Realizability of point processes

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Abstract

There are various situations in which it is natural to ask whether a given collection of k functions, $\rho_j(\mathbf{r}_1, \ldots, \mathbf{r}_j)$, $j = 1, \ldots, k$, defined on a set X, are the first k correlation functions of a point process on X. Here we describe some necessary and sufficient conditions on the ρ_j's for this to be true. Our primary examples are $X = \mathbb{R}^d$, $X = \mathbb{Z}^d$, and X an arbitrary finite set. In particular, we extend a result by Ambartzumian and Sukiasian showing realizability at sufficiently small densities $\rho_1(\mathbf{r})$. Typically if any realizing process exists there will be many (even an uncountable number); in this case we prove, when X is a finite set, the existence of a realizing Gibbs measure with k body potentials which maximizes the entropy among all realizing measures. We also investigate in detail a simple example in which a uniform density ρ and translation invariant ρ_2 are specified on $\mathbb{Z}$; there is a gap between our best upper bound on possible values of ρ and the largest ρ for which realizability can be established.

1 Introduction

A *point process* in a set X is a random collection of points in X, whose distribution is described by a probability measure μ on the set of all possible point collections. Here we will take X to be $\mathbb{R}^d$, a lattice such as $\mathbb{Z}^d$, the torus $\mathbb{T}^d$, a lattice on the torus, or an open subset of any of these. We always assume that any bounded subset of X contains only finitely many points of the collection (this is of course automatically true if X is a lattice); the collection of points is then necessarily countable and we will write it as $\{\mathbf{x}_1, \mathbf{x}_2, \ldots\}$, with the understanding that the $\mathbf{x}_i$ are all distinct.

Well known examples of point processes are Gibbs measures for equilibrium systems of statistical mechanics. The points of the process are then interpreted as the positions of particles; because the particle configuration

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is identified with a subset of physical space, the models satisfy an exclusion principle: no two particles can occupy the same position. Point processes are also used to model phenomena other than those of statistical mechanics, such as trains of neural spikes [1, 2], departure times from queues [3], and positions of stars in galaxies [4].

In many of these cases the quantities of primary interest, partly because they are the ones most accessible to experiment, are the low order correlations, such as the one particle density $\rho_1(\mathbf{r}_1)$ and the pair density $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$. These may be defined in terms of expectations (averages), with respect to the measure μ, of products of the (random) *empirical field* η describing the process. For continuum systems, i.e., when X is $\mathbb{R}^d$ or an open subset of $\mathbb{R}^d$, η is defined by

$$\eta(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{x}_i), \tag{1.1}$$

where δ is the Dirac delta function and the $\mathbf{x}_i$'s are as above the (random) positions of the points of the process. Then, with $\langle \cdot \rangle$ denoting expectation with respect to μ,

$$\rho_1(\mathbf{r}_1) = \langle \eta(\mathbf{r}_1) \rangle, \tag{1.2}$$

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \langle \eta(\mathbf{r}_1)\eta(\mathbf{r}_2) \rangle - \rho_1(\mathbf{r}_1)\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{1.3}$$

and so on; in general,

$$\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \left\langle \sum_{i_1 \neq i_2 \neq \cdots \neq i_n} \prod_{k=1}^{n} \delta(\mathbf{r}_k - \mathbf{x}_{i_k}) \right\rangle. \tag{1.4}$$

Equation (1.4) defines ρ_n as a measure, and we will always assume that this measure assigns finite mass to any bounded set in $\mathbb{R}^{dn}$ (which means that the number of particles in a bounded set in $\mathbb{R}^d$ is a random variable with finite moments up to order n). In many cases this measure is absolutely continuous with respect to Lebesgue measure and we identify $\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ with its density, i.e., $\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) d\mathbf{r}_1 \ldots d\mathbf{r}_n$ is the probability of finding a particle in the infinitesimal box $d\mathbf{r}_i$ at $\mathbf{r}_i$ for $i = 1, \ldots, n$. We will assume that, whenever possible, ρ_n is extended by continuity to be defined at points where two of its arguments coincide. The ρ_n, here and in the lattice case discussed in the next paragraph, are often referred to as the n-particle distribution functions or correlation functions.

When X is discrete, a finite set or a lattice, we will also use the notation (1.1) and the definitions (1.2)–(1.4), interpreting $\delta(\mathbf{r}-\mathbf{x}_i)$ as the Kronecker delta $\delta_{\mathbf{r},\mathbf{x}_i}$, so that $\eta(\mathbf{r})$ has value 0 or 1, depending on whether the site $\mathbf{r} \in X$ is empty or occupied. Note that if $n \geq 2$ then $\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)$, $\mathbf{r}_i \in X$, vanishes whenever $\mathbf{r}_i = \mathbf{r}_j$ for some $i \neq j$, and that for distinct sites $\mathbf{r}_1,\ldots,\mathbf{r}_n$, $\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)$ is the probability of having particles at these sites.

In this paper we shall study the following *realizability problem:* given functions $\rho_1(\mathbf{r}_1)$, $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$, …, $\rho_k(\mathbf{r}_1,\ldots,\mathbf{r}_k)$, nonnegative and symmetric, does there exist a point process for which these are the correlations? Since only a finite number of correlations are prescribed, the problem may be regarded as an infinite dimensional version of the standard truncated moment problem [5]. The full realizability problem, in which all the correlations ρ_j, $j = 1, 2, \ldots$ are given, was studied by A. Lenard [6].

Realizability, and the related question of fully describing the realizing process, are long standing problems in the classical theory of fluids [7], recently revived by Torquato, Stillinger, et al. [8, 9]. An important ingredient in that theory is the introduction of various approximation schemes for computing $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$, such as the Percus-Yevick and hyper-netted chain approximations [7]. It is then of primary interest to determine whether or not the resulting functions (ρ_1,ρ_2) in fact correspond to any point process, that is, are in some sense internally consistent. If so they can provide rigorous bounds for the entropy of the system under consideration. A novel application of the realizability problem to the determination of the maximal density of sphere packing in high dimensions is discussed in [10].

Applications of the problem of describing a point process from its low order correlations occur in other contexts, for example, in the study of neural spikes [1, 2]. In this and other physical situations it is natural to consider a closely related problem in which the ρ_j, $j = 1, 2, \ldots, k$, are specified only on part of the domain X; for example, on the lattice we might only specify the nearest neighbor correlations. See [11] for a similar problem in error correcting codes. We will not consider this case further here, except for some comments at the end of section 6.

An important special case is that in which X is $\mathbb{R}^d$, $\mathbb{Z}^d$, or a periodic version of one of these (a torus), and the point process is translation invariant. The specified correlation functions will then also be translation invariant and may be written in the form

$$\rho_1(\mathbf{r}_1) = \rho, \tag{1.5}$$

$$\rho_j(\mathbf{r}_1,\ldots,\mathbf{r}_j) = \rho^j g_j(\mathbf{r}_2-\mathbf{r}_1,\ldots,\mathbf{r}_j-\mathbf{r}_1), \qquad j=2,\ldots,k. \tag{1.6}$$

As we often work with $k = 2$, we write $g(\mathbf{r}) \equiv g_2(\mathbf{r})$. We will often state our arguments and results in the translation invariant case, but these may frequently be extended to the more general situation; when we do not impose translation invariance we will use a notation similar to (1.6):

$$\rho_j(\mathbf{r}_1,\ldots,\mathbf{r}_j) = \prod_{i=1}^{j} \rho_i(\mathbf{r}_i)\; G_j(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_j), \qquad j=2,\ldots,k. \tag{1.7}$$

We now make some general remarks in order to put the realizability problem in context. First, we observe that if the correlations (1.5)–(1.6) can be realized for some density ρ, then they can also be realized, for the same functions $g_2,\ldots,g_k$, for any ρ' with $0 \leq \rho' < \rho$ [12]. To see this, note that if $\eta_0(\mathbf{r}) = \sum \delta(\mathbf{r}-\mathbf{x}_i)$ is the empirical field with density ρ, then $\eta(\mathbf{r}) = \sum Q_i\delta(\mathbf{r}-\mathbf{x}_i)$, where the Q_i are independent, identically distributed Bernoulli random variables with expectation ρ'/ρ, is a field with density ρ' having the same value for all g_j's. In other words, the new measure is constructed by independently choosing to delete or retain each point in a configuration, keeping a point with probability ρ'/ρ. (We will refer to this construction as *thinning*.) In this light it is thus natural to pose the realizability problem in the following form: given the g_j, $j = 2,\ldots,k$, what is the least upper bound $\bar{\rho}$ of the densities for which they can be realized? It is of course possible in the continuum case to have $\bar{\rho} = \infty$; for example, if $g_j = 1$ for $j \leq 2 \leq k$ then for any density $\rho > 0$ a Poisson process realizes the correlations. For the lattice systems considered here, on the other hand, we always have $\bar{\rho} \leq 1$.

Lacking a full answer to this question, one may of course ask rather for upper and lower bounds on $\bar{\rho}$. A lower bound $\bar{\rho} \geq \rho_0$ may be obtained by the construction of a process at density ρ_0; we discuss such constructions in sections 3–5 and show that $\bar{\rho} > 0$ under reasonable restrictions on the g_j in (1.6). Upper bounds on $\bar{\rho}$ may be obtained from necessary conditions for realizability, some of which are described in section 2.

Beyond the question of realizability one may ask about the number or more generally about the types of measures which give rise to a specified set of correlations ρ_j, $j = 1, \ldots, k$. A natural question in the theory of fluids, for example, is whether any of these measures are Gibbsian for interactions in a particular class; for example, given ρ_1 and ρ_2, is there a Gibbs measure realizing these correlations which involves only pair interactions? This question is considered in section 6, where we discuss the nature of the realizing measure μ which maximizes the Gibbs-Shannon entropy.

The outline of the rest of this paper is as follows. In section 2, we discuss some necessary conditions for realizability. (In a separate paper [13] we will present general necessary and sufficient conditions.) Sections 3, 4, and 5 cover proofs of realizability: in section 3 we prove a theorem, a generalization of one proven by R. V. Ambartzumian and H. S. Sukiasian [12], showing that if $g-1$ is absolutely integrable and g satisfies a certain stability condition then the pair (ρ, g) is realizable for sufficiently small ρ, with explicitly given higher correlations. In section 4 we show that the construction can be extended to the case in which the third correlation function g_3 is also specified, showing in particular that the realization determined by (ρ, g) alone is not unique; in fact since g_3 can take an uncountable number of values there are at low values of ρ an uncountable number of measures realizing (ρ, g). We note also possible extensions to higher order g_j. In section 5 we give a variant construction for lattice systems, based on the Lee-Yang theorem [14, 15]. In section 6 we show that a problem with specified (ρ, g), on a finite set, e.g., a periodic lattice, may be realized by a Gibbs measure with just one- and two-particle potentials whenever $\rho < \bar{\rho}$. We make some concluding remarks in section 7, and in the appendices discuss in some detail an illustrative one-dimensional example and give some technical proofs.

