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Nearest-neighbor statistics in a one-dimensional random sequential adsorption process

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The probability of finding a nearest neighbor at some radial distance from a reference point in many-particle systems is of fundamental importance in a host of fields in the physical as well as biological sciences. We have derived exact analytical expressions for nearest-neighbor probability functions for particles deposited on a line during a random sequential adsorption process for all densities, i.e., up to the jamming limit. Using these results, we find the mean nearest-neighbor distance λ as a function of the packing fraction and discuss it in light of recent theorems derived for general ergodic and isotropic packings of hard spheres.

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I. INTRODUCTION

There has been a resurgence of interest in *nearest-neighbor distribution functions* of many-particle systems since such knowledge is of basic importance in many applications, including the study of liquids and amorphous solids [1–8], transport processes in heterogeneous materials [9,10], and spatial patterns in biological systems [11]. Generally speaking, nearest-neighbor functions characterize the probability of finding a nearest neighbor at some distance from a reference point in the many-particle system. From such functions one can determine other quantities of fundamental interest, such as the *mean nearest-neighbor distance between particles.*

Hertz [12] was apparently the first to obtain exact expressions for nearest-neighbor functions. He did so for a three-dimensional system of "point" particles, i.e., spatially uncorrelated (Poisson distributed) particles. Deriving analytical expressions for finite-sized interacting particles is considerably more complex. Torquato, Lu, and Rubinstein (TLR) [4] derived exact analytical series representations of nearest-neighbor functions for isotropic distributions of identical interacting D-dimensional spheres at number density ρ in terms of multidimensional integrals over the infinite set of n-particle probability density functions $\rho_1, \rho_2, \ldots, \rho_n$ $(n \to \infty)$. Generally, this series cannot be summed exactly since such complete knowledge of the ρ_n is usually not available.

For an *equilibrium ensemble* of hard rods ($D = 1$), the ρ_n for any n are known exactly, permitting an exact evaluation of the nearest-neighbor functions. In the case of equilibrium ensembles of hard disks ($D = 2$) and hard spheres ($D = 3$), accurate approximations have been developed recently that apply up to the random close-packing density [7,8].

To our knowledge, nearest-neighbor expressions have yet to be obtained for any *nonequilibrium ensemble.* In this paper we derive exact expressions for the nearest-neighbor functions of systems of hard rods deposited on a line during a random sequential adsorption (RSA) process [13–19]. In this process, also known as the *car parking problem*, rods are placed randomly and sequentially on a line such that each rod is adsorbed if it does not overlap any of the rods already adsorbed. The geometrical blocking effects and the irreversible nature of the process result in structures that are distinctly different from corresponding equilibrium configurations, except for low densities [14]. Near the jamming limit (the final state of this process whereby no particles can be added), the kinetics follows an algebraic power law [17].

It will be of interest to examine our exact results in light of some recent general theorems [7] that suggest that the functional nature of the nearest-neighbor functions for RSA particles should be surprisingly different than for corresponding equilibrium particles. We note that our exact one-dimensional results will aid in obtaining approximate nearest-neighbor relations in higher dimensions.

In Sec. II, we define and discuss the nearest-neighbor functions for systems of identical, interacting one-dimensional rods in instances in which the reference point is arbitrary ("void" quantities) and in which the reference point is a rod center ("particle" quantities). In Sec. III, we derive exact expressions for the void nearest-neighbor functions for RSA rods. In Sec. IV, we obtain corresponding results for the particle quantities and find the mean

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nearest-neighbor distance as well. In Sec. V, we graphically present our analytical results and discuss them in relation to the general theorems of Ref. [7]. Monte Carlo simulations of the nearest-neighbor functions for RSA rods are also carried out here. Finally, in Sec. VI, we discuss our results.

II. NEAREST-NEIGHBOR FUNCTIONS

The nearest-neighbor distribution functions defined here for identical rods in one dimension are a specialization of the general case of D-dimensional spheres defined by TLR [4] and are of two primary types. The *particle* distribution functions (denoted by a subscript P) refer to nearest-neighbor quantities measured with respect to an arbitrary rod center, while the *void* distribution functions (denoted by a subscript V) refer to nearest-neighbor quantities measured with respect to an arbitrary point in the system. It should be noted that in the case of the void quantities, the reference point can still lie within a rod. The void functions are identical to those introduced by Reiss, Frisch, and Lebowitz [20] in their scaled-particle theory.

