On the Construction of Particle Distributions with Specified Single and Pair Densities†

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We discuss necessary conditions for the existence of a probability distribution on particle configurations in d-dimensions, i.e., a point process, compatible with a specified density ρ and radial distribution function $g(\mathbf{r})$. In $d = 1$ we give necessary and sufficient criteria on $\rho g(\mathbf{r})$ for the existence of such a point process of renewal (Markov) type. We prove that these conditions are satisfied for the case $g(r) = 0$, $r < D$ and $g(r) = 1$, $r > D$, if and only if $\rho D \le e^{-1}$: the maximum density obtainable from diluting a Poisson process. We then describe briefly necessary and sufficient conditions, valid in every dimension, for $\rho g(r)$ to specify a determinantal point process for which all n-particle densities,$\rho_n(\mathbf{r}_1,...,\mathbf{r}_n)$, are given explicitly as determinants. We give several examples.

1. Introduction

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 d-dimensions.[1] 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 $\rho_2(\mathbf{r}_1,\mathbf{r}_2) = \rho^2 g(\mathbf{r}_1 - \mathbf{r}_2)$; $g(\mathbf{r}) = g(-\mathbf{r})$ is the radial distribution function and $\rho g(\mathbf{r})$ 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 $|\mathbf{r}| \to \infty$, and for isotropic systems, $g(\mathbf{r}) = g(r)$, $r = |\mathbf{r}|$.

The theory of classical equilibrium fluids is based in large part on finding good approximations to $g(r)$.[1] An interesting and important question, which arises in this connection, is the following: Given a $\rho > 0$, what are the conditions on $g(\mathbf{r})$, obtained via some approximate theory or just invented for capturing a certain behavior, to correspond to some actual distribution of particles, i.e., points, in d-dimensional space? That is, does there exist a probability distribution on points in d-dimensions with density ρ, something called by mathematicians a *point process*, whose radial distribution function is given by the proposed $g(\mathbf{r})$? This is the *realizability problem* which has a long history[2,3] and was investigated extensively in a recent series of papers by Stillinger and collaborators.[4−9]

A closely related question discussed some time ago by Lenard[10] is the existence of a point process with specified n-particle densities $\rho_n(\mathbf{r}_1,...,\mathbf{r}_n)$, for all $n = 1, 2,...$. Lenard gave a set of necessary and sufficient (positivity) conditions on the ρ_n for this to be true. From these, one can also obtain an infinite set of conditions in the case where only ρ_1 and ρ_2 are given.[11] These conditions are very hard (or impossible) to check so the real question is whether one can get away with a smaller number of readily checkable conditions.

A simple subset of such positivity conditions, emphasized by Percus[2] and by Stillinger et al.,[4−9] which follow directly from the definitions are

$$\rho > 0,\ g(\mathbf{r}) \ge \mathbf{0} \tag{1.1}$$

$$\hat{S}(\mathbf{k}) = \rho + \rho^2 \int_{\mathbb{R}^d} e^{i\mathbf{k}\cdot\mathbf{r}}[g(\mathbf{r}) - 1]\,d\mathbf{r} \ge 0 \tag{1.2}$$

Conditions (1.1) are obvious, whereas (1.2) ensures that variances of one particle sum functions, $\psi = \sum\phi(\mathbf{r}_i)$, are nonnegative, since it follows from the definition of ρ_2 that

$$\langle(\psi - \langle\psi\rangle)^2\rangle = \left(\frac{1}{2\pi}\right)^d \int d\mathbf{k}\ |\hat{\phi}(\mathbf{k})|^2\hat{S}(\mathbf{k}) \tag{1.3}$$

