Abstracts

On the Realizability of Point Processes with Specified One and Two Particle Densities

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(joint work with O. Costin, T. Kuna and E. R. Speer)

Abstract: We investigate and give partial answers to the following question: given a one particle and pair density, $\rho_1(\mathbf{r}_1)$ and $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$, $\mathbf{r}_1, \mathbf{r}_2 \in \mathbb{R}^d$ (or $\mathbb{Z}^d$), does there exist a point process, i.e. a probability measure on points in $\mathbb{R}^d$ ($\mathbb{Z}^d$), having these densities?

The microscopic structure of macroscopic systems, such as fluids, is best described by the joint n-particle densities $\rho_n(\mathbf{r}_1, ...\mathbf{r}_n)$, where the $\mathbf{r}_1, ..., \mathbf{r}_n$ are position vectors in $\mathbb{R}^d$. The most important of these are the one particle density $\rho_1(\mathbf{r}_1)$ and the pair density $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$. For spatially homogeneous systems, the only ones we shall consider here, $\rho_1(\mathbf{r}_1) = \rho$ and $\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \rho^2 g(\mathbf{r}_1 - \mathbf{r}_2)$ with $g(\mathbf{r}) = g(-\mathbf{r})$; thus $\rho g(\mathbf{r})$ is the density of particles at a displacement $\mathbf{r}$ from the position of a specified particle. For pure fluid phases $g(\mathbf{r}) \to 1$ as $|\mathbf{r}| \to \infty$.

The theory of classical equilibrium fluids is based in large part on finding good approximations to $g(\mathbf{r})$. This leads to an interesting and important question: given a density $\rho > 0$ and a candidate $g(\mathbf{r})$, obtained via some approximate theory or just invented for capturing a certain behavior, do these arise from some actual distribution of particles in d-dimensional space? That is, does there exist a *point process*—a probability measure on sets of points in $\mathbb{R}^d$—with density ρ and with pair density corresponding to the proposed $g(\mathbf{r})$? More generally, what are necessary and sufficient conditions on ρ and $g(\mathbf{r})$ for this to be true? For more background on the long history of this *realizability problem*, see [1] and references therein.

One may also consider the realizability problem on the lattice $\mathbb{Z}^d$. We assume the exclusion condition that each lattice site contains at most one particle. Now ρ is the probability that there is a particle on any fixed site and $\rho^2 g(\mathbf{r}_1 - \mathbf{r}_2)$ the probability that there are particles at $\mathbf{r}_1$ and $\mathbf{r}_2$; the exclusion condition corresponds formally to $g(\mathbf{0}) = 0$. In what follows we will frequently state results for the continuum case, making some comment on the translation to the lattice when that is more complicated than simply replacing integrals by sums.

There are some obvious conditions which ρ and $g(\mathbf{r})$ must satisfy [1]:

$$\rho > 0 \quad \text{and} \quad g(\mathbf{r}) \geq 0; \tag{1}$$

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

$$V_\Lambda \equiv \rho|\Lambda| + \rho^2 \iint\limits_{\Lambda} \left[g(\mathbf{r}_1 - \mathbf{r}_2) - 1\right] d\mathbf{r}_1 d\mathbf{r}_2 \geq \theta(1-\theta). \tag{3}$$

In (3), V_Λ is the variance of the number N_Λ of particles in a region $\Lambda \subset \mathbb{R}^d$ and θ is the fractional part of the mean $\rho|\Lambda|$ of N_Λ: $\rho|\Lambda| = k + \theta$ with $k = 0, 1, \ldots$ and $0 \le \theta < 1$. These conditions may, however, be only the tip of the iceberg. Necessary and sufficient conditions for realizability can be given in the form of an uncountable number of positivity conditions on ρ and $g(\mathbf{r})$ [2]: Given any functions $f_2(\mathbf{r}_1, \mathbf{r}_2)$ and $f_1(\mathbf{r})$ such that, for any n points $\mathbf{r}_1, \ldots, \mathbf{r}_n$, $\sum_{i \neq j} f_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_i f_1(\mathbf{r}_i) + 1 \ge 0$, we must have

$$\rho^2 \iint_{\Lambda} g(\mathbf{r}_1, \mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 + \rho \int_\Lambda f_1(\mathbf{r}) d\mathbf{r} + 1 \ge 0 \tag{4}$$

for all $\Lambda \subset \mathbb{R}^d$. Conditions (1)–(3) may be obtained from (4) by appropriate choices of f_1 and f_2, but clearly represent just a very small subset of the latter equations. Nevertheless, we must confess that we do not have at the present time any example which satisfies (1)–(3) and not (4) in $\mathbb{R}^d$. We do however have such an example on the lattice $\mathbb{Z}$, which we shall now describe. (The conditions for $\mathbb{Z}^d$ corresponding to (1)–(4) are obtained in the obvious way.)

