

The Existence of Pair Potential Corresponding to Specified Density and Pair Correlation

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Abstract

Given a potential of pair interaction and a value of activity, one can consider the Gibbs distribution in a finite domain $\Lambda \subset \mathbb{Z}^d$. It is well known that for small values of activity there exist the infinite volume ($\Lambda \rightarrow \mathbb{Z}^d$) limiting Gibbs distribution and the infinite volume correlation functions. In this paper we consider the converse problem - we show that given ρ_1 and $\rho_2(x)$, where ρ_1 is a constant and $\rho_2(x)$ is a function on \mathbb{Z}^d , which are sufficiently small, there exist a pair potential and a value of activity, for which ρ_1 is the density and $\rho_2(x)$ is the pair correlation function.

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1 Introduction

Let us consider a translation invariant measure μ on the space of particle configurations on the lattice \mathbb{Z}^d . For a given configuration each site can be occupied by one particle or be empty. An m -point correlation function $\rho_m(x_1, \dots, x_m)$ is the probability of finding m different particles at positions $x_1, \dots, x_m \in \mathbb{Z}^d$. The following natural question has been extensively discussed in physical and mathematical literature: given $\rho_1(x_1) \equiv \bar{\rho}_1$ and $\rho_2(x_1, x_2) = \bar{\rho}_2(x_1 - x_2)$, does there exist a measure μ , for which these are the first correlation function (density) and the pair correlation function, respectively?

In the series of papers [3]-[5] Lenard provided a set of relations on the functions ρ_m which are necessary and sufficient for the existence of such a measure. However, given ρ_1

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and ρ_2 , it is not clear how to check if there are some ρ_3, ρ_4, \dots for which these relations hold.

There are several recent papers which demonstrate the existence of particular types of point processes (measures on the space of particle configurations), which correspond to given ρ_1 and ρ_2 under certain conditions on ρ_1 and ρ_2 . In particular, one dimensional point processes of renewal type are considered by Costin and Lebowitz in [2], while determinantal processes are considered by Soshnikov in [8]. In [1] Ambartzumian and Sukiasian prove the existence of a point process corresponding to a sufficiently small density and correlation function. Recently Costin and Lebowitz suggested generalizations of their results. In [9] Stillinger and Torquato consider fields over a space with finitely many points. Besides, for the lattice model, they discuss possible existence of a pair potential for a given density and correlation function using cluster expansion without addressing the issue of convergence.

In this paper we show that if ρ_1 and ρ_2 are small (in a certain sense), there exists a measure on the space of configurations for which ρ_1 is the density and ρ_2 is the pair correlation function. Moreover, this measure is the Gibbs measure corresponding to some pair potential and some value of activity. In a sense, this is the converse of the classical statement that a given potential of pair interaction and a sufficiently small value of activity determine a translation invariant Gibbs measure on the space of particle configurations in \mathbb{Z}^d (or \mathbb{R}^d) and the sequence of infinite volume correlation functions.

2 Notations and Formulation of the Result

We shall consider the following lattice system. Let $\Phi(x)$, $x \in \mathbb{Z}^d$ be a potential of pair interaction and let $U(x_1, \dots, x_n) = \sum_{1 \leq i < j \leq n} \Phi(x_i - x_j)$ be the total potential energy of the configuration (x_1, \dots, x_n) . We assume that $\Phi(x) = \Phi(-x) \geq c_0 > -\infty$ for all x and that $\Phi(0) = +\infty$. The full list of assumptions on $\Phi(x)$ will be given below.

Let Λ be a finite subset of \mathbb{Z}^d . The grand canonical ensemble is defined by a measure on $\bigcup_{n=0}^{\infty} \Lambda^n$, whose restriction on Λ^n is equal to

$$\nu(x_1, \dots, x_n) = \frac{z^n}{n!} e^{-U(x_1, \dots, x_n)} .$$

The parameter $z > 0$ is called the activity. The inverse temperature, which is the factor usually present in front of the function U , is set to be equal to one (or, equivalently, incorporated into the function U). The total mass of the measure is the grand partition function

$$\Xi(\Lambda, z, \Phi) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{(x_1, \dots, x_n) \in \Lambda^n} e^{-U(x_1, \dots, x_n)} .$$

The m -point correlation function is defined as the probability of finding m different par-

ticles at positions $x_1, \dots, x_m \in \Lambda$,

$$\rho_m^\Lambda(x_1, \dots, x_m) = \Xi(\Lambda, z, \Phi)^{-1} \sum_{n=0}^{\infty} \frac{z^{m+n}}{n!} \sum_{(y_1, \dots, y_n) \in \Lambda^n} e^{-U(x_1, \dots, x_m, y_1, \dots, y_n)} .$$

The corresponding measure on the space of all configurations of particles on the set Λ (Gibbs measure) will be denoted by μ^Λ . Given another set $\Lambda_0 \subseteq \Lambda$, we can consider the measure $\mu_{\Lambda_0}^\Lambda$ obtained as a restriction of the measure μ^Λ to the set of particle configurations on Λ_0 .