where $\hat{\phi}(\mathbf{k}) = \int e^{i\mathbf{k}\cdot\mathbf{r}}\phi(\mathbf{r})\,d\mathbf{r}$, and the averages are with respect to the probability distribution of the point process. Simple considerations, see ref 3, show that one should add to (1.1) and (1.2) at least one further requirement: the variance V_Λ of the number of particles N_Λ in a region Λ, which corresponds to $\phi(\mathbf{r})$ being the characteristic function of the region Λ, must be larger than $\theta(1 - \theta)$, where θ is the fractional part of the average number of particles in Λ. That is, if $\langle N_\Lambda\rangle = k + \theta$, for k a nonnegative integer, $k = 0, 1, 2,...$, then

$$V_\Lambda = \langle(N_\Lambda - \langle N_\Lambda\rangle)^2\rangle \ge \theta(1 - \theta) \tag{1.4}$$

The bound (1.4) comes from the fact that N_Λ can only take nonnegative integer values, see ref 3 and Appendix where a more general condition of type (1.4) is proven.

A simple one-dimensional example for which (1.1) and (1.2) are satisfied but (1.4) is violated, is

$$g(r) = \begin{cases} 2(\rho r)^3 & r < \rho^{-1} \\ 1 & r > \rho^{-1} \end{cases} \tag{1.5}$$

A direct computation shows that $\hat{S}(k) \ge 0$, with equality holding for $k = 0$ (see below), whereas the variance in an interval of length $L, L > \rho^{-1}$ is equal to 1/5, which violates (1.4), whenever $\theta(1 - \theta) > 1/5$. It is possible that the condition (1.4) becomes less important in higher dimensions where the minimal variance will go to infinity as the domain grows. For spherical domains it will grow at least like the surface area.[12,13] Note that by choosing the value of r beyond which $g(r) = 1$ as slightly

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smaller than ρ^{-1} (1.1) and (1.2) would still be satisfied but (1.4) would not for some L.

It is however possible, especially for the type of $g(r)$ considered in refs 4–9 that (1) and (2) are enough to ensure realizability. These $g(r)$ have a hard core exclusion, prohibiting the centers of two particles from coming closer than a certain distance D, i.e., $g(r) = 0$ for $r < D$. In particular, it was conjectured in refs 4–8 that it is possible to find a point process with density $\rho > 0$ and a $g(r)$ of the form

$$g(r) = \begin{cases} 0 & r < D \\ 1 & r > D \end{cases} \tag{1.6}$$

as long as $\rho v(D) \leq 2^{-d}$, where $v(D)$ is the volume of a d-dimensional sphere of radius $D/2$. For $\rho v(D) > 2^{-d}$, $\hat{S}(\mathbf{k})$ will be negative for $\mathbf{k} = 0$. (6) also satisfies condition (1.4) for $\rho v(D) \leq 2^{-d}$, although this was not explicitly imposed. There are also heuristic arguments, bolstered by computer simulations[7] and by considerations of the $d \rightarrow \infty$ limit,[14] for the realizability of (1.6) when $\rho v(D) \leq 2^{-d}$.

The case $\rho v(D) = 2^{-d}$, for which $\hat{S}(0) = 0$, is of particular interest, since it yields a system for which the variance V_Λ grows only like the surface area of the boundary of Λ rather than the volume. Such systems are variously called superhomogeneous,[15,17] or hyperuniform.[8] In $d = 1$, the variance in an interval of length L, V_L, can actually be bounded uniformly in L as analyzed in refs 15 and 17. Thus for the example (1.6) with $\rho D = 1/2$

$$V_L = \begin{cases} \rho L(1 - \rho L) & \rho L \leq \dfrac{1}{2} \\ \dfrac{1}{4} & \rho L \geq \dfrac{1}{2} \end{cases} \tag{1.7}$$

This is, by (1.4), the minimum permissible variance when $\rho L = k + (1/2)$, $k = 0, 1, 2, ...$

Inspired by the work of Stillinger and Torquato, we give here a proof of realizability of the model $g(r)$ in (6) for the case $d = 1$ and $\rho v(D) = \rho D \leq e^{-1}$. This is based on a particular construction of the point process as a dilution of a Poisson process with $\rho D = \lambda D \exp[-\lambda D]$, see section 3. It turns out that the new process is a Markov or renewal process.[18–19] This permits us to describe all higher order correlation functions in terms of $g(r)$. We do not know at present whether there exist non renewal point processes for some or all $\rho D \in (e^{-1}, (1/2)]$. We also do not know whether the explicitly constructed process for $\rho D \leq e^{-1}$ is unique. In principle, there can exist more than one process with the same ρ and $g(r)$ but different higher order correlations; see section 5.