We define the nearest-neighbor functions $H_{V(P)}$, $E_{V(P)}$, and $G_{V(P)}$ for the void (particle) quantities as follows:

$$H_V(r)\,dr \tag{1}$$

is the probability that, at an arbitrary point in the system, the center of the nearest particle lies at a distance between r and $r+dr$;

$$H_P(r)\,dr \tag{2}$$

is the probability that, at an arbitrary disk center in the system, the center of the nearest disk lies at a distance between r and $r+dr$;

$$E_V(r) \tag{3}$$

is the probability of finding a region of length $2r$ (centered at some arbitrary point) empty of rod centers;

$$E_P(r) \tag{4}$$

is the probability of finding a region of length $2r$ (centered at some arbitrary disk center) empty of rod centers;

$$2\rho G_V(r)\,dr \tag{5}$$

is the probability that, given a region of length $2r$ centered at an arbitrary point in the system that is empty of rod centers, rod centers are contained in the shell of thickness $2dr$ encompassing the region; and

$$2\rho G_P(r)\,dr \tag{6}$$

is the probability that, given a region of length $2r$ centered on a rod center that is empty of any other rod centers, rod centers are contained in the shell of thickness $2dr$ encompassing the region. The prefactor of 2 in front of $G_V(r,t)$ and $G_P(r,t)$ is the "surface area" of the rod. Although we will be applying these definitions to the case of RSA of hard rods, they are valid for any distribution of hard rods of uniform size.

From the definitions given above, we can see that $E_{V(P)}(r,t)$ is just the cumulative distribution function associated with $H_{V(P)}(r,t)$, so one can write

$$E_{V(P)}(r,t) = 1 - \int_0^r H_{V(P)}(y,t)\,dy. \tag{7}$$

Differentiating the above expression gives the expression

$$H_{V(P)}(r,t) = -\frac{\partial E_{V(P)}(r,t)}{\partial r}. \tag{8}$$

Finally, once one has $E_{V(P)}(r,t)$ and $H_{V(P)}(r,t)$, one can obtain $G_{V(P)}$ via the relation

$$G_{V(P)} = \frac{H_{V(P)}(r,t)}{2\rho E_{V(P)}(r,t)}. \tag{9}$$

Because of these relations, we will concentrate on evaluating $E_{V(P)}(r,t)$ and deriving expressions for $H_{V(P)}(r,t)$ and $G_{V(P)}(r,t)$ from that.

III. THEORY: VOID QUANTITIES

In order to derive expressions for the nearest-neighbor void quantities for one-dimensional RSA, we must first define a few preliminary expressions. Let $n(h,t)$ be the number density of gaps with length between h and $h+dh$ at dimensionless time t. Without loss of generality, we will also assume the rods to have a diameter of unity. Then, the total number density of gaps $N(t)$ at time t is given by

$$N(t) = \int_0^\infty dh\, n(h,t). \tag{10}$$

In one dimension, this must be equal to the number density of rods at time t, $\rho(t)$.

The time evolution of $n(h,t)$ is governed by a rate equation that takes into account the destruction and creation of gaps of length h [15,19,21]. In the case of $h<1$, the gaps cannot be destroyed since a particle cannot be added to the gap. Therefore, there is only a creation term of the form

$$\frac{\partial n(h,t)}{\partial t} = 2\int_{h+1}^\infty dh'\, n(h',t) \qquad (h<1). \tag{11}$$

For $h \geq 1$, gaps can be both created and destroyed and the rate can be written as

$$\frac{\partial n(h,t)}{\partial t} = -(h-1)n(h,t) + 2\int_{h+1}^\infty dh'\, n(h',t) \quad (h \geq 1). \tag{12}$$

In order to solve these equations for $n(h,t)$ as a function of h only, we can introduce the function

$$n(h,t) = \exp[-(h-1)t](Ht) \tag{13}$$

for $h \geq 1$, which after insertion in Eq. (12) and proper account of the initial condition leads to the known solution [15]

$$H(t) = t^2 \exp\left[-2\int_0^t \frac{1-e^{-u}}{u}\,du\right] \tag{14}$$

$$= \exp\{-2[\gamma - \mathrm{Ei}(-t)]\}, \tag{15}$$

where $\mathrm{Ei}(t)$ is the exponential integral of t and $\gamma = 0.577\,21\ldots$ is Euler's constant.

