Diffusion of interacting particles in one dimension

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We study the diffusion of N particles on an infinite line. The particles obey the standard diffusion equation and interact by a hard-core interaction. The problem has an exact solution, from which we derive the single-particle and two-particle probability distributions for arbitrary initial conditions, as expansions in powers of $t^{-1/2}$, where t denotes time. Explicit expressions are given for the moments of the displacement for each of the particles and correlations of displacements between any pair of particles. The mth moment grows as $t^{m/2}$ in the leading order. Correlations in the system are quite strong. Two of the interesting features are as follows. (1) Correlation between the displacements of the central particle and that of any other particle decays with the label distance exponentially, but with a correlation length of the order of N. (2) Correlations of a particle near one edge with those on the other edge are much larger than with those near the center. This implies that the size of the assembly expands quite symmetrically with time as $t^{1/2}$.

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I. INTRODUCTION

The diffusion of interacting particles has been extensively studied due to its numerous applications in biological, chemical, and physical processes [1,2]. Examples of these processes are the flow of ions and water through molecular-sized channels in membranes [3], sliding proteins along DNA [4], transport of adsorbate molecules through zeolites [2], carrier migration in polymers and superionic conductors [5], and migration of adsorbed molecules on surfaces [6]. Recently diffusion of water molecules in carbon nanotubes has also been studied and the results seem to reflect features typical of such diffusion [7].

In one dimension, interactions play a crucial role and alter some qualitative features of the diffusion process, as was first shown in a pioneering study by Harris [8]. He showed that a tagged particle follows a subdiffusive behavior: the mean square displacement grows with time as $t^{1/2}$. The result has been confirmed in subsequent numerical studies for many kinds of models [9,10], and a physical understanding of this behavior has been achieved in these contexts through exact [11] and approximate solutions [9,10,12–16]. In most of the studies, the interaction between particles is taken to be the hard-sphere interaction, which makes the particles impenetrable. This diffusion process is also termed "single-file diffusion" in the literature. The models considered are either lattice models, in which the double occupation of a site is prohibited, or continuum models, in which particle pairs reflect from each other on meeting.

In this paper, we study the continuum model, which was first solved by Rödenbeck *et al.* [11] for arbitrary number N of particles on an infinite line. These authors presented an exact solution of the one-particle probability distribution for an ensemble average over random initial conditions. They also obtained results for a nonzero density of particles and showed that for this model also the mean square displacement varies as $t^{1/2}$ in the long-time limit. This was followed by the work of Aslangul [17], who gave an exact solution for this problem for a finite number of particles, but for one particular initial condition, which is that all the particles start from one point. He obtained the one-particle distribution function and showed that the mean displacement is also nonzero for a finite assembly of particles, growing as $t^{1/2}$ to the right if the particle is in the right half of the assembly, and to the left if the particle is in the left half of the assembly. He also gave an expression for the correlation function of the displacements of the two particles at the two ends of the assembly.

The purpose of this work is to generalize earlier results in the continuum model for N particles on an infinite line for arbitrary initial conditions and to study the general two-particle correlation functions. We develop expansions in powers of $t^{-1/2}$ and obtain to two leading orders (i) the one-particle distribution function for each of the particles, and (ii) the two-particle distribution function for each pair of particles. We present explicit results for the mean displacement and mean sqare displacement, in particular their variations with the position of the particle. We next give a general formula for the correlated moments of the displacements. Numerical evaluation of these correlations reveals several interesting features. Correlations are surprisingly strong and long ranged, and moreover show interesting finite-size effects for the particles in the exterior regions. The paper is organized as follows. In Sec. II, we present the analytical results for the N-particle probability distribution and characterize the one-particle distribution functions by giving formulas for all the moments of displacement for each of the particles. We then present some numerical results for the mean and the mean square displacements. In Sec. III, we study two-particle correlations by calculating the moments of displacement for all pairs of particles. This is followed by numerical evaluation of some of the above quantities to illustrate the nature of correlations in this system. We end the paper with a summary of the results and a discussion in Sec. IV.

