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The realizability problem for point processes: an explicit construction on the $d-$dimensional lattice

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***Abstract*— In this talk we focus on a particular instance of the realizability problem, namely, on the question of establishing whether two given functions $\rho_1(i)$ and $\rho_2(i,j)$ non-negative and symmetric on $\mathbb{Z}^d$ ($d \in \mathbb{N}$) are the first two correlation functions of a translation invariant point process on $\mathbb{Z}^d$. We present a joint work with Emanuele Caglioti and Tobias Kuna, where we provide an explicit construction of such a process for any $d \geq 2$ under some natural assumptions relevant for applications in fluid theory and material science (iso-g processes).**

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I. INTRODUCTION

The realizability problem is an infinite dimensional version of the classical truncated moment problem which naturally arises from applied fields dealing with the analysis of complex systems, and which is still open in many of its aspects. One of the main difficulties in studying such a system is to handle an enormous number of its identical components. This challenge is commonly tackled by evaluating selected characteristics of the system which provide a reasonable picture of its qualitative behaviour. For example, the so-called correlation functions (often just the first two) are the most interesting quantities characterizing particle systems in statistical mechanics and can be estimated through approximation schemes such as Percus-Yevick and hyper-netted chain approximations. The realizability problem exactly addresses the question of determining whether or not the resulting functions represent the actual correlation functions of some random distribution.

Let us give a rigorous formulation of this problem in the setting considered in [1], that is, the realizability problem for point processes on the $d-$dimensional lattice, where d is a positive integer. Recall that a point process on $\mathbb{Z}^d$ is a random collection of points in $\mathbb{Z}^d$, whose distribution is described by a probability measure on the set of all possible point collections. In the following we will consider only simple point processes, i.e., countable collections of distinct points in $\mathbb{Z}^d$, and so we will omit "simple" as no confusion can arise. Then the set of all possible point processes on $\mathbb{Z}^d$ can be seen as the set of all counting functions $\{0,1\}^{\mathbb{Z}^d}$. The first and second *correlation functions* of a point process $P = \{P_{\mathbf{i}}\}_{\mathbf{i}\in\mathbb{Z}^d}$ on the $d-$dimensional lattice, $P_{\mathbf{i}} \in \{0,1\}$, whose distribution is described by the probability μ, are defined as

$$\begin{cases} \rho_1^{\mu}(\mathbf{i}) := \mathbb{E}_{\mu}(P_{\mathbf{i}}) \\ \rho_2^{\mu}(\mathbf{i},\mathbf{j}) := \mathbb{E}_{\mu}(P_{\mathbf{i}}P_{\mathbf{j}}) - \mathbb{E}_{\mu}(P_{\mathbf{i}})\delta(\mathbf{i}-\mathbf{j}) \end{cases},$$

where $\mathbf{i},\mathbf{j} \in \mathbb{Z}^d$, δ is the Dirac delta function and $\mathbb{E}_{\mu}$ denotes the expectation w.r.t. μ.

The *truncated realizability problem* in this setting addresses the following question: given two functions $\rho_1(\mathbf{i})$ and $\rho_2(\mathbf{i},\mathbf{j})$ non-negative and symmetric for all $\mathbf{i},\mathbf{j} \in \mathbb{Z}^d$, does there exist a point process P with distribution μ for which these are the correspondent first and second correlation functions, i.e., $\rho_1(\mathbf{i}) = \rho_1^{\mu}(\mathbf{i})$ and $\rho_2(\mathbf{i},\mathbf{j}) = \rho_2^{\mu}(\mathbf{i},\mathbf{j})$ for all $\mathbf{i},\mathbf{j} \in \mathbb{Z}^d$? Clearly, the problem can be posed for any finite sequence of non-negative and symmetric functions $(\rho_k(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_k))_{k=1}^n$ with $n \in \mathbb{N}$, but for simplicity we will just focus on the case $n = 2$. We should mention that when this question is asked for a given infinite sequence $(\rho_k)_{k=1}^{\infty}$, then the problem is addressed as full realizability problem (see e.g., [9] for a systematic study of the full case for point processes and [4] for recent developments).