2 Necessary conditions for realizability

Clearly, from (1.4), realizability requires that

$$\rho_j(\mathbf{r}_1, \ldots, \mathbf{r}_j) \geq 0, \qquad j = 1, \ldots, k. \tag{2.1}$$

We also know that the covariance matrix of the field $\eta(\mathbf{r})$,

$$\begin{aligned} S(\mathbf{r}_1, \mathbf{r}_2) &= \langle \eta(\mathbf{r}_1)\eta(\mathbf{r}_2)\rangle - \langle \eta(\mathbf{r}_1)\rangle\langle \eta(\mathbf{r}_2)\rangle \\ &= \rho_2(\mathbf{r}_1, \mathbf{r}_2) + \rho_1(\mathbf{r}_1)\delta(\mathbf{r}_1 - \mathbf{r}_2) - \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2), \end{aligned} \tag{2.2}$$

must be positive semi-definite, i.e., for all functions φ with bounded support,

$$\int\int \varphi(\mathbf{r}_1)\bar{\varphi}(\mathbf{r}_2)S(\mathbf{r}_1,\mathbf{r}_2)\,d\mathbf{r}_1 d\mathbf{r}_2 \geq 0. \tag{2.3}$$

If we take $\varphi(\mathbf{r}) = \mathbb{1}_\Lambda e^{i\mathbf{kr}}$ for Λ a bounded subset of X then (2.3) becomes

$$\int_\Lambda \rho_1(\mathbf{r}_1)\,d\mathbf{r}_1 + \int_\Lambda\int_\Lambda e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\left[\rho_2(\mathbf{r}_1,\mathbf{r}_2) - \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\right]d\mathbf{r}_1 d\mathbf{r}_2 \geq 0; \tag{2.4}$$

conversely, if (2.4) holds for all $\mathbf{k} \in \mathbb{R}^d$ and all Λ, then (2.3) holds for all φ.

In the translation invariant case (2.4) is equivalent to the nonnegativity of the infinite volume structure function $\hat{S}(\mathbf{k})$:

$$\hat{S}(\mathbf{k}) \equiv \rho + \rho^2 \int_{\mathbb{R}^d} e^{i\mathbf{k}\cdot\mathbf{r}}\left[g(\mathbf{r}) - 1\right]d\mathbf{r} \geq 0. \tag{2.5}$$

Here we assume $\int_{\mathbb{R}^d} |g(\mathbf{r}) - 1|\,d\mathbf{r} < \infty$; otherwise (2.5) holds in the sense of generalized functions, cf. [16]. There are corresponding conditions on the torus $\mathbb{T}^d$, the lattice $\mathbb{Z}^d$, and the periodic lattice. If equality holds in (2.5) for some $\mathbf{k}$ then clearly ρ is maximal: $\rho = \bar{\rho}$.

We note also a necessary condition due to Yamada [17]: if N_Λ denotes the number of of particles in a region $\Lambda \subset X$, and if θ is the fractional part of the mean of N_Λ, so that $\langle N_\Lambda \rangle = k + \theta$ with $k = 0, 1, \ldots$ and $0 \leq \theta < 1$, then the variance V_Λ of N_Λ,

$$\begin{aligned} V_\Lambda &\equiv \int_\Lambda\int_\Lambda S(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \\ &= \int_\Lambda \rho_1(\mathbf{r}_1)\,d\mathbf{r}_1 + \int_\Lambda\int_\Lambda \left[\rho_2(\mathbf{r}_1,\mathbf{r}_2) - \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\right]d\mathbf{r}_1 d\mathbf{r}_2, \end{aligned} \tag{2.6}$$

must satisfy

$$V_\Lambda \geq \theta(1-\theta), \tag{2.7}$$

because N_Λ is an integer:

$$V_\Lambda = \langle (N_\Lambda - k)^2 \rangle - \theta^2 = \theta(1-\theta) + \Big\langle \big((N_\Lambda - k)(N_\Lambda - k - 1)\big) \Big\rangle \geq \theta(1-\theta). \tag{2.8}$$

The above necessary conditions all follow from the more general conditions that we prove in [13]. In summary these say that, given any functions

$f_2(\mathbf{r}_1, \mathbf{r}_2)$, $f_1(\mathbf{r})$ and constant f_0 such that, for any n points $\mathbf{r}_1, \ldots, \mathbf{r}_n$ in X, $\sum_{i,j} f_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_i f_1(\mathbf{r}_i) + f_0 \geq 0$, we must have

$$\iint_{\Lambda\times\Lambda} \rho_2(\mathbf{r}_1, \mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 + \int_\Lambda \rho_1(\mathbf{r}) f_1(\mathbf{r}) d\mathbf{r} + f_0 \geq 0, \qquad (2.9)$$

for all $\Lambda \subset \mathbb{R}^d$. We prove in fact that in the case $k = 2$, i.e. for the case that only ρ_1 and ρ_2 are given, (2.9) is also a sufficient condition for realizability under some mild assumptions on the point process.

We remark that in the case $k = 2$ all restrictions on ρ and g beyond those arising from nonnegativity of ρ and of the covariance matrix S of (2.2) are due to the fact that we want $\eta(\mathbf{r})$ to be a point process, since we can always find a Gaussian process realizing any ρ_1, ρ_2 with $S > 0$ [18].

We also note that for $g(\mathbf{r}) \leq 1$ one has

$$\hat{S}(\mathbf{k}) \geq \hat{S}(\mathbf{0}) = \lim_{\Lambda\to\infty} \frac{1}{|\Lambda|} V_\Lambda. \qquad (2.10)$$

Hence equality in (2.5) implies that the variance V_Λ is growing slower than the volume. Processes with this property are called *superhomogeneous* and are of independent interest, see [19, 8, 20]. As noted above, superhomogeneity can hold, for a given $g(\mathbf{r})$, only at the maximal density $\rho = \bar{\rho}$.

3 Realizability for small density

In this section we show the realizability of a given translation invariant ρ and $g(\mathbf{r})$, $\mathbf{r} \in \mathbb{R}^d$, for sufficiently small ρ. Our arguments extend immediately to the lattice $\mathbb{Z}^d$ and to the torus, as well as to non-translation invariant $\rho_1(\mathbf{r})$, $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$. Our results are an extension of those given by R. V. Ambartzumian and H. S. Sukiasian [12], and are based closely on the key idea of that paper: given ρ and $g(\mathbf{r})$ satisfying suitable conditions, one proves the existence of a translation invariant process for which the correlation functions ρ_n, $n = 1, 2, 3, \ldots$, are given by

$$\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) \;=\; \rho^n \prod_{1\leq i<j\leq n} g(\mathbf{r}_i - \mathbf{r}_j), \qquad (3.1)$$

and which therefore solves the realization problem for ρ and g. The ansatz (3.1) for the dependence on ρ and g of the higher order correlations (which determines the point process uniquely) is arguably the simplest one possible. It corresponds, for $n = 3$, to the well-known Kirkwood superposition approximation in the theory of equilibrium fluids [7]. Here, however, we are not talking of an approximation to a particular given point process but rather of constructing a realizing process or measure μ whose correlations have the form (3.1).

To find a point process corresponding to (3.1), Ambartzumian and Sukiasian used the inclusion-exclusion principle which, for any point process, relates the correlation functions ρ_n to the probability densities $p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ for finding exactly n particles, with positions $\mathbf{r}_1, \ldots, \mathbf{r}_n$, in a region $\Lambda \subset \mathbb{R}^d$:

$$
\begin{aligned}
p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n) \\
&= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{\Lambda^k} \rho_{n+k}(\mathbf{r}_1, \ldots, \mathbf{r}_n, \mathbf{x}_1, \ldots, \mathbf{x}_k)\, d\mathbf{x}_1 \ldots d\mathbf{x}_k. \qquad (3.2)
\end{aligned}
$$

Inserting the ansatz (3.1) in (3.2), one finds an expression for the proposed densities:

$$
\begin{aligned}
p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n) \;&\equiv\; \rho^n \prod_{1 \le i < j \le n} g(\mathbf{r}_j - \mathbf{r}_i) \\
&\times \sum_{k=0}^{\infty} \frac{(-\rho)^k}{k!} \int_{\Lambda^k} \prod_{1 \le i < j \le k} g(\mathbf{x}_j - \mathbf{x}_i) \prod_{\substack{i=1,\ldots,n \\ j=1,\ldots,k}} g(\mathbf{x}_j - \mathbf{r}_i)\, d\mathbf{x}_1 \ldots d\mathbf{x}_k. \qquad (3.3)
\end{aligned}
$$

It remains to verify that (3.3) in fact defines the probability densities of a point process.

First, note that the quantities $p_n^\Lambda(\mathbf{r}_1, ..., \mathbf{r}_n)$ are well defined by (3.3) for any value of ρ whenever there is, for every region Λ, a constant M_Λ such that (3.1) satisfies

$$
|\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)| \le M_\Lambda^n, \qquad (3.4)
$$

for $\mathbf{r}_1, \ldots, \mathbf{r}_n$ in Λ. The condition (3.4) is easily verified for many g (see, e.g., Theorem 3.1 below). The remaining problem is to prove that the p_n^Λ are all nonnegative. If this is done, then in each region Λ the collection p_n^Λ, $n = 1, 2, \ldots$, determines a measure μ^Λ defining a point process; if $\Lambda \subset \Lambda'$ then μ^Λ and $\mu^{\Lambda'}$ are compatible and by general arguments (Kolmogorov's projective limit theorem) there exists an infinite volume realizing measure μ.

Ambartzumian and Sukiasian considered only the case $g(\mathbf{r}) \le 1$, $r \in \mathbb{R}^d$. For this case they constructed a cluster expansion of the Penrose-Ruelle type and obtained inequalities of the Groeneveld-Lieb-Penrose type to show nonnegativity of each term in a reorganized expansion of the p_n^Λ. In order to extend their result to g's which can be bigger than one, when the cluster expansion is no longer positive term by term, we need to use a different approach. Recall the definition of the standard grand canonical partition function, in the region Λ, of a particle system with fugacity z, one-particle potential $V^{(1)}(\mathbf{y})$, pair potential $V(\mathbf{r})$, and inverse temperature $\beta = 1$ [15]:

$$\begin{aligned} \Xi_\Lambda(z, V^{(1)}, V) &= \sum_{k=0}^{\infty} \frac{z^k}{k!} \int_\Lambda \cdots \int_\Lambda \\ &\times \exp\Biggl\{-\Biggl[\sum_{1\le i\le k} V^{(1)}(\mathbf{y}_i) + \sum_{1\le i<j\le k} V(\mathbf{y}_i - \mathbf{y}_j)\Biggr]\Biggr\} d\mathbf{y}_1 \cdots d\mathbf{y}_k. \end{aligned} \tag{3.5}$$

Then (3.3) takes the form

$$p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \Biggl[\rho^n \prod_{1\le i<j\le n} g(\mathbf{r}_i - \mathbf{r}_j)\Biggr] \Xi_\Lambda(-\rho, V^{(1)}, V), \tag{3.6}$$

with $V(\mathbf{r}) = -\log(g(\mathbf{r}))$ and $V^{(1)}(\mathbf{y})\bigl(= V^{(1)}(\mathbf{y}; \mathbf{r}_1, \ldots, \mathbf{r}_n)\bigr) = \sum_{i=1}^n V(\mathbf{y} - \mathbf{r}_i)$. Note that in (3.6) the one-particle potential $V^{(1)}$, and hence also the partition function $\Xi_\Lambda(z, V^{(1)}, V)$, is different for each $p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n)$, depending explicitly on n and on the particle positions $\mathbf{r}_1, ..., \mathbf{r}_n$. The condition (3.4) implies that $\Xi_\Lambda(z, V^{(1)}, V)$ is an entire function of z.