We note that one-dimensional renewal processes, described in section 2, and determinantal processes for arbitrary dimension, described in section 4, are the only examples we know for which one can explicitly (and easily) construct higher order correlations from ρ_1 and ρ_2. In some cases these processes correspond to the distribution of particles in equilibrium systems. There is also a formula for the entropy of a renewal process in terms of $g(r)$.[19]

2. Renewal Processes

A translational invariant one-dimensional particle system with density $\rho > 0$, is described by a renewal process (RP) whenever the conditional probability density of finding a particle (or point) at a position q on the line, given the configuration of all particles to the left of q, say,..., $q_{-1} < q_0 < q$, depends only on $x = q - q_1$.[18,19] Let us call that density $P_1(x)$. In other words, given that there is a particle at q, $P_1(x)$ is the probability density that the *first* particle to the right (left) of q is at $q + x$ (or at $q - x$). This corresponds, if we think of the points as events in time, to a Markov process. Clearly

$$\int_0^\infty P_1(x)\, dx = 1, \int_0^\infty xP(x)\, dx = \rho^{-1} \tag{2.1}$$

Calling $P_n(x)$ the probability density for finding the nth particle at a distance x to the right of the specified position of a given particle we have

$$P_n(x) = \int_0^x P_{n-1}(x-y)P_1(y)\, dy, \quad n = 2, 3,... \tag{2.2}$$

By the definition of $\rho g(r)$ we have

$$\rho g(r) = \sum_{n=1}^{\infty} P_n(r) \tag{2.3}$$

Taking the Laplace transform of (2.3), using (2.2), then gives

$$\rho\bar{g}(s) \equiv \rho\sum_{n=1}^{\infty} e^{-sr} g(r)\, dr = \sum_{n=1}^{\infty} [\bar{P}_1(s)]^n$$
$$= \bar{P}_1(s)/[1 - \bar{P}_1(s)] \tag{2.4}$$

Conversely, a given ρ and $g(r)$ will be realizable as a renewal point process if and only if

$$\bar{Q}(s) = \rho\bar{g}(s)/[1 + \rho\bar{g}(s)] \tag{2.5}$$

is the Laplace transform of a probability density, $P_1(r) \geq 0$, satisfying (2.1). We will show in the next section that for the one-dimensional $g(r)$ given in (1.6) this is true when and only when $\rho D \leq e^{-1}$.

It is clear from the definition of a renewal process that the higher order correlation functions of such a system can be readily expressed in terms of ρ and $g(r)$. More specifically given points $x_1 < x_2 < ... < x_n$ on the line we have for $n = 3, 4,...$

$$\rho_n(x_1,..., x_n)/\rho_{n-1}(x_1,..., x_{n-1}) = \rho g(x_n - x_{n-1}) \tag{2.6}$$

since the left side is just the particle density at x_n given that there are particles at $x_1,..., x_{n-1}$. Thus

$$\rho_3(x_1, x_2, x_3) = \rho^3 g(x_2 - x_1)g(x_3 - x_2),\ x_1 < x_2 < x_3 \tag{2.7}$$

etc.

There is also a simple expression for s, the entropy per unit length of a renewal process.[18,19] It is given by the following formula,

$$s = -\rho\int_0^\infty P_1(r)\log[P_1(r)/W_0(r)]\, dr + \rho \tag{2.8}$$

where $W_0(r) = \int_r^\infty P_1(y)\, dy$ is the probability that there is no particle between q and $(q + r)$.