II. PROBABLITY DISTRIBUTION AND SINGLE-PARTICLE MOMENTS

For the sake of completeness, we first present a derivation of the probability distribution, which is a little different from

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that of earlier papers [11,17]. The distribution function $Q(x_1,x_2,\ldots,x_N;t)$ obeys the usual diffusion equation

$$\frac{\partial Q}{\partial t}=\sum_i \frac{\partial^2 Q}{\partial^2 x_i}. \quad (1)$$

Interactions among the particles are incorporated through the conditions

$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_{i+1}}\right)Q\,(x_1,x_2,\ldots,x_N;t)\Big|_{x_i=x_{i+1}}=0, \quad (2)$$

which physically imply that the particles cannot cross each other. If $\{\phi_n(x)e^{-\lambda_n t}\}$ denotes the complete set of the single-particle solutions with the desired boundary conditions, then the N-particle solution obeying the conditions of Eq. (2) can be written as

$$Q(x_1,x_2,\ldots,x_N;t)=\sum_{\{n_i\}}A(\{n_i\})D_{n_1,n_2,\ldots}(x_1,x_2,\ldots;t), \quad (3)$$

where $D_{n_1,n_2,\ldots}(x_1,x_2,\ldots;t)$ is a completely symmetrized product of one-particle solutions, given as

$$D_{n_1,n_2,\ldots}(x_1,x_2,\ldots;t)=\sum_P \phi_{n_1}(x_1^P)\cdots\phi_{n_N}(x_N^P)\exp\left(-\sum_i \lambda_{n_i}t\right), \quad (4)$$

where P represents permutations of $(x_1,x_2,\ldots,x_N)$ and x_j^P is the j coordinate in permutation P. The summation is over all the permutations. The coefficients $A(\{n_i\})$ are determined from the initial conditions. The above solution is valid for a given sector of the coordinates. If the initial positions of the particles are $X_1<X_2<\ldots<X_N$ for particles 1, 2,..., N, respectively, then $Q(x_1,x_2,\ldots,x_N;t)$ is nonzero only in the sector $x_1<x_2<\cdots<x_N$. For the infinite line, the one-particle eigenfunctions and eigenvalues are: $\phi_k(x)=\exp(ikx)/\sqrt{2\pi}$; $\lambda_k=Dk^2$. Using these one obtains,

$$Q(x_1,x_2,\ldots,x_N;t)=(2\pi)^{-N/2}\sum_{\{k_j\}}A(\{k_j\})\times\sum_P \exp\left(-Dt\sum_j k_j^2+i\sum k_jx_j\right). \quad (5)$$

If we take

$$A(\{k_j\})=\exp\left(-i\sum_j k_jX_j\right), \quad (6)$$

it is easily seen that the required initial condition is achieved for the above sector of $\{x_j\}$'s. Performing the summation over k's, one gets

$$Q(x_1,x_2,\ldots,x_N;t)=\frac{1}{(4\pi Dt)^{N/2}}\sum_P \times\exp\left(-\frac{1}{4Dt}\sum_i (x_i-X_i^P)^2\right)\times\prod_{i=1}^{N-1}\theta(x_{i+1}-x_i). \quad (7)$$

We now integrate this distribution function to characterize various one-particle and two-particle distribution functions. For this purpose, we first consider the mth moment of the displacement of the kth particle,

$$p_m(k,t)=\frac{1}{(4\pi Dt)^{N/2}}\sum_P \int_{-\infty}^{\infty}dx_1\int_{x_1}^{\infty}dx_2\cdots\times\int_{x_{N-1}}^{\infty}dx_N(x_k-X_k)^m\exp\left(-\frac{1}{4Dt}\sum_i (x_i-X_i^P)^2\right). \quad (8)$$

Introducing the variables $u_i=(x_i-X_i^P)/\sqrt{4Dt}$ and changing the order of integrations to keep the integration over u_k as the last, one arrives at the form

$$p_m(k,t)=(4Dt)^{m/2}\sum_P \int_{-\infty}^{\infty}\frac{du_k}{\sqrt{\pi}}e^{-u_k^2}(u_k-Y_k^P-Y_k)^m\times\int_{-\infty}^{u_k+\eta_{k,k-1}^P}\frac{du_{k-1}}{\sqrt{\pi}}e^{-u_{k-1}^2}\cdots\int_{-\infty}^{u_2+\eta_{2,1}^P}\frac{du_1}{\sqrt{\pi}}e^{-u_1^2}\times\int_{u_k+\eta_{k,k+1}^P}^{\infty}\frac{du_{k+1}}{\sqrt{\pi}}e^{-u_{k+1}^2}\cdots\int_{u_{N-1}+\eta_{N-1,N}^P}^{\infty}\frac{du_N}{\sqrt{\pi}}e^{-u_N^2}, \quad (9)$$

where $Y_i=X_i/\sqrt{4Dt}$, $Y_i^P=X_i^P/\sqrt{4Dt}$, and $\eta_{ij}^P=Y_i^P-Y_j^P$. For clarity of the procedure, we choose to write this result compactly by defining the following two sequences of iterated functions:

$$c^1\mathrm{Erf}(x)=\int_x^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}=\frac{1-\mathrm{erf}(x)}{2},$$

$$c^2\mathrm{Erf}(x,\eta_1)=\int_x^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}c^1\mathrm{Erf}(u+\eta_1),$$