For $h < 1$, the gap distribution function is then given by

$$n(h,t) = 2\int_0^t dt'\,\frac{H(t')}{t'}e^{-ht'}. \tag{16}$$

The density of adsorbed rods can then be calculated from Eq. (10) by substituting the expression for $n(h,t)$ in Eq. (16) and integrating with respect to h to give

$$\rho(t) = \int_0^t dt'\,\frac{H(t')}{t'^2}. \tag{17}$$

Knowledge of the gap distribution function allows us to calculate the void quantities. Let us first look at $E_V(r,t)$. For $r < 1/2$, the only region prohibited will be those regions that are within a distance r from each rod center. Since $r < 1/2$, we do not have to worry about multiple overlaps and we can immediately write down

$$E_V(r,t) = 1 - 2r\rho(t) \qquad (r \leq 1/2), \tag{18}$$

$$H_V(r,t) = 2\rho(t) \qquad (r \leq 1/2), \tag{19}$$

$$G_V(r,t) = \frac{1}{1-2r\rho(t)} \qquad (r \leq 1/2). \tag{20}$$

In the case of $r \geq 1/2$, we know that $E_V(r,t)$ is the probability of finding a void of radius r (or diameter $2r$) empty of rod centers. Thus we must consider all gaps between particle centers that are larger than $2r-1$. The total contribution of a gap of size h will be $h-(2r-1)$ and the total probability of finding a void of radius r can be written

$$E_V(r,t) = \int_{2r-1}^{\infty} [h-(2r-1)]\,n(h,t)\,dh. \tag{21}$$

In the case of $r \geq 1$ we can substitute in the expression for $n(h,t)$ in terms of $H(t)$ to get

$$E_V(r,t) = \int_{2r-1}^{\infty} [h-(2r-1)]\,H(t)e^{-(h-1)t}\,dh \tag{22}$$

$$= H(t)\int_0^{\infty} xe^{-[x+2(r-1)]t}\,dx \tag{23}$$

$$= \frac{H(t)}{t^2}e^{-2(r-1)t} \qquad (r \geq 1). \tag{24}$$

Using Eqs. (8) and (9), we can now also write

$$H_V(r,t) = -\frac{\partial E_V}{\partial r} = 2\frac{H(t)}{t}e^{-2(r-1)t} \qquad (r \geq 1) \tag{25}$$

and

$$G_V(r,t) = \frac{H_V(r,t)}{2\rho(t)E_V(r,t)} = \frac{t}{\rho(t)}. \tag{26}$$

In the case of $1/2 \leq r \leq 1$, the integrals can no longer be done analytically due to the nature of $n(h,t)$. However, the expressions can be written down fairly simply in terms of integrals to give

$$E_V(r,t) = 1 - 2(1-r)\rho(t) - 2\int_0^t dt'\,\frac{H(t')}{t'^3}\left[1-e^{-(2r-1)t'}\right] \qquad (1/2 \leq r \leq 1), \tag{27}$$

$$H_V(r,t) = 2\int_0^t dt'\,\frac{H(t')}{t'^2}(2e^{-(2r-1)t'}-1) \qquad (1/2 \leq r \leq 1), \tag{28}$$

with $G_V(r,t)$ readily determined from $E_V(r,t)$ and $H_V(r,t)$.

IV. THEORY: PARTICLE QUANTITIES

For $0 \leq r \leq 1$, we have simply

$$E_P(r,t) = 1, \tag{29}$$

$$H_P(r,t) = 0, \tag{30}$$

$$G_P(r,t) = 0, \tag{31}$$

reflecting the impenetrability of the particles. In order to derive expressions for the particle nearest-neighbor functions for $r > 1$, we must introduce the *two-gap* distribution function $n(h,h',t)$, which is defined as the number density of *neighboring* gaps of size h and h'. Clearly, we have

$$n(h,t) = \int_0^{\infty} dh'\,n(h,h',t). \tag{32}$$

Using the $n(h,h',t)$ defined in this manner, we can now write

$$E_P(r,t) = \frac{1}{\rho(t)}\int_{r-1}^{\infty} dh \int_{r-1}^{\infty} dh'\,n(h,h',t) \tag{33}$$

when $r \geq 1$.

We can absorb the h (or h') dependence in $n(h,h',t)$ in a manner similar to that for $n(h,t)$ by using the following ansatz:

$$n(h,h',t) = \begin{cases} H(h;1,t)e^{-(h'-1)t} & (h \leq 1,\ h' \geq 1) \quad (34) \\ H(h';1,t)e^{-(h-1)t} & (h \geq 1,\ h' \leq 1) \quad (35) \\ H(1,t)e^{-(h+h'-2)t} & (h \geq 1,\ h' \geq 1) \quad (36) \\ H(h,h';1,t) & (h \leq 1,\ h' \leq 1). \quad (37) \end{cases}$$