We can realize an RP as an equilibrium system of particles in $d = 1$ in which only nearest neighbors interact: there are no interactions between nonnearest neighbor particles, whatever the distances between them. For such an interaction $u(r)$, $P_1(r)$ is given by[1]

$$P_1(r) = Ce^{-\beta[pr+u(r)]}, \quad r > 0 \tag{2.9}$$

where β is the reciprocal temperature, $p = p(\beta,\rho)$ is the pressure and $C = [\int_0^\infty e^{-\beta[pr+u(r)]}\, dr]^{-1}$ is a normalization constant.

Conversely given $P_1(r)$ we can always define a $\beta u(r)$ and the corresponding βp by inverting (2.9).

A well-known example of such an equilibrium system with only pair interactions is that of hard rods with diameter D, $u(r) = \infty$ for $r < D$, $u(r) = 0$ for $r > D$. For this system $P_1(r) = 0$, for $r < D$, and

$$P_1(r) = \beta p e^{-\beta p(r-D)}, \quad \text{for } r \geq D \tag{2.10}$$

with

$$\beta p = \rho[1 - \rho D]^{-1} \tag{2.11}$$

Equation 2.7 then gives the well-known formula for the entropy density of this system[1]

$$s = -\rho \log[\rho/(1 - \rho D)] + \rho \tag{2.12}$$

3. Realizability of (1.6) as an RP

By general theorems, a necessary and sufficient condition for a function of s to be the Laplace transform of a nonnegative density is that it be "completely monotone" for all $s \geq 0$.[20] That is, it is required that its derivatives alternate in sign for all $s \geq 0$. Thus, for g to define a renewal process, it is necessary and sufficient that $\bar{Q}(s)$ in (2.5) have the property that

$$(-1)^k \bar{Q}^{(k)}(s) > 0, \text{ for all } k = 0, 1, 2,..., \text{ and all } s \geq 0 \tag{3.1}$$

where $f^{(k)}(s) \equiv d^k f(s)/ds^k$.

For the $g(r)$ in (1.6)

$$\bar{g}(s) = \rho \int_D^\infty e^{-sr}\, dr = \rho s^{-1} e^{-sD} \tag{3.2}$$

and the corresponding $\bar{Q}(s)$ in (2.5) is

$$\bar{Q}(s) = \rho e^{-sD}/[s + \rho e^{-sD}] \tag{3.3}$$

It can be shown that (3.1) will be satisfied by (3.3) if and only if $\rho D \leq e^{-1}$.[21] Here we provide a simple construction of this point process by starting with a Poisson process on the line, $x \in (-\infty,\infty)$, with density λ and removing points which are too close ending up with a density $\rho = \lambda e^{-\lambda D}$ and the step $g(r)$ of (1.6).

The procedure is as follows. Denote the points of the Poisson process, by ..., $-x_2$, $-x_1$, x_0, x_1, x_2, x_3, ..., with $x_i \leq x_{i+1}$. Then if $(x_{i+1} - x_i) < D$, x_i is removed; if $(x_{i+1} - x_i) \geq D$, x_i stays. Now the probability that $(x_{i+1} - x_i)$ is greater than D is $e^{-\lambda D}$ so the density of remaining points is

$$\rho D = \lambda D e^{-\lambda D} \leq e^{-1} \tag{3.4}$$

The last inequality follows from the fact that ye^{-y} has its maximum value e^{-1} at $y = 1$. Note that for $\rho D < e^{-1}$ there are two different values of λ which lead to the same RP with density ρ (see below).

The new translation invariant process with density ρ clearly has $g(r) = 0$ for $r < D$. To see that $g(r) = 1$ for $r > D$ we note that, given a surviving point at position q, the density of other surviving points at $q + r$ is, for $r \geq D$, just the density of points for the Poisson processes which have survived, i.e., $\lambda e^{-\lambda D} = \rho$.

