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Exact Determination of the Two-Point Cluster Function for One-Dimensional Continuum Percolation

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The two-point cluster function $C_2(r_1, r_2)$ provides a measure of clustering in continuum models of disordered many-particle systems and thus is a useful signature of the microstructure. For a two-phase disordered medium, $C_2(r_1, r_2)$ is defined to be the probability of finding two points at positions r_1 and r_2 in the *same cluster of one of the phases*. An exact analytical expression is found for the two-point cluster function $C_2(r_1, r_2)$ of a one-dimensional continuum-percolation model of Poisson-distributed rods (for an arbitrary number density) using renewal theory. We also give asymptotic formulas for the tail probabilities. Along the way we find exact results for other cluster statistics of this continuum percolation model, such as the cluster size distribution, mean number of clusters, and two-point blocking function.

KEY WORDS: Percolation; clustering; point processes; Poisson statistics.

1. INTRODUCTION

The problem of physical clustering of particles in *continuum* (off-lattice) models of disordered many-body systems has received considerable attention.[1-8] A singularly important case of physical clustering occurs at the percolation transition, i.e., the point at which a sample-spanning cluster first appears. The study of clustering behavior of particles in continuum systems is of importance in phenomena such as conduction in dispersions, flow in porous media, elastic behavior of composites, sol–gel transition in

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polymer systems, aggregation of colloids and microemulsions, and the structure of liquid water, to mention but some examples.

Various transport and mechanical properties of two-phase random media have been expressed rigorously in terms of the n-point probability function $S_n(r_1,..., r_n)$, which gives the probability of simultaneously finding n points with positions $r_1,..., r_n$ in one of the phases.[9–11] However, lower-order S_n (e.g., S_1, S_2, S_3) do not reflect information about clustering within the media. For example, for suspensions of identical spheres, S_2 is insensitive to the percolation transition.[5]

Recently, Torquato *et al.*[5] introduced the cluster analogs of the S_n. In particular, at the two-point level, the quantity $C_2(r_1, r_2)$ is defined to be the probability of finding both points r_1 and r_2 in the *same cluster of one of the phases.* This is referred to as the *two-point cluster function* and is a useful signature of the microstructure insofar as it reflects clustering information.[3] These authors found an exact series representation of C_2 in terms of the n-particle *connectedness functions.* The two-point cluster function has been evaluated analytically for the so-called sticky-sphere model[5] and numerically for overlapping spheres (i.e., Poisson-distributed spheres).[7]

The latter model of overlapping spheres is a prototypical continuum percolation problem.[1–4,6–8] The analytical evaluation of C_2 for such systems, however, is mathematically intractable for two and higher spatial dimensions because it is an intrinsically many-body problem, i.e., it involves the unknown infinite set of n-particle connectedness functions.

In this paper we determine the two-point cluster function C_2 exactly for a one-dimensional Poisson distribution of rods at an arbitrary intensity (number density) using renewal theory.[12] We also give asymptotic formulas for the tail probabilities as the distance between the two points tends to $+\infty$. Along the way we find exact results for other cluster statistics of this continuum percolation model, such as the cluster size distribution, mean number of clusters, and two-point blocking function. We note that an exact determination of C_2 for this one-dimensional model can be employed to test and develop approximations of it for Poisson-distributed particles in higher dimensions.

In Section 2 we describe the model and present our analysis to obtain the two-point cluster function and other cluster statistics. In Section 3 we discuss our results and make concluding remarks.

[3] There is currently no known rigorous way to relate C_2 to bulk properties of random media. However, approximate property predictions for suspensions have been suggested that incorporate the average cluster sizes, obtainable, for example, from spatial moments of C_2.