$$c^{m+1}\mathrm{Erf}(x,\eta_m,\eta_{m-1},\ldots,\eta_1)=\int_x^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}c^m\mathrm{Erf}(u+\eta_m,\eta_{m-1},\ldots,\eta_1), \quad (10)$$

and

$$g^1\mathrm{Erf}(x)=\int_{-\infty}^{x}\frac{du}{\sqrt{\pi}}e^{-u^2}=\frac{1+\mathrm{erf}(x)}{2},$$

$$g^2\mathrm{Erf}(x,\eta_1)=\int_{-\infty}^{x}\frac{du}{\sqrt{\pi}}e^{-u^2}g^1\mathrm{Erf}(u+\eta_1),$$

$$g^{m+1}\mathrm{Erf}(x,\eta_m,\eta_{m-1},\ldots,\eta_1)=\int_{-\infty}^{x}\frac{du}{\sqrt{\pi}}e^{-u^2}g^m\mathrm{Erf}(u+\eta_m,\eta_{m-1},\ldots,\eta_1). \quad (11)$$

Then

$$p_m(k,t) = (4Dt)^{m/2}\sum_P \int_{-\infty}^{\infty} \frac{du_k}{\sqrt{\pi}} e^{-u_k^2}(u_k - Y_k^P - Y_k)^m \times g^{k-1}\mathrm{Erf}(u + \eta_{k,k-1}^P, \eta_{k-1,k-2}^P, \dots, \eta_{2,1}^P) \times c^{N-k}\mathrm{Erf}(u + \eta_{k,k+1}^P, \eta_{k+1,k+2}^P, \dots, \eta_{N-1,N}^P). \quad (12)$$

From the above expression, it is easy to develop an expansion in powers of $t^{-1/2}$. This is done by expanding the functions in the integrand in powers of $\eta_{k,j}^P$ and Y_i^P, as they each carry the factor of $(4Dt)^{-1/2}$. Noting that $\Sigma_P \eta_{k,j}^P = 0$, we obtain the first two terms as

$$p_m(k,t) = (4Dt)^{m/2}N!\int_{-\infty}^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}u^m g^{k-1}\mathrm{Erf}(u,0,0,\dots,0)c^{N-k}\mathrm{Erf}(u,0,0,\dots,0) + m(4Dt)^{(m-1)/2} \times \sum_P (X_k^P - X_k)\int_{-\infty}^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}u^{m-1}g^{k-1}\mathrm{Erf}(u,0,0,\dots,0)c^{N-k}\mathrm{Erf}(u,0,0,\dots,0) + O(t^{(m-2)/2}). \quad (13)$$

These equations are further simplified by noting that

$$c^m\mathrm{Erf}(u,0,\dots,0) = \frac{1}{m!}[c^1\mathrm{Erf}(u)]^m,$$

$$g^m\mathrm{Erf}(u,0,\dots,0) = \frac{1}{m!}[g^1\mathrm{Erf}(u)]^m. \quad (14)$$

This allows us to write

$$p_m(k,t) = \frac{N!}{(k-1)!(N-k)!}(4Dt)^{m/2}E_m(k-1,N-k) + \frac{(N-1)!}{(k-1)!(N-k)!}m(4Dt)^{(m-1)/2}\sum_l (X_l - X_k) \times E_{m-1}(k-1,N-k), \quad (15)$$

where

$$E_m(I,J) = \left(\frac{1}{2^{I+J}}\right)\int_{-\infty}^{\infty}\frac{du}{\sqrt{\pi}}e^{-u^2}u^m[1+\mathrm{erf}(u)]^I[1-\mathrm{erf}(u)]^J. \quad (16)$$

The above formula characterizes the single-particle distribution of the displacement of the kth particle by giving all its moments in the long-time limit. Note that the first term is independent of the initial conditions and agrees with the result given by Aslangul [17]. The physical features are largely associated with the first two moments of the particle displacements. The mean displacement of the kth particle is

$$\langle x_k\rangle = \langle X\rangle + \sqrt{4Dt}v_N(k), \quad (17)$$

$$v_N(k) = \frac{N!}{(k-1)!(N-k)!}E_1(k-1,N-k), \quad (18)$$

where $<X>$ denotes the average over the initial positions of all the particles. As noted by Aslangul, the nonzero value of the mean displacement is one clear effect of interactions in a finite assembly of particles. This is basically the effect of asymmetry, a particle on the right of center is pushed right, as its motion to the left is blocked by more particles than the number blocking it from the right. Similarly, the particles on the left side of the center are pushed left in a symmetric manner, as $E_1(I,J) = -E_1(J,I)$ and $E_1(I,J) > 0$ for $I > J$. The mean displacement increases as $(4Dt)^{1/2}$ and, in Fig. 1, we show the variation of the coefficient $v_N(k)$ with particle number, for some values of N. The variation is shown for the right side of the assembly with $l = k - k_M$, where k_M labels the central particle. For particles near the center of the assembly, the moments can be approximately evaluated analytically for large N in the following manner. Considering an assembly of an odd number of particles, we write $k = (N+1)/2 + l$; then the moments of displacement in terms of l are