Suppose now that $\log \Xi_\Lambda(z, V^{(1)}, V)$ is analytic in z in some domain Ω containing the origin; then $\Xi_\Lambda(z, V^{(1)}, V)$ can not vanish in Ω. In particular, if (a, b) is the largest interval on the real axis which contains the origin and is contained in Ω, then $\Xi_\Lambda(z, V^{(1)}, V) > 0$ for $a < z < b$, since $\Xi_\Lambda(0, V^{(1)}, V) = 1$. We will apply this observation by finding a domain Ω—a disk centered at the origin, of radius R—such that for all Λ, all n, and all $\mathbf{r}_1, \ldots, \mathbf{r}_n$, $\log \Xi_\Lambda(z, V^{(1)}, V)$ is analytic in Ω; then since $g(\mathbf{r}) \ge 0$, all $p_n^\Lambda(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ will be nonnegative for $0 \le \rho \le R$.

These considerations lead to our main result. We write

$$C(g) \equiv \int_{\mathbb{R}^d} |g(\mathbf{x}) - 1| d\mathbf{x}. \tag{3.7}$$

Theorem 3.1 *Let g be a non-negative even function on $\mathbb{R}^d$, and suppose that (i) $C(g) < \infty$ and (ii) there exists a constant b, $1 \le b < \infty$, such that* *for all* $n \geq 1$,

$$\prod_{i=1}^{n} g(\mathbf{x}_0 - \mathbf{x}_i) \leq b \qquad (3.8)$$

whenever $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n$ *satisfy* $\prod_{i<j} g(\mathbf{x}_i - \mathbf{x}_j) > 0$. *Then (3.4) is satisfied, and* (ρ, g) *is realizable, for all* ρ *satisfying*

$$0 \leq \rho \leq (ebC(g))^{-1}. \qquad (3.9)$$

For completeness we state the analogous result on the lattice.

Theorem 3.2 *Let* g *be an even non-negative function on* $\mathbb{Z}^d$, *and suppose that* $C(g) := \sum_{x\in\mathbb{Z}^d} |g(x) - 1| < \infty$. *Let* b *be a constant, with* $1 \leq b < \infty$, *such that* $\prod_{i=1}^{n} g(x_i) \leq b$ *whenever* $x_1, \ldots, x_n$ *satisfy* $\prod_{i<j} g(x_i - x_j) > 0$. *Then* (ρ, g) *is realizable for all* ρ *satisfying* $0 \leq \rho \leq (ebC(g))^{-1}$.

Remark 3.3 (a) The fact that (3.4) holds under hypothesis (ii) of the theorem, with constant $M_\Lambda = \rho b^{1/2}$ independent of Λ, is immediate. In the language of statistical mechanics, this says that the interaction V is *stable*.
(b) If $g \leq 1$ then hypothesis (ii) holds with $b = 1$, and we recover the result of [12].
(c) Hypothesis (ii) also holds if there exists (I) a $D > 0$ such that $g(\mathbf{r}) = 0$ when $|\mathbf{r}| \leq D$, and (II) a nonnegative decreasing function ψ on $[D, \infty)$, satisfying $\int_0^\infty t^{d-1}\psi(t)\,dt < \infty$, such that $(g(\mathbf{r}) - 1) \leq \psi(|\mathbf{r}|)$ [15]. In the language of statistical mechanics, (I) says that $V(\mathbf{r})$ has a *hard core*; (II) says that $V(\mathbf{r})$ is *lower regular* [21]. In this case one easily obtains an explicit possible value for the constant b.
(d) Note that, despite the use of results from equilibrium systems, there is no reason to expect the realizing measure μ giving rise to the ρ_n of (3.1) to be a Gibbs measure with pair potential (unless $g(\mathbf{r}) \equiv 1$, in which case $V(\mathbf{r}) = 0$ and μ corresponds to a Poisson process).

Proof of Theorem 3.1: Denote by k_m^Λ the m^{th} correlation function for a grand canonical ensemble in Λ with pair potential V, one-particle potential $V^{(1)}$, inverse temperature $\beta = 1$, and activity z; as for the partition function (3.5) for this system, these correlation functions depend through $V^{(1)}$ on $\mathbf{r}_1, \ldots, \mathbf{r}_n$. By the above remarks it suffices to establish analyticity of k_1^Λ in a disk $|z| < R$ with $R = (ebC(g))^{-1}$, because from

$$\frac{d}{dz} \log\left(\Xi_\Lambda(z, V^{(1)}, V)\right) = \frac{1}{z}\int_\Lambda k_1^\Lambda(\mathbf{x})\,d\mathbf{x} \qquad (3.10)$$

it follows that $\log \Xi_\Lambda(z, V^{(1)}, V)$ is also analytic in this disk.

To establish the analyticity of k_1^Λ we in fact show analyticity of all k_m^Λ; we proceed as in the classical proof, following in particular section 4.2 of [15]. In this proof the Kirkwood-Salsburg equations for the correlation functions are written in an appropriately chosen Banach space in the form $k^\Lambda = z\psi + z\mathcal{K}k^\Lambda$ for some operator $\mathcal{K}$ and fixed vector ψ. One shows that $\|z\mathcal{K}\| < 1$ when $|z| < R$, so that $I - z\mathcal{K}$ is then invertible via a power series in z, and a unique solution, analytic in z, exists. The primary change in the proof required in our case is that one must introduce a dependence of the operator $\mathcal{K}$ on the sites $\mathbf{r}_1, \ldots, \mathbf{r}_n$. We leave the details to appendix B, which is probably best read with [15] in hand. ■

We next state a generalization of Theorem 3.1 to non-translation invariant systems; the proof is omitted. Let $X \subset \mathbb{R}^d$ be open, and recall the notation $\rho_2(\mathbf{x}, \mathbf{y}) = \rho_1(\mathbf{x})\rho_1(\mathbf{y})G_2(\mathbf{x}, \mathbf{y})$ of (1.7).

Theorem 3.4 *Let ρ_1 and G_2 be non-negative functions on X and $X \times X$, respectively, with G_2 symmetric, and suppose that there exists a constant b, with $1 \le b < \infty$, such that for all $n \ge 1$, $\prod_{i=1}^n G_2(\mathbf{x}_0, \mathbf{x}_i) \le b$ whenever $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n \in X$ satisfy $\prod_{i<j} \rho_2(\mathbf{x}_i - \mathbf{x}_j) > 0$. Then the pair (ρ_1, ρ_2) is realizable if*

$$eb \sup_{\mathbf{x} \in X} \left(\int_X |G_2(\mathbf{x}, \mathbf{y}) - 1| \rho_1(\mathbf{y}) d\mathbf{y} \right) \le 1. \tag{3.11}$$

3.1 Decay of correlations

We are interested in the decay of the truncated correlation functions u_k for the realizing measure specified by (3.1), defined recursively by [15]

$$\rho_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \sum_{k=1}^{n} \sum_{\{I_1, \ldots, I_k\} \in \mathcal{P}_k(n)} \prod_{j=1}^{k} u_{|I_j|}((\mathbf{r}_i)_{i \in I_j}), \tag{3.12}$$

where $\mathcal{P}_k(n)$ denotes the set of all partitions of $\{1, \ldots, n\}$ in k disjoint sets. We consider only the case in which $X = \mathbb{R}^d$ and ρ_1 and ρ_2 are translation invariant; then $u_1(\mathbf{r}_1) = \rho$ and $u_2(\mathbf{r}_1, \mathbf{r}_2) = \rho^2[g(\mathbf{r}_1 - \mathbf{r}_2) - 1]$. For the correlation functions (3.1) the corresponding truncated correlation functions have the form

$$u_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \rho^n \sum_{G \in \mathcal{G}_c(n)} \prod_{\{i,j\} \in G} \big(g(\mathbf{r}_i - \mathbf{r}_j) - 1 \big), \tag{3.13}$$

with $\mathcal{G}_c(n)$ the set of all connected subgraphs of the complete graph with vertex set $\{1, 2, \ldots, n\}$.

Let $\mathcal{T}(n)$ denote the set of all undirected trees on $\{1, \ldots, n\}$. Then from (3.13) and an estimate of Penrose [22],

$$|u_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)| \leq \rho^n b^{n-2} \sum_{T \in \mathcal{T}(n)} \prod_{\{i,j\} \in T} \big|g(\mathbf{r}_i - \mathbf{r}_j) - 1\big|, \tag{3.14}$$

where b is defined as in Theorem 3.1. Using $|\mathcal{T}(n)| = n^{n-2}$ we then obtain the L^1 decay property

$$\int_{X^n} \big|u_{n+1}(\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_n)\big|\, d^n\mathbf{r} \leq \rho^{n+1}((n+1)b)^{n-1} C(g)^n. \tag{3.15}$$

Compare Theorem 4.4.8 of [15].

One may also establish a pointwise decay bound: if $|g(\mathbf{r}) - 1|$ decays polynomially or exponentially, then $u_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ also decays polynomially or exponentially, respectively, with $\max_{1 \leq i < j \leq n} |\mathbf{r}_i - \mathbf{r}_j|$. For example, if $|g(\mathbf{r}) - 1| \leq D_1 e^{-D_2|\mathbf{r}|}$ for some $D_1, D_2 > 0$ and all $\mathbf{r}$, then

$$|u_n(\mathbf{r}_1, \ldots, \mathbf{r}_n)| \leq (nb)^{n-2} D_1^{n-1} \rho^n e^{-D_2 L}, \tag{3.16}$$

where L is the minimal length of a tree connecting all points $\mathbf{r}_1, \ldots, \mathbf{r}_n$ and the length of a tree T is $\sum_{\{i,j\} \in T} |\mathbf{r}_i - \mathbf{r}_j|$.

This decay implies that the realizing measure is mixing and therefore ergodic.

4 Triplet correlation function

We now consider briefly the application of the ideas of section 3 to the realization problem under the specification of $\rho_1, \ldots, \rho_k$ for $k > 2$. For simplicity we discuss only the case $k = 3$ and restrict our considerations to translation invariant correlations in $\mathbb{R}^d$ which have densities with respect to Lebesgue measure. Other cases can be treated analogously. We adopt the notation

$$\begin{aligned} \rho_3(\mathbf{x}, \mathbf{y}, \mathbf{z}) &= \rho^3 g_3(\mathbf{y} - \mathbf{x}, \mathbf{z} - \mathbf{x}) \\ &= \rho^3 g(\mathbf{y} - \mathbf{x}) g(\mathbf{z} - \mathbf{x}) g(\mathbf{z} - \mathbf{y}) \tilde{g}_3(\mathbf{y} - \mathbf{x}, \mathbf{z} - \mathbf{x}); \end{aligned} \tag{4.1}$$

the first equation here is just (1.6), and the second is justified by the fact that, from the definition (1.4), $\rho_2(\mathbf{x}, \mathbf{y})$ cannot vanish on a set S of positive (Lebesgue) measure unless $\rho_3(\mathbf{x}, \mathbf{y}, \mathbf{z})$ vanishes, for almost all $\mathbf{z}$, if $(\mathbf{x}, \mathbf{y}) \in S$.

