem differently to obviate this confusion. The conclusions of Section 3.2 provide the basis for the variational principle defined in (1.3.13-1.3.15).

Existence and differentiability of the inverse map for $m \geq 1$ also leads to the hierarchy of generalized OZ equations connecting $2m$-...$m$-particle densities and generalized direct correlation functions. This is shown in Section 3.3. It should be noted that this generalization is cardinally different from the one considered in [25] and has not been studied yet.

## 1.4 NOTATION

(i) $(\Lambda, dx)$ designates a complete $\sigma$-finite measure space. For every $k \in \mathbb{N}$, $d^k x$ is the completion of the product measure $dx^{\otimes k}$ on $\Lambda^k$. The wording "almost everywhere" ("a.e.") is always understood relative to the measure $d^k x$, unless specified otherwise, with $k$ obvious from the context. The $[d^k x]$ measure of a (measurable) set $E \subset \Lambda^k$ is denoted by $|E|$, with $k$ again obvious from the context.

(ii) Let $m, N \in \mathbb{N}$, and $N \geq m$. For a function $v : \Lambda^m \to \mathbb{R}$, we define a function $\hat{C}_{N,m} v : \Lambda^N \to \mathbb{R}$ by

$$(\hat{C}_{N,m} v)(x_1, ..., x_N) := \sum_{1 \leq i_1 < \cdots < i_m \leq N} v(x_{i_1}, ..., x_{i_m}). \tag{1.4.1}$$

For example, $(\hat{C}_{N,1} v)(x_1, ..., x_N) = \sum_{i=1}^N v(x_i)$, $(\hat{C}_{N,2} v)(x_1, ..., x_N) = \sum_{1 \leq i < j \leq N} v(x_i, x_j)$, and so on. The number $m \in \mathbb{N}$ is fixed throughout this treatise, unless specified otherwise. In Chapter 3, $S_N$, $U_N$, and $V_N$ designate the functions on $\Lambda^N$ defined by (1.2.1), with $v$ replaced by $s$ or $u$ when appropriate. In addition, $S$, $U$, and $V$ indicate the corresponding sequences of functions $V := (V_N \mid N = 0, 1, 2, ...)$.

(iii) A set $E \subset \Lambda^N$ is called symmetric if $(x_1, ..., x_N) \in E$ implies $(x_{\sigma(1)}, ..., x_{\sigma(N)}) \in E$ for all permutations $\sigma$ of $(1, ..., N)$. A function $f$ defined on a symmetric set $E$ is symmetric if $f(x_1, ..., x_N) = f(x_{\sigma(1)}, ...x_{\sigma(N)})$ for all permutations $\sigma$ of $(1, ..., N)$. If, in addition, $\left|\Lambda^N \setminus E\right| = 0$, then we say that $f$ is symmetric a.e.

(iv) For two sets $A$ and $B$, let us write $A \sim B$ if $|A \Delta B| = 0$, where $\Delta$ is a symmetric difference [4, p. 3]. It is easy to check that $A \sim B$ and $B \sim C$ imply $A \sim C$.

(v) For any function $f$, $f_+ := \max(f, 0)$, $f_- := \max(-f, 0)$.

## 2.0 THE INVERSE CONJECTURE IN THE CANONICAL ENSEMBLE

### 2.1 STATEMENT OF THE PROBLEM ANS ASSUMPTIONS

In this chapter the inverse conjecture in the canonical formulation for $m \geq 1$ is proved. Accordingly, we consider a system of $N$ identical particles immersed in a thermal bath described in Section 1.1. Note, that the energy $W$ is a finite function, and so $|W^{-1}(\infty)| = 0$. This means that hard-core regions are not allowed. This was also an assumption in [1] in the authors' treatment of the case $m = 1$ for the Canonical formulation.

Given a symmetric function $\rho^{(m)} : \Lambda^m \to (0, \infty) \in L^1(\Lambda^m, d^m x)$, with $\|\rho^{(m)}\|_{1(d^m x)} = \frac{N!}{(N-m)!}$, and $W : \Lambda^N \to \infty$, the inverse conjecture claims that there exists a unique (up to an additive constant) function $v$ such that $\rho_v^{(m)} = \rho^{(m)}$ a.e. The forthcoming proof of this assertion is based on the following assumptions.

(i) The partition function for the system governed by energy $W$ is finite, that is $Z(0) < \infty$. This condition must be satisfied by all physically meaningful energies $W$. By implication, $Z(c) < \infty$ for all $c \in \mathbb{R}$.

(ii) There is a symmetric probability density $(0, \infty) \leftarrow \Lambda^N : P \in L^1(\Lambda^N, d^N x)$ such that $\rho^{(m)} = \rho_P^{(m)}$ a.e. on $\Lambda^m$, where for every $k \in \mathbb{N}$:

$$\rho_P^{(k)} := \frac{N!}{(N-k)!} \int_{\Lambda^{N-m}} P(\cdot, x_{m+1}, ..., x_N). \tag{2.1.1}$$

Note that $\rho_F^{(k)} \in L^1(\Lambda^k, d^k x)$, with $||\rho_F^{(k)}||_{1(d^k x)} = \frac{N!}{(N-k)!}$. A common example of such a situation is when $(\Lambda, dx)$ is a space of coarse-grained coordinates, and $P$ is a mean-field probability density on it. In general, if $\rho^{(m)}$ came from a real world (i.e. measured or calculated), then it must be an $m$-variable reduction of some probability density $P$.

(iii) Certainly, for a solution to the inverse problem to be possible, there are must be a condition connecting given $\rho^{(m)}$ and $W$. To illustrate why this is so, let us suppose for a moment that $|W^{-1}(\infty)| > 0$, and $|\{P = 0\}| > 0$. Let us take $P = \rho^{(m)} \otimes F$, with $\|F\|_{1(d^{N-m}x)} > 0$. Suppose that $\rho^{(m)} > 0$ on some set $E_m \subset \Lambda^m$, and that $W = \infty$ on $E_m \otimes \Lambda^{N-m}$. Then, for any finite $v$, $\rho_v^{(m)} = [Z(v)]^{-1} \int_{\Lambda^{N-m}} e^{-W-V} d^{N-m}x = 0$ a.e. on $E_m$, and so no solutions to the inverse problem exist.

We impose the following integrability condition connecting $W$ and $\rho^{(m)}$:

$$\mathcal{F}_+(P) := \int_{\Lambda^N} P(W + \ln P)_+ d^N x < \infty. \tag{2.1.2}$$

Note, that this condition would exclude the illustrative example given above.

(iv) The probability density $P$ has the property that for a.e. $x_N$ in some subset $B \subset \Lambda$ of positive $dx$ measure, there is a constant $\gamma(x_N) > 0$ such that

$$P(\cdot, x_N) \geq \gamma(x_N)\rho^{(N-1)} \text{ a.e. on } \Lambda^{N-1}. \tag{2.1.3}$$

This property holds for arbitrary small perturbations in $L^1(\Lambda^N, d^N x)$ ( and in $L^\infty(\Lambda^N, d^N x)$ if $dx$ is finite and $P$ is bounded) to any symmetric probability density $P$. (See Theorem 2.3.10 in the next section. )

## 2.2 EXISTENCE AND UNIQUENESS

Consider the following set of functions on $\Lambda^m$:

$$\mathcal{C} := \{s \in L^1(\Lambda^m, \rho^{(m)} d^m x) \mid s \text{ is a.e. finite and symmetric}, Z(s) < \infty\}, \tag{2.2.1}$$

and a functional on $\mathcal{C}$:

$$\Im(s) := \frac{\exp\left[-\frac{1}{m!}\int_{\Lambda^m} s\rho^{(m)} d^m x\right]}{Z(s)}, \quad \forall s \in \mathcal{C}. \tag{2.2.2}$$

Note, that $\mathcal{C} \neq \emptyset$ because $\mathbb{R} \in \mathcal{C}$ by assumption (i), and that $0 < \Im(s) < \infty$ for every $s \in \mathcal{C}$. It will be shown here that functional $\Im$ admits a unique maximizer on $\mathcal{C}$, and that every maximizer is a solution. Finally, the uniqueness of solutions will be proved. The choice of the functional $\Im$ is not accidental, considering that $\ln \Im(s) = \mathcal{A}_{\rho^{(m)}}(s)$, and that formally, maximizers of $\mathcal{A}_{\rho^{(m)}}$ are solutions to the inverse problem and vise versa (see Section 1.3).

**Lemma 2.2.1.** *The set $\mathcal{C}$ is convex, and $\log \Im$ is concave on $\mathcal{C}$. More precisely,*

$$\log \Im(\lambda v + (1-\lambda)u) \geq \lambda \log \Im(v) + (1-\lambda) \log \Im(u) \tag{2.2.3}$$

*for every $\lambda \in (0,1)$ and every $v, u \in \mathcal{C}$, with equality if and only if $v-u$ is a.e. a constant.*

*Proof.* Let $v, u \in \mathcal{C}$ and $\lambda \in (0,1)$. Then $s := \lambda v + (1-\lambda)u \in L^1(\Lambda^m, \rho^{(m)} d^m x)$ and is symmetric. Let $V = \hat{C}_{N,m} v$ and $U = \hat{C}_{N,m} u$. By Holder's inequality,

$$\int_{\Lambda^N} e^{-\lambda V - (1-\lambda)U} e^{-W} d^N x \leq ||e^{-V} e^{-W}||_1^{\lambda} ||e^{-U} e^{-W}||_1^{(1-\lambda)} < \infty. \tag{2.2.4}$$

Thus, $s \in \mathcal{C}$, and so the set $\mathcal{C}$ is convex.

From (2.2.2), $\log \mathcal{F}_P(V) = -\frac{1}{m!} \int_{\Lambda^N} s \rho^{(m)} d^m x - \log Z(s)$. Since the first term is linear, (2.2.3) holds if and only if $\log Z(s) \leq \lambda \log Z(v) + (1-\lambda) \log Z(u)$. But this inequality is equivalent to (2.2.4). Moreover, (2.2.4) is an equality if and only if $V - U$ is a constant a.e. $[d^N x]$ [4, Theorem 6.2]. (We have used the fact that measures $d^N x$ and $e^{-W} d^N x$ are absolutely continues with respect to each other.) However, by Corollary 2.3.4, $V-U$ is a constant a.e. $[d^N x]$ if and only if $v - u$ is a constant a.e. $[d^m x]$. □

**Lemma 2.2.2.** *The functional $\Im$ is bounded on $\mathcal{C}$. Precisely,* $0 < \Im(s) \leq \exp[\mathcal{F}_+(P)] < \infty$ *for every $s \in \mathcal{C}$.*

*Proof.* Let $s \in \mathcal{C}$, and $S = \hat{C}_{N,m} s$. Then,

$$\begin{aligned} &\int_{\Lambda^N} P \,|(W + \ln P)_+ + S|\, d^N x \leq \mathcal{F}_+(P) + \int_{\Lambda^N} P \hat{C}_{N,m} |s| d^N x \\ &= \mathcal{F}_+(P) + \frac{1}{m!} \int_{\Lambda^m} \rho^{(m)} |s| d^m x, \end{aligned} \tag{2.2.5}$$

which is finite by (2.1.2). Therefore, by Jensen's inequality for the measure $[P d^N x]$ [26, Theorem 3.3]:

$$\begin{aligned} Z(s) &= \int_{\Lambda^N} P e^{-[W + \ln P + S]} d^N x \geq \exp\left[ -\int_{\Lambda^N} P \left( [W + \ln P]_+ + S \right) d^N x \right] \\ &= \exp[-\mathcal{F}_+(P)] \exp\left[ -\frac{1}{m!} \int_{\Lambda^m} s \rho^{(m)} d^m x \right]. \end{aligned} \tag{2.2.6}$$

The last inequality implies that $\Im(s) \leq \exp[\mathcal{F}_+(P)]$. □

From now on, we set

$$M := \sup_{s\in\mathcal{C}} \Im(s) \in (0,\infty). \tag{2.2.7}$$

Let $(v_n) \in \mathcal{C}$ be a maximizing sequence for $\Im$, i.e. $\lim_{n\to\infty} \Im(v_n) = M$, and set $V_n = \hat{C}_{N,m} v_n$. Since $\Im(s) = \Im(s+c)$ for any $s \in \mathcal{C}$ and $c \in \mathbb{R}$, by adding a suitable constant to each $v_n$, it can be assumed that $Z(v_n) = \|e^{-V_n/2}\|_{2(e^{-W}d^Nx)} = 1$. Therefore, by reflexivity of $L^2(\Lambda^N, e^{-W}d^Nx)$, there is a subsequence (still denoted by $(v_n)$) and $\Pi \in L^2(\Lambda^N, e^{-W}d^Nx)$ such that $(e^{-V_n/2})$ converges weakly to $\Pi$ [27, Theorem 3.18]. After a modification on a set of zero measure, it can be assumed that $\Pi$ takes values in $[0,\infty)$.

**Lemma 2.2.3.** *$e^{-V_n/2} \to \Pi$ in $L^2(\Lambda^N, e^{-W}d^Nx)$. (In particular, $\int_{\Lambda^N} \Pi^2 e^{-W} = 1$.)*

*Proof.* For convenience, let us define $\Pi_n := e^{-V_n/2}$. It suffices to show that $1 = \lim_{n\to\infty} \|\Pi_n\|_{2(e^{-W}d^Nx)} = \|\Pi\|_{2(e^{-W}d^Nx)}$. The weak convergence implies

$$1 = \lim_{n\to\infty} ||\Pi_n||_{2(e^{-W}d^Nx)} \geq ||\Pi||_{2(e^{-W}d^Nx)}. \tag{2.2.8}$$

Let $\varepsilon > 0$ be fixed. There is $n_0 \in \mathbb{N}$ such that for each $n \geq n_0$,

$$e^{-\frac{1}{m!}\int_{\Lambda^m} v_n \rho^{(m)} d^m x} = \Im(v_n) > M(1-\varepsilon). \tag{2.2.9}$$

By Mazur's theorem [28, Theorem 3.13], there is a sequence of convex combinations $(\widetilde{\Pi}_n | n \geq n_0)$, i.e.

$$\widetilde{\Pi}_n = \sum_{k=n_0}^{n} \lambda_k^{(n)} \Pi_k, \quad \lambda_k^{(n)} \geq 0 \quad \forall\, n_0 \leq k \leq n, \quad \text{and} \sum_{k=n_0}^{n} \lambda_k^{(n)} = 1, \tag{2.2.10}$$

such that $\lim_{n\to\infty} \|\widetilde{\Pi}_n - \Pi\|_{2(e^{-W}d^Nx)} = 0$. For every $n \geq n_0$ choose $j_n, k_n \in \{n_0, ..., n\}$ such that $\langle \Pi_{j_n}, \Pi_{k_n}\rangle \leq \langle \Pi_j, \Pi_k\rangle$ for every $j,k \in \{n_0,...,n\}$, where $\langle\cdot,\cdot\rangle$ denotes the inner product of $L^2(\Lambda^N; e^{-W}d^Nx)$. Then,

$$\|\widetilde{\Pi}_n\|^2_{2,e^{-W}d^Nx} = \sum_{j,k=n_0}^{n} \lambda_j^{(n)}\lambda_k^{(n)} \langle \Pi_j, \Pi_k\rangle \geq \left(\sum_{j,k=n_0}^{n} \lambda_j^{(n)}\lambda_k^{(n)}\right) \langle \Pi_{j_n}, \Pi_{k_n}\rangle = \langle \Pi_{j_n}, \Pi_{k_n}\rangle. \tag{2.2.11}$$

Since $\langle \Pi_{j_n}, \Pi_{k_n} \rangle = \int_{\Lambda^N} e^{-\frac{V_{j_n}+V_{k_n}}{2} - W} d^N x$, (2.2.11) reads

$$\|\widetilde{\Pi}_n\|^2_{2(e^{-W}d^N x)} \geq Z(y_n), \tag{2.2.12}$$

where $y_n := \frac{v_{j_n}+v_{k_n}}{2} \in \mathcal{C}$ (because $\mathcal{C}$ is convex by Lemma 2.2.1). Therefore, using (2.2.9),

$$M \geq \frac{e^{-\frac{1}{m!}\int_{\Lambda^m}(v_{j_n}+v_{k_n})/2\,\rho^{(m)} d^m x}}{Z(y_n)} = \frac{(\Im(v_{j_n})\Im(v_{k_n}))^{\frac{1}{2}}}{Z(y_n)} > \frac{M(1-\varepsilon)}{Z(y_n)}. \tag{2.2.13}$$

Inequalities (2.2.12) and (2.2.13) imply that $\|\widetilde{\Pi}_n\|^2_{2(e^{-W}d^N x)} \geq Z(y_n) > 1-\varepsilon$. Therefore, in view of (2.2.8), $1 \geq \|\Pi\|^2_{2(e^{-W}d^N x)} = \lim_{n\to\infty} \|\widetilde{\Pi}_n\|^2_{2(e^{-W}d^N x)} \geq 1-\varepsilon$ for any $\varepsilon > 0$. Thus, $\|\Pi||_{2(e^{-W}d^N x)}\| = 1$. □

**Theorem 2.2.4.** *There is $v \in \mathcal{C}$ such that $\Im(v) = \sup_{s\in\mathcal{C}} \Im(s) = M$. Moreover, if also $u \in \mathcal{C}$, and $\Im(u) = M$, then $v - u$ is a.e. a constant on $\Lambda^m$.*

*Proof.* (1) It follows from Lemma 2.2.3 (and the fact that $d^N x$ and $e^{-W}d^N x$ have the same zero measure sets) that there is a subsequence (still denoted $(v_n)$) such that $e^{-V_n/2} \to \Pi$ a.e. on $\Lambda^N$ [26, Theorem 3.12]. If $E_N \subset \Lambda^N$ is the set on which $e^{-V_n/2}$ converges to $\Pi$, then $|\Lambda^N \setminus E_N| = 0$. Let

$$V := \begin{cases} -2\ln\Pi & \text{on } E_N \\ r & \text{on } \Lambda^N \setminus E_N, \end{cases} \tag{2.2.14}$$

where $r$ is an arbitrary real number, and $\ln 0 := -\infty$. Then, $V_n \to V$ on $E_N$, and so a.e. on $\Lambda^N$.

(2) In this step we prove that $V_- \in L^1(\Lambda^N; Pd^N x)$. By Lemma 2.2.3,

$$1 = \int_{\Lambda^N} \Pi^2 d^N x = \int_{\Lambda^N} e^{-V-W} d^N x \geq \int_{\Lambda^N} e^{-V-(W+\log P)_+} P d^N x. \tag{2.2.15}$$

The relations $e^t \geq t_+$ and $(-t)_+ = t_-$ for $t \in \mathbb{R}$ together with (2.2.15) imply that $\int_{\Lambda^N} (V + (W+\log P)_+)_- \, P d^N x \leq 1$. Particularly,

$$(V + (W+\log P)_+)_- \in L^1(\Lambda^N; P d^N x). \tag{2.2.16}$$

Next, using $(t+s)_- \leq t_- + s_-$ for $t \in \overline{\mathbb{R}}$ and $s \in \mathbb{R}$, with $t = V + (W+\log P)_+$ and $s = -(W+\log P)_+$, we obtain $V_- \leq (V + (W+\log P)_+)_- + (W+\log P)_+$. Therefore, by (2.1.2) and (2.2.16), $V_- \in L^1(\Lambda^N; P d^N x)$.

(3) Next, we show $V_+ \in L^1(\Lambda^N; Pd^N x)$. For $k, \ell \in \mathbb{N}$, let us define

$$V^k := \min(V, k), \qquad \phi^\ell := \min(W + \log P, \ell). \tag{2.2.17}$$

We have that

$$0 \le W + \log P - \phi^\ell \le (W + \log P)_+ \tag{2.2.18}$$

because $W + \log P - \phi^\ell = 0$ when $W + \log P \le \ell$, and
$0 < W + \log P - \phi^\ell = (W + \log P)_+ - \ell < (W + \log P)_+$ when $W + \log P > \ell$. In particularly, $W + \log P - \phi^\ell \in L^1(\Lambda^N; Pd^N x)$ by (2.1.2). Moreover,

$$\lim_{\ell \to \infty} \int_{\Lambda^N} (W + \log P - \phi^\ell) P = 0 \tag{2.2.19}$$

by dominated convergence. Since also $V^k = -V_- + V_+^k \in L^1(\Lambda^N; Pd^N x)$ by step (2), it follows that $(V^k - V_n)/2 - W - \log P + \phi^\ell \in L^1(\Lambda^N; Pd^N x)$. Therefore, by Jensen's inequality

$$e^{-\int_{\Lambda^N} \frac{V_n}{2} Pd^N x} e^{\int_{\Lambda^N} \left(\frac{V^k}{2} - W - \log P + \phi^\ell\right) Pd^N x} \le \\ \int_{\Lambda^N} e^{-\left(\frac{(V_n - V^k)}{2} + W + \log P - \phi^\ell\right)} Pd^N x = \int_{\Lambda^N} e^{-\frac{V_n}{2}} e^{\frac{V^k}{2} + \phi^\ell} e^{-W} d^N x. \tag{2.2.20}$$

Next, we will show that $e^{\frac{V^k}{2} + \phi_\ell} \in L^2(\Lambda^N, e^{-W} d^N x)$. Indeed, $\phi^\ell \le W + \log P$ on $S$ implies $e^{\phi^\ell - W} \le P$ a.e., and therefore, $e^{\phi^\ell - W} \in L^1(\Lambda^N, d^N x)$. Also, $\phi^\ell \le \ell$, $V^k \le k$ imply $V^k + 2\phi^\ell - W \le k + \ell + \phi^\ell - W$. Therefore, $e^{V^k + 2\phi^\ell - W} \le e^{k+\ell} e^{\phi^\ell - W} \in L^1(\Lambda^N, d^N x)$. Equivalently,

$$e^{\frac{V^k}{2} + \phi^\ell} \in L^2(\Lambda^N, e^{-W} d^N x). \tag{2.2.21}$$

With $k, \ell$ being held fixed, let $n \to \infty$. Since, $\int_{\Lambda^N} \frac{1}{2} V_n Pd^N x = \frac{1}{2m!} \int_{\Lambda^m} v_n \rho^{(m)} d^{(m)} x$, the leftmost hand side of (2.2.20) converges to $\sqrt{M} e^{\int_{\Lambda^N} (\frac{U^k}{2} - W - \log P + \phi^\ell) Pd^N x}$. By (2.2.21) and weak convergence, the rightmost hand side of (2.2.20) converges to

$$\int_{\Lambda^N} e^{-\frac{(V - V^k)}{2}} e^{\phi^\ell - W} d^N x = \int_{\Lambda^N} e^{-\frac{(V - V^k)}{2}} e^{-(W + \log P - \phi^\ell)} Pd^N x \le 1, \tag{2.2.22}$$

where the last inequality follows by $V - V^k \ge 0$, $W + \log P - \phi_\ell \ge 0$, and $\int_{\Lambda^N} P = 1$. This yields

$$\sqrt{M} e^{\int_{\Lambda^N} \frac{V^k}{2} Pd^N x} e^{-\int_{\Lambda^N} (W + \log P - \phi_\ell) Pd^N x} \le 1. \tag{2.2.23}$$

With $k$ being held fixed, let $\ell \to \infty$ in (2.2.23). Then, by (2.2.19), we obtain $\sqrt{M} e^{\int_{\Lambda^N} \frac{V^k}{2} P d^N x} \leq 1$. Equivalently, using $V^k = -V_- + V_+^k$,

$$M \leq e^{-\int_{\Lambda^N} V^k P d^N x} = e^{-\int_{\Lambda^N} V_+^k P d^N x} e^{\int_{\Lambda^N} V_- P d^N x}. \tag{2.2.24}$$

Now, $V_+^k$ is increasing to $V_+$ pointwise. Thus, by monotone convergence, $\lim_{k\to\infty} \int_{\Lambda^N} V_+^k P d^N x = \int_{\Lambda^N} V_+ P d^N x$. Taking $k \to \infty$ in (2.2.24) results into

$$0 < M \leq e^{-\int_{\Lambda^N} V_+ P d^N x} e^{\int_{\Lambda^N} V_- P d^N x}. \tag{2.2.25}$$

Since $V_- \in L^1(\Lambda^N, P d^N x)$ by Step (2), (2.2.25) shows that $V_+$ (and therefore $V$) belongs to $L^1(\Lambda^N; P d^N x)$.