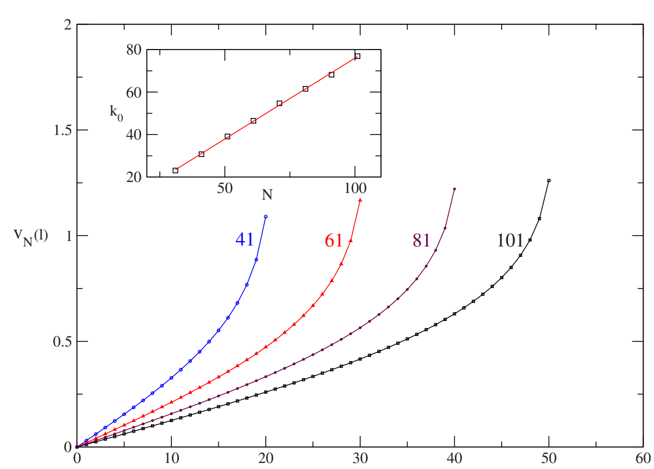

FIG. 1. (Color online) Plots of $v_N(l)$ with l ($l = k - k_M$, where k_M labels the central particle) according to Eq. (18) for four values of N as indicated. The inset shows the variation of the inverse slopes k_0 of these plots with N. These vary linearly with N.

$$\langle x_l^m\rangle = N(4Dt)^{m/2}\frac{(N-1)!}{\left(\frac{N-1}{2}-l\right)!\left(\frac{N+1}{2}-l\right)!}\frac{1}{2^{N-1}}\int_{-\infty}^{\infty}u^m e^{-u^2}\times[1-\text{erf}^2(u)]^{(N-1)/2}\left[\frac{1+\text{erf}(u)}{1-\text{erf}(u)}\right]^l. \quad (19)$$

Due to the factor $[1-\text{erf}^2(u)]^{(N-1)/2}$ the integrand is nonzero in a very narrow region around zero. Thus, for large N and small l, we can expand other factors in powers of u to obtain

$$\langle x_l^m\rangle/(4Dt)^{m/2} \approx N\frac{1}{\sqrt{2\pi N}}\exp(-l^2/2N)\int_{-\infty}^{\infty}u^m e^{-(2N/\pi)u^2}\times\left(1+\frac{4ul}{\sqrt{\pi}}\right). \quad (20)$$

Setting $m=1$, we obtain to the leading order

$$v_N(l) = \frac{\pi l}{2N}. \quad (21)$$

This shows that near the center $v_N(l)$ rises linearly with l, with a slope decreasing as $1/N$. As shown in Fig. 1, the numerical data conform to this variation of $v_N(l)$. The variation of the inverse slope, k_0 with N is shown in the inset of Fig. 1, which also agrees with the analytical evaluation. Toward the edge $v_N(k)$ rises rapidly as expected on physical grounds. As shown by Aslangul [17], for the edge particles, v_N should grow as $\sqrt{\log N}$ for large N, which we verified by numerical evaluation.

In this paper, we have numerically evaluated the formulas for $v_N(k)$ and other quantities involved in mean-square displacement and correlation functions for N up to 101. In principle, these formulas can be computed for arbitrarily large values of N, but there are practical numerical problems. These formulas involve two factors, a combinatorial factor which becomes huge even for moderately large N, and an integral containing functions raised to powers of order N, which make the integrands extremely small. So a judicious manipulation between the two factors is required for the correct computation of these formulas. The approximate analytic evaluation of the formulas indicates the basic trends these quantities follow at large N, and we believe that our computations up to $N=101$ establish these, though computations for larger N would certainly be desirable. Moreover, there is now intrinsic interest in finite-size effects in small assemblies under nonequilibrium conditions.