In analogy with (3.1) we make now the ansatz

$$\rho_n(\mathbf{r}_1,\dots,\mathbf{r}_n) \;:=\; \rho^n \prod_{1\le i<j\le n} g(\mathbf{r}_i-\mathbf{r}_j) \prod_{1\le i<j<k\le n} \tilde g_3(\mathbf{r}_k-\mathbf{r}_i,\mathbf{r}_j-\mathbf{r}_i) \quad (4.2)$$

for the higher correlation functions ($n \ge 4$). As before, the probability densities p_n^Λ for the point process defined by (4.2) can be written in terms of the correlations via the inclusion-exclusion principle (3.2) and thus in terms of a grand-canonical partition function $\Xi_\Lambda(z, V^{(1)}, V^{(2)}, V^{(3)})$ for a particle system in Λ with fugacity z, one particle potential $V^{(1)}$, non-translation-invariant pair potential $V^{(2)}$, and translation invariant triplet potential $V^{(3)}$:

$$\begin{aligned} p_n^\Lambda(\mathbf{r}_1,\dots,\mathbf{r}_n) \;=\; & \rho^n \prod_{1\le i<j\le n} g(\mathbf{r}_j-\mathbf{r}_i) \prod_{1\le i<j<k\le n} \tilde g_3(\mathbf{r}_j-\mathbf{r}_i,\mathbf{r}_k-\mathbf{r}_i) \\ & \times \Xi_\Lambda(-\rho, V^{(1)}, V^{(2)}, V^{(3)}), \end{aligned} \quad (4.3)$$

where

$$V^{(3)}(\mathbf{x},\mathbf{y},\mathbf{z}) \;:=\; -\ln(\tilde g_3(\mathbf{y}-\mathbf{x},\mathbf{z}-\mathbf{x})), \quad (4.4)$$

$$V^{(2)}(\mathbf{x},\mathbf{y}) \;:=\; -\ln(g(\mathbf{y}-\mathbf{x})) + \sum_{1\le i\le n} V^{(3)}(\mathbf{x},\mathbf{y},\mathbf{r}_i), \quad (4.5)$$

$$V^{(1)}(\mathbf{x}) \;:=\; \sum_{1\le i\le n} V^{(2)}(\mathbf{x}-\mathbf{r}_i) + \sum_{1\le i<j\le n} V^{(3)}(\mathbf{x},\mathbf{r}_i,\mathbf{r}_j). \quad (4.6)$$

In order to proceed as in section 3 we have to show that there exists a domain for z, independent of $\mathbf{r}_1,\dots,\mathbf{r}_n$, in which $\ln \Xi_\Lambda(z, V^{(1)}, V^{(2)}, V^{(3)})$ is analytic. Now, however, we must work with the cluster expansion for both the pair and the triplet interactions, as in [23]. We give a result in which the hypotheses have been chosen to keep the proof simple and are thus far from optimal. We let v_d denote the volume of the sphere in $\mathbb{R}^d$ of diameter 1 and write

$$C_3(\tilde g_3) = \sup_{\mathbf{x},\mathbf{y}\in\mathbb{R}^d} \max\{\, |\tilde g_3(\mathbf{x},\mathbf{y})-1|, |\tilde g_3(\mathbf{x},\mathbf{y})-1|^{1/3}\,\}. \quad (4.7)$$

Proposition 4.1 *Let g and $\tilde g_3$ be be given, and assume that (i) g satisfies the conditions of Remark 3.3(c), and $C(g) < \infty$; (ii) there exists a $D_3 > 0$ such that $\tilde g_3(\mathbf{x}_2-\mathbf{x}_1,\mathbf{x}_3-\mathbf{x}_1) = 1$ if $|\mathbf{x}_i-\mathbf{x}_j| > D_3$ for some i,j,k, and $C_3(\tilde g_3) < \infty$. Then $(\rho, g, \tilde g_3)$ is realizable whenever*

$$0 \le \rho \le \Big[ebb_3\,(1+bC_3(\tilde g_3))^{(3D_3/D)^{2d}}\,\big(C(g)+v_d(D_3/2)^d C_3(\tilde g_3)\big)\Big]^{-1}, \quad (4.8)$$

where b is defined as in Theorem 3.1 and b_3 is a constant such that

$$\prod_{j=1}^{n}\prod_{i=j+1}^{n}\tilde{g}_3(\mathbf{x}_i-\mathbf{x}_0,\mathbf{x}_j-\mathbf{x}_0)\le b_3 \tag{4.9}$$

for all n and all $\mathbf{x}_0,\mathbf{x}_1,\ldots,\mathbf{x}_n$ with $|\mathbf{x}_i-\mathbf{x}_j|>D$ for $0\le i<j\le n$. .

Remark 4.2 (a) Without loss of generality we may assume that $D_3>D$, since otherwise $\tilde{g}_3=1$ and the proposition reduces to Theorem 3.1.
(b) Since there can be at most

$$N:=\left(\frac{2D_3+D}{D}\right)^d\le\left(\frac{3D_3}{D}\right)^d \tag{4.10}$$

points within a distance D_3 of x_0, all separated from x_0 and from each other by a distance at least D, we may in particular take

$$b_3=(1+C_3(\tilde{g}_3))^{(3D_3/D)^{2d}}.$$

Note that with this choice the upper bound of (4.8) converges as $C_3(\tilde{g}_3)\searrow 0$ to the upper bound of (3.9).

Proof of Theorem 4.1: The proof is a fairly straightforward extension of the proof of Theorem 3.1. We sketch some details in appendix B. ■

Finally we would like to point out a consequence of Proposition 4.1 which illustrates the fact that the same (finite) family of correlation functions may be realized by distinct measures, and in fact by mutually singular measures, where two measures are called *mutually singular* if configurations of points typical for one of the realizing point process are atypical for the other one, i.e., if there exists a set of point configurations A such that A has probability 1 for one measure and probability 0 for the other.

Corollary 4.3 *Let g be a function fulfilling the conditions of Remark 3.3(c). Then for any ρ satisfying the bound (3.9) of Theorem 3.1 with strict inequality there exist uncountably many distinct and in fact mutually singular realizations of (ρ,g) by point processes.*

Proof: Under the hypotheses one may choose $\tilde{g}_3$ quite arbitrarily, subject only to a condition that $C_3(\tilde{g}_3)$ be sufficiently small (how small depends on D_3), and still have ρ satisfy the bound (4.8). Thus there are certainly uncountably many realizations with distinct three point functions. To show that these are mutually singular one first establishes, following the procedure of subsection 3.1, the decay of the truncated correlation functions for the measure constructed in Proposition 4.1. A direct consequence of this decay is that the corresponding realizing point process is mixing and therefore ergodic. Since any two translation invariant ergodic measures are either identical or mutually singular, the result follows. ■

5 The Lee-Yang approach

While for given ρ_j we cannot in general improve the region of realizability beyond that described in section 3 and 4, there are special situations in which more can be said. One class of examples is treated in appendix A. In this section we consider a lattice gas on a countable set X, e.g., $X = \mathbb{Z}^d$, with $G_2(\mathbf{x}, \mathbf{y}) \geq 1$ for $\mathbf{x}, \mathbf{y} \in X$, $\mathbf{x} \neq \mathbf{y}$. This enables us to to establish realizability using techniques developed for proving the Lee-Yang theorem [14].

Theorem 5.1 *Let X be a countable set and suppose that $G_2(\mathbf{x}, \mathbf{y}) \geq 1$ for all $\mathbf{x}, \mathbf{y} \in X$ with $\mathbf{x} \neq \mathbf{y}$ and that*

$$b := \sup_{\mathbf{x}\in X} \prod_{\mathbf{y}\in X\setminus\{\mathbf{x}\}} G_2(\mathbf{x}, \mathbf{y}) < \infty. \tag{5.1}$$

Then (ρ, G_2) is realizable for all

$$0 \leq \rho \leq b^{-1}. \tag{5.2}$$

The condition (5.2) improves the result of Theorem 3.2, increasing the upper bound on ρ by a factor of $eC(g)$, with $C(g) = \sum_{\mathbf{x}\in\mathbb{Z}^d} |g(x) - 1|$ as in that theorem. Note that $C(g) \geq 1$ since $g(0) = 0$.

Proof: We again use the ansatz (3.1) for the higher correlation functions. Let Λ be a finite subset of X; then (5.1) implies that ρ_n fulfills the bound (3.4) with $M_\Lambda = \rho b^{1/2}$. Hence we can write the probability densities p_n^Λ in terms of the correlation functions via (3.2). Since the correlation function $\rho_{n+k}(\mathbf{r}_1, \ldots, \mathbf{r}_n, \mathbf{x}_1, \ldots, \mathbf{x}_k)$ vanishes when any of its arguments coincide, one can work with the variables $\xi := \{\mathbf{r}_1, \ldots, \mathbf{r}_n\}$ and $\gamma = \{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$, where ξ and γ vary over all finite subsets of Λ with $\gamma \cap \xi = \emptyset$. Then (3.2) may be written in terms of γ and ξ as $p_n^\Lambda(\xi) = \rho_n(\xi)\Xi_n^\Lambda(\xi)$, where

$$\Xi_n^\Lambda(\xi) = \sum_{\gamma \subset \Lambda \setminus \xi} (-\rho)^{|\gamma|} \prod_{\substack{\mathbf{y}\in\gamma \\ \mathbf{x}\in\gamma\setminus\{\mathbf{y}\}}} G_2(\mathbf{x},\mathbf{y})^{1/2} \prod_{\substack{\mathbf{r}\in\xi \\ \mathbf{y}\in\gamma}} G_2(\mathbf{r},\mathbf{y}) \tag{5.3}$$

(compare (3.5)–(3.6)). As before the main problem is to verify that $p_n^\Lambda \geq 0$. To apply techniques used for the Lee-Yang theorem we write p_n^Λ in terms of the set $\sigma = (\Lambda \setminus \xi) \setminus \gamma$ of empty sites rather than in terms of γ. Writing $\tilde{\Lambda} := \Lambda \setminus \xi$ we obtain

$$\begin{aligned} \Xi_n^\Lambda(\xi) \;&=\; (-\rho)^{|\tilde\Lambda|} \prod_{\mathbf{y}\in\tilde\Lambda} \left(\prod_{\mathbf{r}\in\xi} G_2(\mathbf{r},\mathbf{y}) \prod_{\mathbf{x}\in\tilde\Lambda\setminus\{\mathbf{y}\}} G_2(\mathbf{x},\mathbf{y})^{1/2} \right) \qquad (5.4) \\ &\cdot \sum_{\sigma\subset\tilde\Lambda} \prod_{\mathbf{y}\in\sigma} \left(-\rho^{-1} \prod_{\mathbf{r}\in\xi} G_2(\mathbf{r},\mathbf{y})^{-1} \prod_{\mathbf{x}\in\tilde\Lambda\setminus\{\mathbf{y}\}} G_2(\mathbf{x},\mathbf{y})^{-1/2} \prod_{\mathbf{x}\in\tilde\Lambda\setminus\sigma} G_2(\mathbf{x},\mathbf{y})^{-1/2} \right). \end{aligned}$$