This follows the notations used in [21], where the 1 in the argument denotes a one-particle cluster. With the gap size dependence taken into account, we can write down the time evolution equation for $n(h,h',t)$ as [21]

$$\frac{\partial}{\partial t}n(h,h',t) = -[k(h)+k(h')]n(h,h',t) + \int_{h+1}^{\infty} dh''\, n(h'',h',t) + \int_{h'+1}^{\infty} dh''\, n(h,h'',t) + n(h+h'+1,t), \quad (38)$$

where

$$k = \begin{cases} h-1, & h \geq 1 \\ 0, & h < 1. \end{cases} \quad (39)$$

For $r \geq 2$, we know that $h \geq 1$, $h' \geq 1$, and Eq. (38) reduces to

$$\frac{\partial}{\partial t}H(1;t) = H(t)e^{-2t} + 2H(1,t)\frac{e^{-t}}{t}, \quad (40)$$

which can be integrated to give

$$H(1;t) = H(t)\frac{1-e^{-2t}}{2}. \quad (41)$$

Using Eq. (33), we can now write down

$$E_P(r,t) = \frac{1}{\rho(t)}\frac{H(1,t)}{t^2}e^{-2(r-2)t} \qquad (r \geq 2), \quad (42)$$

$$H_P(r,t) = \frac{2t}{\rho(t)}\frac{H(1,t)}{t^2}e^{-2(r-2)t} \qquad (r \geq 2), \quad (43)$$

$$G_P(r,t) = \frac{H_P(r,t)}{2\rho(t)E_P(r,t)} = \frac{t}{\rho(t)} \qquad (r \geq 2). \quad (44)$$

So, for $r \geq 2$, $G_P(r,t) = G_V(r,t)$ and is independent of r.

In order to solve the case in which $1 \leq r \leq 2$, we must solve Eq. (38) in the cases where h or h' can be less than 1. These can be written in terms of quadratures as

$$H(h,1;t) = H(t)\frac{1-e^{-2t}}{2}e^{(1-h)t} - \frac{1-h}{2}\sqrt{H(t)} \times \int_0^t dt_1\, \sqrt{H(t_1)}(1-e^{-2t_1})e^{(1-h)t_1} \quad (45)$$

and

$$H(h,h';1;t) = \int_0^t dt_1\, H(t_1)e^{(-h+h')t_1} + \int_0^t dt_1\, \sqrt{H(t_1)}\frac{e^{-h't_1}}{t_1}\int_0^{t_1} dt_2 \frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\sqrt{H(t_2)}e^{-ht_2} + \int_0^t dt_1\, \sqrt{H(t_1)}\frac{e^{-ht_1}}{t_1}\int_0^{t_1} dt_2 \frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\sqrt{H(t_2)}e^{-h't_2}. \quad (46)$$

Using these expressions, the results for $1 \leq r \leq 2$ can now be written down as

$$\begin{aligned}\rho(t)E_P(r,t) &= \int_{r-1}^{1}\int_{r-1}^{1} dh\, dh'\, n(h,h',t) + 2\int_{r-1}^{1} dh \int_1^{\infty} dh'\, n(h,h',t) + \int_1^{\infty}\int_1^{\infty} dh\, dh'\, n(h,h',t) \\ &= \int_0^t dt_1\, \frac{H(t_1)}{t_1^2}\left[e^{-2(r-1)t_1} - (1-e^{-2t_1})\left(\frac{1-e^{-(r-1)t_1}}{t_1}\right)\right] \\ &\quad -2\int_0^t dt_1 \left(\frac{1-e^{-(r-1)t_1}}{t_1}\right)\frac{\sqrt{H(t_1)}}{t_1}\int_0^{t_1} dt_2 \left[\left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right)\sqrt{H(t_2)}\left(\frac{e^{-(r-1)t_2}-e^{-t_2}}{t_2}\right)\right]. \end{aligned} \quad (47)$$

From this expression, we also have

$$\begin{aligned}\rho(t)H_P(r,t) &= -\rho(t)\frac{\partial}{\partial r}E_P(r,t) \\ &= \int_0^t dt_1 \frac{H(t_1)}{t_1}\left[2e^{-2(r-1)t_1} + (1-e^{-2t_1})\frac{e^{-(r-1)t_1}}{t_1}\right] \\ &\quad +2\int_0^t dt_1 \frac{\sqrt{H(t_1)}}{t_1}e^{-(r-1)t_1}\int_0^{t_1} dt_2\, \sqrt{H(t_2)}\left(\frac{e^{-(r-1)t_2}-e^{-t_2}}{t_2}\right)\left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right) \\ &\quad -2\int_0^t dt_1 \left(\frac{1-e^{-(r-1)t_1}}{t_1}\right)\int_0^{t_1} dt_2\, \sqrt{H(t_2)}e^{-(r-1)t_2}\left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right) \end{aligned} \quad (48)$$

and

$$G_P(r,t) = \frac{1}{2\rho(t)}\frac{H_P(r,t)}{E_P(r,t)}. \quad (49)$$

Finally, knowledge of $E_P(r,t)$ allows us to calculate the mean nearest-neighbor distance $\lambda(t)$ as in Ref. [4] according to the relation