Keeping in mind that the correlation functions associated to a point process are the factorial moments of its distribution, it should be clear now that the realizability problem for point processes on $\mathbb{Z}^d$ is nothing but a moment problem posed for measures supported on the set of all possible point processes on the $d-$dimensional lattice, so it can be regarded as an infinite-dimensional moment problem. This reinterpretation has been recently used as a powerful approach in several particular instances of the realizability problem, see e.g., [2], [5], [6], [7], [8].

In [1] we consider the important special case of *translation invariant point processes*, which actually contains all the essential difficulties of the problem. In this case the realizability problem asks if, for given $\rho \in \mathbb{R}^+$ and $g : \mathbb{Z}^d \to \mathbb{R}^+$ symmetric, there exists a translation invariant point process on $\mathbb{Z}^d$ with distribution μ such that

$$\begin{cases} \rho_1^{\mu}(\mathbf{i}) = \rho \\ \rho_2^{\mu}(\mathbf{i},\mathbf{j}) = \rho^2 g(\mathbf{i}-\mathbf{j}) \end{cases}. \tag{1}$$

If such a process exists, then it is said to be *realizing* (ρ, g) and the latter is called a *realizable* pair on $\mathbb{Z}^d$. The function g is known in fluid theory as *radial distribution*. The realizability problem is in fact a longstanding problem in the classical theory of fluids (see e.g., [3], [11]), but it has been investigated in many other contexts such as stochastic geometry [8], spatial statistics [14], spatial ecology [10], just to name a few. In particular, Stillinger and Torquato developed fascinating applications in the study of heterogeneous

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materials and mesoscopic structures based on the solvability of the realizability problem (see e.g., [12], [13], [15]).

II. ISO-g^α PROCESSES ON $\mathbb{Z}^d$: OUR CONSTRUCTION

In [1] we explicitly construct a point process on the $d-$dimensional lattice with $d \geq 2$ such that, for given $\alpha \geq 0$ and $\rho > 0$, (1) holds for $g = g^{(\alpha)}$ defined as follows:

$$g^{(\alpha)}(\mathbf{x}) := \begin{cases} 0 & \text{if } \mathbf{x} = 0 \\ \alpha & \text{if } |\mathbf{x}| = 1 \\ 1 & \text{if } |\mathbf{x}| > 1 \end{cases}, \ \mathbf{x} \in \mathbb{Z}^d. \tag{2}$$

Such a process is then a realizing process for (ρ, g^α) and it is usually referred to as *iso-$g^{(\alpha)}$ process*. The realizability problem for iso-$g^{(\alpha)}$ processes has been extensively studied for the case $\alpha = 0$ by Stillinger and Torquato, e.g., in [12]. The function $g^{(0)}$ describes a model with on-site and nearest neighbour exclusion and with no correlation for pairs of sites separated by two or more lattice spacings. For any fixed $\alpha \geq 0$, explicit constructions of iso-$g^{(\alpha)}$ processes in the case $d = 1$ were provided in [6, Appendix 1] but to the best of our knowledge no constructions were introduced before in higher dimensions.

Let us then briefly review the multi-dimensional construction we propose in [1], which is actually a very natural method to build a point process on $\mathbb{Z}^d$ with $d \geq 2$ starting from a point process on $\mathbb{Z}$. Given $\alpha \geq 0$, we call *basic process with density* γ (in short $BP\gamma$) a point process defined on $\mathbb{Z}$ and realizing $(\gamma, g^{(\alpha)})$. For any $j = 1, \ldots, d$ we independently define a point process $B^{(j)}$ on $\mathbb{Z}^d$ such that for any fixed $i_1, \ldots, i_{j-1}, i_{j+1}, \ldots, i_d \in \mathbb{Z}$, $\{B^{(j)}_{i_1,\ldots,i_d}\}_{i_j \in \mathbb{Z}}$ is a $BP\gamma$ in the variable i_j. In other words, the process $B^{(j)}$ can be seen as a sequence of parallel $BP\gamma$'s independent one from each other. Using the simple but special structure of each of the $B^{(j)}$'s and their independence, we show in [1, Section 2.1] that the point process $P := \{P_{i_1,\ldots,i_d}\}_{(i_1,\ldots,i_d) \in \mathbb{Z}^d}$ with $P_{i_1,\ldots,i_d} := B^{(1)}_{i_1,\ldots,i_d} \cdots B^{(d)}_{i_1,\ldots,i_d}$ is a realizing process for the pair $(\gamma^d, g^{(\alpha)})$.