Given a potential of pair interaction $\Phi(x)$, we define $g(x) = e^{-\Phi(x)} - 1$, $x \in \mathbb{Z}^d$. We shall make the following standard assumptions:

$$g(x) \geq -a > -1 \quad \text{for } x \neq 0. \quad (1)$$

$$g(0) = -1; \quad g(x) = g(-x) \quad \text{for all } x; \quad \sum_{x \neq 0} |g(x)| \leq c < \infty. \quad (2)$$

Clearly, any function $g(x)$ which satisfies (1)-(2) defines a potential of pair interaction via

$$\Phi(x) = -\ln(g(x) + 1) .$$

It is well known ([7], [6]) that when $\Lambda \rightarrow \mathbb{Z}^d$ in a suitable manner (for example, $\Lambda = [-k, k]^d$ and $k \rightarrow \infty$) the following two limits exist for sufficiently small z :

(a) There is a probability measure $\mu^{\mathbb{Z}^d}$ on the space of all configurations on \mathbb{Z}^d , such that

$$\mu_{\Lambda_0}^\Lambda \rightarrow \mu_{\Lambda_0}^{\mathbb{Z}^d} \quad \text{as } \Lambda \rightarrow \mathbb{Z}^d \quad (3)$$

for any finite set $\Lambda_0 \subset \mathbb{Z}^d$.

(b) All the correlation functions converge to the infinite volume correlation functions. Namely,

$$\rho_m^\Lambda(x_1, \dots, x_m) \rightarrow \rho_m(x_1, \dots, x_m) \quad \text{as } \Lambda \rightarrow \mathbb{Z}^d. \quad (4)$$

The infinite volume correlation functions are the probabilities with respect to the measure $\mu^{\mathbb{Z}^d}$ of finding m different particles at positions $x_1, \dots, x_m \in \mathbb{Z}^d$. To make these statements precise we formulate them as a lemma.

Lemma 2.1. ([7], [6]) *Assuming that (1) and (2) hold, there is a positive $\bar{z} = \bar{z}(a, c)$, such that (3) and (4) hold for all $0 < z \leq \bar{z}$ when $\Lambda = [-k, k]^d$ and $k \rightarrow \infty$.*

Thus, a pair potential defines a sequence of infinite volume correlation functions for sufficiently small values of activity. Note that $\rho_m(x_1, \dots, x_m) = 0$ if $x_i = x_j$ for $i \neq j$, since two distinct particles can not occupy the same position. Also note that all the correlation functions are translation invariant,

$$\rho_m(x_1, \dots, x_m) = \rho_m(0, x_2 - x_1, \dots, x_m - x_1) .$$

Thus, ρ_1 is a constant, ρ_2 can be considered as a function of one variable, etc. Let $\bar{\rho}_m$ be the function of $m - 1$ variables, such that

$$\rho_m(x_1, \dots, x_m) = \bar{\rho}_m(x_2 - x_1, \dots, x_m - x_1) . \quad (5)$$

The main result of this paper is the following theorem.

Theorem 2.2. *Let $0 < r < 1$ be a constant. Given any sufficiently small constant $\bar{\rho}_1$ and any function $\bar{\rho}_2(x)$, such that $\bar{\rho}_2(0) = 0$ and $\sum_{x \neq 0} |\bar{\rho}_2(x) - \bar{\rho}_1^2| \leq r\bar{\rho}_1^2$, there are a potential $\Phi(x)$, which satisfies (1)-(2), and a value of activity z , such that $\bar{\rho}_1$ and $\bar{\rho}_2(x)$ are the first and the second correlation functions respectively for the system defined by (z, Φ) .*

Remark 1. Let $\xi(x)$ be a random field with values 0 and 1 (which is the same as a measure on the space of particle configurations), and let $\bar{\rho}_1$ and $\bar{\rho}_2(x)$ be its first two correlation functions. Then

$$E(\xi(x) - \bar{\rho}_1)(\xi(0) - \bar{\rho}_1) = \begin{cases} \bar{\rho}_1 - \bar{\rho}_1^2 & \text{if } x = 0 \\ \bar{\rho}_2(x) - \bar{\rho}_1^2 & \text{otherwise.} \end{cases}$$

The positive definiteness of this function, which is necessary for the existence of the field $\xi(x)$ with the given $\bar{\rho}_1$ and $\bar{\rho}_2(x)$, is clearly guaranteed by the conditions of the theorem if $\bar{\rho}_1$ is sufficiently small.

Remark 2. As will seen from the proof of the theorem, the pair potential and the activity corresponding to given $\bar{\rho}_1$ and $\bar{\rho}_2(x)$ are unique, if we restrict consideration to sufficiently small values of Φ and z . The method of the proof allows one to explore the properties of the pair potential based on the properties of the correlation function.

The outline of the proof is the following. In Sections 3 and 4, assuming that a pair potential and a value of the activity exist, we express the correlation functions (or, rather, the cluster functions, which are closely related to the correlation functions) in terms of the pair potential and the activity. This relationship can be viewed as an equation for unknown Φ and z . In Section 5 we use the contracting mapping principle to demonstrate that this equation has a solution. In Section 6 we provide the technical estimates needed to prove that the right hand side of the equation on Φ and z is indeed a contraction.

3 Cluster Functions and Ursell Functions

In this section we shall obtain a useful expression for cluster functions in terms of the pair potential. The cluster functions are closely related to the correlation functions. Some of the general known facts will be stated in this section without proofs. The reader is referred to Chapter 4 of [7] for a more detailed exposition.