Next, we write the expression for the mean-square displacement of the kth particle,

$$p_2(k,t) = (4Dt)d_N(k) - (4Dt)^{1/2}\frac{2v_N(k)}{N}\sum_l (X_k - X_l), \quad (22)$$

where $d_N(k)$ can be read off from Eq. (15). Note that the $t^{1/2}$ term is negative for all values of k and represents a substantial correction for the particle toward the edges at early times. The coefficient $d_N(k)$ is symmetric about the central particle for which it is the minimum. In Fig. 2, we show its

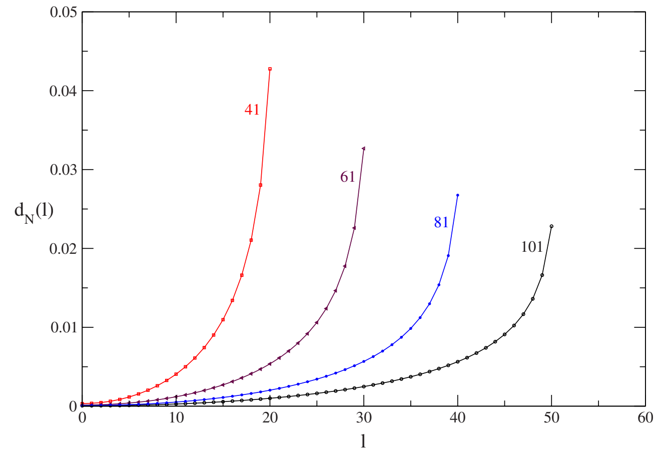

FIG. 2. (Color online) $d_N(l)$ vs l according to Eq. (20) for four values of N. The particle labels l are the same as in Fig. 1.

variation with l for some values of N. For small l and large N, we can use Eq. (20) to deduce

$$d_N(l) = d_N(0) + b_N l^2, \quad (23)$$

with $d_N(0)=\pi^{3/2}/8N$ and $b_N=3\pi^{3/2}/4N^2$. For small l, the results shown in Fig. 2 fit this variation very well. Our result on $1/N$ variation of $d_N(0)$ agree with the results of Harris [8] and Aslangul [17]. The variations of $d_N(0)$ and b_N with N are exhibited in Fig. 3, the latter in the inset. The coefficient $d_N(0)$ is expected to decrease as $1/N$; thus we show the best fit of the numerical results with this variation. Similarly we show the fit of the data for b_N with the analytically derived variation of $1/N^2$. The quality of these fits is not good enough to establish these variations quantitatively. Clearly, computations for larger N are required to confirm the analytical results.

III. CORRELATIONS

As mentioned above, a very significant effect of interactions is to induce rather strong correlations among the

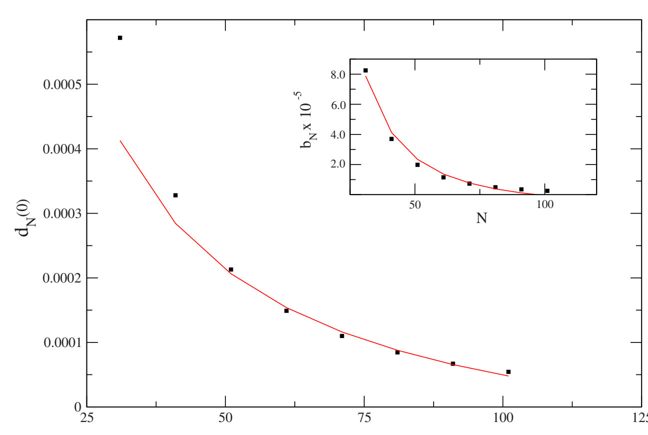

FIG. 3. (Color online) Numerical results for $d_N(0)$ and b_N (inset). Analytically $d_N(0)$ should decrease as $1/N$ for large N. The line shows the best fit with this variation. The line in the inset shows the best fit for b_N according to the analytically derived variation as $1/N^2$.

particles. A good measure of this is the correlator $C_N(k,k+r,t)=\langle \Delta x_k \Delta x_{k+r}\rangle$, where $\Delta x_k = x_k - X_k$. After the change of variables as in Eq. (9), this is given by

$$C_N(k,k+r,t) = (4Dt)^{1/2}\sum_P \int_{-\infty}^{\infty} \frac{du_1}{\sqrt{\pi}} e^{-u_1^2} \times \int_{u_1+\eta_{1,2}^P}^{\infty} \frac{du_2}{\sqrt{\pi}} e^{-u_2^2} \cdots \int_{u_{k-1}+\eta_{k-1,k}^P}^{\infty} \frac{du_k}{\sqrt{\pi}} e^{-u_k^2} \times (u_k - Y_k^P - Y_k) \cdots \int_{u_{k+r-1}+\eta_{k+r-1,k+r}^P}^{\infty} \frac{du_{k+r}}{\sqrt{\pi}} e^{-u_{k+r}^2} \times (u_{k+r} - Y_{k+r}^P - Y_{k+r}) \cdots \int_{u_{N-1}+\eta_{N-1,N}^P}^{\infty} \frac{du_N}{\sqrt{\pi}} e^{-u_N^2}. \tag{24}$$