It is clear from the above construction that the new process satisfies the conditions at the beginning of sec. 2 and so is an RP with $P_1(r) = Q(r)$, the inverse Laplace transform of $\bar{Q}(s)$ in (3.3). To compute $Q(r)$ we use units in which $\rho = 1$. Define

$$Q(r) = Q(y + nD) = w_n(y), \quad \text{for } nD \leq r < (n + 1)D \tag{3.5}$$

and $0 \leq y \leq D$, $n = 0, 1, 2,....$ It is then easy to deduce from (3.3) that

$$w_{n+1}(y) = w_{n+1}(0) - \int_0^y w_n(x)\, dx,\ n \geq 0 \tag{3.6}$$

with

$$w_0(y) = 0,\ w_1(y) = 1,\ w_2(y) = 1 - y,\ ... \tag{3.7}$$

Furthermore

$$w_{n+1}(0) = w_n(D) \text{ for } n \geq 1 \tag{3.8}$$

i.e., $Q(r)$ is continuous for $r > D$.

Define now

$$\psi(\lambda; y) = \sum_{n=1}^\infty \lambda^n w_n(y) \tag{3.9}$$

It follows then from (6) that

$$\psi(\lambda, y) = \psi(\lambda; 0) - \lambda \int_0^y \psi(\lambda; x)\, dx \tag{3.10}$$

and thus

$$\psi(\lambda; y) = \psi(\lambda; 0) e^{-\lambda y} \tag{3.11}$$

Putting $y = D$ then yields

$$\psi(\lambda; D) = \psi(\lambda;0) e^{-\lambda D} = \frac{1}{\lambda}[\psi(\lambda; 0) - \lambda] \tag{3.12}$$

where the last equality follows from (3.8) and (3.7). This gives

$$\psi(\lambda; 0) = \frac{\lambda}{1 - \lambda e^{-\lambda D}} \tag{3.13}$$

The positivity of $Q(r)$ is equivalent to the requirement that all the coefficients C_j in the expansion of

$$\psi(\lambda; 0) = \sum_{j=0}^\infty C_j \lambda^j \tag{3.14}$$

are positive. This again leads to the requirement that $D \leq e^{-1}$, with the explicit formula (due to E. Speer)

$$w_n(y) = \sum_{k=1}^n [(n - k)D + y]^{k-1} (-1)^{k-1}/(k - 1)!,\ D \leq e^{-1} \tag{3.15}$$

4. Determinantal Point Process

We review here briefly how one can obtain point processes from a $g(\mathbf{r})$ satisfying certain inequalities in any dimension. The construction of such processes is a subject of great current interest in mathematics and we refer the reader to[22] for more information. We again restrict ourselves to homogeneous systems and choose units in which $\rho = 1$. Let $B(\mathbf{r})$ be a complex function such that

$$B(\mathbf{r}) = B^*(-\mathbf{r}),\ B(0) = 1 \tag{4.1}$$

and

$$0 \leq \hat{B}(k) \equiv \int_{\mathbb{R}^d} e^{-i\mathbf{k}\cdot\mathbf{r}} B(r)\, d\mathbf{r} \leq 1 \tag{4.2}$$

It can then be proven that conditions (4.1) and (4.2) are necessary and sufficient for the existence of a point process with n-particle densities given by the determinants[22]

$$\rho_n(\mathbf{r}_1,...,\mathbf{r}_n) = \begin{bmatrix} 1 & B(\mathbf{r}_{12}) & \cdots & B(\mathbf{r}_{1n}) \\ B(\mathbf{r}_{21}) & 1 & \cdots & B(\mathbf{r}_{2n}) \\ & \cdots & & \\ B(\mathbf{r}_{n1}) & B(\mathbf{r}_{n2}) & \cdots & 1 \end{bmatrix} \quad (4.3)$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. In particular we have

$$g(\mathbf{r}) = 1 - |B(\mathbf{r})|^2 \quad (4.4)$$

with $g(0) = 0$, $g(r) \leq 1$.