Let A be the complex vector space of sequences ψ ,

$$\psi = (\psi_m(x_1, \dots, x_m))_{m \geq 0}$$

such that, for each $m \geq 1$, ψ_m is a bounded function on \mathbb{Z}^{md} , and ψ_0 is a complex number. It will be convenient to represent a finite sequence (x_1, \dots, x_m) by a single letter $X = (x_1, \dots, x_m)$. We shall write

$$\psi(X) = \psi_m(x_1, \dots, x_m).$$

Let now $\psi^1, \psi^2 \in A$. We define

$$\psi^1 * \psi^2(X) = \sum_{Y \subseteq X} \psi^1(Y) \psi^2(X \setminus Y),$$

where the summation is over all subsequences Y of X and $X \setminus Y$ is the subsequence of X obtained by striking out the elements of Y in X .

Let A_+ be the subspace of A formed by the elements ψ such that $\psi_0 = 0$. Let $\mathbf{1}$ be the unit element of A ($\mathbf{1}_0 = 1, \mathbf{1}_m \equiv 0$ for $m \geq 1$).

We define the mapping Γ of A_+ onto $\mathbf{1} + A_+$:

$$\Gamma\varphi = \mathbf{1} + \varphi + \frac{\varphi * \varphi}{2!} + \frac{\varphi * \varphi * \varphi}{3!} + \dots$$

The mapping Γ has an inverse Γ^{-1} on $\mathbf{1} + A_+$:

$$\Gamma^{-1}(\mathbf{1} + \varphi') = \varphi' - \frac{\varphi' * \varphi'}{2} + \frac{\varphi' * \varphi' * \varphi'}{3} - \dots$$

It is easy to see that $\Gamma\varphi(X)$ is the sum of the products $\varphi(X_1) \dots \varphi(X_r)$ corresponding to all the partitions of X into subsequences X_1, \dots, X_r . If $\varphi \in A_+$ and $\psi = \Gamma\varphi$, the first few components of ψ are

$$\psi_0 = 1; \quad \psi_1(x_1) = \varphi_1(x_1); \quad \psi_2(x_1, x_2) = \varphi_2(x_1, x_2) + \varphi_1(x_1)\varphi_1(x_2).$$

Let Φ be a pair correlation function which satisfies (1)-(2), and let $z \leq \bar{z}(a, c)$. Note that the sequence of correlation functions $\rho = (\rho_m)_{m \geq 0}$ (with $\rho_0 = 1$) is an element of $\mathbf{1} + A_+$.

Definition 3.1. *The cluster functions $\omega_m(x_1, \dots, x_m)$, $m \geq 1$ are defined by*

$$\omega = \Gamma^{-1}\rho.$$

Thus,

$$\omega_1(x_1) = \rho_1(x_1); \quad \omega_2(x_1, x_2) = \rho_2(x_1, x_2) - \rho_1(x_1)\rho_1(x_2),$$

or, equivalently,

$$\bar{\omega}_1 = \bar{\rho}_1; \quad \bar{\omega}_2(x) = \bar{\rho}_2(x) - \bar{\rho}_1^2$$

where $\bar{\omega}_m$ are defined as in (5).

Let $\psi \in \mathbf{1} + A_+$ be defined by

$$\psi_0 = 1; \quad \psi_m(x_1, \dots, x_m) = e^{-U(x_1, \dots, x_m)} .$$

Define also

$$\varphi = \Gamma^{-1}\psi .$$

Definition 3.2. *The functions ψ_m and φ_m are called Boltzmann factors and Ursell functions, respectively.*

Lemma 3.3. *([7]) The cluster functions can be expressed in terms of the Ursell functions as follows*

$$\omega_m(x_1, \dots, x_m) = z^m \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \varphi_{m+n}(x_1, \dots, x_m, y_1, \dots, y_n) .$$

We shall later need certain estimates on the Ursell functions in terms of the potential. To this end we obtain a recurrence formula on a set of functions related to the Ursell functions. Given $X = (x_1, \dots, x_m)$, we define the operator $D_X : A \rightarrow A$ by

$$(D_X \psi)_n(y_1, \dots, y_n) = \psi_{m+n}(x_1, \dots, x_m, y_1, \dots, y_n) .$$

Then define

$$\tilde{\varphi}_X = \psi^{-1} * D_X \psi ,$$

where ψ is the sequence of Boltzmann factors, and ψ^{-1} is such that $\psi^{-1} * \psi = \mathbf{1}$. It can be seen that

$$\varphi_{1+n}(x_1, y_1, \dots, y_n) = \tilde{\varphi}_{x_1}(y_1, \dots, y_n) \quad (6)$$

and that the functions $\tilde{\varphi}_X$ satisfy a certain recurrence relation, which we state here as a lemma.