$$\lambda(t) = 1 + \int_1^\infty dr\, E_P(r,t). \tag{50}$$

We emphasize that $\lambda(t)$ is not the mean distance between the successive centers on the line, i.e.,

$$\lambda(t) \neq 1 + \frac{1-\rho(t)}{\rho(t)}.$$

Substitution of expression (47) into (50) yields

$$\begin{aligned}\lambda(t) = {} & 1 + \frac{(1-e^{-2t})H(t)}{4t^3\rho(t)} + \frac{1}{\rho(t)}\int_0^t dt_1 \frac{H(t_1)}{t_1^2}\left[2\left(\frac{1-e^{-t_1}}{t_1}\right)-1\right]\left[\frac{1-e^{-2t_1}}{2t_1}\right] \\ & -\frac{2}{\rho(t)}\int_0^t dt_1 \frac{\sqrt{H(t_1)}}{t_1^2}\int_0^{t_1} dt_2 \left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right)\frac{\sqrt{H(t_2)}}{t_2} \\ & \times\left[\left(\frac{1-e^{-t_2}}{t_2}\right) - e^{-t_2} + e^{-t_2}\left(\frac{1-e^{-t_1}}{t_1}\right) - \left(\frac{1-e^{-(t_1+t_2)}}{t_1+t_2}\right)\right].\end{aligned} \tag{51}$$

At small times and densities $[\rho(t) \simeq t - t^2]$, this reduces to

$$\lambda(t) = \frac{1}{2\rho(t)} + \frac{1}{2} + O([\rho(t)]^2) = \frac{1}{2t} + 1 + O(t^2). \tag{52}$$

This has the same leading-order low-density behavior as the equilibrium hard-rod mean nearest-neighbor distance $\lambda_{\rm eq}$ at number density ρ, where

$$\lambda_{\rm eq} = \frac{1}{2} + \frac{1}{2\rho} \tag{53}$$

for *all* values of ρ.

V. DISCUSSION OF RESULTS AND COMPARISON TO COMPUTER SIMULATIONS

In this section, we present graphically our analytical results for the nearest-neighbor functions. These results are compared to corresponding Monte Carlo simulations, which are carried out here. Our results are also discussed in light of some recent general theorems [7].

The computer simulations were carried out using systems of 10^6 particles on a unit line with periodic boundary conditions. The particle radius was determined by the volume fraction of particles desired. The results were averaged over 2000 different samples for volume fractions of 0.5, 0.6, and 0.72 corresponding to a wide range of times in the RSA process. A smaller number of runs were also done at $\rho = 0.747$ in order to obtain results closer to the jamming limit.

A. Void quantities

The results for $H_V(r,t)$ for a wide range of volume fractions are shown in Fig. 1. The results for the simulation data match the theoretical curves almost perfectly, with the difference being smaller than the errors associated with the simulation data. The values of $E_V(r,t)$ (Fig. 2) show a similar correspondence, confirming the theoretical expressions. The graph of $G_V(r,t)$ (Fig. 3), although simply obtained from $E_V(r,t)$ and $H_V(r,t)$, is insightful because it shows that $G_V(r,t)$ is indeed constant for values of $r > 1$. The curve in the computer simulation data for $G_V(r,t) > 2$ is due to the fact that the value of $E_V(r,t)$ is so small in that range that we were unable to get good enough statistics to calculate an accurate value of $G_V(r,t)$.

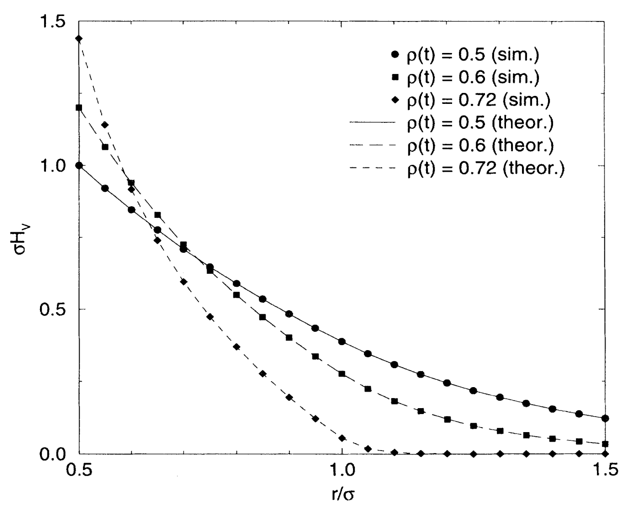

FIG. 1. Computer simulation data and analytical expressions for $H_V(r,t)$ for various values of $\rho(t)$.