Clearly the prefactor here is non-negative in general and is positive for $\rho > 0$. To prove that the sum is non-negative we rewrite it in the form

$$\sum_{\sigma\subset\tilde\Lambda} \prod_{\mathbf{y}\in\sigma} \left(z_{\mathbf{y}} \prod_{\mathbf{x}\in\tilde\Lambda\setminus\sigma} A_{\mathbf{r},\mathbf{y}} \right), \tag{5.5}$$

where

$$z_{\mathbf{y}} \;:=\; -\rho^{-1} \prod_{\mathbf{r}\in\xi} G_2(\mathbf{r},\mathbf{y})^{-1} \prod_{\mathbf{x}\in\tilde\Lambda\setminus\{\mathbf{y}\})} G_2(\mathbf{x},\mathbf{y})^{-1/2}, \tag{5.6}$$

$$A_{\mathbf{x},\mathbf{y}} \;:=\; G_2(\mathbf{x},\mathbf{y})^{-1/2}. \tag{5.7}$$

Note that from $G_2(\mathbf{x},\mathbf{y}) \geq 1$ for $\mathbf{x} \neq \mathbf{y}$ it follows that $-1 \leq A_{\mathbf{x},\mathbf{y}} \leq 1$. Then Proposition 5.1.1. of [15] implies that (5.5) is not zero if $|z_{\mathbf{y}}| > 1$ for all $\mathbf{y} \in \Lambda \setminus \xi$. $|z_{\mathbf{y}}|$ can be bounded below by $\rho^{-1} \prod_{\mathbf{x}\in\Lambda\setminus\{\mathbf{y}\}} G_2(\mathbf{x},\mathbf{y})^{-1} \geq (\rho b)^{-1}$. We have thus shown that $\Xi_n^\Lambda(\xi)$ has no zeros for $0 < \rho < 1/b$. But $\Xi_n^\Lambda(\xi) = 1$ for $\rho = 0$, so that $\Xi_n^\Lambda(\xi)$ and hence $p_n^\Lambda(\xi)$ is non-negative for all $0 \leq \rho \leq 1/b$. ■

6 Gibbsian measures

In this section we ask whether a specified set of correlation functions ρ_j, $j = 1, \dots, k$, which can be realized by at least one point process, can also be realized by a Gibbs measure involving at most k-particle potentials. Here we will first consider this problem for the case in which our system lives on a finite set Λ, e.g., a subset of the lattice. On a finite set every measure is Gibbsian in a general sense, so the important restriction is to be Gibbsian for a set of potentials involving at most k particles: we will say that a measure ν on $\{0,1\}^\Lambda$ is *k-Gibbsian* if it has the form

$$\nu(\eta) = Z^{-1} \exp\left\{ -\sum_{j=1}^{k} \sum_{\mathbf{x}_1 \neq \mathbf{x}_2 \neq \cdots \neq \mathbf{x}_j \in \Lambda} \phi^{(j)}(\mathbf{x}_1, \dots, \mathbf{x}_j) \eta(\mathbf{x}_1) \cdots \eta(\mathbf{x}_j) \right\}, \quad (6.1)$$

where $\eta \in \{0,1\}^\Lambda$, Z is a normalization constant, and $-\infty < \phi^{(j)} \leq \infty$.

As in (1.7) we write, for $j = 2, \dots, k$,

$$\rho_j(\mathbf{x}_1, \dots, \mathbf{x}_j) = \prod_{i=1}^{j} \rho_1(\mathbf{x}_i)\, G_j(\mathbf{x}_1, \dots, \mathbf{x}_j), \qquad \mathbf{x}_1, \dots, \mathbf{x}_j \in \Lambda, \quad (6.2)$$

and again think in terms of specifying the G_j, $j = 2, \dots k$, and asking for what densities $\rho_1(\mathbf{x})$ the correlations (6.2) may be realized by a k-Gibbs measure. We will prove that this is possible whenever $\rho_1(\mathbf{x})$ satisfies $\rho_1(\mathbf{x}) < \bar{\rho}_1(\mathbf{x})$ for all $\mathbf{x} \in \Lambda$, with equality allowed if $\bar{\rho}_1(\mathbf{x}) = 0$, for some $\bar{\rho}_1$ with the property that $\bar{\rho}_1$ and the G_j, $j = 2, \dots, k$, are realizable. The proof is presented only for $k = 2$, but the result could easily be extended to general k.

The key ingredient in the argument is the fact that Gibbs measures are those which maximize the Gibbs-Shannon entropy of the measure μ,

$$S(\mu) \equiv -\sum_{\underline{\eta}} \mu(\underline{\eta}) \log \mu(\underline{\eta}) \quad (6.3)$$

subject to some specified constraints [15]. In particular, if one can use the method of Lagrange multipliers to find a measure which maximizes the entropy, subject to the constraint of a given ρ_1 and ρ_2, then the maximizing measure will be 2-Gibbsian and the Lagrange multipliers obtained in this way will be the desired one body and pair potentials [25]. Here we verify that if $\rho_1(\mathbf{x}) < \bar{\rho}_1(\mathbf{x})$ (with equality allowed if $\bar{\rho}_1(\mathbf{x}) = 0$, as described above) then the method of Lagrange multipliers will indeed apply.

Theorem 6.1 *Suppose that the pair* $(\bar{\rho}_1, G_2)$ *is realizable on* Λ*. If* ρ_1 *satisfies* $0 \le \rho_1(\mathbf{x}) \le \bar{\rho}_1(\mathbf{x})$ *for all* $\mathbf{x} \in \Lambda$*, with* $\rho_1(\mathbf{x}) < \bar{\rho}_1(\mathbf{x})$ *unless* $\bar{\rho}_1(\mathbf{x}) = 0$*, then* (ρ_1, G_2) *is realizable by a 2-Gibbsian measure* ν *for some uniquely determined potentials* $\phi^{(1)}(\mathbf{x})$*,* $\mathbf{x} \in \Lambda$ *and* $\phi^{(2)}(\mathbf{x}, \mathbf{y})$*,* $\mathbf{x}, \mathbf{y} \in \Lambda, \mathbf{x} \neq \mathbf{y}$*. Moreover,* ν *maximizes the Gibbs-Shannon entropy (6.3) over all measures* μ *realizing* (ρ_1, G_2)*.*

Proof: We begin with a preliminary remark. Suppose that we have verified the theorem in the case in which all $\rho_1(\mathbf{x})$ (and hence also all $\bar{\rho}_1(\mathbf{x})$) are strictly positive. Then the case in which, say, $\rho_1(\mathbf{x}) = 0$ for $\mathbf{x} \in \Lambda' \subset \Lambda$, is a direct corollary: we obtain immediately a 2-Gibbsian measure on $\{0,1\}^{\Lambda \setminus \Lambda'}$ realizing the correlations there, and then take $\phi^{(1)}(\mathbf{x}) = \infty$ for $\mathbf{x} \in \Lambda'$. Similarly, if $G_2(\mathbf{x}, \mathbf{y}) = 0$ for some pair of sites $\mathbf{x}, \mathbf{y} \in \Lambda$, $\mathbf{x} \neq \mathbf{y}$, with $\rho_1(\mathbf{x})$ and $\rho_1(\mathbf{y})$ nonzero, then we set $\phi^{(2)}(\mathbf{x}, \mathbf{y}) = \infty$, which guarantees that if ν is given by (6.1) then $\nu(\eta) = 0$ whenever $\eta(\mathbf{x}) = \eta(\mathbf{y}) = 1$. Thus in the remainder of the proof we will assume that $\rho_1(\mathbf{x}) > 0$ for all $\mathbf{x} \in \Lambda$ and prove the existence of a realizing measure ν, of the form (6.1) with *finite* potentials and with $k = 2$, on the set of configurations

$$\mathcal{C}_{G_2} := \{\eta \mid \eta(\mathbf{x})\eta(\mathbf{y}) = 0 \text{ if } G_2(\mathbf{x}, \mathbf{y}) = 0, \mathbf{x} \neq \mathbf{y}\}\,. \tag{6.4}$$

We now turn to the main body of the proof. For any η we let $|\eta| = \sum_{\mathbf{x} \in \Lambda} \eta(\mathbf{x})$ be the number of particles in the configuration η. We first show that there exists a measure μ^* realizing (ρ_1, G_2) for which $\mu^*(\eta) > 0$ whenever $\eta \in \mathcal{C}_{G_2}$ and $|\eta| \le 2$. By hypothesis there exists a measure $\bar{\mu}$ realizing $(\bar{\rho}_1, G_2)$. We may thin this measure as in section 1, deleting a particle at the site $\mathbf{x}$ with probability $1 - \rho_1(\mathbf{x})/\bar{\rho}_1(\mathbf{x})$, independently for each site, to obtain a measure μ^* realizing (ρ_1, G_2). Now we observe that if $\eta \in \mathcal{C}_{G_2}$ and $|\eta| \le 2$ then $\mu^*(\eta) > 0$. For example, if $|\eta| = 2$ with $\eta(\mathbf{x}) = \eta(\mathbf{y}) = 1$ for $\mathbf{x} \neq \mathbf{y}$, then $G_2(\mathbf{x}, \mathbf{y}) > 0$ by (6.4) and hence, since $\bar{\mu}$ realizes $(\bar{\rho}_1, G_2)$, $\bar{\mu}(\tilde{\eta}) > 0$ at least for one $\tilde{\eta}$ with $\tilde{\eta}(\mathbf{x}) = \tilde{\eta}(\mathbf{y}) = 1$, and there is a positive probability that η will result from $\tilde{\eta}$ applying the thinning process.

Next we construct a measure $\hat{\mu}$ realizing (ρ_1, G_2) for which $\hat{\mu}(\eta) > 0$ for all $\eta \in \mathcal{C}_{G_2}$. We first fix $\epsilon > 0$ and for $|\eta| > 2$ define $\hat{\mu}(\eta) = \mu^*(\eta) + \epsilon$. Now the condition that $\hat{\mu}$ realize (ρ_1, G_2) is that

$$\begin{aligned}\sum_{\eta\in\mathcal{C}_{G_2}} \hat{\mu}(\eta) &= 1, &(6.5)\\ \sum_{\eta\in\mathcal{C}_{G_2}} \eta(\mathbf{x})\hat{\mu}(\eta) &= \rho_1(\mathbf{x}), \qquad \mathbf{x}\in\Lambda, &(6.6)\\ \sum_{\eta\in\mathcal{C}_{G_2}} \eta(\mathbf{x})\eta(\mathbf{y})\hat{\mu}(\eta) &= \rho_1(\mathbf{x})\rho_1(\mathbf{y})G_2(\mathbf{x},\mathbf{y}), \qquad \mathbf{x},\mathbf{y}\in\Lambda, \mathbf{x}\neq\mathbf{y}. &(6.7)\end{aligned}$$

Equations (6.5)–(6.7) may be regarded as a system of linear equations for the (as yet) undefined $\hat{\mu}(\eta)$, $|\eta|\le 2$; note that the number of these unknowns is the same as the number of equations. The coefficient matrix in this system is (after an appropriate ordering of the η, $|\eta|<2$) upper triangular, with unit diagonal; thus these equations can be solved uniquely for the $\hat{\mu}(\eta)$, $|\eta|\le 2$, in terms of these given $\hat{\mu}(\eta)$, $|\eta|>2$. The resulting $\hat{\mu}$ will differ from μ^* by a perturbation of order ϵ; in particular, since $\mu^*(\eta)>0$ for $|\eta|\le 2$, we can by choice of ϵ guarantee that also $\hat{\mu}(\eta)>0$ for $|\eta|\le 2$. But $\hat{\mu}(\eta)>0$ for $|\eta|>2$ by construction, so that $\hat{\mu}$ has the desired properties.