(4) Since $V_n \to V$ a.e., it follows from Theorem 2.3.3 in the next section that there is a.e. finite measurable function $v$ on $\Lambda^m$ such that $v_n \to v$ a.e. on $\Lambda^m$. In particular, $v$ is symmetric, and $V = \hat{C}_{N,m} v$. It is at this point that assumption (iv) in Section 2.1 is used. To wit, equation (2.1.3) and Theorem 2.3.8 imply that $v \in L^1(\Lambda^m, \rho^{(m)} d^m x)$. Since also $Z(v) = 1$ by (2.2.15), $v \in \mathcal{C}$, and therefore (2.2.25) implies that $\Im(v) = M$.

(5) Suppose that $u \in \mathcal{C}$, and $\Im(u) = M$. Let $\lambda \in (0,1)$. Then, $\ln \Im[\lambda v + (1-\lambda)u] = \lambda \ln \Im(v) + (1-\lambda)\Im(u)$. Therefore, by Lemma 2.2.1, $v - u$ is a.e. a constant. □

**Theorem 2.2.5.** *There is $v \in \mathcal{C}$ such that $\rho^{(m)} = \rho_v^{(m)}$ a.e. on $\Lambda^m$.*

*Proof.* By Theorem 2.2.4, there is $v \in \mathcal{C}$ such that $\Im(v) = M$. Let $\xi \in L^\infty(\Lambda^m, d^m x)$ be an a.e finite and symmetric function, and set $\Xi = \hat{C}_{N,m}\xi$, $V = \hat{C}_{N,m} v$. Then, $\|\Xi\|_{\infty(d^N x)} \leq \binom{N}{m} ||\xi||_{\infty(d^m x)}$, and so $\Xi \in L^\infty(\Lambda^N, d^N x)$.

For every $t \in \mathbb{R}$, $v + t\xi \in \mathcal{C}$, and therefore, $\Im(v+t\xi) \leq \Im(v)$. The function $t \mapsto \Im(v+t\xi)$ is smooth. This is obvious for the numerator in (2.2.2). The same property for the denominator follows by a theorem on differentiation of parameter-dependent integrals [4, Theorem 2.27]. ($\Xi \in L^\infty(\Lambda^N, d^N x)$ is used here.) Thus, $\frac{d}{dt}\Im(v+t\xi)_{|t=0} = 0$. This gives

$$\Im(v) \left[ \frac{\int_{\Lambda^N} e^{-V-W} \Xi d^N x}{Z(v)} - \int_{\Lambda^N} \Xi P d^N x \right] = 0. \tag{2.2.26}$$

By symmetry, (2.2.26) amounts to $\int_{\Lambda^m} \xi(\rho_v^{(m)} - \rho^{(m)}) d^m x = 0$. Choosing $\xi = \mathrm{sign}\left(\rho_v^{(m)} - \rho^{(m)}\right)$ (with $\mathrm{sign}(0) := 0$), we obtain $\int_{\Lambda^m} |\rho_U^{(m)} - \rho^{(m)}| d^m x = 0$, and so $\rho_v^{(m)} = \rho^{(m)}$ a.e. on $\Lambda^m$. □

**Theorem 2.2.6.** *Under conditions (i)-(iv) stated in Section 2.1, there is $v \in \mathcal{C}$ such that $\rho_v^{(m)} = \rho^{(m)}$ a.e. on $\Lambda^m$. Moreover, if there is another $u \in \mathcal{C}$ satisfying $\rho_u^{(m)} = \rho^{(m)}$ a.e., then $v - u$ is a.e. a constant.*

*Proof.* By Theorem 2.2.4, there is $v \in \mathcal{C}$ such that $\rho_v^{(m)} = \rho^{(m)}$ a.e. on $\Lambda^m$. Suppose that $u \in \mathcal{C}$, and $\rho_u^{(m)} = \rho^{(m)}$ a.e. on $\Lambda^m$. Let us set $V := \hat{C}_{N,m}v$, $U := \hat{C}_{N,m}u$. First, we notice that

$$\begin{aligned}&\frac{1}{Z(v)}\int_{\Lambda^N} e^{-W-V}|V-U|d^Nx = \int_{\Lambda^N} G_v|V-U|d^Nx \leq \\ &\int_{\Lambda^N} G_v\hat{C}_{N,m}(|v|+|u|)d^Nx = \frac{1}{m!}\int_{\Lambda^m}\rho^{(m)}(|v|+|u|)d^mx < \infty.\end{aligned} \tag{2.2.27}$$

Therefore, by Jensen's inequality [26, Theorem 3.3],

$$\begin{aligned}&\frac{Z(u)}{Z(v)} = \frac{1}{Z(v)}\int_{\Lambda^N} e^{-W-V+(V-U)}d^Nx = \int_{\Lambda^N} G_v\exp[V-U]d^Nx \\ &\geq \exp\left[\int_{\Lambda^N} G_v(V-U)d^Nx\right] = \exp\left[\frac{1}{m!}\int_{\Lambda^m}\rho^{(m)}(v-u)d^{(m)}x\right].\end{aligned} \tag{2.2.28}$$

Interchanging $v$ and $u$, we also obtain:

$$\frac{Z(v)}{Z(u)} \geq \exp\left[-\frac{1}{m!}\int_{\Lambda^m}\rho^{(m)}(v-u)d^{(m)}x\right]. \tag{2.2.29}$$

However, the last two inequalities are simultaneously satisfied if and only if they are both equalities. In particular,

$$\int_{\Lambda^N} G_v\exp[V-U]d^Nx = \exp\left[\int_{\Lambda^N} G_v(V-U)d^Nx\right], \tag{2.2.30}$$

which is true if and only if $V - U$ is a constant a.e. $[e^{-W-V}d^Nx]$ [26, Theorem 3.3], and so a.e. $[d^Nx]$ (using the fact that $W$ and $V$ are a.e. finite). Finally, by Corollary 2.3.4 in the next section $V - U$ is a constant a.e. $[d^Nx]$ on $\Lambda^N$ if and only if $v - u$ is a constant a.e. $[d^mx]$ on $\Lambda^m$. □

## 2.3 SOME MEASURE-THEORETIC PROPERTIES OF U-STATISTICS

### 2.3.1 Introduction

This sections contains the theorems needed to finish the proof of the inverse conjecture in the canonical formulation. For a function $u : \Lambda^m \to \mathbb{R}$, let us define the generalized $N$-mean of order $m$ with kernel $u$ as

$$(G_{N,m}u)(x_1, ..., x_N) = \binom{N}{m}^{-1} \sum_{1 \le i_1 < \cdots < i_m \le N} u(x_{i_1}, ..., x_{i_m}). \tag{2.3.1}$$

If $u$ is an $m$-particle interaction, its generalized $N$-mean is the additional potential (apart from a multiplicative constant) for the system of particles studied in the previous section. (Note that $\binom{N}{m} G_{N,m}u = \hat{C}_{N,m}u$.) However, if $(x_1, ..., x_N)$ are replaced with random variables, the generalized $N$-mean in (2.3.1) becomes a U-statistic. U-statistics were introduced by Hoeffding as unbiased estimators of regular functionals [29]. Since then, they have been extensively studied, and numerous applications have been found for them [30, 31]. In common statistical usage, the kernel $u$ is given, and the limit properties of U-statistics are studied as sampling size $N$ goes to infinity. These issues are different from the ones dealt with in the inverse problem. Nevertheless, it should be expected that some applications require a measure-theoretic setting in which the properties of U-statistics provided here are useful.

In the following, we investigate whether various measure-theoretic properties of the kernels (such as a.e. convergence of sequences, measurability, essential boundedness, and integrability with respect to probability measures) can be deduced from the analogous properties of the generalized means, and vice versa. In Section 2.3.2, it is proved that a sequence of generalized $N$-means converges a.e. on $\Lambda^N$ if and only if the corresponding sequence of their kernels converges a.e. on $\Lambda^m$ (Theorem 2.3.3). Despite its apparent simplicity, the "only if" part of this statement is not easy to verify. The difficulty lies in the fact that convergence holds only a.e. on $\Lambda^N$. This can be illustrated on a simple example. Suppose that $G_{N,1}u_n \to U$ everywhere on $\Lambda^N$. Then, for every $x \in \Lambda$, $u_n(x) \to U(x, ..., x)$. However, the same approach cannot be used if the convergence holds only a.e. because the diagonal may be (and often is) a set of measure zero.

The equivalence of measurability and essential boundedness of generalized means and their kernels is established in Theorem 2.3.5. Section 2.3.4 is concerned with integrability issues. The general problem is as follows. A symmetric probability density $P$ on $\Lambda^N$ induces a marginal symmetric probability density $\rho^{(m)}$ on $\Lambda^m$ upon integrating $P$ with respect to any set of $N-m$ variables. If $1 \leq m < N$ and $1 \leq r < \infty$, is it true that a generalized $N$-mean of order $m$ is in $L^r(\Lambda^N; Pd^N x)$ if and only if its kernel is in $L^r(\Lambda^m; \rho^{(m)} d^m x)$? While the "if" part of this question is easy to verify, the "only if" part does not hold in general (Example 2.3.1). However, an extra condition on $P$ given in Theorem 2.3.8 ensures that the answer to the above question is positive. This condition holds in some arbitrarily small perturbations in $L^1(\Lambda^N; d^N x)$ (and in $L^\infty(\Lambda^N; d^N x)$, if measure $dx$ is finite, and $P$ is essentially bounded) of any symmetric probability density (Theorem 2.3.10).

In this section the following definitions will be used. Subsets of $d^k x$ measure zero will be called *null* sets, and their complements *co-null*.

Let $1 \leq m < N$ be integers. Then for any $(x_{m+1}, ..., x_N) \in \Lambda^{N-m}$ and any $E \subset \Lambda^N$, the $(x_{m+1}, ..., x_N)$-section of $E$ is

$$E_{x_{m+1},...,x_N} := \{(x_1, ..., x_m) \in \Lambda^m : (x_1, ..., x_N) \in E\}. \tag{2.3.2}$$

To shorten the presentation, it will be useful to define the operator $\hat{B}_{N,m}$, transforming a set $E_m \subset \Lambda^m$ into a set $\hat{B}_{N,m} E_m \subset \Lambda^N$:

$$\begin{aligned} &\hat{B}_{N,m} E_m := \\ &\{(x_1, ..., x_N) \in \Lambda^N : (x_{i_1}, ..., x_{i_m}) \in E_m \ \forall \ 1 \leq i_1 < \cdots < i_m \leq N\}. \end{aligned} \tag{2.3.3}$$

For ease of future argument, we need to extend the definition of $G_{N,m} u$ to the case where $0 = m \leq N$, and $u \equiv c \in \mathbb{R}$. In this case, we define $G_{N,0} u = c$.

It should be emphasized that, with the exception of Section 4, the kernel $u$ in (2.3.1) is not assumed to be symmetric, as is customarily done for U-statistics.

### 2.3.2 Almost everywhere convergence

In this subsection we address the question of whether the a.e. convergence of a sequence of generalized means $G_{N,m}u_n$ implies the a.e. convergence of their kernels $u_n$. In particular, if this is true, then the a.e. limit of a sequence of generalized $N$-means is a generalized $N$-mean.

The following two simple lemmas will be crucial for the development of all subsequent arguments.

**Lemma 2.3.1.** *Let $1 \leq k \leq N$ be integers, and let $T_k$ be a co-null subset of $\Lambda^k$. Then, the set $T_N = \hat{B}_{N,k}T_k$ is co-null in $\Lambda^N$.*

*Proof.*

$$T_N = \bigcap_{1 \leq i_1 < \cdots < i_k \leq N} T_{i_1,\ldots,i_k}, \tag{2.3.4}$$

where $T_{i_1,\ldots,i_k} := \{(x_1, ..., x_N) \in \Lambda^N : (x_{i_1}, ..., x_{i_k}) \in T_k\}$. Therefore,

$$\left|\Lambda^N \setminus T_N\right| \leq \sum_{1 \leq i_1 < \cdots < i_k \leq N} \left|\Lambda^N \setminus T_{i_1,\ldots,i_k}\right| = \binom{N}{k} \left|\left(\Lambda^k \setminus T_k\right) \otimes \Lambda^{N-k}\right| = 0. \tag{2.3.5}$$

□

**Lemma 2.3.2.** *For any integers $0 \leq k \leq m \leq N$, $G_{N,m}G_{m,k} = G_{N,k}$.*

*Proof.* If $0 = k \leq m \leq N$, and $u \equiv c \in \mathbb{R}$ then, $G_{N,0}u = c$ by definition. On the other hand, $G_{N,m}G_{m,0}u = G_{N,m}c = c$.

Suppose that $1 \leq k \leq m \leq N$, and let $u : \Lambda^k \to \mathbb{R}$ be any function. By a simple combinatorial argument

$$\begin{gathered}\left(G_{N,m}G_{m,k}u\right)(x_1, ..., x_N) = \binom{N}{m}^{-1} \binom{m}{k}^{-1} \binom{N-k}{m-k} \sum_{1 \leq i_1 < \cdots < i_k \leq N} u(x_{i_1}, ..., x_{i_k}) = \\ \binom{N}{k}^{-1} \sum_{1 \leq i_1 < \cdots < i_k \leq N} u(x_{i_1}, ..., x_{i_k}) = G_{N,k}(x_1, ..., x_N).\end{gathered} \tag{2.3.6}$$

The first equality follows because for every $1 \leq i_1 < \cdots < i_k \leq N$, the term $u(x_{i_1}, ..., x_{i_k})$ appears exactly $\binom{N-k}{m-k}$ times. □

**Theorem 2.3.3.** *Let $1 \le m \le N$ be integers,and let $(u_n)$ be a sequence of finite functions on $\Lambda^m$. Then the following is true.*

*There is a finite function $U$ on $\Lambda^N$ such that $G_{N,m}u_n \to U$ a.e. if and only if there is a finite function $u$ on $\Lambda^m$ such that $u_n \to u$ a.e.*

**Remark 2.3.1.** The statement is still true with $U$, $u$ and $u_n$ are a.e. finite. However, we chose them to be everywhere finite to avoid cluttering the proof with non-essential details.

*Proof of Theorem 2.3.3.* Since there is nothing to prove when $m = N$, we will assume that $1 \le m < N$. Suppose first that there exists a finite $u$ such that $u_n \to u$ on some co-null set $E_m \subset \Lambda^m$. Then the set $E_N = \hat{B}_{N,m}E_m \subset \Lambda^N$ is co-null by Lemma 2.3.1. Moreover, $G_{N,m}u_n \to G_{N,m}u$ on $E_N$.

Conversely, suppose that there exists a finite $U$ such that $G_{N,m}u_n \to U$ on some co-null set $E \subset \Lambda^N$.

*Case 1:* $m = 1$. Let us fix $(\tilde{x}_2, ..., \tilde{x}_N) \in \Lambda^{N-1}$ such that $|\Lambda \setminus E_{\tilde{x}_2,...,\tilde{x}_N}| = 0$. (This is possible because the a.e. section of a co-null set is co-null by the Fubini-Tonelli theorem [4, Theorem 2.39].) By the definition of the set $E$, for every $x \in E_{\tilde{x}_2,...,\tilde{x}_N}$:

$$u_n(x) + \sum_{j=2}^{N} u_n(\tilde{x}_j) \to NU(x, \tilde{x}_2, ..., \tilde{x}_N). \tag{2.3.7}$$

Thus, for any $(y_1, ..., y_N) \in E^N_{\tilde{x}_2,...,\tilde{x}_N}$ :

$$\sum_{i=1}^{N} u_n(y_i) + N\sum_{j=2}^{N} u_n(\tilde{x}_j) \to N\sum_{i=1}^{N} U(y_i, \tilde{x}_2, ..., \tilde{x}_N), \tag{2.3.8}$$

where we have summed (2.3.7) over $i$ after replacing $x$ with $y_i$. Let us fix $(y_1, ..., y_N) \in E^N_{\tilde{x}_2,...,\tilde{x}_N} \cap E$. Then, (2.3.8) holds together with $\sum_{i=1}^{N} u_n(y_i) \to NU(y_1, ..., y_N)$. Thus,

$$\sum_{i=2}^{N} u_n(\tilde{x}_i) \to \sum_{i=1}^{N} U(y_i, \tilde{x}_2, ..., \tilde{x}_N) - U(y_1, ..., y_N) =: C. \tag{2.3.9}$$

Using this result in (2.3.7), we finally obtain:

$$u_n(x) \to NU(x, \tilde{x}_2, ..., \tilde{x}_N) - C \quad \forall x \in E_{\tilde{x}_2,...,\tilde{x}_N}. \tag{2.3.10}$$

*Case 2:* $2 \leq m < N$. The proof for this case will proceed by induction on $m$. Let us define $M := \min(m, N-m)$. Suppose that the "only if" statement of the theorem is true for $m-1$. By the Fubini-Tonelli theorem, we can fix $(\tilde{x}_{m+1}, ..., \tilde{x}_N) \in \Lambda^{N-m}$ such that $\left|\Lambda^m \setminus E_{\tilde{x}_{m+1},...,\tilde{x}_N}\right| = 0$. By the definition of the set $E$:

$$(G_{N,m}u_n)(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) \to U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) \quad \text{on } E_{\tilde{x}_{m+1},...,\tilde{x}_N}. \tag{2.3.11}$$

Using the functions $v_n^{(m-k)} : \Lambda^{m-k} \to \mathbb{R}$, $1 \leq k \leq m-1$, and constants $v_n^{(0)} \in \mathbb{R}$ defined as:

$$\begin{aligned} v_n^{(m-k)} &:= \\ &\sum_{1 \leq j_1 < \cdots < j_k \leq N-m} u_n(\cdot, \tilde{x}_{m+j_1}, ..., \tilde{x}_{m+j_k}) \quad \text{if } \ 1 \leq k \leq m-1, \\ v_n^{(0)} &:= \sum_{1 \leq j_1 < \cdots < j_m \leq N-m} u_n(\tilde{x}_{m+j_1}, ..., \tilde{x}_{m+j_m}), \end{aligned} \tag{2.3.12}$$

the left hand side of (2.3.11) can be rewritten as

$$\begin{aligned} &\binom{N}{m} (G_{N,m}u_n)(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) = \\ &\qquad \left[ u_n + \sum_{k=1}^{M} \binom{m}{m-k} G_{m,m-k} v_n^{(m-k)} \right]. \end{aligned} \tag{2.3.13}$$

By Lemma 2.3.2, $G_{m,m-k} = G_{m,m-1}G_{m-1,m-k}$, $1 \leq k \leq m$. Thus, the right hand side of (2.3.13) simplifies to: $u_n + (G_{m,m-1}\omega_n)$, where $\omega_n : \Lambda^{m-1} \to \mathbb{R}$ is

$$\omega_n := \sum_{k=1}^{M} \binom{m}{m-k} G_{m-1,m-k} v_n^{(m-k)}. \tag{2.3.14}$$

Then, in view of (2.3.11), we obtain that

$$u_n + G_{m,m-1}\omega_n \to \binom{N}{m} U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) \ \text{ on } E_{\tilde{x}_{m+1},...,\tilde{x}_N}. \tag{2.3.15}$$

The set $\Omega = \hat{B}_{N,m} E_{\tilde{x}_{m+1},...,\tilde{x}_N} \subset \Lambda^N$ is co-null by Lemma 2.3.1. Moreover, applying the operator $G_{N,m}$ to both sides of (2.3.15), gives that on $\Omega$:

$$\begin{aligned} &G_{N,m}u_n + G_{N,m}G_{m,m-1}\omega_n = \\ &G_{N,m}u_n + G_{N,m-1}\omega_n \to \binom{N}{m} G_{N,m}U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N). \end{aligned} \tag{2.3.16}$$

(Lemma 2.3.2 was used in the equality.) Since (2.3.16) and $G_{N,m}u_n \to U$ both hold on $\Omega \cap E$, we further obtain that

$$G_{N,m-1}\omega_n \to \binom{N}{m} G_{N,m}U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) - U \quad \text{on } \Omega \cap E. \tag{2.3.17}$$

Now, the induction hypothesis implies that there is a finite function $\omega : \Lambda^{m-1} \to \mathbb{R}$ such that $\omega_n \to \omega$ a.e. Further, by the "if" statement of the theorem there is a co-null set $E_m \subset \Lambda^m$ and a finite function $\phi : \Lambda^m \to \mathbb{R}$ such that $G_{m,m-1}\omega_n \to \phi$ on $E_m$. Using this result in (2.3.15), we finally obtain:

$$u_n \to \binom{N}{m} U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N) - \phi \quad \text{on } E_m \cap E_{\tilde{x}_{m+1},...,\tilde{x}_N}. \tag{2.3.18}$$

□

**Corollary 2.3.4.** *Let $1 \leq m \leq N$ be integers, and $u$ be a finite function on $\Lambda^m$. Then, $G_{N,m}u = 0$ a.e. if and only if $u = 0$ a.e. In particular, the linear operator $G_{N,m}$ is injective.*

*Proof.* It is easy to verify, using Lemma 2.3.1, that $G_{N,m}u = 0$ a.e. if $u = 0$ a.e. For the converse, let us define a sequence $(v_n)$ by $v_n = u$ if $n$ is odd and $v_n = 0$ if $n$ is even. Since $G_{N,m}v_n \to 0$ a.e., Theorem 2.3.3 implies that there is a finite function $v$ on $\Lambda^m$ such that $v_n \to v$ a.e. Then, $v = u = 0$ a.e. by the definition of sequence $(v_n)$. □

### 2.3.3 Measurability and essential boundedness

**Theorem 2.3.5.** *Let $1 \leq m \leq N$ be integers, and $u : \Lambda^m \to \mathbb{R}$ be a function. Let $U := G_{N,m}u$. Then,*

*(i) $U$ is measurable if and only if $u$ is measurable.*

*(ii) $U \in L^\infty(\Lambda^N; d^N x)$ if and only if $u \in L^\infty(\Lambda^m; d^m x)$. Moreover, there is a constant $C(N,m)$ such that $||U||_{\infty,d^N x} \leq ||u||_{\infty,d^m x} \leq C(N,m)||U||_{\infty,d^N x}$, with $C(N,1) = 1$. In particular, $G_{N,m}$ is an isomorphism from $L^\infty(\Lambda^m; d^m x)$ onto a closed subspace of $L^\infty(\Lambda^N; d^N x)$.*

*Proof.* "In particular" part is the direct consequence of Theorem 2.3.3 and Corollary 2.3.4. The conclusion holds trivially for $m = N$, so let us assume that $1 \leq m < N$. Since the proofs of (i) and (ii) are very similar, we will only show (ii). However, it will be clear that (i) is established by a shorter version of the same argument.