2. MODEL AND ANALYSIS

2.1. Poisson Model

A point process on $\mathfrak{R}^d$ is a collection of random points in $\mathfrak{R}^d$. If we regard each one of these random points as the center of a sphere of radius r and consider the union V of all those spheres (i.e., *the particle phase*), then we obtain a model for the spatial distribution of the particle phase in $\mathfrak{R}^d$. Obviously, the random region V can be written as the union of countably many disjoint random regions V_i, where each V_i is a connected subset of $\mathfrak{R}^d$. Then, each V_i is called a cluster.

We are interested, for arbitrary deterministic points x and y in $\mathfrak{R}^d$, in the probabilities

$$S_1(x) = \mathscr{P}\{x \in V\}$$
$$S_2(x, y) = \mathscr{P}\{x \in V \text{ and } y \in V\}$$
$$C_2(x, y) = \mathscr{P}\{x \in V_i \text{ and } y \in V_i \text{ for some } i\}$$
$$B_2(x, y) = \mathscr{P}\{x \in V_i \text{ and } y \in V_j \text{ for some } i \text{ and } j, i \neq j\}$$

The first is the probability that x is covered by the particles (particle phase volume fraction), the second is the probability that x and y are covered, the third is the probability that x and y fall in the same cluster, and the fourth, the two-point *blocking function*, is the probability that x and y are in different clusters. Whereas the one- and two-point probability functions S_1 and S_2 are easy to compute, the two-point cluster function C_2 is difficult to obtain. Note that given C_2, one can obtain the two-point blocking function from the relation

$$B_2 = S_2 - C_2 \tag{1}$$

For example, in the case of a Poisson point process with mean measure μ,

$$S_1(x) = 1 - \exp[-\mu(B(x, r)] \tag{2}$$

$$S_2(x, y) = 1 - \exp[-\mu(B(x, r)] - \exp[-\mu(B(y, r)] + \exp[-\mu(B(x, r) \cup B(y, r))] \tag{3}$$

where $B(x, r)$ is the sphere of radius r centered at x. The first follows from the argument that x is covered if and only if $B(x, r)$ has at least one point of the process, the probability of which is the complement of the probability that there are no points in $B(x, r)$. Similarly, $S_2(x, y)$ is the probability that both $B(x, r)$ and $B(y, r)$ have at least one point each. However,

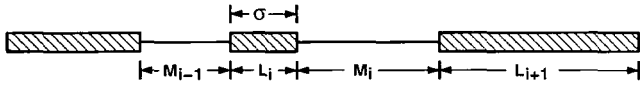

Fig. 1. Schematic of a Poisson distribution of rods of length σ. M_i is the length of the ith gap and L_i is the length of the ith cluster.

$C_2(x, y)$ is not so easy: it is the probability that the point process has a chain of points $x_1,..., x_n$ such that

$$|x-x_1| \leqslant r, \qquad |x_1-x_2| \leqslant 2r,..., \qquad |x_{n-1}-x_n| \leqslant 2r, \qquad |x_n-y| \leqslant r$$

and such probabilities (to our knowledge) have never been computed for a Poisson point process with arbitrary intensity.

Indeed, our aim is to compute C_2 in the simple case of dimension one and for a Poisson point process with constant intensity. This could be accomplished by evaluating the aforementioned series representation of C_2 in terms of the n-particle connectedness functions.[5] Instead we use the well-known results for Geiger counters of type II to write down the distribution of cluster sizes, and then use renewal theory to do the rest.[12] In particular, we give some asymptotic formulas for the tail probabilies.

Consider a Poisson point process on $\Re$ with intensity ρ. The number of points in a Borel set B has the Poisson distribution with mean $\rho \cdot |B|$, where $|B|$ is the Lebesgue measure of B. Each point is to serve as the center of an interval of length σ (where $\sigma > 0$ is a fixed constant) that we refer to as a "rod." The union of all of these rods is the set V. Connected components of V are now intervals or "clusters," each with some random length L_i. The empty intervals between the clusters (gaps) have random lengths M_i, so that the gaps and clusters alternate as illustrated in Fig. 1. It is easy to see that the M_i are independent and identically distributed exponential variables with mean $1/\rho$, i.e., $\mathscr{E}(M) = 1/\rho$. The L_i are independent of the M_i and are again independent and identically distributed.