Finally we show that the Gibbsian measure we seek is the measure which maximizes $S(\mu)$ (see (6.3)) among all measures realizing (ρ_1, G_2). Let ν be such a maximizer; ν is unique by the strict concavity of S. We first observe that ν must lie in the interior of $\mathcal{C}_{G_2}$, i.e., that $\nu(\eta)>0$ for all $\eta\in\mathcal{C}_{G_2}$; otherwise define $\nu_t=(1-t)\nu+t\hat{\nu}$ and note that then

$$\frac{d}{dt}S(\nu_t)\bigg|_{t=0} = -\sum_{\eta\in\mathcal{C}_{G_2}} \log\nu(\eta) = \infty, \tag{6.8}$$

so that $S(\nu_t)>S(\nu)$ for some $t>0$ and ν cannot maximize S. Hence ν may be obtained by the method of Lagrange multipliers, with (6.5)–(6.7) (written for ν rather than $\hat{\mu}$) as constraints. A simple computation shows that the $\nu(\eta)$ then have the form (6.1) with $k=2$, where the $\phi^{(1)}(\mathbf{x})$ and $\phi^{(2)}(\mathbf{x},\mathbf{y})$ are the Lagrange multipliers associated with (6.6) and (6.7), respectively (the multiplier for (6.5) is related to the factor Z).

To verify uniqueness of the potentials, note that any 2-Gibbsian measure realizing (ρ_1, G_2) with, say, potentials $\psi^{(1)}$ and $\psi^{(2)}$, must satisfy the Lagrange multiplier equations with these potentials as multipliers and is hence an extremum of the entropy. From the uniqueness of the extremum and the non-degeneracy of the constraint equations (6.5)–(6.7) it follows that these multipliers are uniquely defined, i.e., that $\psi^{(1)}=\phi^{(1)}$ and $\psi^{(2)}=\phi^{(2)}$. ∎

6.1 Infinite volume

It is natural to ask if there exists an analogue of Theorem 6.1 for an infinite lattice, such as $\mathbb{Z}^d$, for example when the given correlation functions are defined from the beginning on $\mathbb{Z}^d$ as translation invariant quantities, i.e., $\rho_1(\mathbf{x}) = \rho$, $G_2(\mathbf{x}, \mathbf{y}) = g(\mathbf{y} - \mathbf{x})$ as in (1.5), (1.6); on $\mathbb{Z}^d$ we will call a measure 2-Gibbsian if it satisfies the DLR equations for an interaction with only one and two body potentials. A result in this direction is due to L. Koralov [26]; using cluster expansion techniques, he has established the existence of an infinite-volume 2-Gibbsian measure in the lattice case for $k = 2$, ρ small, and g sufficiently close to 1—specifically, for $\sum_{\mathbf{r}\neq 0} |g(\mathbf{r}) - 1| \leq 1$.

An attractive alternative approach would be to apply Theorem 6.1 in large boxes $\Lambda \subset \mathbb{Z}^d$ to obtain potentials $\phi_\Lambda^{(1)}(\mathbf{x})$ and $\phi_\Lambda^{(2)}(\mathbf{x}, \mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \Lambda$, realizing (ρ, g) in Λ, and then to show that under suitable restrictions on ρ and g the $\Lambda \nearrow \mathbb{Z}^d$ limits of these potentials exist and are summable and translation invariant. We do not know how to carry out such a program, as we have no control on the behavior of the ϕ_Λ as Λ changes. In fact we do not know if the 2-Gibbsian measures ν_Λ realizing (ρ, g) in Λ converge as $\Lambda \nearrow \mathbb{Z}^d$ to any measure ν on $\mathbb{Z}^d$. Any sequence of such measures must have a (weakly) convergent subsequence, however, by compactness, and the limiting measure ν will realize the translation invariant (ρ, g) on $\mathbb{Z}^d$. In [27] we showed that any such realizing measure which is translation invariant and Gibbsian, with summable potentials, is necessarily a 2-Gibbsian measure with uniquely determined potentials which maximizes the entropy density among all realizing translation invariant measures.

It follows from the above that if there is in fact a translation invariant entropy maximizing 2-Gibbsian measure ν on $\mathbb{Z}^d$, realizing (ρ, g), with summable translation invariant potentials $\psi^{(1)}$ and $\psi^{(2)}(\mathbf{x} - \mathbf{y})$ ($\psi^{(1)}$ is just the chemical potential), then the conditional measure $\nu(\cdot|\eta_{\Lambda^c})$ on Λ, for a specified configuration η_{Λ^c} on $\mathbb{Z}^d \setminus \Lambda$, will be the 2-Gibbsian measure which maximizes the entropy for $(\rho_1(x|\eta_{\Lambda^c}), G_2(x, y|\eta_{\Lambda^c}))$, the one and two particle distributions obtained from $\nu(\eta_\Lambda|\eta_{\Lambda^c})$. If furthermore this measure is unique for these potentials, then clearly $\nu(\cdot|\eta_{\Lambda^c}) \to \nu$ for every η_{Λ^c} as $\Lambda \nearrow \mathbb{Z}^d$.

To obtain translation invariant measures we may take for the domain Λ in Theorem 6.1 a periodic lattice $\mathbb{L}$, where $\mathbb{L} = \{-L+1, \ldots, L\}^d$ with periodic boundary conditions, and find a measure $\nu_\mathbb{L}$ realizing $(\rho, \rho g_\mathbb{L})$ for some periodic $g_\mathbb{L}(\mathbf{r})$ defined for those $\mathbf{r}$ satisfying $|r_i| \leq L$, $i = 1, \ldots, d$, and such that $g_\mathbb{L}(\mathbf{r}) \to g(\mathbf{r})$ as $L \nearrow \infty$. In this case any subsequence limit ν of

$\nu_{\mathbb{L}}$ will be translation invariant in $\mathbb{Z}^d$ and realize $(\rho, \rho g)$. Conversely, from a translation invariant μ we can construct $\mu_{\mathbb{L}}$ by first projecting μ into a cubical box Λ of side $2L$ to obtain μ_Λ, then defining, for η a configuration in Λ or equivalently $\mathbb{L}$, $\mu_{\mathbb{L}}(\eta) = (2L)^{-d}\sum_{\mathbf{x}\in\mathbb{L}}\mu(\tau_{\mathbf{x}}\eta)$, where τ is the shift operator on $\mathbb{L}$. This yields a periodic measure $\mu_{\mathbb{L}}$ with density ρ and with $\tilde{g}_{\mathbb{L}}(\mathbf{r}) = g(\mathbf{r}) + O(1/L)$ for fixed $\mathbf{r}$.

The real question then is whether any subsequence limit of the $\nu_{\mathbb{L}}$ will be a 2-Gibbs measure with summable pair potentials. To answer this requires some control of the potentials $\phi_\Lambda^{(2)}(\mathbf{x}-\mathbf{y})$, which we lack at present (see question 4 at section 7).

7 Concluding remarks

There are clearly many natural questions left unanswered by our results. We list some of them for the case of a specified ρ and $g(\mathbf{r})$.

1) Is there any practical way to bridge the gap between the obvious necessary conditions described in section 2 and the sufficiency conditions given in sections 3 and 5?

2) When is the measure defined by (3.1) Gibbsian or quasi-Gibbsian?

3) Can one extend Theorem 6.1 to continuum systems in a finite domain $\Lambda \subset \mathbb{R}^d$? We expect this to be true under some reasonable assumptions on $g(\mathbf{r})$, e.g., the hard core condition that $g(\mathbf{r}) = 0$ for $r < D$, $D > 0$, under which there can only be a finite number of particles in Λ.

4) What can one say about the existence and nature of an entropy maximizing measure on $\mathbb{Z}^d$ for (ρ, g)? In particular are there situations for $\rho < \bar{\rho}$ when such a measure is not a translation invariant 2-Gibbsian measure? As pointed out at the end of section 6, if the answer to this question is no then the ν obtained from the periodic $\nu_{\mathbb{L}}$ of formula (6.1) will be the 2-Gibbs entropy maximizing measure on $\mathbb{Z}^d$.

5) What happens to the realizability problem if one does not specify $g(\mathbf{r})$ for all $\mathbf{r} \in \mathbb{Z}^d$ (or $\mathbb{R}^d$), but only for $\mathbf{r}$ in some finite domain, say $|\mathbf{r}| \le R$? (This question was mentioned briefly in section1.) As the notation indicates, we are still considering translation invariant correlations; we may in addition require that the two-point correlations $\rho_2(\mathbf{x}, \mathbf{y})$ of the realizing measure all be translation invariant and approach ρ^2 as $|\mathbf{x}-\mathbf{y}| \to \infty$. This is the problem discussed in [11] for $\mathbf{r} \in \mathbb{Z}$, or just on a ring. It turns out that, at least for the case $\mathbf{r} \in \mathbb{Z}$ and specified $(\rho, g(1), \ldots, g(k))$, one can compute, via

a finite number of operations, whether the correlations are realizable. On the d dimensional periodic lattice $\mathbb{L}$, for general d, the entropy maximizing measure $\nu_{\mathbb{L}}$ in (6.1) will now contain only a finite number of terms, so that the transition to an entropy maximizing 2-Gibbs measure on $\mathbb{Z}^d$ with only finite range potentials appears feasible. This will be described in a separate publication.

A Simple examples

In this appendix we collect some realizability results for certain concretely given g. Let us first mention a realizability problem in $\mathbb{R}^d$ which has been extensively studied by Torquato and Stillinger [8, 9]: to determine for which densities ρ there exists a translation invariant point process on $\mathbb{R}^d$ with

$$g(\mathbf{r}) = \begin{cases} 0, & \text{if } |\mathbf{r}| \leq 1, \\ 1, & \text{if } |\mathbf{r}| > 1. \end{cases} \tag{A.1}$$

Condition (2.5) implies that (ρ, g) can be only realized if $\rho \leq (v_d 2^d)^{-1}$, where v_d is the volume of the ball with diameter 1 in $\mathbb{R}^d$ ($v_1 = 1$, $v_2 = \pi/4$, etc.). In the other direction, Theorem 4.1 implies that for general d these correlations are indeed realizable if $\rho \leq e^{-1} v_d^{-1} 2^{-d}$. Thus the maximum density $\bar{\rho}(d)$ for which g is realizable satisfies $e^{-1} \leq 2^d v_d \bar{\rho}(d) \leq 1$. In one dimension we can say more: a simple construction of [28] shows realizability by a renewal process if $\rho \leq 1/e$ (it is also shown in [28] that $1/e$ is the maximal density for which a renewal process can realize g). A more complicated construction [27], using hidden Markov processes, gives realizability for all $\rho \leq 0.395$, so that $0.395 \leq \bar{\rho}(1) \leq 0.5$. The gap between these upper and lower bounds remains as a challenge to further rigorous analysis; Torquato and Stillinger conjecture, in part from simulation results of [9], that in low dimensions the process may in fact have $\bar{\rho}(d) = 2^{-d} v_d^{-1}$.