Suppose first that $u \in L^\infty(\Lambda^m; d^m x)$. Then, $U$ is a finite sum of measurable functions. Namely, $U = \sum_{1\leq i_1<\cdots<i_m\leq N} U_{i_1,\ldots,i_m}$, where $U_{i_1,\ldots,i_m}(x_1, \ldots, x_N) := u(x_{i_1}, \ldots, x_{i_m})$. Moreover, the set $E_m \subset \Lambda^m$ on which $|u| \leq ||u||_{\infty,d^m x}$ is co-null. It follows that $|U| \leq ||u||_{\infty,d^m x}$ on the co-null set $\hat{B}_{N,m}E_m \subset \Lambda^N$, and so $||U||_{\infty,d^N x} \leq ||u||_{\infty,d^m x}$.

Conversely, suppose that $U \in L^\infty(\Lambda^N; d^N x)$.

*Case 1*: $m = 1$. The Fubini-Tonelli theorem implies that there is $(\tilde{x}_2, \ldots, \tilde{x}_N) \in \Lambda^{N-1}$ such that $U(\cdot, \tilde{x}_2, \ldots, \tilde{x}_N) = u(\cdot) + \sum_{i=2}^N u(\tilde{x}_i) \in L^\infty(\Lambda; dx))$, and so $u \in L^\infty(\Lambda; dx)$.

Next, we will show that $||u||_{\infty,dx} = ||U||_{\infty,d^N x}$. In view of the "if" part of the theorem, it suffices to prove that $||U||_{\infty,d^N x} \geq ||u||_{\infty,dx}$.

Let $s :=$ ess sup $u$, and $S :=$ ess sup $U$. For every $\epsilon > 0$, the measure of the set $A_\epsilon := \{x \in \Lambda : u(x) > s - \epsilon\}$ is strictly positive. Since the set $E := \{(x_1, \ldots, x_N) \in \Lambda^N : U(x_1, \ldots, x_N) \leq S\} \subset \Lambda^N$ is co-null, it follows that $\left|A_\epsilon^N \cap E\right| > 0$. Moreover, for every $(x_1, \ldots, x_N) \in A_\epsilon^N \cap E$, $S \geq U(x_1, \ldots, x_N) > s - \epsilon$. Thus, $S \geq s$. Similarly, ess inf $U \leq$ ess inf $u$, and so $||U||_{\infty,d^N x} \geq ||u||_{\infty,dx}$.

*Case 2*: $2 \leq m < N$. The proof will proceed by induction on $m$. Suppose that the "only if" statement of the theorem holds for $m - 1$. The Fubini-Tonelli theorem implies that there is $(\tilde{x}_{m+1}, \ldots, \tilde{x}_N) \in \Lambda^{N-m}$ such that $U(\cdot, \tilde{x}_{m+1}, \ldots, \tilde{x}_N) \in L^\infty(\Lambda^m; d^m x)$, with

$$||U(\cdot, \tilde{x}_{m+1}, \ldots, \tilde{x}_N)||_{\infty,d^m x} \leq ||U||_{\infty,d^N x}. \tag{2.3.19}$$

By the proof of Theorem 2.3.3 (see (2.3.11 - 2.3.15) ), there is $\omega : \Lambda^{m-1} \to \mathbb{R}$ such that

$$\binom{N}{m} U(\cdot, \tilde{x}_{m+1}, \ldots, \tilde{x}_N) = u + G_{m,m-1}\omega. \tag{2.3.20}$$

Applying $G_{N,m}$ to both sides of (2.3.20), and using Lemma 2.3.2 yield:

$$G_{N,m-1}\omega = \binom{N}{m} G_{N,m} U(\cdot, \tilde{x}_{m+1}, \ldots, \tilde{x}_N) - U. \tag{2.3.21}$$

Therefore, by the "if" statement of the theorem and (2.3.19), $G_{N,m-1}\omega \in L^\infty(\Lambda^N; d^N x)$, with

$$
\begin{aligned}
||G_{N,m-1}\omega||_{\infty,d^N x} &\le \binom{N}{m} ||U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N)||_{\infty,d^m x} + ||U||_{\infty,d^N x} \\
&\le \left(\binom{N}{m} + 1\right) ||U||_{\infty,d^N x}.
\end{aligned}
\tag{2.3.22}
$$

Then, the induction hypothesis implies that $\omega \in L^\infty(\Lambda^{m-1}; d^{m-1}x)$, and

$$
||\omega||_{\infty,d^{m-1}x} \le C(N, m-1) \left(\binom{N}{m} + 1\right) ||U||_{\infty,d^N x} \tag{2.3.23}
$$

for some constant $C(N, m-1)$. Next, using the "if" part of the theorem again, we infer that $G_{m,m-1}\omega \in L^\infty(\Lambda^m; d^m x)$, and $||G_{m,m-1}\omega||_{\infty,d^m x} \le ||\omega||_{\infty,d^{m-1}x}$. This result, together with (2.3.20), (2.3.19), and (2.3.23), yield that $u \in L^\infty(\Lambda^m; d^m x)$, and

$$
\begin{aligned}
||u||_{\infty,d^m x} &\le \binom{N}{m} ||U(\cdot, \tilde{x}_{m+1}, ..., \tilde{x}_N)||_{\infty,d^m x} + ||\omega||_{\infty,d^{m-1}x} \\
&\le \left[\binom{N}{m} (1 + C(N, m-1)) + C(N, m-1)\right] ||U||_{\infty,d^N x}.
\end{aligned}
\tag{2.3.24}
$$

□

### 2.3.4 Integrability

Let $N \ge 2$ and $P$ be a symmetric probability density on $\Lambda^N$. That is, $P$ is a nonnegative, symmetric function, and $\int_{\Lambda^N} P = 1$. For every $1 \le m < N$, the marginal probability density on $\Lambda^m$ is defined as

$$
\rho^{(m)} := \int_{\Lambda^{N-m}} P(\cdot, x_{m+1}, ..., x_N) dx_{m+1} \cdots dx_N \quad \text{a.e. on } \Lambda^m. \tag{2.3.25}
$$

Note that $\rho^{(m)}$ is symmetric a.e. on $\Lambda^m$. In this section we will discuss the relationship between integrability of generalized $N$-means with respect to measure $Pd^N x$ and integrability of their kernels with respect to measure $\rho^{(m)} d^m x$.

It is easy to convince oneself that $u \in L^r(\Lambda^m; \rho^{(m)} d^m x)$ implies that $G_{N,m}u \in L^r(\Lambda^N; Pd^N x)$ for $1 \le r < \infty$. However, the converse is not obvious and, in fact, is not true in general. This situation is illustrated with the following example.

**Example 2.3.1.** Consider a $\sigma$-finite measure space $(\Lambda; d\mu)$, where $\Lambda = \mathbb{N}$, and $d\mu$ is the counting measure. Let us define the probability density $P$ on $\Lambda^2$ by the formula:

$$P(i,j) := \begin{cases} \frac{1}{(i+j)^2} & \text{if } |i-j| = 1 \\ 0 & \text{if } |i-j| \neq 1 \end{cases} \tag{2.3.26}$$

Then, $P$ is symmetric, and

$$\int_{\Lambda^2} P d^2\mu = 2\sum_{i=1}^{\infty} \frac{1}{(2i+1)^2} < \infty. \tag{2.3.27}$$

(That $\int_{\Lambda^2} P d^2\mu \neq 1$ is immaterial.) For every $i \geq 2$, the marginal probability density $\rho^{(1)}(i)$ is calculated to be

$$\rho^{(1)}(i) = \sum_{j=1}^{\infty} P(i,j) = \frac{1}{(2i+1)^2} + \frac{1}{(2i-1)^2} > \frac{1}{(2i+1)^2}. \tag{2.3.28}$$

Let us define $u : \Lambda \to \mathbb{R}$ by $u(i) = 2(-1)^i i$. Then, $|u(i) + u(j)| = 2$ whenever $|i - j| = 1$. Thus, using (2.3.26) and (2.3.28), we find that

$$\int_{\Lambda^2} P|G_{2,1}u| d^2\mu = 2\sum_{i=1}^{\infty} \frac{1}{(2i+1)^2} < \infty, \tag{2.3.29}$$

but

$$\int_{\Lambda} \rho^{(1)}|u| d\mu > 2\sum_{i=2}^{\infty} \frac{i}{(2i+1)^2} = \infty. \tag{2.3.30}$$

In spite of Example 2.3.1, an extra condition on $P$ ensures that a generalized $N$-mean of order $m$ is in $L^1(\Lambda^N; Pd^N x)$ if and only if its kernel is in $L^1(\Lambda^m; \rho^{(m)} d^m x)$. The generality of this condition is addressed in Theorem 2.3.10. We begin with two lemmas that will be used in the proof of Theorem 2.3.8, the main result of this section.

**Lemma 2.3.6.** *Let $1 \leq m \leq N-1$ be integers, $A \subset \Lambda$ be a subset of positive measure, and $\gamma : A \to (0, \infty)$ be a measurable function. If,*

$$\rho^{(m+1)}(x_1, ..., x_{m+1}) \geq \gamma(x_{m+1})\rho^{(m)}(x_1, ..., x_m) \tag{2.3.31}$$

*for a.e. $(x_1, ..., x_{m+1}) \in \Lambda^m \otimes A$, then*

$$\rho^{(m)}(x_1, ..., x_m) \geq \gamma(x_m)\rho^{(m-1)}(x_1, ..., x_{m-1}) \tag{2.3.32}$$

*for a.e. $(x_1, ..., x_m) \in \Lambda^{m-1} \otimes A$.*

*Proof.* Let $E_{m+1} \subset \Lambda^{m+1}$ be a co-null set such that (2.3.31) holds on $E_{m+1} \cap (\Lambda^m \otimes A)$. By the Fubini-Tonelli theorem, there is a co-null set $E_m \subset \Lambda^m$ such that for every $(x_1, ..., x_{m-1}, x_{m+1}) \in E_m$ both sides of (2.3.31) are integrable functions of $x_m$, and the section $(E_{m+1})_{x_1,...,x_{m-1},x_{m+1}} \subset \Lambda$ is co-null. If $(x_1, ..., x_{m-1}, x_{m+1}) \in E_m \cap (\Lambda^{m-1} \otimes A)$, and $x_m \in (E_{m+1})_{x_1,...,x_{m-1},x_{m+1}}$, then $(x_1, ..., x_{m+1}) \in E_{m+1} \cap (\Lambda^m \otimes A)$, and so inequality (2.3.31) holds. Thus, integrating both sides of (2.3.31) with respect to $x_m$, and subsequently renaming $m+1$ with $m$ yield:

$$\rho^{(m)}(x_1, ..., x_m) \geq \gamma(x_m)\rho^{(m-1)}(x_1, ..., x_{m-1}) \tag{2.3.33}$$

for every $(x_1, ..., x_m) \in E_m \cap (\Lambda^{m-1} \otimes A)$. □

**Lemma 2.3.7.** *Let $1 \leq m \leq N-1$ be integers, $A \subset \Lambda$ be a subset of positive measure, and $\gamma : A \to (0, \infty)$ be a measurable function. Suppose that*

$$P(x_1, ..., x_N) \geq \gamma(x_N)\rho^{(N-1)}(x_1, ..., x_{N-1}) \tag{2.3.34}$$

*for a.e. $(x_1, ..., x_N) \in \Lambda^{N-1} \otimes A$. Then,*

$$P(x_1, ..., x_N) \geq \gamma(x_N) \cdots \gamma(x_{m+1})\rho^{(m)}(x_1, ..., x_m) \tag{2.3.35}$$

*for a.e. $(x_1, ..., x_N) \in \Lambda^m \otimes A^{N-m}$.*

*Proof.* Inequality (2.3.35) clearly holds when $m = N-1$. Suppose that it is satisfied for some $2 \leq m \leq N-1$. We will show that it then holds for $m-1$, and so the lemma will follow by induction.

Using Lemma 2.3.6, we infer from (2.3.34) by induction that

$$\rho^{(m)}(x_1, ..., x_m) \geq \gamma(x_m)\rho^{(m-1)}(x_1, ..., x_{m-1}) \tag{2.3.36}$$

for a.e. $(x_1, ..., x_m) \in \Lambda^{m-1} \otimes A$. Therefore, in view of (2.3.35),

$$P(x_1, ..., x_N) \geq \gamma(x_N) \cdots \gamma(x_m)\rho^{(m-1)}(x_1, ..., x_{m-1}) \tag{2.3.37}$$

for a.e. $(x_1, ..., x_N) \in \Lambda^{m-1} \otimes A^{N-m+1}$. □

**Theorem 2.3.8.** *Suppose $N \geq 2$ is an integer, and that for every $x_N$ in some subset $A \subset \Lambda$ of positive measure, there is a constant $\gamma(x_N) > 0$ such that*

$$P(\cdot, x_N) \geq \gamma(x_N)\rho^{(N-1)} \quad a.e. \ on \ \Lambda^{N-1}. \tag{2.3.38}$$

*Let $1 \leq m \leq N$ be integers, $1 \leq r < \infty$, and $u : \Lambda^m \to \mathbb{R}$ be a function. Define $U := G_{N,m}u$. Then,*
*$U \in L^r(\Lambda^N; Pd^N x)$ if and only if $u \in L^r(\Lambda^m; \rho^{(m)} d^m x)$. Moreover, there is a constant $C := C(N, m, r, P)$ such that*
*$||U||_{r,Pd^N x} \leq ||u||_{r,\rho^{(m)}d^m x} \leq C||U||_{r,Pd^N x}$. In particular, $G_{N,m}$ is an isomorphism from $L^r(\Lambda^m; d^m x)$ onto a closed subspace of $L^r(\Lambda^N; d^N x)$.*

**Remark 2.3.2.** The condition on $P$ at the beginning of Theorem 2.3.8 can be replaced with another, seemingly stronger, but in fact equivalent, assumption. To be specific, we can assume that

$$P \geq \rho^{(N-1)} \otimes \gamma \ \text{ a.e. on } \Lambda^{N-1} \otimes A, \tag{2.3.39}$$

where $A \subset \Lambda$ is some subset of positive measure, and $\gamma : A \to (0, \infty)$ is a measurable function.

Indeed, the condition on $P$ stated in Theorem 2.3.8 is equivalent to: ess inf $f(\cdot, x_N) > 0$ for every $x_N \in A$, where $f$ is a measurable function on $\Lambda^N$ defined by

$$f = \begin{cases} P/(\rho^{(N-1)} \otimes 1) & \text{if } \rho^{(N-1)} \otimes 1 > 0, \\ 1 & \text{if } \rho^{(N-1)} \otimes 1 = 0. \end{cases} \tag{2.3.40}$$

Moreover, (2.3.38) holds with $\gamma(x_N)$ replaced by ess inf $f(\cdot, x_N)$, a measurable function. However, if $\gamma$ in (2.3.38) is $dx$ measurable, then $g := P - \rho^{(N-1)} \otimes \gamma$ is $d^N x$ measurable. Let $T := \{(x_1, ..., x_N) \in \Lambda^N : g(x_1, ..., x_N) \geq 0\}$. Arguing by contradiction, it is easy to see that $|\Lambda^{N-1} \otimes A \setminus T| = 0$, i.e. (2.3.39) holds a.e. on $\Lambda^{N-1} \otimes A$.

*Proof of Theorem 2.3.8.* The "in particular" part is the direct consequence of Theorem 2.3.3 and Corollary 2.3.4. Since there is nothing to prove when $m = N$, we will assume that $1 \leq m < N$.

For the "if" part of the theorem, suppose that $u \in L^r(\Lambda^m; d^m x)$. Then,

$$\begin{aligned} &||U||^r_{r,Pd^Nx} = \int_{\Lambda^N} |G_{N,m}u|^r P \leq \\ &\binom{N}{m}^{-1} \sum_{1\leq i_1<\cdots<i_m\leq N} \int_{\Lambda^N} |u(x_{i_1},...,x_{i_m})|^r P dx_1 \cdots dx_N = \\ &\int_{\Lambda^m} |u|^r \rho^{(m)} = ||u||^r_{r,\rho^{(m)}d^m x}. \end{aligned} \tag{2.3.41}$$

For the "only if" part, we will use the condition on $P$, as stated in Remark 2.3.2. Suppose that $U \in L^r(\Lambda^N; Pd^N x)$. Since $\gamma$ is positive on $A$, there is $\varepsilon > 0$ such that the set $A_\varepsilon := \{x \in A : \gamma(x) > \varepsilon\}$ has positive measure. Thus, in view of Lemma 2.3.7, for every $1 \leq m \leq N-1$:

$$\begin{aligned} &P(x_1, ..., x_N) \geq \\ &\gamma(x_N)\cdots\gamma(x_{m+1})\rho^{(m)}(x_1,...,x_m) > \varepsilon^{N-m}\rho^{(m)}(x_1,...,x_m) \end{aligned} \tag{2.3.42}$$

for a.e. $(x_1, ..., x_N) \in \Lambda^m \otimes A_\varepsilon^{N-m}$. Note, that $|A_\varepsilon| < \infty$ because the integration of (2.3.42) gives $1 \geq \int_{\Lambda^m\otimes A_\varepsilon^{N-m}} P \geq (\varepsilon|A_\varepsilon|)^{N-m}$.

**Lemma 2.3.9.** *Let $\alpha := (\varepsilon|A_\varepsilon|)^{-1}$. For every $1 \leq m \leq N-1$, the set*

$$\begin{aligned} &T_{N-m} := \{(x_{m+1}, ..., x_N) \in A_\varepsilon^{N-m} : \\ &U(\cdot, x_{m+1}, ..., x_N) \textit{ is measurable and} \\ &||U(\cdot, x_{m+1}, ..., x_N)||^r_{r,\rho^{(m)}d^m x} \leq \alpha^{N-m}||U||^r_{r,Pd^N x}\} \end{aligned} \tag{2.3.43}$$

*is not a set of measure zero. In particular, it is not empty.*

*Proof.* Suppose that $|T_{N-m}| = 0$. This means that

$$||U||^r_{r,Pd^Nx} < \alpha^{m-N} \int_{\Lambda^m} |U(\cdot, x_{m+1}, ..., x_N)|^r \rho^{(m)} d^m x \tag{2.3.44}$$

for a.e. $(x_{m+1}, ..., x_N) \in A^{N-m}_{\varepsilon}$. Integration over $A^{N-m}_{\varepsilon}$ in the last inequality, and (2.3.42) give:

$$\begin{aligned} ||U||^r_{r,Pd^Nx} &< \varepsilon^{N-m} \int_{\Lambda^m \otimes A^{N-m}_{\varepsilon}} |U(x_1, ..., x_N)|^r \rho^{(m)}(x_1, ..., x_m) d^N x \\ &< \int_{\Lambda^m \otimes A^{N-m}_{\varepsilon}} |U|^r P d^N x \leq ||U||^r_{r,Pd^Nx}, \end{aligned} \tag{2.3.45}$$

a contradiction. Thus, $T_{N-m}$ can not be a set of measure zero. □

*Case 1:* $m = 1$. Let us fix $(\tilde{x}_2, ..., \tilde{x}_N) \in T_{N-1}$, a non-empty set by Lemma 2.3.9. Then,

$$NU(\cdot, \tilde{x}_2, ..., \tilde{x}_N) = u + \sum_{i=2}^{N} u(\tilde{x}_i) := u + \tilde{c}. \tag{2.3.46}$$

By the definition of the set $T_{N-1}$ given in (2.3.43),

$$||U(\cdot, \tilde{x}_2, ..., \tilde{x}_N)||_{r,\rho^{(1)}dx} \leq \alpha^{\frac{N-1}{r}} ||U||_{r,Pd^Nx}. \tag{2.3.47}$$

To get an estimate on $\tilde{c}$, let us apply $G_{N,1}$ to both sides of 2.3.46, with the result $\tilde{c} = NG_{N,1}U(\cdot, \tilde{x}_2, ..., \tilde{x}_N) - U$. Then, the "if" part of the theorem and (2.3.47) imply that

$$\begin{aligned} |\tilde{c}| &\leq N||G_{N,1}U(\cdot, \tilde{x}_2, ..., \tilde{x}_N)||_{r,Pd^Nx} + ||U||_{r,Pd^Nx} \\ &\leq N||U(\cdot, \tilde{x}_2, ..., \tilde{x}_N)||_{r,\rho^{(1)}dx} + ||U||_{r,Pd^Nx} \\ &\leq \left[N\alpha^{\frac{N-1}{r}} + 1\right] ||U||_{r,Pd^Nx}. \end{aligned} \tag{2.3.48}$$

Finally, we infer from (2.3.46), (2.3.47), and (2.3.48) that

$$\begin{aligned} ||u||_{r,\rho^{(1)}dx} &\leq N||U(\cdot, \tilde{x}_2, ..., \tilde{x}_N)||_{r,\rho^{(1)}dx} + |\tilde{c}| \\ &\leq \left(2N\alpha^{\frac{N-1}{r}} + 1\right) ||U||_{r,Pd^Nx}. \end{aligned} \tag{2.3.49}$$

Note that the constant in the round brackets depends on $P$ through $\alpha$.