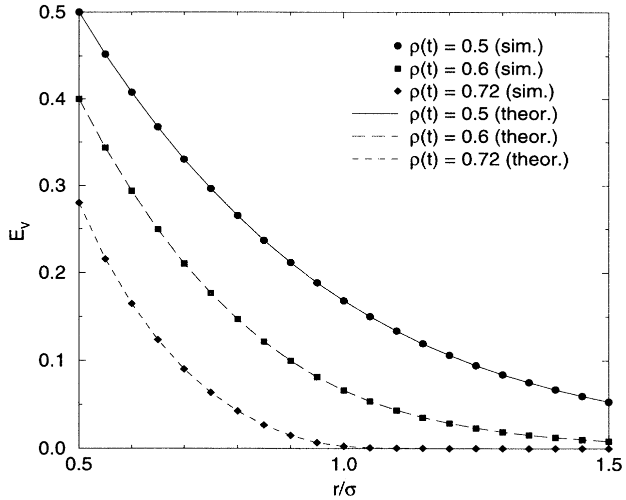

FIG. 2. Computer simulation data and analytical expressions for $E_V(r,t)$ for various values of $\rho(t)$.

B. Particle quantities

The results for $H_P(r,t)$ and $E_P(r,t)$ are shown in Figs. 4 and 5, respectively. These show a clear match with the theory. The results for $G_P(r,t)$ are shown in Fig. 6 and are even more interesting. For long times (large values of ρ) there is an initial downward curvature at $r=1$. This can be predicted by looking at the value of $\partial G_P(r,t)/\partial r$ for $r=1^+$. First, we can write

$$\frac{\partial G_P(r,t)}{\partial r} = \frac{1}{2\rho(t)E_P(r,t)^2} \times\{[H_P(r,t)]^2 + E_P(r,t)H_P'(r,t)\}. \tag{54}$$

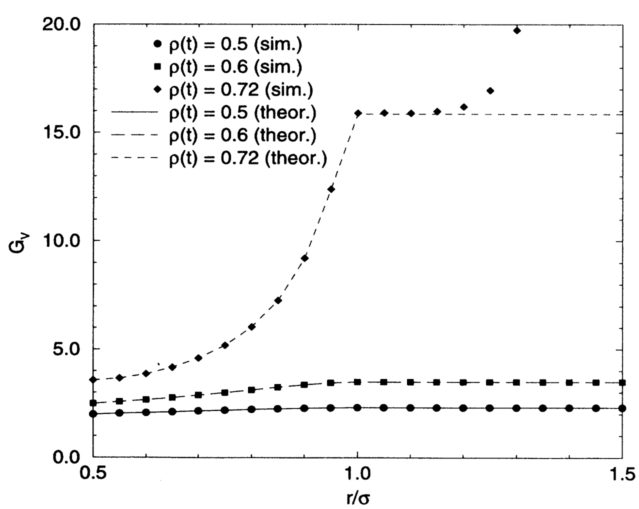

FIG. 3. Computer simulation data and analytical expressions for $G_V(r,t)$ for various values of $\rho(t)$.

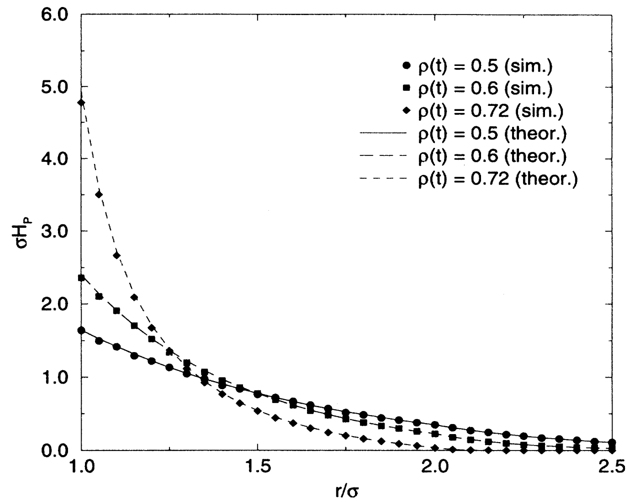

FIG. 4. Computer simulation data and analytical expressions for $H_P(r,t)$ for various values of $\rho(t)$.