Lemma 3.4. *([7]) The functions $\tilde{\varphi}_X$ satisfy the following recurrence relation*

$$\tilde{\varphi}_X(Y) = \exp\left(-\sum_{i=2}^m \Phi(x_i - x_1)\right) \sum_{S \subseteq Y} \prod_{j, y_j \in S} (\exp(-\Phi(y_j - x_1)) - 1) \tilde{\varphi}_{S \cup X \setminus x_1}(Y \setminus S) , \quad (7)$$

where $X = (x_1, \dots, x_m)$, $m \geq 1$, $Y = (y_1, \dots, y_n)$, $n \geq 0$, and $\tilde{\varphi}_X(Y) = \mathbf{1}$ if $m = 0$.

4 Equations Relating the Potential, the Activity, and the Cluster Functions

In this section we shall recast the main theorem in terms of the cluster functions and examine a system of equations, which relates the first two cluster functions with the pair potential and the activity.

First, Theorem 2.2 can clearly be re-formulated as follows

Proposition 4.1. *Let $0 < r < 1$ be a constant. Given any sufficiently small constant $\bar{\omega}_1$ and any function $\bar{\omega}_2(x)$, such that $\bar{\omega}_2(0) = -\bar{\omega}_1^2$ and $\sum_{x \neq 0} |\bar{\omega}_2(x)| \leq r \bar{\omega}_1^2$, there are a potential $\Phi(x)$, which satisfies (1)-(2), and a value of activity z , such that $\bar{\omega}_1$ and $\bar{\omega}_2(x)$ are the first and the second cluster functions respectively for the system defined by (z, Φ) .*

Consider the power expansions for ω_1 and ω_2 , which are provided by Lemma 3.3. Let us single out the first term in both expansions. Note the translation invariance of the functions ω_m and φ_m and the fact that $\varphi(x_1, x_2) = g(x_1 - x_2)$.

$$\bar{\omega}_1 = z + z^2 \sum_{n=1}^{\infty} \frac{z^{n-1}}{n!} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \varphi_{1+n}(0, y_1, \dots, y_n) , \quad (8)$$

$$\bar{\omega}_2(x) = z^2 g(x) + z^3 \sum_{n=1}^{\infty} \frac{z^{n-1}}{n!} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \varphi_{2+n}(0, x, y_1, \dots, y_n) . \quad (9)$$

Let

$$A(z, g) = \sum_{n=1}^{\infty} \frac{z^{n-1}}{n!} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \varphi_{1+n}(0, y_1, \dots, y_n) ,$$

$$B(z, g)(x) = \sum_{n=1}^{\infty} \frac{z^{n-1}}{n!} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \varphi_{2+n}(0, x, y_1, \dots, y_n) .$$

Thus the equations (8) and (9) can be rewritten as follows

$$z = \bar{\omega}_1 - z^2 A(z, g) , \quad (10)$$

$$g = \frac{\bar{\omega}_2}{z^2} - z B(z, g) . \quad (11)$$

Instead of looking at (10)-(11) as a formula defining $\bar{\omega}_1$ and $\bar{\omega}_2$ by a given pair potential and the activity, we can instead consider the functions $\bar{\omega}_1$ and $\bar{\omega}_2$ fixed, and g and z unknown. Thus, Proposition 4.1 follows from the following.

Proposition 4.2. *If $\bar{\omega}_1$ and $\bar{\omega}_2$ satisfy the assumptions of Proposition 4.1, then the system (10)-(11) has a solution (z, g) , such that the function g satisfies (1)-(2) and $z \leq \bar{z}(a, c)$.*

5 Proof of the Main Result

This section is devoted to the proof of Proposition 4.2. We shall need the following notations. Let \mathcal{G} be the space of functions g , which satisfy (2) with some $c < \infty$. Let $\|g\| = \sum_{x \neq 0} |g(x)|$. This is not a norm, since \mathcal{G} is not a linear space, however $d(g_1, g_2) = \|g_1 - g_2\|$ is a metric on the space \mathcal{G} . Let \mathcal{G}_c be the set of elements of \mathcal{G} for which $\|g\| \leq c$. Note that if $c < 1$ then all elements of \mathcal{G}_c satisfy (1) with $a = c$.

We also define $I_{z_0}^{a_1, a_2} = [a_1 z_0, a_2 z_0]$. Let $D = I_{z_0}^{a_1, a_2} \times \mathcal{G}_c$. Note that if $c < 1$ then $(z, g) \in D$ implies that $z \leq \bar{z}(c, c)$ if z_0 is sufficiently small. Thus, the infinite volume correlation functions and cluster functions are correctly defined for $(z, g) \in D$ if z_0 is sufficiently small.

Let us define an operator Q on the space of pairs $(z, g) \in D$ by $Q(z, g) = (z', g')$, where

$$z' = \bar{\omega}_1 - z^2 A(z, g) , \quad (12)$$

$$g'(x) = \frac{\bar{\omega}_2(x)}{z^2} - zB(z, g)(x) \quad \text{for } x \neq 0; \quad g'(0) = -1 . \quad (13)$$

We shall prove the following lemma.