We again develop a large-time expansion in powers of $t^{-1/2}$ by expanding the above expression in terms of $\eta_{i,j}^P$ and Y_i. Denoting the first term, which is of order t, by $C_N^{(1)}(k,k+r,t)$, we obtain

$$C_N^{(1)}(k,k+r,t) = (4Dt)N! \int_{-\infty}^{\infty} \frac{du_1}{\sqrt{\pi}} e^{-u_1^2} \int_{u_1}^{\infty} \frac{du_2}{\sqrt{\pi}} e^{-u_2^2} \cdots \times \int_{u_{k-1}}^{\infty} \frac{du_k}{\sqrt{\pi}} e^{-u_k^2} u_k \times \int_{u_k}^{\infty} \frac{du_{k+1}}{\sqrt{\pi}} e^{-u_{k+1}^2} \cdots \int_{u_{k+r-1}}^{\infty} \frac{du_{k+r}}{\sqrt{\pi}} e^{-u_{k+r}^2} u_{k+r} \times \int_{u_{k+r}}^{\infty} \frac{du_{k+r+1}}{\sqrt{\pi}} e^{-u_{k+r+1}^2} \cdots \int_{u_{N-1}}^{\infty} \frac{du_N}{\sqrt{\pi}} e^{-u_N^2}. \tag{25}$$

Now integrations over all variables other than u_k and u_{k+r} can be carried out as demonstrated below:

$$C_N^{(1)}(k,k+r,t) = (4Dt)N! \int_{-\infty}^{\infty} \frac{du_1}{\sqrt{\pi}} e^{-u_1^2} \cdots \times \int_{u_{k-1}}^{\infty} \frac{du_k}{\sqrt{\pi}} e^{-u_k^2} u_k F(u_k), \tag{26}$$

where

$$F(u_k) = \frac{1}{(N-k-r)!} \int_{u_k}^{\infty} \frac{du_{k+1}}{\sqrt{\pi}} e^{-u_{k+1}^2} \cdots \int_{u_{k+r-1}}^{\infty} \frac{du_{k+r}}{\sqrt{\pi}} e^{-u_{k+r}^2} u_{k+r} \times [c^1 \mathrm{Erf}(u_{k+r})]^{N-k-r}. \tag{27}$$

By changing the order of integration over the first $k-1$ variables, followed by a similar change of order for the nexr $r-1$ variables, one finds

$$C_N^{(1)}(k,k+r,t) = (4Dt)\frac{N!}{(k-1)!(N-k-r)!} \int_{-\infty}^{\infty} \times \frac{du}{\sqrt{\pi}} e^{-u^2} u [g^1 \mathrm{Erf}(u)]^{k-1} \int_u^{\infty} \frac{du_1}{\sqrt{\pi}} e^{-u_1^2} \cdots \times \int_{u_{k-1}}^{\infty} \frac{dv}{\sqrt{\pi}} e^{-v^2} v [c^1 \mathrm{Erf}(v)]^{N-k-r} = (4Dt)\frac{N!}{(k-1)!(r-1)!(N-k-r)!} E_3(N,k,r), \tag{28}$$

where

$$E_3(N,k,r) = \frac{1}{2^{N-2}} \int_{-\infty}^{\infty} \frac{du}{\sqrt{\pi}} e^{-u^2} u \times [1+\mathrm{erf}(u)]^{k-1} \int_u^{\infty} \frac{dv}{\sqrt{\pi}} e^{-v^2} v [\mathrm{erf}(v) - \mathrm{erf}(u)]^{r-1} [1-\mathrm{erf}(v)]^{N-k-r}. \tag{29}$$

The next order terms proportional to $(4Dt)^{1/2}$ in $C_N(k,k+r,t)$ are seen to be

$$\sum_l (X_l - X_k)\langle \Delta x_{k+r}\rangle_1 + \sum_l (X_l - X_{k+r})\langle \Delta x_k\rangle_1, \tag{30}$$

where the subscript 1 on the averages in the above formulas denote the leading $t^{1/2}$ contribution. This allows us to write

$$G_N(k,k+r;t) = \langle \Delta x_k \Delta x_{k+r}\rangle - \langle \Delta x_k\rangle\langle \Delta x_{k+r}\rangle = 4Dt\left(\frac{N!}{(k-1)!(r-1)!(N-k-r)!} E_3(N,k,r) - v_N(k) v_N(k+r)\right). \tag{31}$$