2.2. Distribution of L

The common distribution of the L_i is given by, writing L for L_1,

$$\mathscr{P}\{L > t\} = e^{-\rho t} \sum_{n=1}^{\infty} \frac{(\rho t)^{n-1}}{(n-1)!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} \left(1 - k\frac{\sigma}{t}\right)_+^{n-1} \tag{4}$$

where for all integers $n \geqslant 0$,

$$x_+^n = \begin{cases} 0 & \text{if } x < 0 \\ x^n & \text{if } x \geqslant 0 \end{cases}$$

This result is obtained by piecing together the results in Feller[12] under the heading of *waiting for large gaps in Poisson traffic*. In particular, for $t < \sigma$, we have $\mathscr{P}\{L > t\} = 1$, as it should be (since every cluster has at least the length σ), and the mean and variance of L are

$$\mathscr{E}(L) = \frac{e^{\rho\sigma} - 1}{\rho}, \qquad \mathrm{Var}(L) = \frac{e^{2\rho\sigma} - 1 - 2\rho\sigma e^{\rho\sigma}}{\rho^2} \tag{5}$$

We note that the *mean density of clusters* in the thermodynamic limit, denoted by n_c, is given by the simple expression

$$n_c = \frac{1}{\mathscr{E}(L) + \mathscr{E}(M)} = \rho e^{-\rho\sigma}$$

In one dimension, this clearly is equal to the *mean density of gaps*.

2.3. Coverage Probabilities

We consider the probability $C_2(x, y)$ that fixed points $x < y$ fall in the same occupied interval, i.e., the same cluster. To this end, we shall use renewal theory associated with the sequence S_n defined by

$$S_0 = 0, \qquad S_{n+1} = S_n + L_{n+1} + M_{n+1}, \qquad n \geqslant 0 \tag{6}$$

Generally, renewal theory is concerned with the partial sums S_n, $n \geqslant 1$, of a sequence of positive, independent, identically distributed random variables W_n, $n \geqslant 1$. So, $S_n = W_1 + \cdots + W_n$, $n \geqslant 1$, and we put $S_0 = 0$. The distribution function F^{n*} of S_n is the n-fold convolution of the common distribution function F of the W_n. The expected number of S_n that belong to the interval $[0, t]$ is given by the so-called renewal function

$$R(t) = \sum_{n=0}^{\infty} F^{n*}(t) \tag{7}$$

The main limit theorem (see Feller[12] for this and other facts below) states that $R(t+\tau) - R(t)$, the expected number of S_n that fall in the interval $(t, t+\tau]$, converges to $\tau/\mathscr{E}(W)$. From this, one obtains the workhorse of the theory:

$$\lim_{t \to \infty} \int_0^t R(ds)\, g(t-s) = \frac{1}{\mathscr{E}(W)} \int_0^t g(s)\, ds \tag{8}$$

provided that g is directly Riemann integrable. In fact, this condition on g is satisfied if g is decreasing and Riemann integrable.

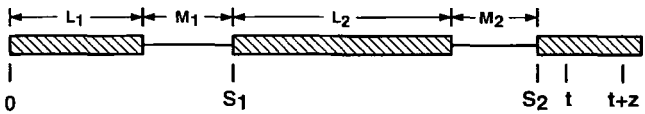

Fig. 2. Schematic indicating definitions for the renewal process described in the text.

Returning to (6), we note that (S_n) is in fact a renewal process with intervals $W_n = L_n + M_n$, since the sequences of random variables L_i and M_i are independent and identically distributed. The intervals W_n between the S_n have the distribution

$$F(s) = \mathscr{P}\{L + M \leqslant s\}, \qquad s \geqslant 0 \tag{9}$$

where $L = L_1$ and $M = M_1$ are independent, L has the distribution specified by (1), and M is exponential with mean $1/\rho$.