Suppose that for $r \in \mathbb{Z}$ we define

$$g(r) = \begin{cases} 0, & \text{for } r = 0, \pm 1, \\ 1, & \text{for } |r| \ge 2. \end{cases} \tag{5}$$

This g describes a model with on-site and nearest neighbor exclusion and with no correlation, on the pair level, for sites separated by two or more lattice spacings. It is then easy to check that (1)–(3) are satisfied for for $\rho \le 1/3$, but a simple argument shows that in fact there is a critical density $\rho_c < 1/3$ such that the process is not realizable for $\rho > \rho_c$ (a numerical calculation indicates that $\rho_c < 0.3287$). On the other hand it is easy to construct explicitly a realization of (5) for $\rho \le 1/4$: Start with a Bernoulli measure on $\mathbb{Z}$ with density λ and then remove any particle from an occupied site x if and only if site $x+1$ is also occupied. This will yield a translation invariant state with density $\rho = \lambda(1-\lambda) \le 1/4$ and with $g(r)$ given by (5). Whether (5) is realizable for any $\rho > 1/4$ (i.e., whether or not $\rho_c > 1/4$) is a complete mystery to us at present. We can show, however, that the state constructed above corresponds to a *renewal* process, for which the sequence of interparticle distances is Markovian, and that such a renewal process with $g(\mathbf{r})$ given by (5) cannot exist for $\rho > 1/4$. (The corresponding result on $\mathbb{R}$ is discussed in [1], where it is shown that a renewal process exists with

$$g(r) = \begin{cases} 0, & \text{for } |r| \le 1, \\ 1, & \text{for } |r| > 1. \end{cases} \tag{6}$$

if and only if $\rho \le 1/e$. Here the maximum ρ consistent with (1)–(3) is 1/2.)

Let us now state a general theorem about realizability of a given ρ and $g(\mathbf{r})$, $\mathbf{r} \in \mathbb{R}^d$.

Theorem: *Let*

$$g(\mathbf{r}) = \begin{cases} 0, & |\mathbf{r}| \le D, \\ \exp(-\varphi(\mathbf{r})), & |\mathbf{r}| > D, \end{cases}$$

where for some $\Phi \geq 0$,

$$\sum_{i=1}^{n} \varphi(\mathbf{r}_i) \geq -2\Phi \quad \text{whenever} \quad |\mathbf{r}_i - \mathbf{r}_j| \geq D, \quad 1 \leq i < j \leq n. \tag{7}$$

Then ρ *and* $g(\mathbf{r})$ *are realizable whenever*

$$\rho \leq \left(e^{1+2\Phi} \int_{\mathbb{R}^d} |g(\mathbf{r}) - 1| \, d\mathbf{r} \right)^{-1}. \tag{8}$$

Note that condition (7) is satisfied for any $D \geq 0$ (and $\Phi = 0$) if $\varphi(\mathbf{r}) \geq 0$ for all r, and for $D > 0$ (i.e., with a hard core) if $\varphi(\mathbf{r})$ decays faster than $|\mathbf{r}|^{-(d+\epsilon)}$ for $|r| \to \infty$ [3]. A similar theorem holds in the lattice case $\mathbb{Z}^d$; the integral has to be replaced by a sum and the hard core condition is automatically satisfied because at most one particle can occupy any site. The theorem is a generalization of a result of R. V. Ambartzumian and H. S. Sukiasian (A-S) [4], who considered only the case $\varphi \geq 0$ ($g \leq 1$). For the example (5) the theorem gives existence only for $\rho \leq (3e)^{-1}$, so it is clearly not optimal. Readers with a statistical mechanics background will recognize the right hand side of (8) as the Ruelle-Penrose lower bound for the radius of convergence of the fugacity expansion for an equilibrium system with pair potential φ given by $g(\mathbf{r}) = e^{-\varphi(\mathbf{r})}$ [3].

The construction by A-S of the point process corresponding to ρ and $g(\mathbf{r})$, which we follow, does not in general yield a Gibbs measure. The existence of a Gibbs measure with a decaying pair potential which realizes a given ρ and $g(\mathbf{r})$ was proven by L. Koralov for lattice gases when ρ is sufficiently small and $\sum_{\mathbf{r}} |g(\mathbf{r}) - 1| < 2$ [5]. In general, if any measure realizes ρ and $g(\mathbf{r})$ then we can ask for the measure which maximizes the entropy subject to the constraint of the given ρ and g; this should "formally" be a Gibbs measure with some pair potential [6]. There is no guarantee, however, that this potential would have any good decay property.

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References

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