Lemma 5.1. *Let $0 < r < 1$ be a constant. There exist positive constants $a_1 < 1$, $a_2 > 1$, and $c < 1$ such that the equation $(z, g) = Q(z, g)$ has a solution $(z, g) \in D$ for all sufficiently small z_0 if $\bar{\omega}_1 = z_0$, $\bar{\omega}_2(0) = -z_0^2$, and $\sum_{x \neq 0} |\bar{\omega}_2(x)| \leq rz_0^2$.*

Before we prove this lemma, let us verify that it implies Proposition 4.2. Let $0 < r < 1$ be fixed and let $\bar{\omega}_1$ be sufficiently small for the statement of Lemma 5.1 to be valid. Let $\bar{\omega}_2$ be such that $\bar{\omega}_2(0) = -\bar{\omega}_1^2$ and $\sum_{x \neq 0} |\bar{\omega}_2(x)| \leq r\bar{\omega}_1^2$. Let (z, g) be the solution of $(z, g) = Q(z, g)$, whose existence is guaranteed by Lemma 5.1. Let $\bar{\omega}'_1$ and $\bar{\omega}'_2$ be the first two cluster functions corresponding to the pair (z, g) . Note that $\bar{\omega}_1$ and $\bar{\omega}'_1$ satisfy the same equation

$$z = \bar{\omega}_1 - z^2 A(z, g) ; \quad z = \bar{\omega}'_1 - z^2 A(z, g) .$$

Therefore, $\bar{\omega}_1 = \bar{\omega}'_1$. The functions $\bar{\omega}_2$ and $\bar{\omega}'_2$ also satisfy the same equation

$$g(x) = \frac{\bar{\omega}_2(x)}{z^2} - zB(z, g)(x) ; \quad g(x) = \frac{\bar{\omega}'_2(x)}{z^2} - zB(z, g)(x) ; \quad \text{for } x \neq 0 .$$

Thus, $\bar{\omega}_2(x) = \bar{\omega}'_2(x)$ for $x \neq 0$. The fact that $\bar{\omega}_2(0) = \bar{\omega}'_2(0)$ follows from

$$\bar{\omega}_2(0) = -\bar{\omega}_1^2 = -\bar{\omega}'_1{}^2 = \bar{\omega}'_2(0) .$$

Thus it remains to prove Lemma 5.1. The proof will be based on the fact that for small z_0 the operator $Q : D \rightarrow D$ is a contraction in an appropriate metric. Define

$$d_{z_0}(z_1, z_2) = \frac{h|z_1 - z_2|}{z_0} .$$

The value of the constant h will be specified later. Now the metric on D is given by

$$\rho((z_1, g_1), (z_2, g_2)) = d_{z_0}(z_1, z_2) + d(g_1, g_2) .$$

Lemma 5.1 clearly follows from the contracting mapping principle and the following lemma

Lemma 5.2. *Let $0 < r < 1$ be a constant. There exist positive constants $a_1 < 1$, $a_2 > 1$, and $c < 1$ such that for all sufficiently small z_0 the operator Q acts from the domain D into itself and is uniformly contracting in the metric ρ for some value of $h > 0$, provided that $\bar{\omega}_1 = z_0$, $\bar{\omega}_2(0) = -z_0^2$, and $\sum_{x \neq 0} |\bar{\omega}_2(x)| \leq rz_0^2$.*

Proof. Take $c = \frac{r+2}{3}$, $a_1 = \sqrt{\frac{2r}{r+1}}$, $a_2 = 2$. We shall need certain estimates on the values of $A(z, g)$ and $B(z, g)$ for $(z, g) \in D$. Namely, there exist universal constants u_1, \dots, u_6 , such that for sufficiently small z_0 we have

$$\sup_{(z,g) \in D} |A(z, g)| \leq u_1 . \quad (14)$$

$$\sup_{(z,g) \in D} \sum_{x \neq 0} |B(z, g)(x)| \leq u_2 . \quad (15)$$

$$\sup_{(z_1, g), (z_2, g) \in D} |A(z_1, g) - A(z_2, g)| \leq u_3 |z_1 - z_2| . \quad (16)$$

$$\sup_{(z, g_1), (z, g_2) \in D} |A(z, g_1) - A(z, g_2)| \leq u_4 d(g_1, g_2) . \quad (17)$$

$$\sup_{(z_1, g), (z_2, g) \in D} \sum_{x \neq 0} |B(z_1, g)(x) - B(z_2, g)(x)| \leq u_5 |z_1 - z_2| . \quad (18)$$

$$\sup_{(z, g_1), (z, g_2) \in D} \sum_{x \neq 0} |B(z, g_1)(x) - B(z, g_2)(x)| \leq u_6 d(g_1, g_2) . \quad (19)$$

These estimates follow from Lemma 6.1 below. For now, assuming that they are true, we continue with the proof of Lemma 5.2. The fact that $QD \subseteq D$ is guaranteed by the inequalities

$$z_0 + (a_2 z_0)^2 u_1 \leq a_2 z_0 , \quad (20)$$

$$z_0 - (a_2 z_0)^2 u_1 \geq a_1 z_0 , \quad (21)$$

$$\frac{r z_0^2}{(a_1 z_0)^2} + a_2 z_0 u_2 \leq c . \quad (22)$$

It is clear that (20)-(22) hold for sufficiently small z_0 . Let us now demonstrate that for some h and for all sufficiently small z_0 we have

$$\rho(Q(z_1, g_1), Q(z_2, g_2)) \leq \frac{1}{2} \rho((z_1, g_1), (z_2, g_2)) \quad \text{if } (z_1, g_1), (z_2, g_2) \in D. \quad (23)$$