*Case 2:* $2 \leq m < N$. Similarly to the proofs for this case in the previous two theorems, we will use induction on $m$. Suppose that the "only if" statement of the theorem holds for

$m-1$. Let us fix $(\tilde{x}_{m+1},...,\tilde{x}_N) \in T_{N-m}$, a non-empty set by Lemma 2.3.9. As was shown previously, (see (2.3.11 - 2.3.15) ), there is $\omega : \Lambda^{m-1} \to \mathbb{R}$ such that

$$\binom{N}{m} U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N) = u + G_{m,m-1}\omega. \tag{2.3.50}$$

By the definition of the set $T_{N-m}$ given in (2.3.43),

$$||U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N)||_{r,\rho^{(m)}d^m x} \leq \alpha^{\frac{N-m}{r}} ||U||_{r,Pd^N x}. \tag{2.3.51}$$

An estimate on $||G_{m,m-1}\omega||_{r,\rho^{(m)}d^m x}$ will follow by induction. Applying $G_{N,m}$ to both sides of (2.3.50) and using Lemma 2.3.2 yield:

$$G_{N,m-1}\omega = \binom{N}{m} G_{N,m} U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N) - U. \tag{2.3.52}$$

The last equation shows that $G_{N,m-1}\omega$ is measurable. In addition, using the "if" statement of the theorem and (2.3.51), we estimate:

$$\begin{aligned} ||G_{N,m-1}\omega||_{r,Pd^N x} &\leq \binom{N}{m} ||G_{N,m} U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N)||_{r,Pd^N x} + ||U||_{r,Pd^N x} \\ &\leq \binom{N}{m} ||U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N)||_{r,\rho^{(m)}d^m x} + ||U||_{r,Pd^N x} \\ &\leq \left[ \binom{N}{m} \alpha^{\frac{N-m}{r}} + 1 \right] ||U||_{r,Pd^N x}. \end{aligned} \tag{2.3.53}$$

The last inequality allows us to conclude from the induction hypothesis that
$\omega \in L^r(\Lambda^{m-1}; \rho^{(m-1)} d^{m-1} x)$, and

$$||\omega||_{r,\rho^{(m-1)}d^{m-1}x} \leq \tilde{C} \left[ \binom{N}{m} \alpha^{\frac{N-m}{r}} + 1 \right] ||U||_{r,Pd^N x} \tag{2.3.54}$$

for some constant $\tilde{C} = \tilde{C}(N, m-1, r, P)$. Using the "if" statement of the theorem one more time, we infer that $G_{m,m-1}\omega \in L^r(\Lambda^m; \rho^{(m)} d^m x)$,and $||G_{m,m-1}\omega||_{r,\rho^{(m)}d^m x} \leq ||\omega||_{r,\rho^{(m-1)}d^{m-1}x}$. This inequality, together with (2.3.50), (2.3.51), and (2.3.54), finally give that
$u \in L^r(\Lambda^m; \rho^{(m)} d^m x)$, and

$$\begin{aligned} ||u||_{r,\rho^{(m)}d^m x} &\leq \binom{N}{m} ||U(\cdot, \tilde{x}_{m+1},...,\tilde{x}_N)||_{r,\rho^{(m)}dx} + \\ ||G_{m,m-1}\omega||_{r,\rho^{(m)}dx} &\leq \left[ \binom{N}{m} \alpha^{\frac{N-m}{r}} (1 + \tilde{C}) + \tilde{C} \right] ||U||_{r,Pd^N x}. \end{aligned} \tag{2.3.55}$$

□

The next theorem shows that any symmetric probability density on $\Lambda^N$ can be approximated in $L^1(\Lambda^N; d^N x)$ by an arbitrarily close symmetric probability density satisfying condition (2.3.38). Moreover, if measure $dx$ is finite and $P \in L^\infty(\Lambda^N; d^N x)$, then this approximation is in $L^\infty(\Lambda^N; d^N x)$.

**Theorem 2.3.10.** *If $N \geq 2$ and $P$ is a symmetric probability density on $\Lambda^N$, there is a sequence $(P_n)$ of symmetric probability densities on $\Lambda^N$ such that $P_n$ satisfies (2.3.38), and $P_n \to P$ in $L^1(\Lambda^N; d^N x)$. If, in addition, measure $dx$ is finite, and $P$ is essentially bounded, then $P_n \to P$ in $L^\infty(\Lambda^N; d^N x)$.*

*Proof.* It suffices to prove the theorem when measure $dx$ is finite, and $P$ is essentially bounded. Indeed, since $(\Lambda; dx)$ is $\sigma$-finite, $\Lambda = \cup_{n=1}^\infty E_n$, where $|E_n| < \infty \; \forall n$, and $E_n \subset E_{n+1}$. Then, by dominated convergence, any symmetric probability density $P$ can be approximated in $L^1(\Lambda^N; d^N x)$ by a sequence of symmetric probability densities $P_n \chi_{E_n} / ||P_n \chi_{E_n}||_{1,d^N x}$, where $\chi_{E_n}$ is the characteristic function of the set $E_n$, and $P_n = \min\{P, n\}$.

In accordance with the above comment, suppose that $|\Lambda| < \infty$, and $P$ is essentially bounded. Then, there is $c > 0$ such that $\rho^{(N-1)} \leq c$ a.e. on $\Lambda^{N-1}$. If $Q_n := \max\{P, \frac{1}{n}\}$, then $P_n := \frac{Q_n}{||Q_n||_{1,d^N x}}$ is a symmetric probability density on $\Lambda^N$, and $P_n \to P$ in $L^1(\Lambda^N; d^N x)$ by dominated convergence. In addition, since $-\frac{1}{n} \leq P - P_n \leq ||P||_{\infty,d^N x} \left(1 - 1/||Q_n||_{1,d^N x}\right)$ on some co-null set for $n$ large enough, $P_n \to P$ in $L^\infty(\Lambda^N; d^N x)$.

It remains to check that $P_n$ satisfies (2.3.38). For this, we notice that

$$P_n \geq \frac{1}{n||Q_n||_{1,d^N x}} \geq \frac{1}{n + |\Lambda|^N}. \tag{2.3.56}$$

Also, a.e. on $\Lambda^{N-1}$:

$$\begin{aligned} \rho_n^{(N-1)} &= \frac{\int_\Lambda Q_n(\cdot, x_N) dx_N}{||Q_n||_{1,d^N x}} \leq \frac{\rho^{(N-1)} + \frac{1}{n}|\Lambda|}{||Q_n||_{1,d^N x}} \\ &\leq \rho^{(N-1)} + \frac{1}{n}|\Lambda| \leq c + \frac{1}{n}|\Lambda|. \end{aligned} \tag{2.3.57}$$

From (2.3.56) and (2.3.57) it follows that for every $x_N \in \Lambda$

$$P_n(\cdot, x_N) \geq \alpha_n \rho_n^{(N-1)}(\cdot) \quad \text{a.e on } \Lambda^{N-1}, \tag{2.3.58}$$

with $\alpha_n := \left[\left(n + |\Lambda|^N\right)\left(c + \frac{1}{n}|\Lambda|\right)\right]^{-1}$. Thus, (2.3.38) is satisfied by $P_n$ with $A = \Lambda$, and $\gamma \equiv \alpha_n$. $\square$

# 3.0 THE INVERSE PROBLEM IN THE GRAND CANONICAL ENSEMBLE

## 3.1 INVERSE CONJECTURE

### 3.1.1 Statement of the problem and assumptions

In this chapter, the inverse problem is formulated for the grand canonical distribution. Accordingly, we have in mind a system of identical particles that can be in different particle number states, as described in Section 1.2. Suppose we are given a measurable symmetric energy function $W := \{W_N : \Lambda^N \to (-\infty, \infty] \mid N = 0, 1, 2, ...\}$ and a symmetric function $\rho^{(m)} : \Lambda^m \to [0, \infty) \in L^1(\Lambda^m, d^m x)$, with $||\rho^{(m)}||_{1(d^m x)} > 0$. The inverse conjecture asserts the existence of a unique function $v$, such that $\rho_v^{(m)} = \rho^{(m)}$ a.e.

This section contains the detailed proof of the inverse conjecture in the grand canonical formulation for $m \geq 1$, stated rigorously in Theorem 3.1.11. Note, that contrary to the case of the canonical ensemble, $|W_N^{-1}(\infty)|$ can be positive, which means that hard-cores are allowed now. The proof is based on the outline in [1, Section 4], and many of the arguments are variations of the methods found in [11, 1]. However, unlike in [1, Section 4], we do not require that the measure $|\Lambda|$ is finite, or that the ensemble is truncated (i.e. $W_N = \infty$ for all $N > \tilde{N}$). Let us start by stating carefully all the assumptions used in the proof.

(i) The first one concerns the structure of hard-core regions defined by
$Q_N := \{(x_1, ..., x_N) \in \Lambda^N \mid W_N(x_1, ..., x_N) = \infty\}$ for every $N \in \mathbb{N}$. First, it will be assumed that $|\Lambda^m \setminus Q_m| > 0$. Next, we will require that

$$\left|Q_N^{i_1,...,i_m} \setminus Q_N\right| = 0 \ \ \forall N > m, \ \ \forall 1 \leq i_1 < \cdots < i_m \leq N, \tag{3.1.1}$$

where

$$Q_N^{i_1,...,i_m} := \{(x_1, ..., x_N) \in \Lambda^N \mid (x_{i_1}, ..., x_{i_m}) \in Q_m\}. \tag{3.1.2}$$

In particular, $Q_N^{1,...,m} = Q_m \otimes \Lambda^{N-m}$, and so $|Q_m \otimes \Lambda^{N-m} \setminus Q_N| = 0$. Condition (3.1.1) means that adding more particles to the system will not make the hard-core regions smaller. It is clearly satisfied when $W_N$ is a sum of 2- to $m$- particle interactions (which can always be rewritten as a sum of $m$-particle ones).

The next three conditions are analogous to (i), (ii), and (iii) in Section 2.1.

(ii) The partition function of the system governed by energy $W$ augmented by a constant function is finite. In other words, $\Xi(c) < \infty$ for all $c \in \mathbb{R}$.

(iii) Let us define the following set of functions in $\mathbb{L}^1(d\mu)$:

$$\begin{aligned}\mathcal{D} := \{&F \in \mathbb{L}^1(d\mu) \mid F_0 > 0, F_N \geq 0 \text{ and is symmetric a.e. } [d^N x] \text{ for every } N \in \mathbb{N},\\ &|||F|||_{1(d\mu)} = 1, 0 < n_m(F) < \infty\},\end{aligned} \tag{3.1.3}$$

where

$$n_m(F) := \langle \frac{N!}{(N-m)!} \rangle_F = \sum_{N=m}^{\infty} \frac{1}{(N-m)!} \int_{\Lambda^N} F_N d^N x. \tag{3.1.4}$$

For every $F \in \mathcal{D}$, it is possible to define an $m$-variable reduction according to:

$$\rho_F^{(m)} := F_m + \sum_{N=m+1}^{\infty} \frac{1}{(N-m)!} \int_{\Lambda^{N-m}} F_N(\cdot, x_{m+1}, ..., x_N). \tag{3.1.5}$$

Note, that because $n_m(F) < \infty$, the Fubini-Tonelli theorem and monotone convergence assure that $\rho_F^{(m)} \in L^1(\Lambda^m, d^m x)$ with $||\rho_F^{(m)}||_{1(d^m x)} = n_m(F)$. Let us assume that there is a probability density $P \in \mathcal{D}$ such that $\rho^{(m)} = \rho_P^{(m)}$ a.e. $[d^m x]$. In particular, $\|\rho^{(m)}\|_{1(d^m x)} = n_m(P) =: n_m$.

(iv)

$$\mathcal{F}_+(P) := \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} P_N(W_N + \ln P_N)_+ d^N x < \infty. \tag{3.1.6}$$

(v) Let $\{\rho^{(m)} = 0\} := \{(x_1, ..., x_m) \in \Lambda^m \mid \rho^{(m)}(x_1, ..., x_m) = 0\}$, and assume that $|\{\rho^{(m)} = 0\} \setminus Q_m\}| = 0$. Note, that this condition is necessary to have $\rho^{(m)} = \rho_v^{(m)}$ a.e. for any finite $v$. (However, it was not stated in [1].)

(vi) The final assumption is a version of (iv) for $m$ particles. Expressly,

$$\int_{\Lambda^m} (W_m + \ln \rho^{(m)})_+ \rho^{(m)} d^m x < \infty. \tag{3.1.7}$$

We finish with two lemmas that follow directly from the conditions stated above.

**Lemma 3.1.1.** *Conditions (i), (iv), and (v) ensure that $Q_m \sim \{\rho^{(m)} = 0\} \sim \{\rho_v^{(m)} = 0\}$ for any finite $v$ with $\Xi(v) < \infty$ and $n_m(v) < \infty$. In particular, disregarding some set of zero measure, $\rho^{(m)}$ and $\rho_v^{(m)}$ vanish on the same set.*

*Proof.* Suppose that $|E_m| := |Q_m \setminus \{\rho^{(m)} = 0\}| > 0$. Then, there is $N \geq m$ such that

$$0 < \int_{E_m \otimes \Lambda^{N-m}} P_N d^N x \leq \int_{Q_m \otimes \Lambda^{N-m}} P_N d^N x \leq \int_{Q_N} P_N d^N x, \tag{3.1.8}$$

where the last inequality follows from (i). Therefore, $|Q_N \setminus \{P_N = 0\}| > 0$, a contradiction with (iv). In view of (v), this implies that $Q_m \sim \{\rho^{(m)} = 0\}$. Moreover, $|\{\rho_v^{(m)} = 0\} \setminus Q_m| = 0$ by the definition of $\rho_v^{(m)}$, and $|Q_m \setminus \{\rho_v^{(m)} = 0\}| = 0$ by (3.1.8) with $P_N$ replaced by $(G_v)_N$. Therefore, $\{\rho_v^{(m)} = 0\} \sim Q_m \sim \{\rho^{(m)} = 0\}$. □

**Lemma 3.1.2.** *Under condition (ii), $n_k(c) < \infty$ for all $k \in \mathbb{N}$ and every $c \in \mathbb{R}$.*

*Proof.* Let $c \in \mathbb{R}$, and define $C_N := 0$ if $1 \leq N < m$, $C_N := \hat{C}_{N,m} c = \binom{N}{m} c$ if $N \geq m$, and $Z_N := \int_{\Lambda^n} e^{-W_N - C_N} d^N x$.

(1) First, notice that if $\ell < k$, then

$$n_\ell(c) \leq [\Xi(c)]^{-1} \sum_{N=\ell}^{k-1} \frac{1}{(N-\ell)!} Z_N + n_k(c) < \infty. \tag{3.1.9}$$

(2) Next, for every $i \in \mathbb{N}$:

$$\Xi(c) n_{im}(c) = \sum_{N=im}^{\infty} \frac{1}{N!} \frac{N!}{(N-im)!} Z_N \leq \sum_{N=im}^{\infty} \frac{1}{N!} \left( \frac{N!}{(N-m)!} \right)^i Z_N. \tag{3.1.10}$$

Since $x^k < e^x$ if $x$ is large enough, there is $N_0 \geq mi$ such that

$$\begin{aligned} &\sum_{N=N_0}^{\infty} \frac{1}{N!} \left( \frac{N!}{(N-m)!} \right)^i Z_N \leq \sum_{N=N_0}^{\infty} \frac{1}{N!} e^{\binom{N}{m} m!} Z_N = \\ &\sum_{N=N_0}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - \hat{C}_{N,m}(c-m!)} d^N x < \Xi(c - m!), \end{aligned} \tag{3.1.11}$$

which is finite by assumption (ii). Thus, $n_{im}(c) < \infty$ for every $i \in \mathbb{N}$, which, together with step (1) implies that $n_k(c) < \infty$ for every $k \in \mathbb{N}$.

$\square$

### 3.1.2 Existence and uniqueness

Let us define a set of functions on $\Lambda^m$:

$$\mathcal{C} := \{s \in L^1(\Lambda^m, \rho^{(m)} d^m x) \mid s \text{ is a.e. finite and symmetric, } \Xi(s) < \infty,\ n_m(s) < \infty\}, \tag{3.1.12}$$

and a functional on $\mathcal{C}$:

$$\Im(s) := \frac{\exp\left[-\frac{1}{m!}\int_{\Lambda^m} s\rho^{(m)} d^m x\right]}{\Xi(s)}, \quad \forall s \in \mathcal{C}. \tag{3.1.13}$$

Note, that $\mathcal{C} \neq \emptyset$ because $\mathbb{R} \in \mathcal{C}$ by assumption (ii) and Lemma 3.1.2 in the previous subsection, and that $0 < \Im(s) < \infty$ for every $s \in \mathcal{C}$. In the following, it will be shown that the only solution to the inverse problem is the unique maximizer of $\Im$ on $\mathcal{C}$.

**Lemma 3.1.3.** *$\mathcal{C}$ is convex, and $\ln \Im$ is concave on $\mathcal{C}$.*

*Proof.* Let $u, v \in \mathcal{C}$, and $0 < \lambda < 1$. Then $s := \lambda u + (1-\lambda)v \in L^1(\Lambda^m, \rho^{(m)} d^m x)$ and is symmetric. Moreover, by the generalized Holder's inequality (Theorem A.0.3)

$$\Xi(s) = \left|\left|\left|e^{-\lambda u - (1-\lambda)v}\right|\right|\right|_{1(e^{-W} d\mu)} \leq \Xi(u)^{\lambda} \Xi(v)^{1-\lambda} < \infty. \tag{3.1.14}$$

Similarly,

$$n_m(s) \leq \Xi(s) n_m(s) \leq \left[\Xi(u) n_m(u)\right]^{\lambda} \left[\Xi(v) n_m(v)\right]^{1-\lambda} < \infty. \tag{3.1.15}$$

Finally, $\ln \Im(s) = -\frac{1}{m!}\int_{\Lambda^m} s\rho^{(m)} d^m x - \ln \Xi(s)$. Since the first term is linear, it suffices to show that $\ln \Xi(s) \leq \lambda \ln \Xi(u) + (1-\lambda) \ln \Xi(v)$. But this inequality is equivalent to 3.1.14. $\square$

**Lemma 3.1.4.** *$\Im$ is bounded on $\mathcal{C}$. Precisely,* $0 < \Im(s) \leq \exp[\mathcal{F}_+(P)] < \infty$ *for every $s \in \mathcal{C}$.*

*Proof.* Let $s \in \mathcal{C}$. Then,

$$\begin{aligned}\Xi(s) \geq 1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} P_N \exp[-W_N - \ln P_N - S_N] d^N x = \\ \langle \exp[-W - \ln P - S] \rangle_P \geq \langle \exp\{-[W + \ln P]_+ - S\} \rangle_P.\end{aligned} \tag{3.1.16}$$

Note that

$$\begin{aligned}|||(W + \ln P)_+ - S|||_{1(Pd\mu)} \leq \mathcal{F}_+(P) + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} P_N \hat{C}_{N,m} |s| d^N x = \mathcal{F}_+(P) \\ + \frac{1}{m!} \sum_{N=1}^{\infty} \frac{1}{(N-m)!} \int_{\Lambda^N} |s| P_N d^N x = \mathcal{F}_+(P) + \frac{1}{m!} \int_{\Lambda^m} |s| \rho^{(m)} d^m x < \infty,\end{aligned} \tag{3.1.17}$$

where the operation $\hat{C}_{N,m}$ was defined in 1.4.1. In the first equality in 3.1.17, symmetry of $s$ was used, while in the second, monotone convergence was used to interchange summation and integration over $\Lambda^m$. By the generalized Jensen's inequality (Theorem A.0.4) and 3.1.17, it follows from 3.1.16 that

$$\Xi(s) \geq \exp\left\{-\langle [W + \ln P]_+ + S \rangle_P\right\} = \exp\left[-\mathcal{F}_+(P)\right] \exp\left\{-\frac{1}{m!} \int_{\Lambda^m} s \rho^{(m)} d^m x\right\}. \tag{3.1.18}$$

In the last equality, symmetry of $s$ and dominated convergence (to interchange summation and integration) were used. Finally, equation 3.1.18 is equivalent to $\Im(s) \leq \exp[\mathcal{F}_+(P)]$. $\square$

**Lemma 3.1.5.** *For every $F \in \mathcal{D}$, there is $\varepsilon_0 > 0$ such that if $0 \leq \varepsilon < \varepsilon_0$, there exists $F_\varepsilon \in \mathcal{D}$ with $\rho_{F_\varepsilon}^{(m)} = (1 + \varepsilon)\rho_F^{(m)}$. Moreover, $\mathcal{F}_+(F) < \infty$ implies $\mathcal{F}_+(F_\varepsilon) < \infty$.*

*Proof.* For any $1 \leq t < \infty$, let $G_t := \left\{F_0 A_t^{-1}, t F_N A_t^{-1} \mid N \in \mathbb{N}\right\}$, where

$$A_t := F_0 + t \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} F_N d^N x < \infty. \tag{3.1.19}$$

Then, $0 < (G_t)_0 = F_0 A_t^{-1} < 1$, $|||G_t|||_{1(d\mu)} = 1$, and $n_m(G_t) = t A_t^{-1} n_m(F) < \infty$. Therefore, $G_t \in \mathcal{D}$. Further, $\rho_{G_t}^{(m)} = t A_t^{-1} \rho_F^{(m)} = (1 + \gamma(t))\rho_F^{(m)}$, where $\gamma(t) := F_0(t-1)[t(1-F_0) + F_0]^{-1}$. Since $\gamma$ is an increasing function on $[1, \infty)$ converging to $\varepsilon_0 := F_0(1 - F_0)^{-1}$, it can assume any value in $[0, \varepsilon_0)$, corresponding to some $t$ in $[1, \infty)$. For $0 \leq \varepsilon < \varepsilon_0$, let $F_\varepsilon := G_{\gamma^{-1}(\varepsilon)}$. Then, $F_\varepsilon \in \mathcal{D}$, and $\rho_{F_\varepsilon}^{(m)} = \rho_{G_{\gamma^{-1}(\varepsilon)}}^{(m)} = (1 + \varepsilon)\rho_F^{(m)}$.

It remains to prove that if $\mathcal{F}_+(F) < \infty$ then $\mathcal{F}_+(F_\varepsilon) < \infty$ for any $0 \le \varepsilon < \varepsilon_0$. This is equivalent to proving that $\mathcal{F}_+(G_t) < \infty$ for every $1 \le t < \infty$. However,

$$\begin{aligned}\mathcal{F}_+(G_t) &= (1+\gamma(t)) \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} F_N \left[W_N + \ln F_N + \ln(1+\gamma(t))\right]_+ d^N x \\ &\le (1+\gamma(t)) \left[\mathcal{F}_+(F) + (1-F_0)\ln(1+\gamma(t))\right] < \infty.\end{aligned} \tag{3.1.20}$$

□

Let $(v_k) := (v_k)_{k=1}^{\infty}$ be a maximizing sequence in $\mathcal{C}$ for $\Im$, i.e. $0 < \lim_{k\to\infty} \Im(v_k) = R := \sup_{s\in\mathcal{C}} \Im(s) < \infty$.

**Lemma 3.1.6.** *There is $C > 0$ such that $\Xi(v_k) \le C$ and $n_m(v_k) \le C$ for every $k \in \mathbb{N}$.*

*Proof.* (1) Suppose that $\Xi(v_k)$ are not bounded above. Then, there is a subsequence $(v_{j_k})$ such that $\Xi(v_{j_k}) \to \infty$. Since $\Im(v_{j_k}) \to R$, this implies that

$$\exp\left[\frac{1}{m!}\int_{\Lambda^m} v_{j_k} \rho^{(m)} d^m x\right] \to 0. \tag{3.1.21}$$

By Lemma 3.1.5, there is $\varepsilon > 0$ and $P_\varepsilon \in \mathcal{D}$ such that $\rho^{(m)}_{P_\varepsilon} = (1+\varepsilon)\rho^{(m)}$ and $\mathcal{F}_+(P_\varepsilon) < \infty$. Replacing $P$ with $P_\varepsilon$ in the proof of Lemma 3.1.4, we obtain:

$$\Im(v_{j_k}) \le \exp\left[\mathcal{F}_+(P_\varepsilon)\right] \exp\left[\frac{1}{m!}\int_{\Lambda^m} v_{j_k} \rho^{(m)} d^m x\right] \to 0. \tag{3.1.22}$$

Therefore, $\Im(v_{j_k}) \to 0$, a contradiction.