Such a process is called a determinantal point process (DP). It follows that given a $g(\mathbf{r})$, such that the Fourier transform of $B(\mathbf{r}) \equiv [1 - g(r)]^{1/2}$ satisfies (4.2) and $g(0) = 0, 0 \leq g(r) \leq 1$, we can construct a point process with explicit correlations (4.3). This gives a large (uncountable) class of $g(\mathbf{r})$ which have the realizability property. For all details, see ref 22 and references there.

We make two remarks:

1. To obtain a superhomogeneous system[13−17] with $\hat{S}(0) = 0$, for the determinantal point process specified by some $B(\mathbf{r})$, it is necessary and sufficient that $\hat{B}(\mathbf{k})$ be a characteristic function of a set Ω in $\mathbf{k}$-space, i.e. $\hat{B}(\mathbf{k}) = 1$ for $\mathbf{k} \in \Omega$, $\hat{B}(\mathbf{k}) = 0$ otherwise. This is the case for the well-known one-dimensional system of particles on a circle with pair interaction $\phi(r_{ij}) = -e^2\log|r_{ij}|$, at reciprocal temperature $\beta = 2e^{-2}$. For this system, with $\rho = 1$, the infinite volume limit of the radial distribution function is given by $g(r) = 1 - (\sin \pi r/\pi r)^2$ and the variance V_L of the number of particles in an interval of length L grows as log L. This system is sometimes referred to as the Dyson gas: the ρ_n describe the correlations of the eigenvalues of random Gaussian Hermitian matrices.[23,24]

2. To get translation invariant determinantal correlation functions as in (4.3), it is not necessary that B depend only on $\mathbf{r}_{12}$. It is only necessary that $B(\mathbf{r}_1,\mathbf{r}_2) = F(\mathbf{r}_{12})e^{i[\phi(\mathbf{r}_1)-\phi(\mathbf{r}_2)]}$ with $B(\mathbf{r}_1,\mathbf{r}_2)$ satisfying, as an operator, the analogue of (4.1).[22,25] This is the case for a two-dimensional one component plasma[13,23] with $\phi(r_{ij}) = -e^2\log|\, r_{ij}|$, $\beta = 2e^{-2}$. For this system the variance in the number of particles in a disk of radius R grows as R.[13]

5. Example and Discussion

We illustrate here the construction of a DP in d dimensions from a given ρ_1 and ρ_2 which is, in $d = 1$, also an RP. As in the example (1.6) this can be done for only a subset of the parameter for which (1.1), (1.2), and (1.4) are satisfied. On the other hand, everything here can be computed explicitly in an elementary way. Using units in which $\rho = 1$, let

$$g(r) = 1 - e^{-\lambda r}, \lambda \geq 0 \quad (5.1)$$

It is easily checked that this g satisfies (1.1), (1.2) and (1.4), whenever $\lambda \geq \lambda_d$, $\lambda_1 = 2$, $\lambda_3 = (8\pi)^{1/3}$, ... It follows from (4.4) that this g determines a DP with $B = e^{-\lambda r/2}$ whenever $\lambda \geq 2\lambda_d$.

On the other hand, using (2.5), we get for $d = 1$, the Laplace transform

$$\bar{Q}(s) = \lambda/[s^2 + \lambda s + \lambda] \quad (5.2)$$

from which one readily finds, by factorizing the denominator in (5.2) and using criteria (3.1), that (5.1) determines a RP if and only if $\lambda \geq 2\lambda_1 = 4$. For such values of λ, it is then easily found that

$$P_1(r) = \lambda[\lambda^2 - 4\lambda]^{-1/2}e^{-\lambda r}\left\{\exp\left[\frac{-\lambda + \sqrt{\lambda^2 - 4\lambda}}{2}r\right] - \exp\left[\frac{-\lambda + \sqrt{\lambda^2 - 4\lambda}}{2}r\right]\right\}, \quad \lambda > 4 \quad (5.3a)$$

$$P_1(r) = 4re^{-2r}, \quad \lambda = 4 \quad (5.3b)$$

It is now easy to check that (2.6) and (4.3) give the same correlations $\rho_n(x_1,..., x_n)$. In particular for all $\lambda \geq 4$

$$\rho_3(x_1, x_2, x_3) = (1 - e^{-\lambda(x_2-x_1)})(1 - e^{-\lambda(x_3-x_2)}), \quad x_1 \leq x_2 \leq x_3 \quad (5.4)$$