For $r=1^+$, knowing that

$$E_P(r=1^+) = 1, \tag{55}$$

$$\rho(t)H_P(r=1^+) = 4\int_0^t dt_1 \frac{H(t_1)}{t_1}, \tag{56}$$

we can calculate

$$-\rho(t)\frac{\partial H_P(r=1^+,t)}{\partial r} = 6\int_0^t dt_1\, H(t_1) + 4\int_0^t dt_1 \frac{\sqrt{H(t_1)}}{t_1} \times \int_0^{t_1} dt_2\, \sqrt{H(t_2)}\left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right) \tag{57}$$

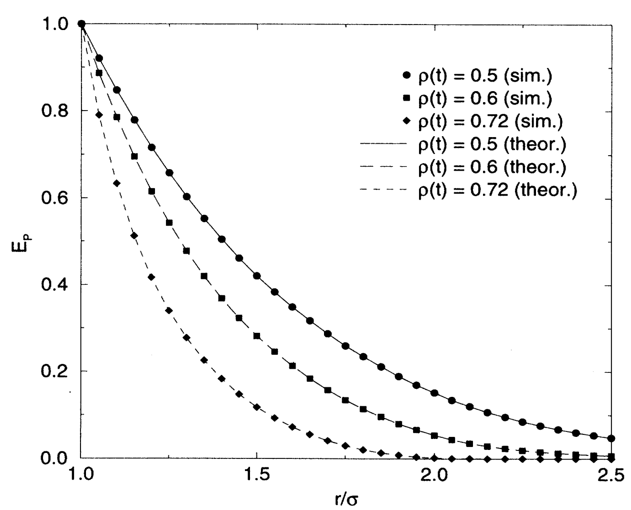

FIG. 5. Computer simulation data and analytical expressions for $E_P(r,t)$ for various values of $\rho(t)$.

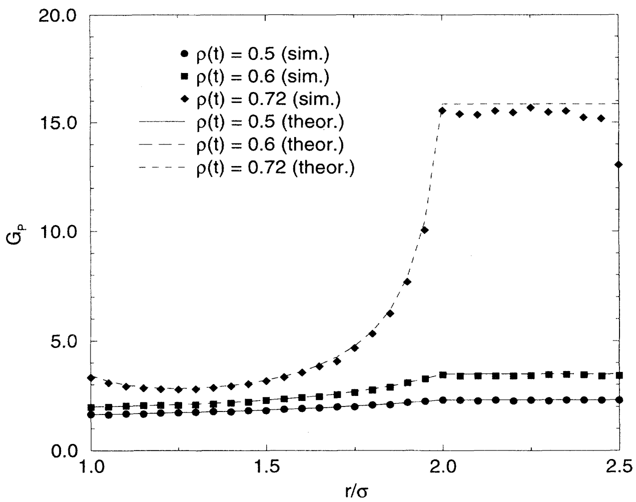

FIG. 6. Computer simulation data and analytical expressions for $G_P(r,t)$ for various values of $\rho(t)$.

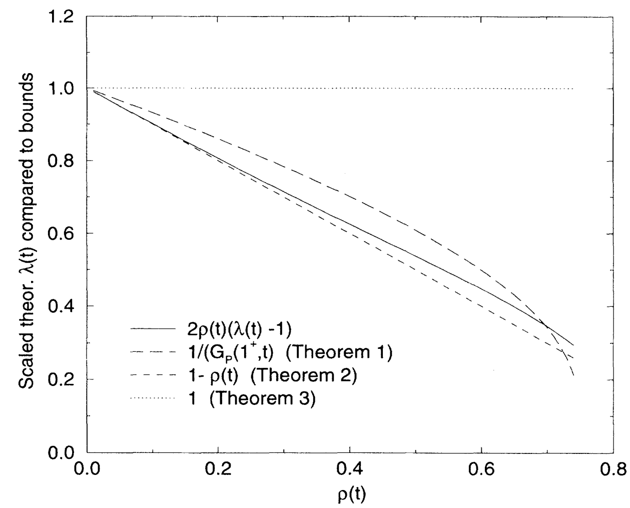

FIG. 7. Comparison between the RSA expression for $2\rho(t)[\lambda(t)-1]$ and the various bounds considered in Theorems 1–3 of Ref. [7] $[1/G_P(1^+,t)$, $1-\rho(t)$, and 1] as a function of $\rho(t)$. The data have been shifted and rescaled as described in the text.

to give

$$\frac{\partial G_P(r=1^+,t)}{\partial r} = \frac{1}{2\rho(t)^3}\left\{\left(4\int_0^t dt_1\,\frac{H(t_1)}{t_1}\right)^2 - 6\rho(t)\int_0^t dt_1\,H(t_1) -4\rho(t)\int_0^t dt_1\frac{\sqrt{H(t_1)}}{t_1} \times\int_0^{t_1} dt_2\,\sqrt{H(t_2)}\left(\frac{1-e^{-2t_2}+2t_2e^{-t_2}}{2t_2}\right)\right\}. \quad (58)$$

For long times, the dominant term will be the second term in the curly brackets, which leads to

$$\frac{\partial G_P(r=1^+,t)}{\partial r} \sim -\frac{3e^{-2\gamma}}{\rho(\infty)^2}t. \quad (59)$$

So, not only does the slope become negative, but as $t\to\infty$, it becomes infinitely negative. Also, for long times $G_P(1^+)\sim \ln t$ and $G_P(r>2)\sim t$, so $G_P(r,t)$ must have a minimum between $r=1$ and $r=2$ for large enough times. The discrepancy between the two curves in Fig. 6 for $r>2$ is due to the fact that the bin widths had to be chosen large enough for there to be a statistically significant amount of data and this width was large enough for the value of $E_V(r,t)$ to change significantly within the bin.