We define, for $t \geqslant 0$ and $z \geqslant 0$,

$$p(t, z) = \mathscr{P}\{S_n \leqslant t \leqslant t + z < S_n + L_{n+1} \text{ for some } n \geqslant 0\} \tag{10}$$

that is, $p(t, z)$ is the probability that the points t and $t + z$ fall in the same cluster, assuming that the origin is taken to be the left endpoint of the cluster with length $L = L_1$ as in Fig. 2.

We note that

$$C_2(x, y) = \lim_{t \to \infty} p(t, y - x), \qquad -\infty < x \leqslant y < \infty \tag{11}$$

Theorem 1. For $-\infty < x \leqslant y < \infty$, introducing the dimensionless distance $r = (y - x)/\sigma$ and dimensionless density $\eta = \rho\sigma$,

$$C_2(r) = e^{-\eta} \sum_{n=1}^{\infty} \sum_{k=0}^{n} (-1)^k \binom{n}{k} e^{-k\eta} h_n(r - k) \tag{12}$$

where

$$h_n(u) = \begin{cases} 1 & \text{if } u \leqslant 0 \\ e^{-\eta u} \displaystyle\sum_{m=0}^{n-1} \frac{(\eta u)^m}{m!} & \text{if } u > 0 \end{cases}$$

Remark 1. The multiple summations of (12) can be rewritten as a single sum as is now described. For a dimensionless distance r in the interval $[m - 1, m]$ and any integer $m \geqslant 1$,

$$C_2(r) = 1 + \sum_{k=1}^{m} (-1)^k e^{-k\eta} \left(\frac{[\eta(r - k + 1)]^{k-1}}{(k-1)!} + \frac{[\eta(r - k + 1)]^k}{k!} \right) \tag{13}$$

Remark 2. For $r=0$ or $x=y$, it is easily seen that

$$C_2(0)=S_1=1-e^{-\eta}$$

which is as mentioned in the Introduction.

Proof of the theorem above follows from the next lemma upon the substitution of $\mathscr{P}\{L>t\}$ by the expression given in (4) and some lengthy but elementary manipulations.

Lemma. For $-\infty<x\leqslant y<\infty$,

$$C_2(r)=\rho e^{-\rho\sigma}\int_{y-x}^{\infty} dt\, \mathscr{P}\{L>t\} \tag{14}$$

Proof. In view of (11), we concentrate on the probability $p(t,z)$ defined by (10):

$$\begin{aligned} p(t,z) &= \sum_{n=0}^{\infty} \mathscr{P}\{S_n\leqslant t<t+z<S_n+L_{n+1}\} \\ &= \sum_{n=0}^{\infty} \mathscr{P}\{S_n\leqslant t, L_{n+1}>t+z-S_n\} \\ &= \sum_{n=0}^{\infty} \int_0^t F^{n*}(ds)\, \mathscr{P}\{L>t+z-s\} \end{aligned}$$

where F^{n*} is the distribution of S_n; here, the first equality is justified by the fact that the intervals $[S_n, S_n+L_{n+1})$ for $n=0, 1, 2,\ldots$ are disjoint, and the third equality uses the fact that L_{n+1} is independent of S_n and has the same distribution as $L=L_1$. Indeed, the distribution F^{n*} of S_n is the n-fold convolution of the distribution F defined by (9). Letting R be the renewal function defined as in (7), we may rewrite the last formula for $p(t,z)$ as

$$p(t,z)=\int_0^t R(ds)\, \mathscr{P}\{L>t-s+z\}$$

Hence, for fixed $z\geqslant 0$, the right side of the formula (11) has the form

$$\lim_{t\to\infty} p(t,z)=\lim_{t\to\infty}\int_0^t R(ds)\, g(t-s) \tag{15}$$

to which we apply the key renewal theorem (8). To that end, we first note that

$$g(u)=\mathscr{P}\{L>u+z\}$$

is a decreasing function of u and it is Riemann integrable:

$$\int_0^\infty du\, g(u) \leqslant \int_0^\infty du\, P\{L > u\} = \mathscr{E}(L) = \frac{e^\eta - 1}{\rho} < \infty$$