Using (5.3) in (2.8) one can also obtain the entropy of this system for $\lambda \geq 4$.

The fact that the DP and RP constructions in the above example yield the same point process might suggest that an RP or DP determines a unique point process. This may indeed be the case. We note, however, that uniqueness is not true in general, as can be seen from considerations of systems with nonreflection invariant correlations. Thus, while we always have, for translation invariant systems, that $g(\mathbf{r}) = g(-\mathbf{r})$, there is no such symmetry for the higher order ρ_n. In particular there is an explicit construction of a translation invariant point processes in $d = 1$ which, when run "backward" will have the same ρ and $g(r)$ as the original process but a ρ_3' obtained from the original one by reflection, i.e. $\rho_3'(x_1, x_2, x_3) = \rho_3(-x_1, -x_2, -x_3) \neq \rho_3(x_1, x_2, x_3)$; see ref 15 for details.

The sufficiency of conditions (1.1), (1.2), and (1.4) (with the generalizations given in the Appendix) remains open although it seems unlikely that any finite number of conditions would suffice for the general case.[2,3,11] The construction of the step $g(r)$ in (1.6) by the dilution of a Poisson process does not seem to work in $d > 1$. On the other hand we have not found any counterexample so far.

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Appendix: Proof of (1.4)

We give here an elementary proof of (1.4) and its generalizations, see also ref 3. Let $P(k)$ = Prob. of having k particles in Λ such that

$$\langle k \rangle = \sum_{k=0}^{\infty} kP(k) = N + \theta, N = 0, 1, 2,..., 0 \leq \theta \leq 1$$

Then the variance

$$\begin{aligned} V_\Lambda &= \sum_k [k - N - \theta]^2 P(k) \\ &= \sum (k - N)^2 P(k) - 2\theta[\langle k \rangle - N] + \theta^2 \\ &= \sum (k - N)^2 P(k) - \theta^2 \\ &\geq \sum (k - N)P(k) - \theta^2 = \theta(1 - \theta) \end{aligned}$$

The inequality follows from the fact that $n^2 \geq n$ for n an integer. Equality occurs when $P(k) = \alpha\delta_{k,N} + (1 - \alpha)\delta_{k,N+1}$, with α determined by θ.

We note that the same argument works also for the variance of a linear combination of the number of particles N_{Λ_i} in regions Λ_i. Let $Y = \sum_{i=1}^{k} m_i N_{\Lambda_i}$, where m_i are integer coefficients, then $\langle (Y - \langle Y\rangle)^2\rangle \geq \theta(1 - \theta)$. In particular consider the difference between the number of particles in a region Λ_1 and a region Λ_2. Letting $\langle (N_{\Lambda_1} - N_{\Lambda_2})\rangle = K + \theta$, $K = 0, \pm 1, \pm 2,...$ we again have

$$V_{1,2} = \langle [N_{\Lambda_1} - N_{\Lambda_2} - K - \theta]^2\rangle \geq \theta(1 - \theta)$$

Note added in proof: We recently learned about ref 26 where it is shown that when $g(r) \leq 1$ and $\rho \leq [e\int_{\mathbb{R}^d}(1 - g(\mathbf{r}))d\mathbf{r}]^{-1}$, the corresponding point process can be realized.[26] We thank Prof. Yu. G. Kondratiev for bringing this work to our attention.

References and Notes

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