(2) Suppose that $n_m(v_k)$ are not bounded above. Then, so is $n_m(v_k)\Xi(v_k) \ge n_m(v_k)$. Therefore, there is a subsequence $(v_{j_k})$ such that $n_m(v_{j_k})\Xi(v_{j_k}) \to \infty$.

Let

$$a := 1 + \sum_{N=1}^{m-1} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N} d^N x, \tag{3.1.23}$$

and

$$B(N) := \begin{cases} \frac{N!}{(N-m)!} & \text{if } N \ge m, \\ 1 & \text{if } 0 \le N < m. \end{cases} \tag{3.1.24}$$

Then (cf. (3.1.16)),

$$\begin{aligned}
&a + n_m(v_{j_k})\Xi(v_{j_k}) \geq \\
&1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} P_N B(N) \exp[-W_N - \ln P_N - (V_{j_k})_N] d^N x = \\
&\langle \exp[-W - \ln P - V_{j_k} + \ln B] \rangle_P \geq \langle \exp\{-[W + \ln P]_+ - V_{j_k} + \ln B\} \rangle_P .
\end{aligned} \tag{3.1.25}$$

Note, that by 3.1.17 $||(W + \ln P)_+ - V_{j_k}||_{1(Pd\mu)} < \infty$. Also,

$$|| \ln B||_{1(Pd\mu)} = \langle \ln B \rangle_P \leq \langle B \rangle_P = ||\rho^{(m)}||_{1(d^m x)} < \infty, \tag{3.1.26}$$

the inequality being due to the fact that $B(N) > 1$ for all $N \geq m$. Thus, by the generalized Jensens inequality (Theorem A.0.4) we obtain from 3.1.25 that (cf. 3.1.18)

$$a + n_m(v_{j_k})\Xi(v_{j_k}) \geq \exp\left[-\mathcal{F}_+(P)\right] \exp\left\{-\frac{1}{m!} \int_{\Lambda^m} v_{j_k} \rho^{(m)} d^m x\right\} \exp\left(\langle \ln B \rangle_P\right), \tag{3.1.27}$$

and so

$$0 < \frac{\exp\left[-\frac{1}{m!} \int_{\Lambda^m} v_{j_k} \rho^{(m)} d^m x\right]}{a + n_m(v_{j_k})\Xi(v_{j_k})} \leq e^{\mathcal{F}_+(P)} e^{-\langle \ln B \rangle_P} < \infty. \tag{3.1.28}$$

Since the denominator in the above ratio goes to infinity, so does the numerator. However, in view of (1), this implies that $\Im(v_{j_k}) \to \infty$, a contradiction. $\square$

Since $(\Xi(v_k))$ is bounded, there is a subsequence (still called $(v_k)$) and a number $1 \leq \Xi_0 < \infty$ such that

$$\Xi(v_k) = |||e^{-V_k/2}|||^2_{2(e^{-W} d\mu)} \to \Xi_0. \tag{3.1.29}$$

By reflexivity [27, Theorem 3.18], there is a further subsequence (also called $(v_k)$) and a function $\Phi \in \mathbb{L}^2(e^{-W} d\mu)$ such that $e^{-V_k/2} \rightharpoonup \Phi \in \mathbb{L}^2(e^{-W} d\mu)$.

**Lemma 3.1.7.** $e^{-V_k/2} \to \Phi$ *in* $\mathbb{L}^2(e^{-W} d\mu)$.

*Proof.* It suffices to show that $\Xi_0 = |||\Phi|||^2_{2(e^{-W}d\mu)}$. By week convergence, $\Xi_0 \geq |||\Phi|||^2_{2(e^{-W}d\mu)}$. The reverse of the last inequality is proved almost exactly as Lemma (), so only an outline will be provided here.

Let $\varepsilon > 0$. Then, there is $k_0 \in \mathbb{N}$ such that $\Im(v_k) > R(1-\varepsilon)$ and $\Xi(v_k) > \Xi_0(1-\varepsilon)$ for every $k \geq k_0$. Application of Mazur's theorem [28, Theorem 3.13] leads to the existence of a sequence $(Y_\ell)_{\ell=1}^\infty \in \mathbb{L}^2(e^{-W}d\mu)$ such that:

$$|||Y_\ell|||^2_{2(e^{-W}d\mu)} \to |||\Phi|||^2_{2(e^{-W}d\mu)}, \quad \text{and } ||Y_\ell|||^2_{2(e^{-W}d\mu)} \geq \Xi(\tilde{v}_\ell) \ \forall \ell \in \mathbb{N}, \tag{3.1.30}$$

where $\tilde{v}_\ell = \frac{1}{2}(v_{i_\ell} + v_{j_\ell})$, and $i_\ell$ and $j_\ell$ are some integers $k_0 + 1 \leq i_\ell \leq j_\ell \leq k_0 + \ell$. Since $\tilde{v}_\ell \in \mathcal{C}$, and $i_\ell, j_\ell > k_0$, we have:

$$R \geq \Im(\tilde{v}_\ell) = \frac{[\Im(v_{i_\ell})\Im(v_{j_\ell})\Xi(v_{i_\ell})\Xi(v_{j_\ell})]^{1/2}}{\Xi(\tilde{v}_\ell)} > \frac{R\Xi_0(1-\varepsilon)^2}{\Xi(\tilde{v}_\ell)}, \tag{3.1.31}$$

from which it follows that $\Xi(\tilde{v}_\ell) > \Xi_0(1-\varepsilon)^2$. In view of (3.1.30), the last inequality implies that $|||\Phi|||^2_{2(e^{-W}d\mu)} = \lim_{\ell\to\infty} |||Y|||^2_{2(e^{-W}d\mu)} \geq \Xi_0(1-\varepsilon)^2$. Since $\varepsilon > 0$ is arbitrary, it follows that $|||\Phi|||^2_{2(e^{-W}d\mu)} \geq \Xi_0$. $\square$

Lemma 3.1.7 implies that $\Phi_0 = 1$, $\Phi_N = 1$ a.e. on $\Lambda^N \setminus Q_N$ if $1 \leq N < m$, and $\Phi_N(x_1, ..., x_N) \in [0, \infty)$ for a.e. $(x_1, ..., x_N) \in \Lambda^N \setminus Q_N$ if $N \geq m$.

**Lemma 3.1.8.** *There is a measurable symmetric function $v : \Lambda^m \to (-\infty, \infty]$ and a subsequence of $(v_k)$ (still referred to as $(v_k)$) such that $e^{-(V_k)_N/2} \to e^{-V_N/2}$ a.e. on $\Lambda^N \setminus Q_N$ for every $N \geq m$, where $V_N = \hat{C}_{N,m}v$. In particular, $e^{-V_k/2} \to e^{-V/2}$ in $\mathbb{L}^2(e^{-W}d\mu)$.*

*Proof.* "In particular" part follows directly from Lemma 3.1.7. The same lemma implies, that for every $N \geq m$, there is a subsequence of $\left(e^{-(V_k)_N/2}\right)$ converging to $\Phi_N$ a.e. on $\Lambda^N \setminus Q_N$. In fact, by a diagonal argument, there is a subsequence of $(v_k)$ (still called $(v_k)$ ) such that $e^{-(V_k)_N/2} \to \Phi_N$ a.e. on $\Lambda^N \setminus Q_N$ for every $N \geq m$.

Let $A_m \subset \Lambda^m \setminus Q_m$ be the set on which $\left(e^{-(V_k)_N/2}\right)$ converges to a finite non-negative number. Then, $A_m$ is a symmetric set, and $|(\Lambda^m \setminus Q_m) \setminus A_m| = 0$. Defining

$$v := \begin{cases} -2\ln\left(\lim_{k\to\infty} \exp[-(v_k)/2]\right) & \text{on } A_m, \\ r & \text{on } \Lambda^m \setminus A_m, \end{cases} \tag{3.1.32}$$

where $\ln 0 := -\infty$, and $r$ is an arbitrary real number, we see that $v$ is a measurable symmetric function taking values in $(-\infty, \infty]$. Moreover, $e^{-v_k/2} \to e^{-v/2}$ on $A_m$ (and so, a.e. on $\Lambda^m \setminus Q_m$). For every $N > m$, let us define the set

$$\Lambda^N \supset A_N := \bigcap_{1 \le i_1 < \cdots < i_m \le N} A_N^{i_1,\ldots,i_m}, \tag{3.1.33}$$

where

$$A_N^{i_1,\ldots,i_m} := \bigcap_{1 \le i_1 < \cdots < i_m \le N} \{(x_1, ..., x_N) \in \Lambda^N \mid (x_{i_1}, ..., x_{i_m}) \in A_m\}. \tag{3.1.34}$$

Then, $e^{-(V_k)_N/2} \to e^{-V_N/2}$ on $A_N$, and $\left|\left(\Lambda^N \setminus Q_N\right) \setminus A_N\right| = 0$. To verify the last claim, we note that for every $1 \le i_1 < \cdots < i_m \le N$:

$$\left|\left(\Lambda^N \setminus Q_N\right) \setminus A_N^{i_1,\ldots,i_m}\right| = \left|\left(\Lambda^N \setminus Q_N\right) \cap Q_N^{i_1,\ldots,i_m}\right| = \left|Q_N^{i_1,\ldots,i_m} \setminus Q_N\right| = 0. \tag{3.1.35}$$

The first equality follows because $\Lambda^N \setminus A_N^{i_1,\ldots,i_m} \supset Q_N^{i_1,\ldots,i_m}$, but

$$|(\Lambda^m \setminus A_m) \setminus Q_m| = |(\Lambda^m \setminus Q_m) \setminus A_m| = 0 \tag{3.1.36}$$

implies that $\left|\left(\Lambda^N \setminus A_N^{i_1,\ldots,i_m}\right) \setminus Q_N^{i_1,\ldots,i_m}\right| = 0$. The second equality in (3.1.35) results from the condition (i) in Subsection 3.1.1. $\square$

**Theorem 3.1.9.** *There is $v \in \mathcal{C}$ such that $\Im(v) = \sup_{s \in \mathcal{C}} \Im(s) = R$. Moreover, if also $u \in \mathcal{C}$, and $\Im(u) = R$, then $u = v$ a.e. $[d^m x]$ on $\Lambda^m \setminus Q_m$.*

*Proof.* Let $v$ be the function stated in Lemma 3.1.8.

(1) Then, $e^{-V/2} \in \mathbb{L}^2(e^{-W} d\mu)$, and so $\Xi(v) = \left|\left|\left|e^{-V/2}\right|\right|\right|^2_{2(e^{-W} d\mu)} < \infty$. In particular, $\int_{\Lambda^m} e^{-W_m - v} d^m x < \infty$. Therefore,

$$\infty > \int_{\Lambda^m} e^{-W_m - v} d^m x \ge \int_{\Lambda^m} e^{-W_m - v - \ln \rho^{(m)}} \rho^{(m)} d^m x \ge \int_{\Lambda^m} (W_m + v + \ln \rho^{(m)})_- d^m x, \tag{3.1.37}$$

where to obtain the last inequality, the fact that $e^t \ge t_+$ if $t \in [-\infty, \infty]$ was used. Since $v_- \le (W_m + v + \ln \rho^{(m)})_- + (W_m + \ln \rho^{(m)})_+$, inequality (3.1.37) and condition (vi) in Subsection 3.1.1 give that $\int_{\Lambda^m} v_- \rho^{(m)} d^m x < \infty$.

(2) By Lemma 3.1.6, there is $C > 0$ such that for every $k \in \mathbb{N}$:

$$\Xi(v_k) n_m(v_k) = \sum_{N=m}^{\infty} \frac{1}{(N-m)!} \left|\left|e^{-(V_k)_N/2}\right|\right|^2_{2(e^{-W_N} d^N x)} \leq C. \tag{3.1.38}$$

Since $\left|\left|e^{-(V_k)_N/2}\right|\right|^2_{2(e^{-W_N} d^N x)} \to \left|\left|e^{-V_N/2}\right|\right|^2_{2(e^{-W_N} d^N x)}$, it is also that

$$\Xi(v) n_m(v) = \sum_{N=m}^{\infty} \frac{1}{(N-m)!} \left|\left|e^{-V_N/2}\right|\right|^2_{2(e^{-W_N} d^N x)} \leq C, \tag{3.1.39}$$

and so $n_m(v) < \infty$.

(3) In this step it will be shown that $v_+ \in L^1(\rho^{(m)} d^m x)$. Let $0 < b := n_m(P) = ||\rho^{(m)}||_{1(d^m x)}$ for the rest of this step. (See assumption (iii) in Subsection 3.1.1 and definitions there.) For every $i \in \mathbb{N}$, let $v^i := \min(v, i)$, and

$$\mathbb{R} \leftarrow \Lambda^m \setminus Q_m : \gamma^i := \min \left[ \left( W_m + \ln \frac{\rho^{(m)}}{b} \right), i \right]. \tag{3.1.40}$$

Note, that $\gamma^i > -\infty$ on $\Lambda^m \setminus Q_m$ because $Q_m \sim \{\rho^{(m)} = 0\}$ by Lemma 3.1.1.

By step (1), we know that $v_- \in L^1(\rho^{(m)} d^m x)$, and so does $v_k - v^i$. Further, on $\Lambda^m \setminus Q_m$:

$$0 \leq W_m + \ln \frac{\rho^{(m)}}{b} - \gamma^i \leq \left( W_m + \ln \frac{\rho^{(m)}}{b} \right)_+ \leq \left( W_m + \ln \rho^{(m)} \right)_+ + (\ln b)_-. \tag{3.1.41}$$

Thus, by assumption (vi) in Subsection 3.1.1, $W_m + \ln \frac{\rho^{(m)}}{b} - \gamma^i \in L^1(\rho^{(m)} d^m x)$. These comments let us use the Jensen's inequality to obtain for all $i, j, k \in \mathbb{N}$:

$$\begin{gathered} \exp \left\{ - \int_{\Lambda^m} \left[ \frac{(v_k - v^i)}{2} + W_m + \ln \frac{\rho^{(m)}}{b} - \gamma^j \right] \frac{\rho^{(m)}}{b} d^m x \right\} \leq \\ \int_{\Lambda^m} \exp \left\{ - \left[ \frac{(v_k - v^i)}{2} + W_m + \ln \frac{\rho^{(m)}}{b} - \gamma^j \right] \right\} \frac{\rho^{(m)}}{b} d^m x \leq \\ \int_{\Lambda^m} \exp \left[ - \frac{(v_k - v^i)}{2} + \gamma^j \right] \exp(-W_m) \, d^m x. \end{gathered} \tag{3.1.42}$$

Since $\int_{\Lambda^m} e^{v^i + 2\gamma^j} e^{-W_m} d^m x \leq e^{i+2j} \int_{\Lambda^m} e^{-W_m} < \infty$, the weak convergence implies that the right most hand side of inequality (3.1.42) converges to

$$\begin{gathered} \int_{\Lambda^m} \exp \left[ - \frac{(v - v^i)}{2} + \gamma^j \right] \exp(-W_m) \, d^m x = \\ \int_{\Lambda^m} \exp \left\{ - \left[ \frac{(v - v^i)}{2} + W_m + \ln \frac{\rho^{(m)}}{b} - \gamma^j \right] \right\} \frac{\rho^{(m)}}{b} d^m x \leq 1 \end{gathered} \tag{3.1.43}$$

as $k$ is taken to infinity. The equality in 3.1.43 holds because $Q_m \sim \{\rho^{(m)} = 0\}$ by Lemma 3.1.1, while the last inequality follows by definitions of $v^i$ and $\gamma^j$. At the same time, the left most hand side of inequality (3.1.42) converges to

$$[R\Xi(v)]^{\frac{m!}{2b}} \exp\left\{\int_{\Lambda^m} \frac{v^i}{2} - \left(W_m + \ln\frac{\rho^{(m)}}{b} - \gamma^j\right)\frac{\rho^{(m)}}{b} d^m x\right\}. \tag{3.1.44}$$

Therefore,

$$\begin{aligned}[R\Xi(v)]^{\frac{m!}{2b}} &\le \exp\left[-\frac{1}{2b}\int_{\Lambda^m}(v_+^i - v_-)\rho^{(m)} d^m x\right] \times \\ \exp&\left\{\int_{\Lambda^m}\left(W_m + \ln\frac{\rho^{(m)}}{b} - \gamma^j\right)\frac{\rho^{(m)}}{b} d^m x\right\},\end{aligned} \tag{3.1.45}$$

where $v_+^i := \min(v_+, i)$. In view of (3.1.41), $\lim_{j\to\infty}\int_{\Lambda^m}\left(W_m + \ln\frac{\rho^{(m)}}{b} - \gamma^j\right)\frac{\rho^{(m)}}{b} d^m x = 0$ by dominated convergence. In addition, $\lim_{i\to\infty}\int_{\Lambda^m} v_+^i \rho^{(m)} d^m x = \int_{\Lambda^m} v_+ \rho^{(m)} d^m x$ by monotone convergence. Thus, taking $i$, $j$ to infinity in (3.1.45) results in

$$0 < [R\Xi(v)]^{\frac{m!}{2b}} \le \exp\left\{-\frac{1}{2b}\int_{\Lambda^m}(v_+ - v_-)\rho^{(m)} d^m x\right\}. \tag{3.1.46}$$

Since $v_- \in L^1(\rho^{(m)} d^m x)$, it is clear from 3.1.46 that $\int_{\Lambda^m} v_+ \rho^{(m)} d^m x < \infty$.

(4) By the last inequality, $|\{v = \infty\} \setminus Q_m| = 0$. Therefore, the definition in (3.1.32) implies that $v$ is symmetric and a.e. finite function. In view of the previous three steps, this means that $v \in \mathcal{C}$. Because the inequality (3.1.46) is equivalent to $0 < R \le \Im(u)$, it is clear that $\Im(u) = R$.

(5) Suppose that $u \in \mathcal{C}$, and $\Im(u) = R$. Let $\lambda \in (0, 1)$. By Lemma 3.1.3, we have that $\ln \Im[\lambda v + (1-\lambda)u] = \lambda \ln \Im(v) + (1-\lambda)\Im(u)$, which is equivalent to
$\Xi[\lambda v + (1-\lambda)u] = \Xi(v)^\lambda \Xi(u)^{1-\lambda}$. Therefore, the generalized Holder's inequality, Lemma A.0.3, implies that there are $\alpha, \beta > 0$ such that $\alpha e^{-V_N/2} = \beta e^{-(U)_N/2}$ a.e. $[e^{-W_N} d^N x]$ for every $N \ge 0$. In particular, $\alpha e^{-v} = \beta e^{-u}$ a.e. on $\Lambda^m \setminus Q_m$ when $N = m$. Taking $N = 0$, we also have that $\alpha = \beta$. Therefore, $v = u$ a.e. on $\Lambda^m \setminus Q_m$. $\square$

The next theorem establishes the existence of solutions to the inverse problem.

**Theorem 3.1.10.** *There is $v \in \mathcal{C}$ such that $\rho^{(m)} = \rho_v^{(m)}$ a.e. on $\Lambda^m$. In fact, $v$ is the maximizer of $\Im$ on $\mathcal{C}$.*

*Proof.* By Theorem 3.1.9, there is $v \in \mathcal{C}$ such that $\Im(v) = R$. Let $\eta := \chi_E \in L^\infty(\Lambda^m, d^m x)$, where $E := \{(x_1, ..., x_m) \in \Lambda^m \mid \rho_v^{(m)}(x_1, ..., x_m) > \rho^{(m)}(x_1, ..., x_m)\}$.

For any $0 < \varepsilon < 1$, $v + \varepsilon\eta \in L^1(\Lambda^m, \rho^{(m)} d^m x)$, and

$$e^{-\frac{1}{m!}\int_{\Lambda^m}(v+\varepsilon\eta)\rho^{(m)}d^m x} = e^{-\frac{1}{m!}\int_{\Lambda^m} v\rho^{(m)}d^m x}\left(1 - \frac{\varepsilon}{m!}\int_{\Lambda^m} \eta\rho^{(m)} d^m x + o(\varepsilon)\right). \tag{3.1.47}$$

We can also write

$$\Xi(v + \varepsilon\eta) = 1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} \left[1 - \varepsilon\eta_N + (\theta_\varepsilon)_N\right] d^N x, \tag{3.1.48}$$

where $\eta_N := \hat{C}_{N,m}\eta$ if $N \geq m$, $\eta_N := 0$ if $0 \leq N < m$, and $(\theta_\varepsilon)_N := \exp(-\varepsilon\eta_N) - 1 + \varepsilon\eta_N$. Since

$$0 \leq (\theta_\varepsilon)_N \leq e^{-\varepsilon\|\eta_N\|_\infty} - 1 + \varepsilon\|\eta_N\|_\infty = o(\varepsilon), \tag{3.1.49}$$

it follows that

$$\lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon} \int_{\Lambda^N} e^{-W_N - V_N} (\theta_\varepsilon)_N d^N x = 0 \quad \forall N \geq m. \tag{3.1.50}$$

At the same time, $0 \leq \varepsilon^{-1}(\theta_\varepsilon)_N \leq \|\eta_N\|_\infty$. Therefore,

$$\begin{aligned} &\frac{1}{\varepsilon}\sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} (\theta_\varepsilon)_N d^N x \leq \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} \|\eta_N\|_\infty d^N x \\ &\leq \sum_{N=m}^{\infty} \frac{1}{(N-m)!} \int_{\Lambda^N} e^{-W_N - V_N} d^N x = n_m(v) < \infty. \end{aligned} \tag{3.1.51}$$

Equations (3.1.50) and (3.1.51) show that

$$\lim_{\varepsilon\to\infty} \frac{1}{\varepsilon} \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} (\theta_\varepsilon)_N d^N x = 0. \tag{3.1.52}$$

Thus, (3.1.48) can be rewritten as

$$\begin{aligned} &\Xi(v + \varepsilon\eta) = \Xi(v) - \varepsilon \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} \eta_N d^N x + o(\varepsilon) = \\ &\Xi(v)\left(1 - \frac{\varepsilon}{m!}\int_{\Lambda^m} \eta\rho_v^{(m)} d^m x + o(\varepsilon)\right). \end{aligned} \tag{3.1.53}$$

Combining equations (3.1.47) and (3.1.52), we obtain:

$$\Im(v + \varepsilon\eta) = \Im(v)\left[1 + \frac{\varepsilon}{m!}\int_{\Lambda^m} \eta(\rho_v^{(m)} - \rho^{(m)}) d^m x + o(\varepsilon)\right], \tag{3.1.54}$$

and so

$$0 \geq \lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon}[\Im(v + \varepsilon\eta) - \Im(v)] = \frac{1}{m!} \int_E |\rho_v^{(m)} - \rho^{(m)}| d^m x. \tag{3.1.55}$$

The last inequality shows that $\rho_v^{(m)} \leq \rho^{(m)}$ a.e. on $\Lambda^m$.