First, taking (14), (16), and (17) into account, we note that

$$\begin{aligned} d_{z_0}(z_1^2 A(z_1, g_1), z_2^2 A(z_2, g_2)) &\leq d_{z_0}(z_1^2 A(z_1, g_1), z_2^2 A(z_1, g_1)) + \\ &d_{z_0}(z_2^2 A(z_1, g_1), z_2^2 A(z_2, g_1)) + d_{z_0}(z_2^2 A(z_2, g_1), z_2^2 A(z_2, g_2)) \leq \\ &\frac{u_1 h |z_1^2 - z_2^2|}{z_0} + \frac{u_3 h (a_2 z_0)^2 |z_1 - z_2|}{z_0} + \frac{u_4 h (a_2 z_0)^2 d(g_1, g_2)}{z_0} . \end{aligned}$$

If h is fixed, the right hand side of this inequality can be estimated from above, for all sufficiently small z_0 , by

$$\frac{1}{6} (d_{z_0}(z_1, z_2) + d(g_1, g_2)).$$

Similarly,

$$\begin{aligned} \sum_{x \neq 0} |z_1 B(z_1, g_1)(x) - z_2 B(z_2, g_2)(x)| &\leq \sum_{x \neq 0} |z_1 B(z_1, g_1)(x) - z_2 B(z_1, g_1)(x)| + \\ \sum_{x \neq 0} |z_2 B(z_1, g_1)(x) - z_2 B(z_2, g_1)(x)| &+ \sum_{x \neq 0} |z_2 B(z_2, g_1)(x) - z_2 B(z_2, g_2)(x)| \leq \\ &u_2 |z_1 - z_2| + u_5 a_2 z_0 |z_1 - z_2| + u_6 a_2 z_0 d(g_1, g_2) . \end{aligned}$$

Again, if h is fixed, the right hand side of this inequality can be estimated from above, for all sufficiently small z_0 , by

$$\frac{1}{6} (d_{z_0}(z_1, z_2) + d(g_1, g_2)).$$

Finally,

$$\sum_{x \neq 0} \left| \frac{\bar{\omega}_2(x)}{z_1^2} - \frac{\bar{\omega}_2(x)}{z_2^2} \right| \leq r z_0^2 \left| \frac{1}{z_1^2} - \frac{1}{z_2^2} \right| \leq \frac{2a_2 |z_1 - z_2|}{a_1^4 z_0} .$$

We can now take $h = \frac{12a_2}{a_1^4}$, which implies that the right hand side of the last inequality can be estimated from above by $\frac{1}{6} d_{z_0}(z_1, z_2)$. We have thus demonstrated the validity of (23), which means that the operator Q is uniformly contracting. This completes the proof of the lemma. \square

6 Estimates on the Ursell Functions

In this section we shall derive certain estimates on the Ursell functions, which, in particular, will imply the inequalities (14)-(19).

Lemma 6.1. *Suppose that the functions $g_1(x)$ and $g_2(x)$ satisfy (2) with $c < 1$. Let $\varphi^k = (\varphi_m^k(x_1, \dots, x_m))_{m \geq 0}$, $k = 1, 2$ be the corresponding Ursell functions. Then there exist constants q_1 and q_2 such that*

$$\begin{aligned} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} |\varphi_{1+n}^k(0, y_1, \dots, y_n)| &\leq n! q_1^{n+1}, \quad k = 1, 2, \\ \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} |\varphi_{1+n}^1(0, y_1, \dots, y_n) - \varphi_{1+n}^2(0, y_1, \dots, y_n)| &\leq n! q_2^{n+1} \|g_1 - g_2\| . \end{aligned}$$

Note that the inequalities (14)-(19) immediately follow from this lemma and the definitions of $A(z, g)$ and $B(z, g)(x)$.

Recall that in Section 3 we introduced the functions $\tilde{\varphi}_X(Y)$, which were closely related to the Ursell functions. Given $g_1(x)$ and $g_2(x)$ which satisfy (2) with $c < 1$, we now define

$$r^k(m, n) = \sup_{(x_1, \dots, x_m)} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} |\tilde{\varphi}_{(x_1, \dots, x_m)}^k(y_1, \dots, y_n)|, \quad k = 1, 2,$$

$$d(m, n) = \sup_{(x_1, \dots, x_m)} \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} |\tilde{\varphi}_{(x_1, \dots, x_m)}^1(y_1, \dots, y_n) - \tilde{\varphi}_{(x_1, \dots, x_m)}^2(y_1, \dots, y_n)| .$$

We shall prove the following lemma.

Lemma 6.2. *Suppose that the functions $g_1(x)$ and $g_2(x)$ satisfy (2) with $c < 1$. Then there exist constants q_1 and q_2 such that*

$$r^k(m, n) \leq n!q_1^{m+n} , \quad k = 1, 2, \quad (24)$$

$$d(m, n) \leq n!q_2^{m+n} \|g_1 - g_2\| . \quad (25)$$

Since we can express the Ursell functions in terms of $\tilde{\varphi}_X(Y)$ via (6), Lemma 6.2 immediately implies Lemma 6.1. It remains to prove Lemma 6.2.

Proof of Lemma 6.2. The estimate (24) follows from (4.27) of [7], and thus we shall not prove it here. We proceed with the proof of (25).