The above minimum can also be predicted from Theorem 1 of [7], which states that for any ergodic ensemble of isotropic packings of identical D-dimensional hard spheres in which $G_P(1^+)\le G_P(r)$, for $1\le r\le\infty$,

$$\lambda \le 1+\frac{1}{D2^D\rho G_P(1^+)}. \quad (60)$$

As $t\to\infty$, $G_P(1^+)\to\infty$ as $\ln t$ and so the bound implies that $\lambda\to 1$. However, we know that for RSA in one dimension λ is strictly larger than 1 due to the fact that there will always be permanent gaps in the system even at the jamming limit. This can be seen in Fig. 7 since the value of $2\rho(t)\lambda-1$ does not go to zero at jamming $[\rho(t)\approx 0.747]$. The data in Fig. 7 have been shifted by 1 and scaled by a factor of $2\rho(t)$ in order to remove the trivial factor of 1 that occurs in Eq. (50) and to elim-

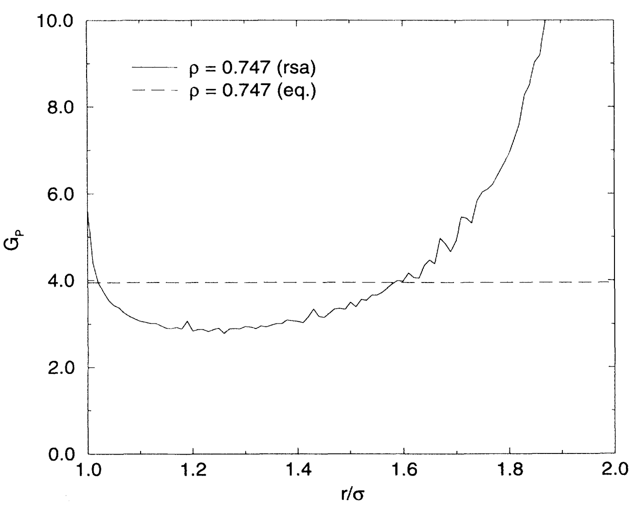

FIG. 8. Comparison of RSA and equilibrium expressions for $G_P(r,t)$ near the RSA jamming limit. In the RSA case, the value of λ is greater than $1+(1-\rho)/2\rho$, so we know that even though $G_P(r,t)>(1-\rho)^{-1}\approx 3.9$ when $r\to 1^+$ and $r=2$, it must become less than that for values of r between 1 and 2.

inate the singularity at $\rho(t = 0) = 0$. Since the RSA process produces rod configurations that are ergodic and isotropic, the condition that $G_P(1^+) \leq G_P(r)$ must be violated at large enough times, resulting in a minimum in $G_P(r)$, as is indeed observed (see Fig. 6).

A similar result can be obtained by looking at Theorem 2 from that same paper [7]. This theorem states that for any ergodic ensemble of isotropic packings of identical D-dimensional hard spheres in which $(1-\rho)^{-1} \leq G_P(r)$ for $1 \leq r \leq \infty$,

$$\lambda \leq 1 + \frac{1-\rho}{D2^D\rho}. \tag{61}$$

For large enough values of ρ for one-dimensional RSA (see Fig. 7) this condition is violated, implying that $G_P(r) \leq (1-\rho)^{-1}$ for some values of r. Theorem 2 gives an idea of the magnitude of the drop in $G_P(r)$. At jamming, $\rho < 1$, so $G_P(r)$ will stay finite for some values of r between 1 and 2, while $G_P(1)$ and $G_P(2)$ become infinite. Figure 8 shows an example of this phenomena for very high densities. Note, finally, that, as required by Theorem 3 of [7], λ is always less than $1 + 1/2\rho$ (see Fig. 7).

VI. CONCLUSION

We have derived analytic expressions for a number of nearest-neighbor distribution functions associated with RSA in one dimension. Computer simulation results agree well with these formulas and the detailed comparison between simulation data and exact solutions provides an interesting calibration before undertaking a numerical study of 2D and 3D systems for which no analytical solutions are known. The results are also used to show the importance of previous results [7] related to general ergodic and isotropic packings of hard spheres.

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