Next, suppose that $\rho_v^{(m)} < \rho^{(m)}$ on some set of positive measure. This implies that there is a potential $\tilde{v} \in \mathcal{C}$ such that $\Im(\tilde{v}) > \Im(v)$, which is impossible. The proof of the last implication for $m \geq 2$ is almost exactly the same as for $m = 1$ and can be found in [11, Lemma 8.6, Proposition 8.7]. □

**Theorem 3.1.11.** *Under the conditions stated in Subsection 3.1.1, there exists an a.e. finite and symmetric function $v$ on $\Lambda^m$ such that $\rho_v^{(m)} = \rho^{(m)}$ a.e. $[d^m x]$. Moreover, if there is another a.e. finite and symmetric function $u$ with $\rho_u^{(m)} = \rho^{(m)}$ a.e., then $v = u$ a.e. on $\Lambda^m \setminus Q_m$.*

**Remark 3.1.1.** Theorem 3.1.11 does not guarantee that, given some interaction $W$ satisfying conditions (i-ii) in Subsection 3.1.1, every non-negative integrable function $\rho^{(m)}$ maps to the potential $v$ defined by $\rho^{(m)} = \rho_v^{(m)}$. Instead, it asserts that this is the case if $\rho^{(m)}$ satisfies conditions (iii-v) in Subsection 3.1.1. However, condition (iii) (and by implication (iv)), though physically natural, can not be verified explicitly.

*Proof of Theorem 3.1.11.* The existence part is settled by Theorem 3.1.10.

(1) For the uniqueness, let us first show that if $v$ is a.e. finite and symmetric, and $\rho_v^{(m)} = \rho^{(m)}$ a.e., then $v \in \mathcal{C}$. Indeed, by the definition of $\rho_v^{(m)}$, $\Xi(v) < \infty$ and $n_m(v) < \infty$. Also, the argument of step (1) in the proof of Theorem 3.1.9 shows that $\int_{\Lambda^m} v_- \rho^{(m)} d^m x < \infty$. To prove that $v_+ \in L^1(\Lambda^m, \rho^{(m)} d^m x)$, we note that

$$\begin{aligned} \infty > \frac{\Xi(0)}{\Xi(v)} &> \frac{1}{\Xi(v)} \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N + V_N} d^N x \\ &\geq \frac{1}{\Xi(v)} \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} (V_N)_+ d^N x. \end{aligned} \tag{3.1.56}$$

However, it is also true that

$$(V_N)_+ \geq V_N = \hat{C}_{N,m} v_+ - \hat{C}_{N,m} v_-, \tag{3.1.57}$$

and that

$$
\begin{aligned}
\langle \hat{C}_{N,m} v_- \rangle_v &= \frac{1}{\Xi(v)} \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} \hat{C}_{N,m} v_- d^N x \\
&= \frac{1}{m!} \int_{\Lambda^m} v_- \rho_v^{(m)} d^m x = \frac{1}{m!} \int_{\Lambda^m} v_- \rho^{(m)} d^m x < \infty.
\end{aligned}
\tag{3.1.58}
$$

Equations (3.1.56-3.1.58) guarantee that $\int_{\Lambda^m} v_+ \rho^{(m)} d^m x = m! \langle \hat{C}_{N,m} v_+ \rangle_v < \infty$, and so $v \in \mathcal{C}$.

(2) Now, we will show that if $u, v \in \mathcal{C}$, and $\rho_v^{(m)} = \rho_u^{(m)}$ a.e., then $u = v$ a.e. on $\Lambda^m \setminus Q_m$. For that purpose, let us write:

$$
\begin{aligned}
&\frac{\Xi(u)}{\Xi(v)} = \frac{1}{\Xi(v)} \left[ 1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N + (V_N - U_N)} d^N x \right] = \\
&\left\langle e^{V-U} \right\rangle_v \geq e^{\langle V-U \rangle_v} = \exp\left\{ \frac{1}{m!} \int_{\Lambda^m} (v-u) \rho_v^{(m)} d^m x \right\},
\end{aligned}
\tag{3.1.59}
$$

where the inequality is due to Theorem A.0.4. In the same manner,

$$
\frac{\Xi(v)}{\Xi(u)} = \left\langle e^{U-V} \right\rangle_u \geq e^{\langle U-V \rangle_u} = \exp\left\{ -\frac{1}{m!} \int_{\Lambda^m} (v-u) \rho_v^{(m)} d^m x \right\}. \tag{3.1.60}
$$

However, the last two inequalities can both be true only if $\left\langle e^{V-U} \right\rangle_v = e^{\langle V-U \rangle_v}$. By the second part of Theorem A.0.4, this implies that $v - u = 0$ a.e. $[e^{-W_m - v} d^m x]$, or equivalently, that $v - u = 0$ a.e. $[d^m x]$ on $\Lambda^m \setminus Q_m$ (because $v$ is a.e. $[d^m x]$ finite). $\square$

## 3.2 DIFFERENTIABILITY OF THE INVERSE MAP

### 3.2.1 Assumptions and preliminaries

In this section we discuss differentiability of the inverse map for $m \geq 1$. The arguments are much easier in the truncated ensemble, and so we will require that $W_N = \infty$ for all $N > N'$ for some $N' > m$. This is true for fluids confined to a finite volume. (The truncation of the ensemble could be replaced by assuming the conclusions of Lemmas 3.2.2 and 3.2.3.) We will also assume that $W$ satisfies conditions (i) and (ii) in Subsection 3.1.1. It will be useful to denote by $L_s^p(\Lambda^N, d^N x)$ the closed subspace of a.e. symmetric functions in $L^p(\Lambda^N, d^N x)$ for $1 \leq p \leq \infty$. It follows from the proof of Lemma 3.1.1 that

$$Q_m \sim \{\rho_v^{(m)} = 0\} \quad \forall v \in L_s^\infty(\Lambda^m, d^m x). \tag{3.2.1}$$

If $v \in L_s^\infty(\Lambda^m, d^m x)$ and $k \in \mathbb{N}$, then by the proof of Lemma 3.1.2, $\Xi(v) < \infty$ and $n_k(v) < \infty$. This shows that $k$-particle densities $\rho_v^{(k)}$ are well-defined by (1.2.5) for all $k \in \mathbb{N}$, and $\int_{\Lambda^k} \rho_v^{(k)} = n_k(v)$. It is also true that $\rho_v^{(k)}$, $k \in \mathbb{N}$, do not depend on the values of $v$ on $Q_m$. In fact, we have the following lemma.

**Lemma 3.2.1.** *If $v, u \in L_s^\infty(\Lambda^m, d^m x)$, and $v - u = 0$ a.e. on $\Lambda^m \setminus Q_m$, then $\rho_v^{(k)} = \rho_u^{(k)}$ a.e. for all $k \in \mathbb{N}$.*

*Proof.* For every $N \geq m$, let

$$E_N := \bigcap_{1 \leq i_1 < \cdots < i_m \leq N} \Lambda^N \setminus Q_N^{i_1,\ldots,i_m}, \tag{3.2.2}$$

where $Q_N^{i_1,\ldots,i_m}$ is defined in (3.1.2). Then,

$$\begin{aligned} &\left|\left(\Lambda^N \setminus Q_N\right) \setminus E_N\right| \leq \sum_{1 \leq i_1 < \cdots < i_m \leq N} \left|\left(\Lambda^N \setminus Q_N\right) \cap Q_N^{i_1,\ldots,i_m}\right| = \\ &\sum_{1 \leq i_1 < \cdots < i_m \leq N} \left|Q_N^{i_1,\ldots,i_m} \setminus Q_N\right| = 0, \end{aligned} \tag{3.2.3}$$

the last equality following from (3.1.1). Suppose that $v, u \in L^\infty_s(\Lambda^m, d^m x)$, and $v - u = 0$ a.e. on $\Lambda^m \setminus Q_m$. For every $N \geq m$

$$\int_{\Lambda^N} e^{-W_N - V_N} d^N x = \int_{\Lambda^N} \chi_{D_N} e^{-W_N - V_N} d^N x, \tag{3.2.4}$$

where $\chi_{D_N}$ is the characteristic function of the set $D_N := \left(\Lambda^N \setminus Q_N\right) \cap E_N$. However, the last integral does not depend on the values of $v$ on $Q_m$ by the definition of the set $E_N$. Thus, $\Xi(v) = \Xi(u)$. Similarly, for every $k \in \mathbb{N}$ and a.e. on $\Lambda^k$:

$$\int_{\Lambda^{N-k}} (G_v)_N d^{N-k} x = \int_{\Lambda^{N-k}} \chi_{D_N} (G_v)_N d^{N-k} x, \tag{3.2.5}$$

where $(G_v)_N$ is defined in (1.2.3). Therefore, $\rho_v^{(k)} = \rho_u^{(k)}$ a.e. on $\Lambda^k$. $\square$

**Definition 3.2.1.** For every $k \in \mathbb{N}$, let

$$M_k := \{f \in L^\infty_s(\Lambda^k, d^k x) \mid \; f = 0 \text{ a.e. on } \Lambda^k \setminus Q_k\}, \tag{3.2.6}$$

and let $\pi_k$ be the quotient map of $L^\infty_s(\Lambda^k, d^k x)$ onto $L^\infty_s(\Lambda^k, d^k x)/M_k$ [28, p. 30]. (Note, that $M_k$ is a closed subspace of $L^\infty_s(\Lambda^k, d^k x)$.) For $\tilde{f}_k = \pi_k(f) \in L^\infty_s(\Lambda^k, d^k x)/M_k$, $\|\tilde{f}_k\|_\infty$ will designate here the quotient norm of $\tilde{f}_k$. It is clear from the definition of the quotient norm [28, p. 32] that $\|\tilde{f}_k\|_\infty = \left\| f_k \restriction (\Lambda^k \setminus Q_k) \right\|_{\infty(d^k x)}$.

In view of Lemma 3.2.1, it is natural to define the $k$-particle densities as functionals on the quotient space $L^\infty_s(\Lambda^m, d^m x)/M_m$. More precisely, For every $v \in L^\infty_s(\Lambda^m, d^m x)$ and $k \in \mathbb{N}$ , we define $\rho^{(k)}(\pi_m(v)) := \rho_v^{(k)}$, with $\rho_v^{(k)}$ given by (1.2.5).

**Lemma 3.2.2.** *For every $v \in L^\infty_s(\Lambda^m, d^m x)$, and every $k \in \mathbb{N}$, there are positive constants $B_{1:k}(v)$ and $B_{2:k}(v)$ such that $B_{1:k}(v)\rho_0^{(k)} \leq \rho_v^{(k)} \leq B_{2:k}(v)\rho_0^{(k)}$ a.e. on $\Lambda^k$.*

*Proof.* Let $v \in L^\infty_s(\Lambda^m, d^m x)$. Then,

$$\Xi(v) \leq 1 + \sum_{N=1}^{N'} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N + \hat{C}_{N,m}\|v\|_\infty} d^N x \leq e^{\hat{C}_{N',m}\|v\|_\infty} \Xi(0). \tag{3.2.7}$$

By the same argument, $e^{-\hat{C}_{N',m}\|v\|_\infty}\Xi(0) \leq \Xi(v) \leq e^{\hat{C}_{N',m}\|v\|_\infty}\Xi(0)$. Therefore, a.e. on $\Lambda^k$:

$$\rho_v^{(k)} \leq \frac{2e^{\hat{C}_{N',m}\|v\|_\infty}}{\Xi(0)} \left[ e^{-W_k} + \sum_{N=k+1}^{N'} \frac{1}{(N-k)!} \int_{\Lambda^N} e^{-W_N} d^{N-k} x \right] = e^{2\hat{C}_{N',m}\|v\|_\infty} \rho_0^{(k)}. \tag{3.2.8}$$

Similarly, $\rho_v^{(k)} \geq e^{-2\hat{C}_{N',m}\|v\|_\infty} \rho_0^{(k)}$. $\square$

**Definition 3.2.2.** (i) Let us define a linear vector space

$$\mathcal{V}_m := \{\omega\rho_0^{(m)} \mid \omega \in L_s^\infty(\Lambda^m, d^m x)\} \subset L_s^1(\Lambda^m, d^m x), \tag{3.2.9}$$

equipped with the norm $\|\omega\rho_0^{(m)}\|_{\mathcal{V}_m} := \|\pi_m(\omega)\|_\infty = \|\omega \restriction \Lambda^m \setminus Q_m\|_{\infty(d^m x)}$. It is easy to check that $\mathcal{V}_m$ is a Banach space.

(ii) Let $\omega, g \in L_s^\infty(\Lambda^m, d^m x)$, and $f = \omega\rho_0^{(m)} \in \mathcal{V}_m$, $\tilde{g} = \pi_m(g) \in L_s^\infty(\Lambda^m, d^m x)/M_m$. Then, $f\tilde{g} := \omega g \rho_0^{(m)} \in \mathcal{V}_m$. Note, that this definition makes sense due to the relation (3.2.1).

According to Lemma 3.2.2, the map $\rho^{(m)}$ defined on $L_s^\infty(\Lambda^m, d^m x)/M_m$ takes values in $\mathcal{V}_m$. Indeed, let $\tilde{v} = \pi_m(v)$ for some $v \in L_s^\infty(\Lambda^m, d^m x)$. Then $\rho^{(m)}(\tilde{v}) = \gamma\rho_0^{(m)}$, where $\gamma = \rho_v^{(m)}/\rho_0^{(m)} \leq B_{2:m}(v)$ a.e. on $\Lambda^m \setminus Q_m$, and $\gamma$ is equal to an arbitrary function in $L_s^\infty(\Lambda^m, d^m x)$ a.e. on $Q_m$.

**Lemma 3.2.3.** *For every $1 \leq k < \ell \leq N'$, there is a positive constant $C_{k,\ell}$ such that $\int_{\Lambda^{\ell-k}} \rho_v^{(\ell)} d^{\ell-k}x \leq C_{k,\ell}\rho_v^{(k)}$ a.e. on $\Lambda^k$ for every $v \in L_s^\infty(\Lambda^m, d^m x)$.*

*Proof.* Let $1 \leq k < \ell \leq N'$. For every $v \in L_s^\infty(\Lambda^m, d^m x)$:

$$\begin{aligned} &\Xi(v) \int_{\Lambda^{\ell-k}} \rho_v^{(\ell)} d^{\ell-k}x = \sum_{N=\ell}^{N'} \frac{1}{(N-\ell)!} \int_{\Lambda^{N-k}} e^{-W_N - V_N} d^{N-k}x \leq \\ &\frac{(N'-k)!}{(N'-\ell)!} \sum_{N=k}^{N'} \frac{1}{(N-k)!} \int_{\Lambda^{N-k}} e^{-W_N - V_N} d^{N-k}x = (N'-k)\cdots(N'-\ell+1)\Xi(v)\rho_v^{(k)}. \end{aligned} \tag{3.2.10}$$

$\square$

### 3.2.2 Differentiability

In this subsection we state sufficient (but not necessary) conditions for the differentiability of the inverse of $\rho^{(m)} : L_s^\infty(\Lambda^m, d^m x)/M_m \to \mathcal{V}_m$. More precisely, it is proved that under these conditions, there is an open set $A$, $0 \in A \subset L_s^\infty(\Lambda^m, d^m x)/M_m$, such that the map $\rho^{(m)} : A \to \mathcal{V}_m$ is a diffeomorphism between $A$ and its image.

**Lemma 3.2.4.** *The map* $\rho^{(m)} : L_s^\infty(\Lambda^m, d^m x)/M_m \to \mathcal{V}_m$ *is continuously differentiable. Given* $v, h \in L^\infty(\Lambda^m, d^m x)$*, set* $\tilde{v} = \pi_m(v)$*,* $\tilde{h} = \pi_m(h)$*. Then, the derivative is given by* $D\rho^{(m)}(\tilde{v})\tilde{h} = -\rho^{(m)}(\tilde{v})[\tilde{h} - K_m(\tilde{v})\tilde{h}]$*, where* $K_m(\tilde{v}) : L_s^\infty(\Lambda^m, d^m x)/M_m \to L_s^\infty(\Lambda^m, d^m x)/M_m$ *is the bounded linear operator that can be written in terms of m-,...,2m-particle densities as*

$$\begin{aligned}
&(K_m(\tilde{v})\tilde{h})(1, ..., m) = \frac{1}{m!}\int_{\Lambda^m} \rho_v^{(m)} h - \\
&\sum_{k=1}^{m} \frac{1}{k!} \sum_{1 \le i_1 < \cdots i_{m-k} \le m} \int_{\Lambda^k} \frac{\rho_v^{(m+k)}(1, ..., m+k)}{\rho_v^{(m)}(1, ..., m)} h(i_1, ..., i_{m-k}, m+1, ..., m+k) \times \\
&d(m+1)\cdots d(m+k) \quad \textit{for a.e. } (1, ..., m) \in \Lambda^m \setminus Q_m.
\end{aligned} \tag{3.2.11}$$

In (3.2.11), $(i, j, ...)$ and $didj\cdots$ stand for $(x_i, x_j, ...)$ and $dx_i dx_j \cdots$ respectively. In particular, when $m = 1$, (3.2.11) reduces to

$$(K_1\tilde{h})(1) = \int_\Lambda \rho_v^{(1)} h - \left[\rho_v^{(1)}(1)\right]^{-1} \int_\Lambda \rho_v^{(2)}(1, 2)h(2)d2, \tag{3.2.12}$$

a well known result in liquid state theory [3, Equation (3.1.6)]. When $m = 2$, (3.2.11) becomes

$$\begin{aligned}
&(K_2\tilde{h})(1, 2) = \frac{1}{2}\int_{\Lambda^2} \rho_v^{(2)} h - \left[\rho_v^{(2)}(1, 2)\right]^{-1} \times \\
&\left\{\int_\Lambda \rho_v^{(3)}(1, 2, 3)[h(1, 3) + h(2, 3)]d3 - \frac{1}{2}\int_{\Lambda^2} \rho_v^{(4)}(1, 2, 3, 4)h(3, 4)d3d4\right\}.
\end{aligned} \tag{3.2.13}$$

**Remark 3.2.1.** It is important to note here that in the *Canonical* formulation for the system of $N$ particles, $K_m(\tilde{v})\tilde{h} \equiv 1$ if $\tilde{h} \equiv 1$. This is easy to verify using the identities $\int_{\Lambda^m} \rho_v^{(m)} d^m x = \frac{N!}{(N-m)!}$, and $\int_{\Lambda^k} \rho_v^{(m+k)}(\cdot, x_1, .., x_k)dx_1 \cdots dx_k = \frac{(N-m)!}{(N-m-k)!}$. Thus, $D\rho^{(m)}(\tilde{v})\tilde{h} \equiv 0$ for all constant functions $\tilde{h} \equiv c$, and so $D\rho^{(m)}(\tilde{v})$ is not injective. This is the reason why the derivative of the inverse map does not exist in the Canonical formulation, the fact known in physics for a long time [12].

*Proof of Lemma 3.2.4.* Let $v, h \in L^\infty(\Lambda^m, d^m x)$, and set $\tilde{v} := \pi(v)$ and $\tilde{h} := \pi(h)$.

(1) Then,

$$\Xi(v+h) = 1 + \sum_{N=1}^{N'} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N}[1 - H_N + \theta(H_N)] d^N x, \tag{3.2.14}$$

where $H_N := \hat{C}_{N,m} h$ if $N \geq m$, $H_N := 0$ if $0 \leq N < m$, and $\theta(H_N) := \exp(-H_N) - 1 + H_N$. Let us define $\widetilde{H}_N := \pi_N(H_N)$. Since the function $x \mapsto e^{-x} - 1 + x$ has its global minimum at 0, we have that

$$\begin{aligned} & 0 \leq \theta(H_N) \leq \\ & \begin{cases} \exp\left(-||\widetilde{H}_N||_\infty\right) - 1 + ||\widetilde{H}_N||_\infty \leq \exp\left[-\binom{N}{m}||\tilde{h}||_\infty\right] - 1 + \binom{N}{m}||\tilde{h}||_\infty & \text{if } H_N \geq 0, \\ \exp\left(||\widetilde{H}_N||_\infty\right) - 1 - ||\widetilde{H}_N||_\infty \leq \exp\left[\binom{N}{m}||\tilde{h}||_\infty\right] - 1 - \binom{N}{m}||\tilde{h}||_\infty & \text{if } H_N < 0 \end{cases} \\ & = o(||\tilde{h}||_\infty). \end{aligned} \tag{3.2.15}$$

It follows that

$$\lim_{||\tilde{h}||_\infty \to 0} \frac{1}{||\tilde{h}||_\infty} \sum_{N=m}^{N'} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} \theta(H_N) d^N x = 0, \tag{3.2.16}$$

and so (3.2.14) can be rewritten as

$$\Xi(v+h) = \Xi(v) \left[1 - \frac{1}{\Xi(v)} \sum_{N=m}^{\infty} \frac{1}{N!} \int_{\Lambda^N} e^{-W_N - V_N} H_N d^N x\right] + o(||\tilde{h}||_\infty). \tag{3.2.17}$$

(2) Similarly,

$$\begin{aligned} & \Xi(v+h)\rho_{v+h}^{(m)} = e^{-W_m - v}[1 - h + \theta(h)] + \\ & \sum_{N=m+1}^{N'} \frac{1}{(N-m)!} \int_{\Lambda^{N-m}} e^{-W_N - V_N}[1 - H_N + \theta(H_N)] d^{N-m} x. \end{aligned} \tag{3.2.18}$$

Let $\varepsilon > 0$. It follows from (3.2.15) that if $\|\tilde{h}\|_\infty$ is small enough, then

$$\begin{aligned} & \left[\|\tilde{h}\|_\infty \rho_0^{(m)}\right]^{-1} \left\{e^{-W_m - v}\theta(h) + \sum_{N=m+1}^{N'} \frac{1}{(N-m)!} \int_{\Lambda^{N-m}} e^{-W_N - V_N} \theta(H_N) d^{N-m} x\right\} \leq \\ & \varepsilon \left[\rho_0^{(m)}\right]^{-1} \left\{e^{-W_m - v} + \sum_{N=m+1}^{N'} \frac{1}{(N-m)!} \int_{\Lambda^{N-m}} e^{-W_N - V_N} d^{N-m} x\right\} = \\ & \varepsilon \left[\rho_0^{(m)}\right]^{-1} \rho_v^{(m)} \Xi(v) \leq \varepsilon B_{2:m}(v) \Xi(v), \end{aligned} \tag{3.2.19}$$

the last inequality being due to Lemma 3.2.2. Therefore, (3.2.18) can be written as

$$\rho_{v+h}^{(m)}\Xi(v+h) = \Xi(v)\times \left\{\rho_v^{(m)} - \frac{1}{\Xi(v)}\left[e^{-W_m-v}h + \sum_{N=m+1}^{\infty}\frac{1}{(N-m)!}\int_{\Lambda^{N-m}} e^{-W_N-V_N}H_N d^{N-m}x\right]\right\} + o(\tilde{h}), \tag{3.2.20}$$

where $\phi = o(\tilde{h})$ means that $\lim_{\|\tilde{h}\|_\infty\to 0}\frac{\|\phi\|_{\mathcal{V}_m}}{\|\tilde{h}\|_\infty} = \lim_{\|\tilde{h}\|_\infty\to 0}\frac{\|[\rho_0^{(m)}]^{-1}\phi\|_\infty}{\|\tilde{h}\|_\infty} = 0$. It is seen from (3.2.17) and (3.2.20) that

$$\rho^{(m)}(\tilde{v}+\tilde{h}) - \rho^{(m)}(\tilde{v}) = D\rho^{(m)}(\tilde{v})\tilde{h} + o(\tilde{h}), \tag{3.2.21}$$

where $D\rho^{(m)}(\tilde{v}) : L^\infty(\Lambda^m d^m x)/M_m \to \mathcal{V}_m$ is the linear map defined by

$$D\rho^{(m)}(\tilde{v})\tilde{h} = \frac{\rho_v^{(m)}}{\Xi(v)}\sum_{N=m}^{\infty}\frac{1}{N!}\int_{\Lambda^N} e^{-W_N-V_N}H_N d^N x - \frac{1}{\Xi(v)}\left[e^{-W_m-v}h + \sum_{N=m+1}^{\infty}\frac{1}{(N-m)!}\int_{\Lambda^{N-m}} e^{-W_N-V_N}H_N d^{N-m}x\right]. \tag{3.2.22}$$

To obtain (3.2.11), notice that the first term on the right hand site of (3.2.22) is equal to $\frac{1}{m!}\rho_v^{(m)}\int_{\Lambda^m}\rho_v^{(m)}hd^m x$. To rewrite the second term, observe that for every $N \geq m$:

$$H_N = \sum_{k=0}^{m}\sum_{1\leq i_1<\cdots i_{m-k}\leq m}\;\sum_{m+1\leq j_1<\cdots j_k\leq N} h(i_1,...,i_{m-k},j_1,...,j_k) \tag{3.2.23}$$

where the corresponding sum over $k$ is set to zero if $N < m+k$, and the third (second) sum disappears if $k=0$ ($k=m$). Using (3.2.23) and symmetry, it can be shown that the second term on the right hand side of (3.2.22), evaluated at $(1,...,m) := (x_1,...,x_m)$, is

$$\sum_{k=0}^{m}\frac{1}{k!}\sum_{1\leq i_1<\cdots i_{m-k}\leq m}\frac{1}{\Xi(v)}\sum_{N=m+k}^{\infty}\frac{1}{(N-m-k)!}\times \int_{\Lambda^{N-m}} e^{-W_N-V_N}(1,...,N)h(i_1,...,i_{m-k},m+1,...,m+k)d(m+1)\cdots dN = \sum_{k=0}^{m}\frac{1}{k!}\sum_{1\leq i_1<\cdots i_{m-k}\leq m}\int_{\Lambda^k}\rho_v^{(m+k)}(1,...,m+k)h(i_1,...,i_{m-k},m+1,...,m+k)\times d(m+1)\cdots d(m+k), \tag{3.2.24}$$

which proves (3.2.11).