III. THE MAXIMAL REALIZABLE DENSITY

The main challenge in the study of the realizability problem for iso-$g^{(\alpha)}$ processes is to find the maximal value of the uniform density ρ for which realizability can be established for a specified $\alpha \geq 0$. In fact, it was proven in [6, Section 1] that for a fixed α the set of realizable densities ρ is an interval $[0, \bar{\rho}_\alpha(d)]$ with $0 < \bar{\rho}_\alpha(d) \leq 1$.

In [1, Section 3.1] we extend to the higher dimensional case the techniques introduced in [6] for getting an upper bound for $\bar{\rho}_\alpha(1)$. Indeed, using that a necessary condition for the realizability of a given pair $(\rho, g^{(\alpha)})$ by an iso$-g^{(\alpha)}$ process on $\mathbb{Z}^d$ is the positive semidefiniteness of its associated covariance matrix, we obtain that $\bar{\rho}_\alpha(d) \leq \frac{1}{1+2d|1-\alpha|}$. for any $d \in \mathbb{N}$ and $\alpha \geq 0$.

Concerning the lower bounds, in [6] the authors discuss certain general methods which, when applied to (2), yield the following lower bounds for $\bar{\rho}_\alpha(d)$ in any dimension $d \in \mathbb{N}$:

$$\bar{\rho}_\alpha(d) \geq r_A(\alpha, d) := \begin{cases} \frac{1}{e(2d+1-2d\alpha)}, & \text{if } 0 \leq \alpha < 1, \\ \frac{1}{\alpha^{2d}}, & \text{if } \alpha \geq 1. \end{cases}$$

For the one-dimensional case, they also develop some explicit constructions of realizing iso-$g^{(\alpha)}$ processes which provide concrete lower bounds for $\bar{\rho}_\alpha(1)$ improving $r_A(\alpha, 1)$.

In [1, Section 3.2] we prove that our $d-$dimensional construction combined with these one-dimensional concrete lower bounds provides the following lower bound for $\bar{\rho}_\alpha(d)$ for any $d \geq 2$ and any $\alpha \geq 0$:

$$\bar{\rho}_\alpha(d) \geq r_C(\alpha, d) := \begin{cases} \frac{1}{(1+\sqrt{1-\alpha})^{2d}}, & \text{if } 0 \leq \alpha < \frac{1}{2}, \\ \frac{1}{(1+\sqrt{2-2\alpha})^{d}}, & \text{if } \frac{1}{2} \leq \alpha \leq 1, \\ \frac{1}{(2\alpha-1)^d}, & \text{if } \alpha \geq 1. \end{cases}$$

For each $d \geq 2$ we also identify the range of values of α for which our lower bound $r_C(\alpha, d)$ improves $r_A(\alpha, d)$ and so provides a better approximation of the feasibility region for the corresponding class of realizability problems:

- if $0 \leq \alpha < \frac{1}{2}$ then $r_C(\alpha, d) \leq r_A(\alpha, d)$
- if $\alpha \geq 1$ then $r_A(\alpha, d) \leq r_C(\alpha, d)$
- if $\frac{1}{2} \leq \alpha \leq 1$ then the relation between the two bounds depends on the dimension d. In fact, there exists $\alpha_C(d) \in \left[\frac{1}{2}, 1\right]$ such that $r_A(\alpha, d) \leq r_C(\alpha, d)$ for all $\alpha \in [\alpha_C(d), 1]$.

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