Thus, g is directly Riemann integrable in the sense of Feller,[12] and the key renewal theorem (8) applies to (15) to yield, recalling that $\mathscr{E}(W) = \mathscr{E}(L+M)$,

$$\begin{aligned}\lim_{t\to\infty} p(t,z) &= \frac{1}{\mathscr{E}(L+M)} \int_0^\infty du\, g(u) \\ &= \frac{1}{(e^\eta - 1)/\rho + 1/\rho} \int_0^\infty du\, \mathscr{P}\{L > u + z\} \\ &= \rho e^{-\eta} \int_z^\infty du\, \mathscr{P}\{L > u\} \qquad (16)\end{aligned}$$

in view of (5) for $\mathscr{E}(L)$ and the fact that $\mathscr{E}(M) = 1/\rho$. The proof of the lemma now follows from (11) and (16).

2.4. Asymptotic Probabilities

We now consider the asymptotic behavior of $C_2(r)$ as the distance r goes to $+\infty$.

Theorem 2. If $\eta = 1$, then

$$C_2(r) \sim 2e^{-1} e^{-\eta r}, \qquad r \to \infty \qquad (17)$$

If $\eta \neq 1$, then

$$C_2(r) \sim \frac{(c-\rho)\, e^{-\eta}}{c(\sigma c - 1)} e^{-c\sigma r}, \qquad r \to \infty \qquad (18)$$

where c is the unique solution of

$$e^{\sigma x} = \frac{e^\eta}{\rho} x, \qquad x \neq \rho \qquad (19)$$

Proof. We start with the asymptotic behavior of $\mathscr{P}\{L > t\}$ as $t \to \infty$. Using the fact that, in a Poisson process with intensity ρ, the intervals are independent exponential variables with parameter ρ, we can write

$$\mathscr{P}\{L > t\} = e^{-\rho t} \cdot 1_{[0,\sigma)}(t) + \int_0^t ds\, f(s)\, \mathscr{P}\{L > t - s\} \qquad (20)$$

where 1_A is the indicator function of the set A and

$$f(s)=\begin{cases}\rho e^{-\rho s} & \text{if} \quad s<\sigma \\ 0 & \text{if} \quad s\geqslant\sigma\end{cases} \tag{21}$$

Note that f is a *defective density function* (with integral $1-e^{-\eta}<1$).[12] Therefore, there is a unique constant $c>0$ such that

$$\int_0^\infty ds\, e^{cs}f(s)=\rho\int_0^\sigma ds\, e^{(c-\rho)s}=1 \tag{22}$$

In fact,

$$c=\rho \qquad \text{if} \quad \eta=1 \tag{23}$$

and otherwise, if $\eta\neq 1$, is the unique solution of (19).

We define a probability density function $\hat{f}$ by

$$\hat{f}(s)=e^{cs}f(s), \qquad s\geqslant 0 \tag{24}$$

and note that we can rewrite (20) as a proper renewal equation:

$$e^{ct}\mathscr{P}\{L>t\}=e^{(c-\rho)t}\cdot 1_{[0,\sigma)}(t)+\int_0^t ds\, \hat{f}(s)\, e^{c(t-s)}\mathscr{P}\{L>t-s\} \tag{25}$$

Solving this and letting $t\to\infty$, by using the key renewal theorem, we get

$$\lim_{t\to\infty} e^{ct}\mathscr{P}\{L>t\}=\frac{1}{\mu}\int_0^\infty ds\, e^{(c-\rho)s}\cdot 1_{[0,\sigma)}(s)=\frac{1}{\rho\mu} \tag{26}$$

in view of (22), where μ is the mean corresponding to the probability density $\hat{f}$, which is

$$\begin{aligned}\mu&=\int_0^\infty ds\, \hat{f}(s)s \\ &=\rho\int_0^\sigma ds\, e^{(c-\rho)s}s=\begin{cases}\eta\sigma/2 & \text{if} \quad \eta=1 \\ (\sigma c-1)/(c-\rho) & \text{if} \quad \eta\neq 1\end{cases}\end{aligned} \tag{27}$$