Next, using equation (3.2.11) and Lemma 3.2.3, we observe that

$$\left\|K_m(\tilde v)\tilde h\right\|_\infty \le \|\tilde h\|_\infty \left(\frac{1}{m!}\int_{\Lambda^m} \rho_v^{(m)} + \sum_{k=1}^{m} \frac{1}{k!}\binom{m}{k} C_{m,m+k}\right), \tag{3.2.25}$$

and so $K_m(\tilde v) : L_s^\infty(\Lambda^m, d^m x)/M_m \to L_s^\infty(\Lambda^m, d^m x)/M_m$ is bounded. Let

$$\|K_m(\tilde v)\|_{\infty,\infty} := \sup_{\|\tilde f\|_\infty \le 1} \|K_m(\tilde v)\tilde f\|_\infty \tag{3.2.26}$$

be the operator norm of $K_m(\tilde v)$. By Definition 3.2.2 and Lemma 3.2.2,

$$\begin{aligned}\left\|D\rho^{(m)}(\tilde v)\tilde h\right\|_{\mathcal{V}_m} &= \left\|\frac{\rho_v^{(m)}}{\rho_0^{(m)}}\left[\tilde h - K_m(\tilde v)\tilde h\right]\right\|_\infty \le \\ B_{2:m}(v)\|\tilde h - K_m(\tilde v)\tilde h\|_\infty &\le \|\tilde h\|_\infty B_{2:m}(v)\left(1 + \|K_m(\tilde v)\|_{\infty,\infty}\right),\end{aligned} \tag{3.2.27}$$

which shows that $D\rho^{(m)}(\tilde v) : L_s^\infty(\Lambda^m, d^m x)/M_m \to \mathcal{V}_m$ is bounded. The fact that $D\rho^{(m)}(\tilde v)$ is continues with respect to $\tilde v$ can be established by the argument similar in nature to (3.2.14-3.2.27). □

**Lemma 3.2.5.** *The operator $D\rho^{(m)}(\tilde v) : L_s^\infty(\Lambda^m, d^m x)/M_m \to \mathcal{V}_m$ is injective for every $\tilde v \in L_s^\infty(\Lambda^m, d^m x)/M_m$. The same is true for*
*$I - K_m(\tilde v) : L_s^\infty(\Lambda^m, d^m x)/M_m \to L_s^\infty(\Lambda^m, d^m x)/M_m$.*

*Proof.* Suppose $v, h \in L_s^\infty(\Lambda^m, d^m x)$, and set $\tilde v := \pi_m(v)$, $\tilde h = \pi_m(h)$. Then,

$$\begin{aligned}&\int_{\Lambda^m} \tilde h D\rho^{(m)}(\tilde v)\tilde h = \frac{1}{m!}\left(\int_{\Lambda^m} \rho_v^{(m)} h\right)^2 - \sum_{k=0}^{m} \frac{1}{(k!)^2}\frac{m!}{(m-k)!}\times \\ &\int_{\Lambda^{m+k}} \rho_v^{(m+k)}(1, ..., m+k)h(1, ..., m-k, m+1, ..., m+k)h(1, ..., m)d1\cdots d(m+k) \\ &= -\frac{m!}{\Xi(v)}\sum_{N=0}^{\infty}\frac{1}{N!}\int_{\Lambda^N} e^{-W_N - V_N}\left[\sum_{1\le i_1<\cdots<i_m\le N} h(i_1, ..., i_m) - \frac{1}{m!}\int_{\Lambda^m}\rho_v^{(m)} h\right]^2 d1\cdots dN.\end{aligned} \tag{3.2.28}$$

In (3.2.28), the sum over $1 \leq i_1 < \cdots < i_m \leq N$ inside the square brackets is set to zero whenever $0 \leq N \leq m-1$. The first equality in 3.2.28 follows directly from (3.2.11) using the symmetry of particle densities. To verify the second equality, notice that for every $N \geq m$:

$$\begin{aligned}\left[\sum_{1\leq i_1<\cdots<i_m\leq N} h(i_1,...,i_m)\right]^2 &= \sum_{k=0}^{m}\left[\sum_{1\leq i_1<\cdots<i_{m-k}\leq N}\ \sum_{1\leq j_1<\cdots<j_k\leq N}\right. \\ &\left.\sum_{1\leq p_1<\cdots<p_k\leq N} h(i_1,...,i_{m-k},j_1,...,j_k)h(i_1,...,i_{m-k},p_1,...,p_k)\right],\end{aligned} \tag{3.2.29}$$

where the corresponding sum over $k$ is set to zero if $N < m+k$, the last two sums inside the square brackets disappear when $k = 0$, while the first one disappear when $k = m$. Also, the sets $\{i_1, ..., i_{m-k}\}$, $\{j_1, ..., j_k\}$, and $\{p_1, ..., p_k\}$ are pair-wise disjoint. Using (3.2.29) and symmetry, the rightmost hand side of (3.2.28) can be rewritten as

$$\begin{aligned}&-\sum_{k=0}^{m}\frac{1}{(k!)^2}\frac{m!}{(m-k)!}\frac{1}{\Xi(v)}\sum_{N=m+k}^{\infty}\frac{1}{(N-m-k)!}\int_{\Lambda^N} e^{-W_N-V_N}\times \\ &h(1,...,m)h(1,...,m-k,m+1,...,m+k)d1\cdots dN + \frac{1}{m!}\left(\int_{\Lambda^m}\rho_v^{(m)}h\right)^2 \\ &= -\sum_{k=0}^{m}\frac{1}{(k!)^2}\frac{m!}{(m-k)!}\int_{\Lambda^{m+k}}\rho_v^{(m+k)}(1,...,m+k)\times \\ &h(1,...,m)h(1,...,m-k,m+1,...,m+k)d1\cdots d(m+k) + \frac{1}{m!}\left(\int_{\Lambda^m}\rho_v^{(m)}h\right)^2,\end{aligned} \tag{3.2.30}$$

which proves (3.2.28).

Suppose that $D\rho^{(m)}(\tilde{v})\tilde{h} = 0$ for some $\tilde{h} = \pi_m(\tilde{h}) \in L_s^\infty(\Lambda^m, d^m x)/M_m$. Then $\int_{\Lambda^m} \tilde{h} D\rho^{(m)}(\tilde{v})\tilde{h} = 0$, and so the summands on the rightmost hand side of (3.2.28) are equal to zero for all $N \geq 0$. When $N = m$, this implies that

$$\int_{\Lambda^m} e^{-W_m-v}\left(h - \frac{1}{m!}\int_{\Lambda^m}\rho_v^{(m)}h\right)^2 d^m x = 0, \tag{3.2.31}$$

which is equivalent to $h = \frac{1}{m!}\int_{\Lambda^m}\rho_v^{(m)}h$ a.e. on $\Lambda^m \setminus Q_m$. However, when $N = 0$, we obtain that $\int_{\Lambda^m}\rho_v^{(m)}h = 0$, and so $h = 0$ a.e. on $\Lambda^m \setminus Q_m$. This means that $\tilde{h} = 0$, and so $D\rho^{(m)}(\tilde{v})$ is injective. It is easy to see that $D\rho^{(m)}(\tilde{v})$ is injective if and only if $I - K_m(\tilde{v})$ is so. $\square$

To ensure that $D\rho^{(1)}(\tilde{v})$ is invertible, it suffices to require that the pair correlation function

$$h_0^{(2)}(x_1,x_2) := g_0^{(2)}(x_1,x_2) - 1 := \frac{\rho_0^{(2)}(x_1,x_2)}{\rho_0^{(1)}(x_1)\rho_0^{(1)}(x_2)} - 1 \tag{3.2.32}$$

is essentially bounded on $(\Lambda \setminus Q_1) \otimes (\Lambda \setminus Q_1)$. This is certainly true for any fluid [3]. The case with $m \geq 2$ is much harder because the operators on the right hand side of (3.2.11) corresponding to $1 \leq k \leq m-1$ are not integral. (See (3.2.13) for the simplest example.) It is possible to construct a proof that $D\rho^{(m)}(\tilde{v})$ is surjective when $\Lambda = \mathbb{R}^\nu$, $\nu \in \mathbb{N}$. However, we do not pursue this here. Instead, we assume that $\|K_m(0)\|_{\infty,\infty} < 1$. This condition is consistent with fluids at low density and high temperature.

**Lemma 3.2.6.** *(i) Suppose there is $C_0 > 0$ such that $g_0^{(2)} \leq C_0$ a.e. on $(\Lambda \setminus Q_1) \otimes (\Lambda \setminus Q_1)$. Then $D\rho^{(1)}(\tilde{v}) : L_s^\infty(\Lambda, dx)/M_1 \to \mathcal{V}_m$ is invertible for every $\tilde{v} \in L_s^\infty(\Lambda, dx)/M_1$.*

*(ii) Suppose that $1 \leq m < N'$, and $\|K_m(0)\|_{\infty,\infty} < 1$. Then, there is an open set $0 \in \Omega \subset L_s^\infty(\Lambda^m, d^m x)/M_m$ such that $D\rho^{(m)}(\tilde{v}) : L_s^\infty(\Lambda^m, d^m x)/M_m \to \mathcal{V}_m$ is invertible for every $\tilde{v} \in \Omega$.*

*Proof.* (i)

(1) Let $v \in L_s^\infty(\Lambda, dx)$, and $\tilde{v} = \pi_1(v)$. We will begin by proving that $K_1(\tilde{v})$ in (3.2.12) is well defined as operator on $L_s^2(\Lambda, \rho_v^{(1)} dx)$ into $L_s^2(\Lambda, \rho_v^{(1)} dx)$. In fact, if $h \in L_s^2(\Lambda, \rho_v^{(1)} dx)$, then for a.e. $x \in \Lambda \setminus Q_1$:

$$\begin{aligned} \left[K_1(\tilde{v})h\right](x) = \int_\Lambda \left[\rho_v^{(1)}(y) - \frac{\rho_v^{(2)}(x,y)}{\rho_v^{(1)}(x)}\right] h(y)dy = \\ \int_{\Lambda\setminus Q_1} \left[1 - g_v^{(2)}(x,y)\right] h(y)\rho_v^{(1)}(y)dy, \end{aligned} \tag{3.2.33}$$

where in the second equality relation (3.2.1) and the fact that $\Lambda \otimes Q_1 \subset Q_2$ were used. Therefore, by Holder's inequality and Lemma 3.2.2,

$$\left|\left[K_1(\tilde{v})h\right](x)\right| \leq (1 + C_v) \|h\|_{2(\rho_v^{(1)} dx)} \quad \text{for a.e. } x \in \Lambda \setminus Q_1, \tag{3.2.34}$$

with $C_v := C_0 B_{2,2}(v) \left[B_{1:1}(v)\right]^{-2}$. Equation (3.2.34) shows that

$$K_1(\tilde{v})h \in L_s^\infty(\Lambda, dx)/M_1 \subset L_s^2(\Lambda, \rho_v^{(1)} dx). \tag{3.2.35}$$

In addition,

$$\begin{aligned}\|1-g_v^{(2)}\|^2_{2(\rho_v^{(1)}dx*\rho_v^{(1)}dy)} &= \int_{\Lambda\setminus Q_1\otimes\Lambda\setminus Q_1}\left(1-g_v^{(2)}(x,y)\right)^2\rho_v^{(1)}dx\rho_v^{(1)}dy\\ &\le\left[(1+C_v)n_1(v)\right]^2<\infty,\end{aligned}\tag{3.2.36}$$

and so $1-g_v^{(2)}\in L_s^2(\Lambda^2,\rho_v^{(1)}dx\rho_v^{(1)}dy)$. Thus, $K_1(\tilde v):L_s^2(\Lambda,\rho_v^{(1)}dx)\to L_s^2(\Lambda,\rho_v^{(1)}dx)$ is a Hilbert-Schmidt operator, which is compact [32, Theorem XI.6.6]. By Fredholm Alternative, it suffices to show that $I-K_1(\tilde v)$ is injective ([27]). This fact can be established in the same way as Lemma 3.2.5 was. Let us quickly review the steps.

For every $h\in L_s^2\left(\Lambda,\rho_v^{(1)}dx\right)$:

$$\begin{aligned}&\int_\Lambda\left[h-K_1(\tilde v)h\right]\rho_v^{(1)}dx=\\ &\frac{1}{\Xi(v)}\sum_{N=0}^{N'}\frac{1}{N!}\int_{\Lambda^N}e^{-W_N-V_N}\left[\sum_i^N h(x_i)-\int_\Lambda\rho_v^{(1)}h\right]^2dx_1\cdots dx_N\end{aligned}\tag{3.2.37}$$

by (3.2.28) with $m=1$. (Note that the left hand side of (3.2.37) makes sense since $L_s^2\left(\Lambda,\rho_v^{(1)}dx\right)\subset L_s^1\left(\Lambda,\rho_v^{(1)}dx\right)$, and the proof of (3.2.28) still applies.)

Suppose that $h-K_1(\tilde v)h=0$ for some $h\in L_s^2(\Lambda,\rho_v^{(1)}dx)$. Then, $\int_\Lambda\left[h-K_1(\tilde v)h\right]\rho_v^{(1)}dx=0$, and so all the summands on the right hand side of (3.2.37) are equal to zero. For $N=1$, we obtain that

$$\int_\Lambda e^{-W_1-v}\left(h-\int_\Lambda\rho_v^{(1)}h\right)^2dx=0,\tag{3.2.38}$$

and so $h=\int_\Lambda\rho_v^{(1)}hdx$ a.e. $[dx]$ on $\Lambda\setminus Q_1$. From $N=0$, we also have that $h=\int_\Lambda\rho_v^{(1)}hdx=0$ a.e. $[dx]$ on $\Lambda\setminus Q_1$. In view of (3.2.1), this is equivalent to $h=0$ a.e. $[\rho_v^{(1)}dx]$ on $\Lambda$. This establishes the fact that $I-K_1(\tilde v)$ is invertible as an operator on (and onto) $L_s^2\left(\Lambda,\rho_v^{(1)}dx\right)$.

(2) Let us go back to our original setting and consider $D\rho^{(1)}(\tilde v):L_s^\infty(\Lambda,dx)/M_1\to\mathcal{V}$. This operator is injective by Lemma (3.2.5). To prove that it is also surjective, let $f=\omega*\rho_0^{(1)}\in\mathcal{V}$, where $\omega\in L^\infty(\Lambda,dx)$. Since, $\gamma:=-\omega\rho_0^{(1)}[\rho_v^{(1)}]^{-1}\in L^\infty(\Lambda,dx)$ by Lemma 3.2.2 it is also in $L^2(\Lambda,\rho_v^{(1)}dx)$. Therefore, by step (1) there is $h\in L^2(\Lambda,\rho_v^{(1)}dx)$ such that $h-K_1(\tilde v)h=\gamma$. Moreover, $h$ is essentially bounded on $(\Lambda\setminus Q_1)$ in view of (3.2.35). Therefore,

$$f=\omega*\rho_0^{(1)}=-\rho^{(1)}(\tilde v)[\tilde h-K_1(\tilde v)\tilde h]=D\rho^{(1)}(\tilde v)\tilde h,\tag{3.2.39}$$

where $\tilde h=\pi_1(h)$. □

(ii) Let $1 \leq m < N'$, and suppose that $\|K_m(0)\|_{\infty,\infty} < 1$. By continuity of $K_m$, there is an open set $\Omega \in L_s^\infty(\Lambda, dx)/M_m$ such that $\|K_m(\tilde{v})\|_{\infty,\infty} < 1$ whenever $\tilde{v} \in \Omega$. Therefore, $I - K_m(\tilde{v})$ is invertible for all $\tilde{v} \in \Omega$. The rest of the proof is just as at the end of step (2) in (i). (See equation (3.2.39).)

**Theorem 3.2.7.** *If either of the conditions (i) or (ii) in Lemma 3.2.6 are satisfied, then there is open set $A \subset L_s^\infty(\Lambda, dx)/M_m$ such that the map $\rho^{(m)} : A \to \rho^{(m)}(A) \subset L_s^\infty(\Lambda^m, d^m x)/M_m {*} \rho_0^{(m)}$ is a diffeomorphism. For every $f \in \rho^{(m)}(A)$, $\left[D(\rho^{(m)})^{-1}\right](f) = D\rho^{(m)}\left[(\rho^{(m)})^{-1}(f)\right]$.*

*Proof.* The proof is a direct consequence of Lemmas 3.2.4 and 3.2.6 and the Inverse Function Theorem for Banach spaces[33, Theorem 5.2.3 and Corollary 5.3.4]. □

## 3.3 GENERALIZED ORNSTEIN-ZERNIKE EQUATIONS

In this section we show that the existence and differentiability (see remark bellow) of the inverse map $\rho^{(m)} \to v$ for $m \geq 1$ leads to the hierarchy of generalized Ornstein-Zernike (OZ) equations, the first member ($m = 1$) being the original OZ relation in (1.3.11) [3].

**Remark 3.3.1.** Strictly speaking, the OZ equation and its generalizations here are based on the fact that $I - K_m$ in (3.2.11 ) is invertible, regardless whether the derivative of the inverse map exists or not. However, besides the value of its own, the OZ equation is often employed inside various functional integration schemes for obtaining other relations in liquid state theory [3, 5]. In such methods, the differentiability of the inverse map is essential and is implicitly assumed.

To continue, we need to say a few words about the notation used in this section. Since $v$-dependent quantities will appear here only with $v = 0$, the subscript 0 in $\rho_0^{(m)}$, $h_0^{(m)}$, $K_m(0)$ etc. will be dropped. Further, a point $(x_1, ..., x_k) \in \Lambda^k$ will often be denoted by $\mathbf{x}$, with $k$ evident from the context. Finally, for a function $v : \Lambda^m \to \mathbb{R}$ and $1 \leq k \leq m$, let us define

$(\hat{P}_{m,m-k}v) : \Lambda^{m+k} \to \mathbb{R}$ as

$$
\begin{aligned}
&(\hat{P}_{m,m-k}v)(x_1, ..., x_{m+k}) := \\
&\begin{cases} \sum_{1\le i_1<\cdots i_{m-k}\le m} v(x_{i_1}, ..., x_{i_{m-k}}, x_{m+1}, ..., x_{m+k}) & \text{if } 1 \le k \le m-1, \\ v(x_{m+1}, ..., x_{2m}) & \text{if } k = m. \end{cases}
\end{aligned} \tag{3.3.1}
$$

Suppose our system is governed by an energy function $W$, and the conditions described in Section 3.2.1 are satisfied. To review, it is assumed that $W$ satisfies conditions (i) and (ii) in Section 3.1.1, and that $W_N = \infty$ for all $N > N'$ for some $N' > m$. The only slight modification in this section is that instead of (3.1.1 ), we will now require that

$$\left|Q_N^{i_1,\ldots,i_k} \setminus Q_N\right| = 0 \quad \forall 2 \le k < N, \quad \forall 1 \le i_1 < \cdots < i_k \le N, \tag{3.3.2}$$

where $Q_N^{i_1,\ldots,i_k}$ is defined by (3.1.2) with $m$ replaced by $k$. This condition has the same interpretation as (3.1.1). Since $W_1$ is just a constant for uniform fluids, we will also assume that $|Q_1| = 0$. By the arguments found in the proof of Lemma 3.1.1, equation (3.3.2) and $|Q_1| = 0$ imply that $\{\rho^{(k)} = 0\} \sim Q_k$ for every $k \in \mathbb{N}$, and that for every $1 \le k \le \ell$:

$$\rho^{(\ell)} = 0 \text{ a.e. on } \bigcup_{1\le i_1<\cdots<i_k\le \ell} Q_\ell^{i_1,\ldots,i_k}. \tag{3.3.3}$$

(For example, $\rho^{(\ell)} = 0$ a.e. on $\Lambda^{\ell-k} \otimes Q_k = Q_\ell^{\ell-k+1,\ldots,\ell}$.)