This continuum problem is, in dimension $d = 1$, related to the following lattice problem: for what densities ρ can the second correlation function $\rho^2 g^{(\alpha)}$, where

$$g^{(\alpha)}(x) = \begin{cases} 0, & \text{if } x = 0, \\ \alpha, & \text{if } |x| = 1, \\ 1, & \text{if } |x| > 1, \end{cases} \tag{A.2}$$

be realized by a point process on $\mathbb{Z}$? From the remarks in section 1 we know that for fixed α the set of realizable densities ρ is an interval $[0, \bar{\rho}_\alpha]$ with $0 < \bar{\rho}_\alpha \leq 1$. There is a superficial similarity between the continuum problem (A.1) and the lattice problem (A.2) for $\alpha = 0$, but there is also a deeper relation. For suppose that η_c is a point process in $\mathbb{R}$ which realizes (A.1) at density ρ. Then, for any $k \in \mathbb{Z}$, define $\eta(k) = N_{(k,k+1]} = \int_{k-1}^{k} \eta_c(x)\, dx$ (that is, $\eta(k)$ is the number of points of the process η_c lying in the interval $(k, k+1]$). Then η_k has value 0 or 1, $\langle \eta_k \rangle = \rho$, and for $j > 0$,

$$\begin{aligned} \langle \eta_k \eta_{k+j} \rangle \;=\; \langle \eta_0 \eta_j \rangle \;&=\; \rho^2 \int_0^1 dx \int_j^{j+1} dy\, g(y-x) \\ &=\; \begin{cases} \rho^2 \displaystyle\int_0^1 dx \int_{1+x}^{2} dy = \rho^2/2, & \text{if } j = 1, \\ \rho^2 \displaystyle\int_0^1 dx \int_j^{j+1} dy = \rho^2, & \text{if } j \geq 2. \end{cases} \end{aligned} \tag{A.3}$$

Thus η solves the lattice problem with the same density ρ and with $\alpha = 1/2$, from which $\bar{\rho}(1) \leq \bar{\rho}_{1/2}$. We will see below that $\bar{\rho}_{1/2} = 1/2$, so that this relation is consistent with the Torquato-Stillinger conjecture $\bar{\rho}(1) = 1/2$, but we see no way of going from the realizability of the lattice problem to that of the continuum and thus establishing the conjecture.

We now discuss the lattice problem (A.2) in some detail, as an illustration of the difficulties to face in the general situation. Clearly $\bar{\rho}_1 = 1$, since for each $\rho \in [0, 1]$ the Bernoulli or product measure ν_ρ realizes (A.2); for $\rho \neq 0, 1$ there are in fact uncountably many mutually inequivalent realizing measures [27], while for $\rho = 0, 1$ the realization is unique. For other values of α, upper bounds on $\bar{\rho}_\alpha$ are provided by (2.5) and (2.7). In particular, (2.5) yields the upper bound $\bar{\rho}_\alpha \leq R_F(\alpha)$, where

$$R_F(\alpha) = \begin{cases} \dfrac{1}{3-2\alpha}, & \text{if } 0 \leq \alpha \leq 1, \\ \dfrac{1}{2\alpha - 1}, & \text{if } 1 \leq \alpha. \end{cases} \tag{A.4}$$

The Yamada condition (2.7) gives an upper bound $\bar{\rho}_\alpha \leq R_Y(\alpha)$; a straightforward but somewhat lengthy computation shows that $R_Y(\alpha) = R_F(\alpha)$ for $\alpha = 1/2$, for $\alpha = (k \pm 1)/2k$, $k = 1, 2, \ldots$, and for $\alpha \geq 1$. For other values of α, $R_Y(\alpha) < R_F(\alpha)$, so that certainly the bound R_F is not always sharp. These bounds, together with several lower bounds for $\bar{\rho}_\alpha$ obtained below,

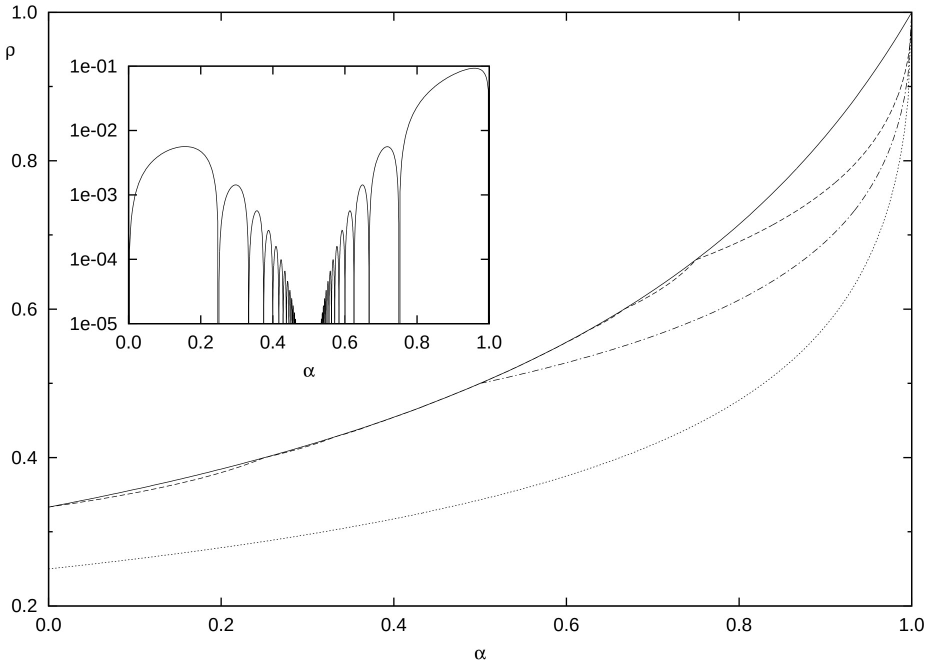

Figure 1: Upper bounds $R_F(\alpha)$ (solid) and $R_Y(\alpha)$ (dashes) for $\bar{\rho}_\alpha$. Lower bounds $r_S(\alpha)$ (dots/dashes) and $r_B(\alpha)$ (dots), for $0 \leq \alpha \leq 1$. The inset plots the difference $R_F(\alpha) - R_Y(\alpha)$ on a logarithmic scale.

are plotted in Figure 1; for values of α at which $R_Y(\alpha) < R_F(\alpha)$, $R_Y(\alpha)$ is determined numerically.

Lower bounds on $\bar{\rho}_\alpha$ come, essentially, from procedures for explicitly realizing the desired process at some value of ρ. For example, from Theorem 3.1, for $\alpha \leq 1$, and Theorem 5.1, for $\alpha \geq 1$, we obtain $\bar{\rho}_\alpha \geq r_A(\alpha)$, where

$$r_A(\alpha) = \begin{cases} \dfrac{1}{e(3-2\alpha)}, & \text{for } 1 \geq \alpha \geq 0, \\ \dfrac{1}{\alpha^2}, & \text{for } \alpha \geq 1. \end{cases} \tag{A.5}$$

Comparison with (A.4) shows that, as might be expected, the lower bounds from these general construction methods do not approach the upper bound very closely. To get better bounds or exact values for $\bar{\rho}_\alpha$ one must turn to more *ad hoc* methods. In this spirit we next describe two families of processes which realize (A.2) and which provide improvements in the lower bounds (A.5). We studied other constructions, partially improving some of the results below, but these are omitted for conciseness.

The first construction, valid for $\alpha \geq 1/2$, achieves a density $\rho = r_S(\alpha)$, where

$$r_S(\alpha) = \begin{cases} \dfrac{1}{1+\sqrt{2-2\alpha}}, & \text{if } 1/2 \leq \alpha \leq 1, \\ \dfrac{1}{2\alpha - 1}, & \text{if } 1 \leq \alpha; \end{cases} \tag{A.6}$$

thus $\bar{\rho}_\alpha \geq r_S(\alpha)$. Comparison of (A.6) with (A.4) shows that $r_S(\alpha) = R_F(\alpha)$ for $\alpha = 1/2$ and $\alpha \geq 1$, so that $\bar{\rho}_\alpha = R_F(\alpha)$ for these values. The measures for these processes are superpositions of two measures of period two. To construct them, we first choose with equal probability one of two partitions of $\mathbb{Z}$, either $\ldots \cup \{-2,-1\} \cup \{0,1\} \cup \{2,3\} \cup \ldots$ or $\ldots \cup \{-1,0\} \cup \{1,2\} \cup \{3,4\} \cup \ldots$, and then assign a configuration to each pair $(i, i+1)$ of sites in the partition independently, taking (η_i, η_{i+1}) to have value $(1,0)$, $(0,1)$ each with probability p, $(0,0)$ with probability q, and $(1,1)$ with probability $(1-p-q)/2$. The optimal choices of parameters which lead to (A.6) are $q = 0$, $p = \sqrt{2-2\alpha}/(1+\sqrt{2-2\alpha})$ for $1/2 \leq \alpha \leq 1$ and $p = 0$, $q = (2\alpha-2)/(2\alpha-1)$ for $\alpha \geq 1$.

The measures constructed above, as superpositions of period-two measures, do not have good mixing properties (this defect will be inherited by measures with lower values of ρ obtained via the thinning process described in section 1). For the case $\alpha = \rho = 1/2$ this decomposability is inevitable; the system is then superhomogeneous (see section 2; in fact the variance of the number of points on any set of consecutive lattice sites is uniformly bounded by 3/4) and the decomposability of any realizing measure then follows from a result of Aizenmann, Goldstein, and Lebowitz [29].

Our second construction is valid for $0 \leq \alpha \leq 1$. For this process we first distribute particles on $\mathbb{Z}$ with a Bernoulli measure such that each site is occupied with probability λ; then if in this initial configuration a site is occupied we delete the particle occupying its left neighbor, if it exists, with probability κ. With the optimal choices $\lambda = 1/(1+\sqrt{1-\alpha})$ and $\kappa = \sqrt{1-\alpha}$ we obtain a realization of (A.2) with density

$$r_B(\alpha) = \frac{1}{(1+\sqrt{1-\alpha})^2}, \tag{A.7}$$

so that $\bar{\rho}_\alpha \geq r_B(\alpha)$. For $\alpha \geq 1/2$ this is of no interest, since $r_B \leq r_S$, but for $0 \leq \alpha < 1/2$ it improves on the bounds (A.5).