In other words,

$$\mathscr{P}\{L>t\}\sim\frac{1}{\rho\mu}e^{-ct}, \qquad t\to\infty \tag{28}$$

using this asymptotic formula in the formula given in the lemma [cf. Eq. (14)] yields

$$C_2(r) \sim \rho e^{-\eta} \frac{1}{c\rho\mu} e^{-c\sigma r}, \qquad r \to \infty \tag{29}$$

This completes the proof in view of (28), and the observation (23).

Remark. The integral of $C_2(r)$ diverges only at the trivial percolation threshold of $\eta = +\infty$ or $S_1 = 1$, since at this critical value $C_2(r)$ equals the constant unity.

3. DISCUSSION AND CONCLUSIONS

In Fig. 3 we plot the two-point cluster function $C_2(r)$ as obtained from (14), as a function of r for three values of S_1, the fraction of space occupied by the rods. As expected, $C_2(r)$ is a monotonically decreasing function of r, tending to zero for large r, and its range increases as S_1 increases. It may not be as obvious that the mth derivative of $C_2(r)$ with respect to r for $m \geqslant 1$ is discontinuous at $r = m$. Mathematically, this property is easily seen from (14). Physically, such discontinuities arise because clusters composed of m rods (and smaller) no longer contribute to $C_2(r)$ as r is made slightly larger than m. In higher dimensions the derivatives are smoother.

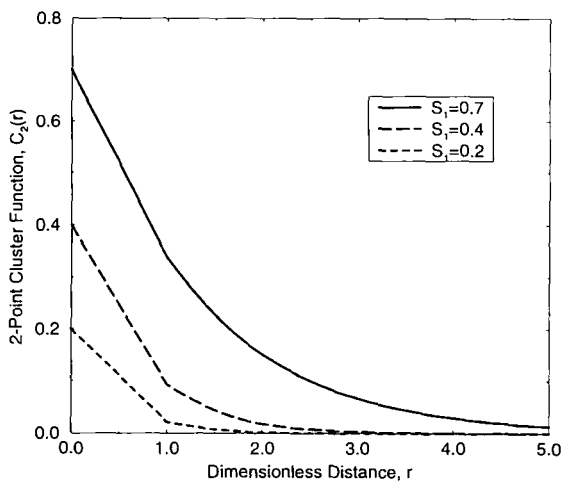

Fig. 3. The two-point cluster function $C_2(r)$, as obtained from (10), as a function of the dimensionless distance r for three values of S_1.

Figure 4 depicts corresponding results for the two-point blocking function $B_2(r)$. Recall that $B_2(r)$ gives the probability that two points separated by a distance r are in *different* clusters. This quantity is easily obtained from (1), using relation (3) for the conventional two-point probability function $S_2(r)$ (the probability that the two points are in the rod space), and formula (14) for $C_2(r)$. The function $B_2(r)$ must be identically zero at $r=0$ and must tend to S_1^2 for large r. It is easily shown [using relations (1), (3), and (14)] that the first spatial derivative of $B_2(r)$ at $r=1$ is continuous.

To summarize, we have obtained an exact analytical expression for the two-point cluster function $C_2(r)$ of a one-dimensional continuum-percolation model of Poisson-distributed rods (for an arbitrary number density) using renewal theory. We also have obtained asymptotic formulas for the tail probabilities as the distance r tends to $+\infty$. Moreover, we have found exact results for other cluster statistics of this continuum percolation model, such as the cluster size distribution, mean number of clusters, and two-point blocking function.