Let us define

$$h^{(2m)}(\mathbf{x}, \mathbf{y}) := \frac{\rho^{(2m)}(\mathbf{x}, \mathbf{y})}{\rho^{(m)}(\mathbf{x})\rho^{(m)}(\mathbf{y})} - 1, \tag{3.3.4}$$

for a.e. $(\mathbf{x}, \mathbf{y}) \in (\Lambda^m \setminus Q_m) \otimes (\Lambda^m \setminus Q_m)$, and

$$h^{(m+k)}(\mathbf{x}, \mathbf{y}) := \frac{\rho^{(m+k)}(\mathbf{x}, \mathbf{y})}{\rho^{(m)}(\mathbf{x})\rho^{(k)}(\mathbf{y})} \tag{3.3.5}$$

for $1 \le k \le m-1$, and a.e. $(\mathbf{x}, \mathbf{y}) \in (\Lambda^m \setminus Q_m) \otimes (\Lambda^k \setminus Q_k)$. Using these definitions and in view of (3.3.3), equation (3.2.11) can be rewritten (with $\tilde{v} = 0 \in L^\infty(\Lambda^m, d^m x)/M_m$, and $\tilde{h} = \tilde{\phi} = \pi_m(\phi) \in L^\infty(\Lambda^m, d^m x)/M_m$) as

$$K_m\tilde{\phi} = -\sum_{k=1}^{m} \frac{1}{k!} \int_{\Lambda^k} h^{(m+k)}(\cdot, \mathbf{x})\rho^{(k)}(\mathbf{x})(\hat{P}_{m,m-k}\phi)(\cdot, \mathbf{x})d^k x. \tag{3.3.6}$$

Note that Lemma 3.2.3 implies that for every $1 \le k \le m$

$$\alpha_k := \left\| \int_{\Lambda^{m+k}} |h^{(m+k)}(\cdot, \mathbf{x})| \rho^{(k)}(\mathbf{x}) d^k x \right\|_\infty < \infty. \tag{3.3.7}$$

It is reasonable to expect that for fluids at high temperature and low density

$$\gamma := \sum_{k=1}^{m} \frac{1}{k!} \binom{m}{k} \alpha_k < 1. \tag{3.3.8}$$

In this case, it follows from (3.3.6) and (3.3.8) that $\|K_m\|_{\infty,\infty} \le \gamma < 1$, and so $I - K_m : L^\infty(\Lambda^m, d^m x)/M_m \to L^\infty(\Lambda^m, d^m x)/M_m$ is invertible, with $(I - K_m)^{-1} = I + \sum_{n=1}^{\infty} (K_m)^n =: I + L_m$.

**Lemma 3.3.1.** *Suppose (3.3.8) is true. Then, for every $n \in \mathbb{N}$ and $1 \le k \le m$, there is $h_n^{(m+k)} \in L^1(\Lambda^{m+k}, \rho^{(m)} d^m x \; \rho^{(k)} d^k y)$, symmetric with respect to the interchange of the first $m - k$, the next $k$, and the last $k$ variables, taken separately, such that*

$$\frac{1}{k!} \left\| \int_{\Lambda^k} |h_n^{(m+k)}(\cdot, \mathbf{x})| \rho^{(k)}(\mathbf{x}) d^k x \right\|_\infty \le \gamma^n, \tag{3.3.9}$$

*and for every $\tilde{\phi} = \pi_m(\phi) \in L_s^\infty(\Lambda^m, d^m x)/M_m$:*

$$(K_m)^n \tilde{\phi} = \sum_{k=1}^{m} \frac{1}{k!} H_{m,n}^k \tilde{\phi}, \tag{3.3.10}$$

*where*

$$\begin{aligned} \left[ H_{m,n}^k \tilde{\phi} \right] (x_1, ..., x_m) = & \sum_{1 \le i_1 < \cdots i_{m-k} \le m} \; \sum_{1 \le j_1 < \cdots j_k \le m} \\ & \int_{\Lambda^k} h_n^{(m+k)}(x_{i_1}, ..., x_{i_{m-k}}, x_{j_1}, ..., x_{j_k}, \mathbf{y}) \rho^{(k)}(\mathbf{y}) \phi(x_{i_1}, ..., x_{i_{m-k}}, \mathbf{y}) d^k y \end{aligned} \tag{3.3.11}$$

*for a.e. $(x_1, ..., x_m) \in \Lambda^m \setminus Q_m$. The sets $\{i_1, ..., i_{m-k}\}$ and $\{j_1, ..., j_k\}$ in (3.3.11) are pairwise disjoint.*

*Proof.* The proof proceeds by induction on $n$, with (3.3.6) as a base case. □

**Theorem 3.3.2.** *Suppose (3.3.8) holds. For every $1 \leq k \leq m$, there is a function $c^{(m+k)} \in L^1(\Lambda^{m+k}, \rho^{(m)} d^m x\ \rho^{(k)} d^m y)$, symmetric with respect to the interchange of the first $m-k$, the next $k$, and the last $k$ variables, taken separately, such that*

$$\left\| \int_{\Lambda^k} |c^{(m+k)}(\cdot, \mathbf{x})| \rho^{(k)}(\mathbf{x}) d^k x \right\|_\infty < \infty \tag{3.3.12}$$

*and*

$$\begin{aligned} \left[(L_m)\tilde{\phi}\right](x_1, ..., x_m) = -\sum_{k=1}^{m} \frac{1}{k!} \sum_{1 \leq i_1 < \cdots i_{m-k} \leq m} \sum_{1 \leq j_1 < \cdots j_k \leq m} \\ \int_{\Lambda^k} c^{(m+k)}(x_{i_1}, ..., x_{i_{m-k}}, x_{j_1}, ..., x_{j_k}, \mathbf{y}) \rho^{(k)}(\mathbf{y}) \phi(x_{i_1}, ..., x_{i_{m-k}}, \mathbf{y}) d^k y \end{aligned} \tag{3.3.13}$$

*for every $\tilde{\phi} = \pi_m(\phi) \in L_s^\infty(\Lambda^m, d^m x)/M_m$ and a.e. $(x_1, ..., x_m) \in \Lambda^m \setminus Q_m$. The sets $\{i_1, ..., i_{m-k}\}$ and $\{j_1, ..., j_k\}$ in (3.3.13) are pair-wise disjoint.*

The functions $c^{(m+k)}$ for $1 \leq k \leq m$ are generalizations to the OZ direct correlation function $c^{(2)}$ corresponding to $m = k = 1$.

**Remark 3.3.2.** Recall that according to Lemma 3.2.4,

$$\begin{aligned} \left[D\rho^{(1)}\right]^{-1} \tilde{\varphi} = -\left[I - K_1\right]^{-1} \left(\varphi[\rho^{(1)}]^{-1}\right) = -[I + L_1] \left(\varphi[\rho^{(1)}]^{-1}\right) = \\ -\frac{\varphi}{\rho^{(1)}} + \int_\Lambda c^{(2)}(\cdot, x) dx. \end{aligned} \tag{3.3.14}$$

In the notation used in [3], (3.3.14) is written as

$$c^{(2)}(x_1, x_2) = \frac{\delta v(x_1)}{\delta \rho^{(1)}(x_2)} + \frac{1}{\rho^{(1)}(x_1)} \delta(x_1 - x_2), \tag{3.3.15}$$

which coincides with the definition (1.3.7) given in the introduction.

*Proof of Theorem 3.3.2.* Let $\tilde{\phi} = \pi_m(\phi) \in L_s^\infty(\Lambda^m, d^m x)/M_m$ and $1 \leq k \leq m$. For every $n \in \mathbb{N}$, let us define $L_{m,n}^k := \sum_{i=1}^n H_{m,n}^k$, and $c_n^{(m+k)} := -\sum_{i=1}^n h_i^{(m+k)}$. By (3.3.9), $\left(L_{m,n}\tilde{\phi}\right)_{n=1}^\infty$ is a Cauchy sequence in $L_s^\infty(\Lambda^m, d^m x)/M_m$. Moreover, since (3.3.9) implies that

$$\|h_n^{(m+k)}\|_{1(\rho^{(m)}d^m x \ \rho^{(k)}d^k x)} \leq \gamma^n \|\rho^{(m)}\|_{1(d^m x)} = \gamma^n n_m, \tag{3.3.16}$$

$\left(c_n^{(m+k)}\right)_{n=1}^\infty$ is a Cauchy sequence in $L^1(\Lambda^{m+k}, \rho^{(m)}d^m x \ \rho^{(k)}d^k y)$. Let

$$c^{(m+k)} = \lim_{n\to\infty} c_n^{(m+k)} \in L^1(\Lambda^{m+k}, \rho^{(m)}d^m x \ \rho^{(k)}d^k y) \tag{3.3.17}$$

and $f_k = \lim_{n\to\infty} L_{m,n}^k \tilde{\phi} \in L_s^\infty(\Lambda^m, d^m x)/M_m$. Then, $c^{(m+k)}$ satisfies (3.3.12) , and it remains to show that:

$$\begin{aligned} f_k = g_k := &\sum_{1\leq i_1<\cdots i_{m-k}\leq m} \sum_{1\leq j_1<\cdots j_k\leq m} \\ &\int_{\Lambda^k} c^{(m+k)}(x_{i_1}, ..., x_{i_{m-k}}, x_{j_1}, ..., x_{j_k}, \mathbf{y})\rho^{(k)}(\mathbf{y})\phi(x_{i_1}, ..., x_{i_{m-k}}, \mathbf{y})d^k y \end{aligned} \tag{3.3.18}$$

for a.e. $(x_1, ..., x_m) \in \Lambda^m \setminus Q_m$. In fact, for every $n \in \mathbb{N}$:

$$\begin{aligned} &\|f_k - g_k\|_{1(\rho^{(m)}d^m x)} \leq \left\|f_k - L_{m,n}^k\right\|_{1(\rho^{(m)}dx)} + \\ &\binom{m}{k} \|\phi\|_\infty \left\|c_n^{(m+k)} - c^{(m+k)}\right\|_{1(\rho^{(m)}d^m x \ \rho^{(k)}d^k y)}. \end{aligned} \tag{3.3.19}$$

Since the right hand side of (3.3.19) converges to zero, (3.3.18) follows. □

Each member of the hierarchy of generalized OZ relations is derived from the identity

$$(I + L_m)(I - K_m)] = I, \tag{3.3.20}$$

using equation (3.3.6) and (3.3.13). Let us derive the first two members of the hierarchy explicitly.

(1) When $m = 1$, (3.3.6) and (3.3.13) reduce to

$$K_1\tilde{\phi} = -\int_\Lambda h^{(2)}(\cdot, x)\rho^{(1)}(x)\phi(x)dx \tag{3.3.21}$$

and

$$L_1\tilde{\phi} = -\int_\Lambda c^{(2)}(\cdot, x)\rho^{(1)}(x)\phi(x)dx \tag{3.3.22}$$

respectively. Substituting the last two equations into the identity $K_1\tilde{\phi} = L_1\tilde{\phi} - L_1K_1\tilde{\phi}$, we obtain for a.e. $x_1 \in \Lambda \setminus Q_1$:

$$\begin{aligned}&\int_\Lambda \left\{ h^{(2)}(x_1, x_2) - c^{(2)}(x_1, x_2) - \int_\Lambda c^{(2)}(x_1, x_3)\rho^{(1)}(x_3)h^{(2)}(x_2, x_3)dx_3 \right\} \\ &\rho^{(1)}(x_2)\phi(x_2)dx_2 = 0.\end{aligned} \tag{3.3.23}$$

Taking $\phi$ to be the sign of the integrand in (3.3.23), we see that for a.e. $(x_1, x_2) \in (\Lambda \setminus Q_1) \otimes (\Lambda \setminus Q_1)$ ):

$$h^{(2)}(x_1, x_2) = c^{(2)}(x_1, x_2) + \int_\Lambda h^{(2)}(x_1, x_3)\rho^{(1)}(x_3)c^{(2)}(x_2, x_3)dx_3, \tag{3.3.24}$$

which is the OZ relation (1.3.11).

(2) For $m = 2$, it will be useful to adopt the notation $\hat{S}F(x_1, x_2) = F(x_1, x_2) + F(x_2, x_1)$ for any function $F(x_1, x_2)$. Then, (3.3.6) and (3.3.13) become

$$\begin{aligned}&\left[K_2\tilde{\phi}\right](x_1, x_2) = -\left\{ \frac{1}{2}\int_{\Lambda^2} h^{(4)}(x_1, x_2, y_1, y_2)\rho^{(2)}(y_1, y_2)\phi(y_1, y_2)dy_1dy_2 + \right. \\ &\left. \int_\Lambda \hat{S}[h^{(3)}(x_1, x_2, y)\rho^{(1)}(y)\phi(x_1, y)]dy \right\}\end{aligned} \tag{3.3.25}$$

and

$$\begin{aligned}&\left[L_2\tilde{\phi}\right](x_1, x_2) = -\left\{ \frac{1}{2}\int_{\Lambda^2} c^{(4)}(x_1, x_2, y_1, y_2)\rho^{(2)}(y_1, y_2)\phi(y_1, y_2)dy_1dy_2 + \right. \\ &\left. \int_\Lambda \hat{S}[c^{(3)}(x_1, x_2, y)\rho^{(1)}(y)]\phi(x_1, y)dy \right\}\end{aligned} \tag{3.3.26}$$

for a.e. $(x_1, x_2) \in \Lambda^2 \setminus Q_2$ respectively. Substituting (3.3.25 and (3.3.26) into the identity $K_2\tilde{\phi} = L_2\tilde{\phi} - L_2K_2\tilde{\phi}$, we obtain the generalized OZ equation:

$$\begin{aligned}&\frac{1}{2}h^{(4)}(x_1, x_2, y_1, y_2) + \hat{S}\left[h^{(3)}(x_1, x_2, y_1)\frac{\rho^{(1)}(y_1)\delta(x_1, y_2)}{\rho^{(2)}(y_1, y_2)}\right] = \\ &\frac{1}{2}c^{(4)}(x_1, x_2, y_1, y_2) + \hat{S}\left[c^{(3)}(x_1, x_2, y_1)\frac{\rho^{(1)}(y_1)\delta(x_1, y_2)}{\rho^{(2)}(y_1, y_2)}\right] + \\ &\frac{1}{4}\int_{\Lambda^2} c^{(4)}(x_1, x_2, z_1, z_2)\rho^{(2)}(z_1, z_2)h^{(4)}(z_1, z_2, y_1, y_2)dz_1dz_2 + \\ &\int_\Lambda c^{(4)}(x_1, x_2, y_1, z)\frac{\rho^{(2)}(y_1, z)\rho^{(1)}(y_2)}{\rho^{(2)}(y_1, y_2)}h^{(3)}(y_1, z, y_2)dz + \\ &\frac{1}{2}\int_\Lambda \hat{S}[c^{(3)}(x_1, x_2, z)\rho^{(1)}(z)h^{(4)}(x_1, z, y_1, y_2)]dz + \\ &\hat{S}\left[c^{(3)}(x_1, x_2, y_1)\frac{\rho^{(1)}(y_1)\rho^{(1)}(y_2)}{\rho^{(2)}(y_1, y_2)}h^{(3)}(x_1, y_1, y_2)\right] + \\ &\int_\Lambda \hat{S}\left[c^{(3)}(x_1, x_2, z)\rho^{(1)}(z)\rho^{(1)}(y_1)h^{(3)}(x_1, z, y_1)\delta(x_1, y_2)\right]dz.\end{aligned} \tag{3.3.27}$$

# APPENDIX

## GENERALIZATIONS OF $L^P$ SPACES FOR GRAND CANONICAL FORMULATION

Let $\Lambda$ be a set, and $d\mu_N$ be a measure on $\Lambda^N$ for every $N \in \mathbb{N}$. For $1 \leq p < \infty$,

$$\mathbb{L}^p(d\mu) = \ell^p \left[ \bigoplus_{N=0}^{\infty} L^p \left( \Lambda^N, d\mu_N/N! \right) \right] \tag{A.0.1}$$

is a sequence of functions $f = (f_0 \in \mathbb{R}, f_N \in L^p(\Lambda^N, d\mu_N) \mid N \in \mathbb{N})$ such that

$$|||f|||_{p(d\mu)} := \left[ \sum_{N=0}^{\infty} \frac{1}{N!} ||f_N||^p_{p(d\mu_N)} \right]^{\frac{1}{p}} < \infty. \tag{A.0.2}$$

In the last equation, $||f_0||_{p(d\mu_0)} := |f_0|$, and $||g_0||_{q(d\mu_0)} := |g_0|$.

**Theorem A.0.3** (Holder's inequality)**.** *Let $p > 1$, and suppose that $f \in \mathbb{L}^p(d\mu)$ and $g \in \mathbb{L}^q(d\mu)$, where $1/q = 1 - 1/p$. Then, $fg \in \mathbb{L}^1(d\mu)$, with*

$$|||fg|||_{1(d\mu)} \leq |||f|||_{p(d\mu)} |||g|||_{q(d\mu)}. \tag{A.0.3}$$

*Moreover, If $|||f|||_{p(d\mu)} > 0$, and $|||g|||_{q(d\mu)} > 0$, then equality holds in A.0.3 if and only if there are $\alpha, \beta > 0$ such that $\alpha f_N^p = \beta g_N^q$ a.e. $[d\mu_N]$ for every $N \geq 0$.*

*Proof.* By Holder's inequality used twice:

$$\begin{aligned} |||fg|||_{1(d\mu)} \leq \sum_{N=0}^{\infty} \frac{1}{N!} ||f_N||_{p(d\mu_N)} ||g_N||_{q(d\mu_N)} \leq \\ \left( \sum_{N=0}^{\infty} \frac{1}{N!} ||f_N||^p_{p(d\mu_N)} \right)^{\frac{1}{p}} \left( \sum_{N=0}^{\infty} \frac{1}{N!} ||g_N||^q_{q(d\mu_N)} \right)^{\frac{1}{q}} = |||f|||_{p(d\mu)} |||g|||_{q(d\mu)}. \end{aligned} \tag{A.0.4}$$

Suppose that $|||f|||_{p(d\mu)} > 0$, $|||g|||_{q(d\mu)} > 0$, and there exist $\alpha, \beta > 0$ such that $\alpha f_N^p = \beta g_N^q$ a.e. $[d\mu_N]$ for every $N \geq 0$. Then, the left and right hand sights of A.0.3 reduce to $\left(\frac{\alpha}{\beta}\right)^{\frac{1}{q}} |||f|||^p_{p(d\mu)}$. Conversely, suppose that A.0.3 is an equality. Then, both inequalities in A.0.4 are equalities. The second one implies that there are $\alpha, \beta > 0$ such that $\alpha ||f_N||^p_{p(d\mu_N)} = \beta ||g_N||^q_{q(d\mu_N)}$ for every $N \geq 0$ [4, Theorem 6.2]. (In particular, $||f_N||_{p(d\mu_N)} = 0$ if and only if $||g_N||_{q(d\mu_N)} = 0$.) In fact, one can take $\alpha = 1/|||f|||^p_{p(d\mu)}$, and $\beta = 1/|||g|||^q_{q(d\mu)}$. The first inequality holds only if $||f_N g_N||_{1(d\mu_N)} = ||f_N||_{p(d\mu_N)} ||g_N||_{q(d\mu_N)}$ for every $N \geq 1$. Therefore, for every $N \geq 1$, either $||f_N||_{p(d\mu_N)} = ||g_N||_{q(d\mu_N)} = 0$ or there are $\alpha_N, \beta_N > 0$ such that $\alpha_N |f_N|^p = \beta_N |g_N|^q$ a.e. $[d\mu_N]$. In the later case, integrating over $\Lambda^N$ gives $\alpha_N ||f_N||^p_{p(d\mu_N)} = \beta_N ||g_N||^q_{q(d\mu_N)}$. In view of the conclusion derived from the second inequality, this means that $\alpha/\beta = \alpha_N/\beta_N$, and so $\alpha |f_N|^p = \beta |g_N|^q$ a.e. $[d\mu_N]$ for every $N \geq 0$. $\square$

**Theorem A.0.4** (Jensen's inequality)**.** *Let $f \in \mathbb{L}^1(d\mu)$, with $|||f|||_{1(d\mu)} = 1$, and $g \in \mathbb{L}^1(f d\mu)$. If $\phi : \mathbb{R} \to \mathbb{R}$ is convex, then*

$$\begin{aligned} \langle \phi(g) \rangle_f := \phi(g_0) f_0 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda_N} \phi(g_N) f_N d\mu_N \geq \\ \phi \left( g_0 f_0 + \sum_{N=1}^{\infty} \frac{1}{N!} \int_{\Lambda_N} g_N f_N d\mu_N \right) = \phi\left(\langle g \rangle_f\right). \end{aligned} \tag{A.0.5}$$

*(In case that $|||\phi(g)|||_{1(fd\mu)} = \infty$, the left hand side of A.0.5 is equal to plus infinity.)*

*Moreover, if $\phi$ is strictly convex, then A.0.5 is an equality if and only if $g_N =< g >_f$ a.e. $[f_N d\mu_N]$ for every $N \geq 0$.*

*Proof.* Let $\beta := \sup_{s<t} \frac{\phi(t)-\phi(s)}{t-s}$. Then, $\phi(s) \geq \phi(t) + \beta(s-t)$ for every $s \in \mathbb{R}$ [26, Theorem 3.3]. In particular,

$$\phi(g_N) \geq \phi(t) + \beta(g_N - t) \text{ a.e. } [f_N d\mu_N] \text{ for every } N \geq 0. \tag{A.0.6}$$

If $|||\phi(g)|||_{1(d\mu)} < \infty$, then integrating over $\Lambda^N$ and summing over $N$ the above inequality gives $\langle \phi(g) \rangle_f \geq \phi(\langle g \rangle_f)$, which is A.0.5. If $|||\phi(g)|||_{1(d\mu)} = \infty$, let us write

$$\phi(g_N) = [\phi(g_N) - \phi(t) - \beta(g_N - t)] + [\phi(t) + \beta(g_N - t)]. \tag{A.0.7}$$

Since the first term on the right hand side of A.0.7 in nonnegative by A.0.6, and the second term is in $\mathbb{L}^1(f d\mu)$, it follows that $\langle \phi(g) \rangle_f = \infty$.

Suppose that $g_N = t \in \mathbb{R}$ a.e. $[f_N d\mu_N]$ for every $N \geq 0$. Then, $< g >_f = t$, and $< \phi(g) >_f = \phi(< g >_f) = \phi(t)t$. Conversely, assume that $\phi$ is strictly convex, and $< \phi(g) >_f = \phi(< g >_f)$. Let $t := < g >_f$. Then,

$$0 = < \phi(g) >_f - \phi(t) = \langle < \phi(g) >_f - \phi(t) - \beta(g-t) \rangle >_f . \tag{A.0.8}$$

This equation holds only if A.0.6 is the equality for every $N \geq 0$. However, since $\phi$ is strictly convex, this is possibly only if $g_0 = t$, and $g_N = t$ a.e. $[f_N d\mu_N]$ for every $N \geq 1$. $\square$

It is easy to check that $\mathbb{L}^p(d\mu)$ is a Banach space with the norm $||| \cdot |||_{p(d\mu)}$. In addition, $\mathbb{L}^2(d\mu)$ is a Hilbert space with the inner product defined by $<< f, g >> := |||fg|||_{1(d\mu)}$ for every $f, g \in \mathbb{L}^2(d\mu)$.

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