The case $\alpha = 0$ merits special discussion. From (A.7), $\bar{\rho}_0 \geq 0.25$; in this case the point process used to obtain r_B is a renewal process and the construction is a lattice version of that given in [28] to establish that $\bar{\rho} \geq 1/e$ for the continuum problem (A.1). A construction based on a hidden Markov process [27] improves this lower bound to $\bar{\rho}_0 > 0.265$. The upper bound $\bar{\rho}_0 \leq R_F(\alpha) = R_Y(\alpha) = 1/3$ can be improved [27] to $\bar{\rho}_0 \leq (326 - \sqrt{3115})/822 \simeq 0.3287$. As in the continuum problem (A.1), it remains a challenge to diminish the rather large gap between these upper and lower bounds.

B Proofs of Theorems 3.1 and 4.1

Completion of the proof of Theorem 3.1 We must show that the functions k_m^Λ are analytic for $|z| < R$. As indicated in section 3, the proof follows closely the proof of Theorem 4.2.3 of [15], and we content ourselves with pointing out a few key steps and the necessary changes. Let E_ξ be the Banach space of all sequences $(\varphi_m)_{m=1}^\infty$, where $\varphi_m : (\mathbb{R}^d)^m \to \mathbb{C}$, for which

$$\|\varphi\|_\xi := \sup_{m\geq 0} \sup_{\mathbf{x}_1,\ldots,\mathbf{x}_m\in\mathbb{R}^d} \xi^{-m}|\varphi_m(\mathbf{x}_1,\ldots,\mathbf{x}_m)| < \infty, \tag{B.1}$$

and let $\chi_m(\mathbf{x}_1,\ldots,\mathbf{x}_m)$ be the characteristic function of the set

$$\left\{ (\mathbf{x}_1,\ldots\mathbf{x}_m) \in (\mathbb{R}^d)^m \;\middle|\; \mathbf{x}_i \in \Lambda,\ \prod_{i=1}^m \left(\prod_{j=i+1}^m g(\mathbf{x}_i - \mathbf{x}_j) \prod_{j=1}^n g(\mathbf{x}_i - \mathbf{r}_j) \right) > 0 \right\}. \tag{B.2}$$

Define the operator $\mathcal{K}$ on $\bigcup_{\xi>0} E_\xi$ by

$$\begin{aligned}(\mathcal{K}\varphi)_{m+1}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{x}) &= \chi_{m+1}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{x}) e^{-V^{(1)}(\mathbf{x})-\sum_{j=1}^m V^{(2)}(\mathbf{x}-\mathbf{x}_j)} \\ &\quad\cdot \sum_{k=\max\{0,1-m\}}^\infty \frac{1}{k!}\int_{\mathbb{R}^{dk}} \prod_{j=1}^k \left(e^{-V^{(2)}(\mathbf{x}-\mathbf{z}_j)} - 1\right) \\ &\quad\cdot \varphi_{m+k}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{z}_1,\ldots,\mathbf{z}_k)\, d\mathbf{z}_1\cdots d\mathbf{z}_k.\end{aligned} \tag{B.3}$$

The factor χ_{m+1} in (B.3) is needed in the estimate (B.4) below because the one-body potential $V^{(1)}$ in (B.3) depends on $\mathbf{r}_1,\ldots,\mathbf{r}_n$, and it is primarily these aspects which distinguish the proof here from that of [15]. Note that, with this factor, $\mathcal{K}$ depends on Λ, on g, and on $\mathbf{r}_1,\ldots,\mathbf{r}_n$. Then

$$\begin{aligned}|(\mathcal{K}\varphi)_{m+1}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{x})| &\leq \|\varphi\|_\xi e^{-V^{(1)}(\mathbf{x})-\sum_{j=1}^m V^{(2)}(\mathbf{x}-\mathbf{x}_j)} \\ &\cdot\chi_{m+1}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{x})\sum_{k=0}^\infty \frac{1}{k!}\int_{\mathbb{R}^{dk}}\prod_{j=1}^k \left|e^{-V^{(2)}(\mathbf{x}-\mathbf{z}_j)}-1\right|\xi^{k+m}d\mathbf{z}_1\cdots d\mathbf{z}_k \\ &\leq \|\varphi\|_\xi \xi^m\, b\exp\left(\xi\int_{\mathbb{R}^d}|g(\mathbf{z})-1|d\mathbf{z}\right), \end{aligned} \tag{B.4}$$

so that

$$\|\mathcal{K}\varphi\|_\xi \leq \xi^{-1} b\exp\left(\xi\int_{\mathbb{R}^d}|g(\mathbf{z})-1|d\mathbf{z}\right)\|\varphi\|_\xi. \tag{B.5}$$

Now as in [15] the sequence of correlation functions k_m^Λ satisfies the Kirkwood-Salsburg equation

$$k^\Lambda = z\psi + z\,\mathcal{K}k^\Lambda \tag{B.6}$$

where $\psi_m = \delta_{m1}$; by an optimal choice of ξ we may insure that $\|z\mathcal{K}\|_\xi < 1$ whenever $|z| < R$. For such z, $I - z\mathcal{K}$ is invertible and the equation (B.6) has a unique solution in E_ξ; one proceeds as in [15]. ■

Proof of Theorem 4.1 As in the proof of Theorem 3.1 we denote by k_m^Λ the m^{th} correlation function for a grand canonical ensemble in Λ with activity z, inverse temperature β, and potentials (4.4)–(4.6) ; we do not write explicitly the dependence of these functions on $\mathbf{r}_1,\ldots,\mathbf{r}_n$. The k^Λ again satisfy the Kirkwood-Salsburg equation (B.6) in the Banach space E_ξ, but with a modified operator $\mathcal{K}$. To define $\mathcal{K}$ we write $\mathbf{u}_i := \mathbf{r}_i$ for $i = 1,\ldots,n$, $\mathbf{u}_i := \mathbf{x}_{i-n}$ for $i = n+1,\ldots,n+m$, and $\mathbf{u}_i := \mathbf{z}_{i-n-m}$ for $i = n+m+1,\ldots,n+m+k$. Then

$$\begin{aligned}(\mathcal{K}\varphi)_{m+1}(\mathbf{x}_1,\ldots,\mathbf{x}_m,\mathbf{x}) &= ze^{-E(\mathbf{x}|\mathbf{u}_1,\ldots,\mathbf{u}_{n+m})}\sum_{k=0}^\infty\frac{1}{k!}\int_{\Lambda^k} \\ &\cdot K(\mathbf{x}|\mathbf{u}_1,\ldots,\mathbf{u}_{n+m+k})\varphi_{m+k}(\mathbf{u}_{m+1},\ldots,\mathbf{u}_{n+m+k})\,d\mathbf{u}_{n+m+1}\cdots d\mathbf{u}_{n+m+k},\end{aligned} \tag{B.7}$$

with

$$
\begin{aligned}
E(\mathbf{x}|\mathbf{u}_1,\ldots,\mathbf{u}_{n+m}) &:= \sum_{i=1}^{n+m} V^{(2)}(\mathbf{x},\mathbf{u}_i) + \sum_{1\le i<j\le n+m} V^{(3)}(\mathbf{x},\mathbf{u}_i,\mathbf{u}_j) \quad \text{(B.8)}\\
K(\mathbf{x}|\mathbf{u}_1,\ldots,\mathbf{u}_{n+m+k}) &:= \chi_{n+m+k+1}(\mathbf{u}_1,\ldots,\mathbf{u}_{n+m+k},\mathbf{x})\\
&\cdot \sum_{\eta\subset\{1,\ldots,k\}} \prod_{i\in\{1,\ldots,k\}\setminus\eta} \left(e^{-V^{(2)}(\mathbf{x},\mathbf{u}_{n+m+i})}-1\right)\\
&\cdot \sum_G \prod_{\{i,j\}\in G} \left(e^{-V^{(3)}(\mathbf{x},\mathbf{u}_i,\mathbf{u}_j)}-1\right) \prod_{i\in\eta} e^{-V^{(2)}(\mathbf{x},\mathbf{u}_{n+m+i})}. \quad \text{(B.9)}
\end{aligned}
$$

Here $\sum_G$ extends over the set of graphs which have vertex set $V_1 \cup V_2$, where $V_1 = \{1,\ldots,m+n\}$ and $V_2 = \{l+m+n \mid l \in \eta\}$ (a graph being identified as a set of edges, i.e., of unordered pairs of vertices), and in which every edge has at least one of its vertices lying in V_2, and every vertex in V_2 has at least one edge incident on it. The derivation of (B.7–B.9) is similar to that of the usual Kirkwood-Salsburg equation [15].

The operator $\mathcal{K}$ can be bounded as follows. First, the hypotheses of the theorem imply that $\chi_{n+m+k+1}(\mathbf{u},\mathbf{x})e^{-E(\mathbf{x}|\mathbf{u})} \le b\ b_3$. Next, since the factor $(e^{-V^{(3)}(\mathbf{x},\mathbf{u}_i,\mathbf{u}_j)}-1)$ in (B.9) vanishes unless $\mathbf{u}_i$ and $\mathbf{u}_j$ lie inside the ball of radius D_3 around $\mathbf{x}$, the sum over η is nonzero only for those η's such that all points $(\mathbf{z}_i)_{i\in\eta}$ are inside this ball. On the other hand, the factor $\chi_{n+m+k+1}(\mathbf{u},\mathbf{x})$ implies that K vanishes unless all the $\mathbf{u}_i$ are separated by a distance at least D, so that we may suppose that there are at most N (see (4.10)) of these points inside the ball. We thus have the bound

$$
\begin{aligned}
&\int_{\Lambda^k} |K(\mathbf{x}|\mathbf{u}_1,\ldots,\mathbf{u}_{n+m+k})|\, d\mathbf{u}_{n+m+1}\cdots d\mathbf{u}_{n+m+k}\\
&\qquad \le \sum_{l=0}^{N} \binom{k}{l} C(g)^{k-l}(v_d(D_3/2)^d)^l \sum_{j=\lceil l/2\rceil}^{M} \binom{M}{j} \hat{C}_3^j b^j\\
&\qquad \le (1+bC_3(\tilde{g}_3))^M \left(C(g)+v_d(D_3/2)^d C_3(\tilde{g}_3)\right)^k. \quad \text{(B.10)}
\end{aligned}
$$

Here $M = N(N-1)/2$, $\hat{C}_3 = \sup_{\mathbf{x},\mathbf{y}\in\mathbb{R}^d} |\tilde{g}_3(\mathbf{x},\mathbf{y})-1|$, $\lceil s\rceil$ is the least integer not smaller than s, and we have used the inequality $\hat{C}_3^j \le C_3(\tilde{g}_3)^j C_3(\tilde{g}_3)^l$, valid for $j \ge l/2$, which follows from (4.7) by considering separately the cases $\hat{C}_3 \ge 1$ and $\hat{C}_3 < 1$.

¿From (4.10) we have that $M \leq (3D_3/D)^{2d}$, and from (B.7) and (B.10) it then follows that the norm of $\mathcal{K}$ in the Banach space E_ξ satisfies

$$\|\mathcal{K}\|_\xi \leq \xi^{-1} b b_3 \left(1 + bC(\tilde{g}_3)\right)^{(3D_3/D)^{2d}} e^{\xi\left(C(g)+v_d(D_3/2)^d C(\tilde{g}_3)\right)}. \tag{B.11}$$

An optimal choice of ξ again shows that $\|z\mathcal{K}\|_\xi < 1$ when $|z| < R_3$, where R_3 denotes the right hand side of (4.8), completing the proof. ■

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