The calculation of the higher-order two-particle moments follows identical manipulation, and the leading-order term is given as

$$\langle (\Delta x_k)^M (\Delta x_{k+r})^L \rangle = (4Dt)^{(M+L)/2} \frac{N!}{(k-1)!(r-1)!(N-k-r)!} \times \int_{-\infty}^{\infty} \frac{du}{\sqrt{\pi}} e^{-u^2} u^M [g^1 \mathrm{Erf}(u)]^{k-1} \times \int_u^{\infty} \frac{dv}{\sqrt{\pi}} e^{-v^2} v^L \left(\frac{\mathrm{erf}(v) - \mathrm{efr}(u)}{2}\right)^{r-1} \times [c^1 \mathrm{Erf}(v)]^{N-k-r}. \tag{32}$$

We now evaluate these correlators numerically. The quantity, $g_N(k_M,l) = G_N(k_M,k_M+l)/4Dt$, which is the time-independent coefficient of the correlation between the displacement of the central particle (labeled k_M) and the displacement of the kth particle, $k=k_M+l$ is shown in Fig. 4 on a logarithmic scale. This is an odd function, so the plot contains only the right side. One finds that these correlations extend right up to the edge of the assembly. In the interior,

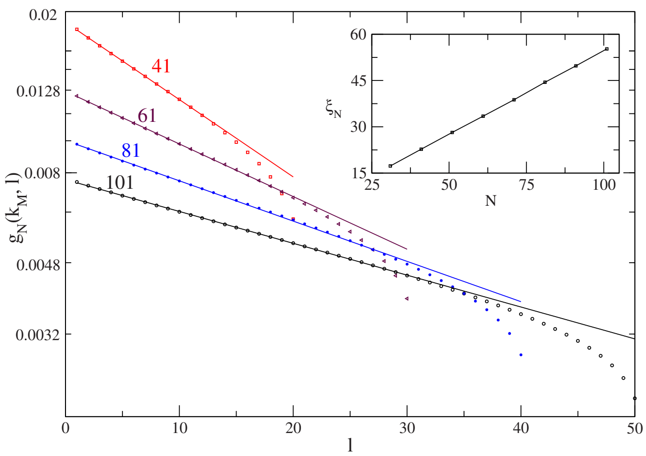

FIG. 4. (Color online) Correlation coefficient $g_N(k_M,l)$ on logarithmic scale for four values of N, shown as symbols. The straight-line fits for small l show that the coefficients decrease exponentially with increasing N. The inset shows the variation of ξ_N with N.

the correlators can be well fitted to an exponential decay, $g_N(k_M,l)=g_0\exp(-l/\xi_N)$. These are seen as straight-line fits for small l in Fig. 4. Quite remarkably, the correlation length ξ_N (measured in terms of particle labels) turns out to be of the order of the number of particles in the assembly. In the inset of Fig. 4, we show the variation of ξ_N with N. It rises linearly with N, being a little larger than $N/2$. We believe that the edge effects cause the deviations from the exponential fits. However, note that the magnitude of the correlator decreases with increasing N.

Next we show in Fig. 5 the correlation coefficient $g_N(e_1,l)=G_N(e_1,l)/4Dt$ between the displacement of the first particle and that of the kth particle ($l=k-k_M$). One finds that the correlations are quite large and extend through the entire assembly. They decrease toward the center, change sign at the center, and increase in magnitude as one goes toward the other edge. As may be noted from the figure, the correlations with the particles in the interior region follow a linear behavior with the particle label, but the invere slope l_0 is again of the order of N. The inset of this figure shows the variation of l_0 with N, which again increases linearly with the system size. These curve also suggest that the deviations from the linearity are due to the edge effects. The magnitude of the correlator between particles at the opposite edges actually increases with N, unlike the correlations in the interior region which decrease with N. This behavior of correlations can be physically understood in the following terms. Whichever way the particle is displaced, it pushes other particles in the same direction. As the effect of pushes of successive particles decreases, the correlation decreases with distance albeit slowly, vanishing at the center due to symmetry. The reason it becomes negative for particles in the other half of the assembly reflects the tendency of the whole assembly to expand. The growth of the correlations in magnitude is related to the larger displacements of the particles near the edges. Stronger correlations between the particles on or near different edges implies that the whole assembly expands in a rather symmetrical manner, and for large N most of the movement occurs near the edges.