In the definition of $d(m, n)$ we can take the supremum over a restricted set of sequences (x_1, \dots, x_m) , namely those sequences, for which all x_i are distinct. Indeed, if $x_i = x_j$ for $i \neq j$, then $\tilde{\varphi}_{(x_1, \dots, x_m)}^1(y_1, \dots, y_n) = \tilde{\varphi}_{(x_1, \dots, x_m)}^2(y_1, \dots, y_n) = 0$, as follows from the definition of $\tilde{\varphi}_X(Y)$.

Let $f_k(x) = e^{-\Phi_k(x)} = g_k(x) + 1$, $k = 1, 2$. We shall need the fact that if \mathcal{X} is any set, which does not contain x_1 , then

$$\prod_{x \in \mathcal{X}} f_k(x - x_1) \leq \exp\left(\sum_{x \in \mathcal{X}} \ln(g_k(x - x_1) + 1)\right) \leq \exp\left(\sum_{x \in \mathcal{X}} g_k(x - x_1)\right) \leq e^c .$$

The proof of (25) will proceed via an induction on $m + n$. Assume that x_1, \dots, x_m are all distinct. From the recurrence relation (7) it follows that

$$\begin{aligned} & \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} |\tilde{\varphi}_{(x_1, \dots, x_m)}^1(y_1, \dots, y_n) - \tilde{\varphi}_{(x_1, \dots, x_m)}^2(y_1, \dots, y_n)| = \\ & \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \left| \prod_{i=2}^m f_1(x_i - x_1) \sum_{S \subseteq Y} \prod_{j, y_j \in S} g_1(y_j - x_1) \tilde{\varphi}_{S \cup X \setminus x_1}^1(Y \setminus S) - \right. \\ & \left. \prod_{i=2}^m f_2(x_i - x_1) \sum_{S \subseteq Y} \prod_{j, y_j \in S} g_2(y_j - x_1) \tilde{\varphi}_{S \cup X \setminus x_1}^2(Y \setminus S) \right| \leq I_1 + I_2, \end{aligned}$$

where

$$I_1 = \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \sum_{S \subseteq Y} \left| \prod_{i=2}^m f_1(x_i - x_1) \prod_{j, y_j \in S} g_1(y_j - x_1) (\tilde{\varphi}_{S \cup X \setminus x_1}^1(Y \setminus S) - \tilde{\varphi}_{S \cup X \setminus x_1}^2(Y \setminus S)) \right| ,$$

$$I_2 = \sum_{y_1, \dots, y_n \in \mathbb{Z}^d} \sum_{S \subseteq Y} \left| \prod_{i=2}^m f_1(x_i - x_1) \prod_{j, y_j \in S} g_1(y_j - x_1) - \right.$$

$$\prod_{i=2}^m f_2(x_i - x_1) \prod_{j, y_j \in S} g_2(y_j - x_1) |\tilde{\varphi}_{S \cup X \setminus x_1}^2(Y \setminus S)|.$$

Note that there are $\frac{n!}{s!(n-s)!}$ subsequences S of the sequence Y , which are of length s . Rearranging the sum, so that to take it over all possible values of s , we see that

$$\begin{aligned} I_1 &\leq \sum_{s=0}^n \frac{n!}{s!(n-s)!} \sum_{y_1, \dots, y_s \in \mathbb{Z}^d} \left| \prod_{i=2}^m f_1(x_i - x_1) \prod_{j=1}^s g_1(y_j - x_1) \right| d(m+s-1, n-s) \leq \\ &\sum_{s=0}^n \frac{n!}{s!(n-s)!} e^c (1+c)^s d(m+s-1, n-s). \end{aligned}$$

Similarly,

$$\begin{aligned} I_2 &\leq \sum_{s=0}^n \frac{n!}{s!(n-s)!} \sum_{y_1, \dots, y_s \in \mathbb{Z}^d} \left| \prod_{i=2}^m f_1(x_i - x_1) \prod_{j=1}^s g_1(y_j - x_1) - \right. \\ &\left. \prod_{i=2}^m f_2(x_i - x_1) \prod_{j=1}^s g_2(y_j - x_1) \right| r(m+s-1, n-s). \end{aligned}$$

Let

$$F_k^{a,b} = \prod_{i=a}^b |f_k(x_i - x_1)|, \quad \text{where } 2 \leq a \leq b \leq m \quad \text{and} \quad k = 1, 2,$$

$$G_k^{a,b} = \prod_{i=a}^b |g_k(y_i - x_1)|, \quad \text{where } 1 \leq a \leq b \leq s \quad \text{and} \quad k = 1, 2.$$

Note that

$$F_k^{a,b} \leq e^c, \quad (26)$$

$$\sum_{y_a, \dots, y_b \in \mathbb{Z}^d} G_k^{a,b} \leq (1+c)^{b-a+1}. \quad (27)$$