The existence of an exact solution for C_2 and related cluster statistics for one-dimensional Poisson distributions of rods can be used to test and develop approximate methods for corresponding quantities in higher dimensions. At first glance it might be difficult to envision how the solution of the one-dimensional problem (with its trivial percolation transition) can be profitably used to study more complex higher-dimensional systems. In order to answer this question, it is useful to recall the exact series

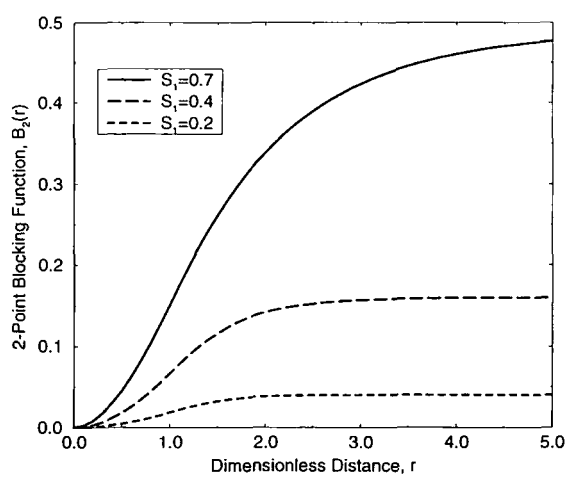

Fig. 4. The two-point blocking function $C_2(r)$, as obtained from (1), (3), and (10), as a function of the dimensionless distance r for three values of S_1.

representation of C_2 for d-dimensional suspensions of spheres obtained by Torquato *et al.*,[5] which, in schematic notation, can be written as

$$C_2(r_1, r_2) = \sum_{n=1}^{\infty} f_n[P_1, P_2, ..., P_n] \tag{30}$$

Here the $P_n(r_1, ..., r_n)$ are the so-called n-particle connectedness functions and the f_n are certain functionals (integrals). The connectedness functions characterize the probability of finding subsets of n spheres connected to one another. These functions have a fundamental role in continuum percolation theory analogous to that of the n-particle distribution functions g_n in the theory of liquids. *Indeed, the P_n are directly obtainable from the g_n by employing a decomposition scheme.*[3,5] For systems of interacting spheres, exact solutions for g_n and thus P_n for $n \geqslant 2$ do not exist for $d \geqslant 2$ and hence one must rely on approximations for them (e.g., as obtained from integral equations). In order to understand the nature of the difficulty of solving the integral equations for g_n for $d \geqslant 2$, Salsburg *et al.*[13] studied one-dimensional systems of interacting particles and found exact expressions for the g_n. Again, how can exact one-dimensional solutions (with their trivial phase transitions) aid in the study of more complex higher-dimensional systems? As discussed by Salsburg *et al.*, one might decide between the use of two numerical methods to solve the integral equations for $d \geqslant 2$ on the basis of the convergence of both methods in the one-dimensional problem, where the solution is known. Haymet[14] solved an integral equation involving the triplet function g_3 in one dimension using approximations for g_3 that are employed in higher dimensions. By comparing his approximate results to the exact result for g_3 he was able to ascertain the best approximation in higher dimensions.

In a future paper we will study analogous approximations for the connectedness functions P_n in higher dimensions. In particular, we shall examine the relationship between the present results and the representation of $C_2(r)$ in terms of the connectedness functions as given by (30). For $d = 1$, since the g_n are known exactly, the P_n are known exactly, for reasons already noted. Therefore, we can carry out one-dimensional analyses similar to that used by Haymet in the context of liquids in order to develop useful approximations for the P_n and hence the two-point cluster function C_2 in higher dimensions.

Finally, we note that the exact one-dimensional solution of C_2 will be of help in computer simulations studies of this quantity in higher dimensions. The precise simulation of systems near their percolation thresholds is nontrivial because of long-range correlations. Algorithms to measure C_2 can be carried out in one dimension and tested against the exact solution.

The advantage of one dimension is that system sizes can be much larger than in higher dimensions and hence errors due to finite-size effects can be better estimated.

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