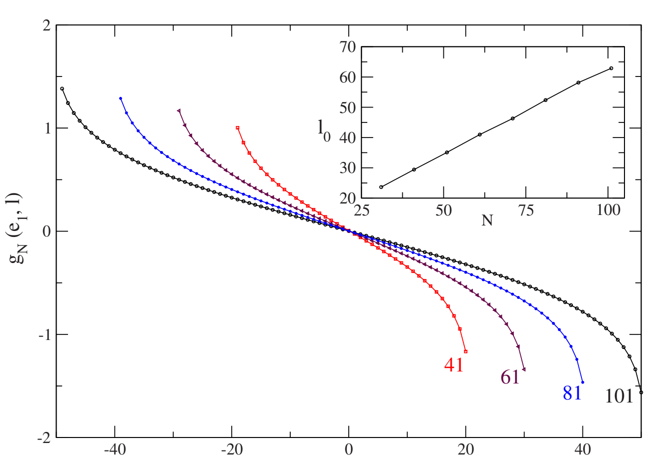

FIG. 5. (Color online) Correlation coefficient $g_N(e_1,l)$ for four values of N. Here e_1 labels the leftmost particle and $l=k-k_M$. The inset shows the variation of the inverse slopes l_0 of the middle linear region of the plots as function of N.

IV. SUMMARY

In conclusion we give a summary of our results along with some discussion. We have studied the dynamical behavior of N interacting particles (hard spheres) diffusing on an infinite line. The joint probability distribution of the positions of the particles with arbitrary initial conditions is obtained exactly. From this we calculate the moments of displacement for each of the particles as a series in powers of $t^{-1/2}$. In the long-time limit the leading term for the mth moment of displacement for any particle goes as $t^{m/2}$. All the moments increase in magnitude as one goes outward from the center of the assembly. In the middle of the assembly, the mean displacement increases linearly and the mean-square displacement increases quadratically with the label index of the particle measured from the center. For particles near the edges moments grow more rapidly.

The correlations in the system are long ranged, spanning the entire assembly. We demonstrate this by studying two cases. One, the correlations of the displacement of a particle with that of the central particle show a rather slow decay with the particle label l, measured from the center. Near the center the variation is exponential, but with a correlation length which is of order $N/2$. Two, the correlations of the displacements of a particle with that of a particle on one edge are much larger than those in the previous case. They are positive when the particle is in the same half as the edge and decrease toward the central particle. On crossing the center they become negative and increase in magnitude with the particle label. This behavior is quite different from an equilibrium assembly of particles in higher dimensions obeying classical or quantum dynamics. Such strong correlations are certainly a feature of one dimension. The other aspect of the problem, apart from the nature of dynamics, is that the assembly here is not in equilibrium. It is expanding with time. The above calculations show that the size of the assembly grows on average as $t^{1/2}$, and the strong correlations ensure that it is symmetrical on the two edges.

Finally we comment on the relation of our study to the subdiffusive $t^{1/4}$ behavior for the root-mean-square displacement of the tagged particle, which has been the prime motivation for the earlier studies. In the present set of results, the diffusion is normal $t^{1/2}$ type, but note that with increasing N, apart from the effects around the edges, the coefficients $v_N(k)$ and $d_N(k)$ tend to zero. This suggests that, in the infinite-particle limit, such behavior gives way to something different in the bulk. The $t^{1/4}$ behavior has been obtained for systems of nonzero density, which may be obtained by considering N particles on a finite line of length L [18] and considering the limit $N,L\to\infty$ with finite density $\rho=N/L \neq 0$. This is a nontrivial limit in our procedure, so it is interesting to examine the additional considerations that have gone into the derivation of the subdiffusive behavior.

We first discuss a rather transparent derivation of Harris's result [8] due to Levitt. Levitt [12] built on the earlier work on the one-dimensional classical gas of hard-sphere particles [19,20], by substituting the single-particle propagators with diffusion propagators on the infinite line. The collision between the particles do not change trajectories, but simply relabel their identification with the particles, which is just the content of Eq. (7). Levitt averages over the initial positions and introduces additional probabilistic arguments for the average number of label changes to arrive at the subdiffusive behavior. Similarly, in the exact study of Rödenbeck *et al.* [11], the distribution function of Eq. (7) is averaged over the initial conditions and a stationarity condition on density is additionally imposed to achieve the $t^{1/4}$ result. Similar assumptions are part of the other physically motivated derivations. Numerical verification of this result also requires similar conditions. For example, Beijeren *et al.* [10] obtained the $t^{1/4}$ result by maintaining a constant density and performing an ensemble average in their simulations. Naturally, the other features associated with finite size, like nonzero mean displacement, expansion of the assembly size, large correlations between particles near edges, etc., are absent in these stationary ensembles.

We conclude with some remarks on the possibility of the experimental verification of our results. Recently some very well-characterized single-file diffusion system have been constructed, where the diffusion of colloidal particles has been studied in one-dimensional channels constructed by photolithography [21] or by optical tweezers [22]. These experiments track the trajectories of single particles and establish the transition from normal diffusion at short times to non-Fickian behavior at large times. The analysis for such trajectories for small expanding assemblies should also yield information on correlation functions studied here. It would also be of interest to study the variation of the diffusive behavior with the position of the particles across the assembly to verify our other results and resolve the issues raised above.

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