Then,

$$\begin{aligned} &\sum_{y_1, \dots, y_s \in \mathbb{Z}^d} \left| \prod_{i=2}^m f_1(x_i - x_1) \prod_{j=1}^s g_1(y_j - x_1) - \prod_{i=2}^m f_2(x_i - x_1) \prod_{j=1}^s g_2(y_j - x_1) \right| \leq \\ &\sum_{y_1, \dots, y_s \in \mathbb{Z}^d} [|f_1(x_2 - x_1) - f_2(x_2 - x_1)| F_1^{3,m} G_1^{1,s} + \\ &F_2^{2,2} |f_1(x_3 - x_1) - f_2(x_3 - x_1)| F_1^{4,m} G_1^{1,s} + \dots + F_2^{2,m-1} |f_1(x_m - x_1) - f_2(x_m - x_1)| G_1^{1,s} + \\ &F_2^{2,m} |g_1(y_1 - x_1) - g_2(y_1 - x_1)| G_1^{2,s} + \dots + F_2^{2,m} G_2^{1,s-1} |g_1(y_s - x_1) - g_2(y_s - x_1)|]. \end{aligned}$$

There are $m + s$ terms inside the square brackets. In addition to (26) and (27) we use the fact that

$$\begin{aligned} |f_1(x_i - x_1) - f_2(x_i - x_1)| &\leq \|g_1 - g_2\|, \quad 2 \leq i \leq m, \\ \sum_{y_i \in \mathbb{Z}^d} |g_1(y_i - x_1) - g_2(y_i - x_1)| &\leq \|g_1 - g_2\|, \quad 1 \leq i \leq n. \end{aligned}$$

Therefore, the entire sum can be estimated from above by

$$(m + s)e^{2c}(1 + c)^s \|g_1 - g_2\|.$$

Therefore,

$$\begin{aligned} I_2 &\leq \sum_{s=0}^n \frac{n!}{s!(n-s)!} (m + s)e^{2c}(1 + c)^s \|g_1 - g_2\| r(m + s - 1, n - s) \leq \\ &\|g_1 - g_2\| (m + n)e^{2c} n! q_1^{m+n-1} \sum_{s=0}^n \frac{(1 + c)^s}{s!} \leq \|g_1 - g_2\| (m + n)e^{1+3c} n! q_1^{m+n-1}. \end{aligned}$$

Combining this with the estimate on I_1 we see that

$$\begin{aligned} d(m, n) &\leq \sum_{s=0}^n \frac{n!}{s!(n-s)!} e^c (1 + c)^s d(m + s - 1, n - s) + \\ &\|g_1 - g_2\| (m + n)e^{1+3c} n! q_1^{m+n-1}. \end{aligned}$$

Let us use induction on $m + n$ to prove that

$$d(m, n) \leq n! q_2^{m+n} \|g_1 - g_2\| (m + n) \quad (28)$$

for some value of q_2 . The statement is obviously true for $m + n = 0$. Assuming that the induction hypothesis holds for all m', n' with $m' + n' \leq m + n - 1$, we obtain

$$\begin{aligned} d(m, n) &\leq \sum_{s=0}^n \frac{n!}{s!(n-s)!} e^c (1 + c)^s (n - s)! q_2^{m+n-1} \|g_1 - g_2\| (m + n - 1) + \\ &\|g_1 - g_2\| (m + n)e^{1+3c} n! q_1^{m+n-1} \leq \\ &\|g_1 - g_2\| (m + n)e^{1+3c} n! (q_1^{m+n-1} + q_2^{m+n-1}). \end{aligned}$$

The expression in the right hand side of this inequality is estimated from above by the right hand side of (28) if $q_2 = 2e^{1+3c} \max(1, q_1)$. Thus, (28) holds for all m, n with this choice of q_2 . Note that we can get rid of the factor $(m + n)$ in the right hand side of (28) by taking a larger value of q_2 . This completes the proof of (25) and of Lemma 6.2. \square

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References

- [1] R. Ambartzumian, H. Sukiasian. *Inclusion-Exclusion and Point Processes*. Acta Applicandae Mathematicae 22; pp 15-31, 1991.
- [2] O. Costin, J. Lebowitz. *On the Construction of Particle Distributions with Specified Single and Pair Densities*. Journal of Physical Chemistry B. 108 (51) (2004), 19614-19618 (cond-mat0405519).
- [3] A. Lenard. *Correlation Functions and the Uniqueness of the State in Classical Statistical Mechanics*. Commun. Math. Phys. 30, pp 35-44 (1973).
- [4] A. Lenard. *States of Classical Statistical Mechanical Systems of Infinitely Many Particles. I*. Arch. Rational Mech. Anal. 59 (1975), no. 3, 219–239.
- [5] A. Lenard. *States of Classical Statistical Mechanical Systems of Infinitely Many Particles. II*. Arch. Rational Mech. Anal. 59 (1975), no. 3, 241–256.
- [6] R. Minlos. *Limiting Gibbs Distribution*. Funktsional’nyi Analiz i Ego Prilozheniya, Vol. 1, No. 2, pp. 60-73, March-April 1967.
- [7] D. Ruelle. *Statistical Mechanics. Rigorous Results*. W.A. Benjamin, inc., 1969.
- [8] A. Soshnikov. *Determinantal Random Point Fields*. Russian Mathematical Surveys, vol.55, No.5, pp.923-975, (2000)
- [9] F. Stillinger, S. Torquato. *Pair Correlation Function Realizability: Lattice Model Implications*. Journal of Physical Chemistry B, 108 (51) (2004) 19589-19594.