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On the Absence of Diffusion in a Semiinfinite One-Dimensional System

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For obvious reasons, the self-diffusion coefficient in bounded many-body systems must be strictly zero, provided that it is defined as the limit of $\langle [R(t) - R(0)]^2 \rangle / (2td)$ when t grows indefinitely [d is the dimensionality, $R(\tau)$ is the position of a given particle at time τ]. Thus, the time integral of the velocity correlation function is strictly zero. A system of hard points on a half-infinite line with a reflective wall at the origin does exhibit this property of absence of diffusion, since each particle has an average position. We study in detail the difference between the velocity correlation functions of the infinite and of the half-infinite systems.

KEY WORDS: Nonequilibrium statistical dynamics; one-dimensional hard-point gas; semiinfinite line; self-diffusion coefficient; dynamics of large systems; long-time behavior.

1. INTRODUCTION

At the IUPAP Meeting at Chicago in 1971, Lebowitz emphasized that the self-diffusion coefficient in a bounded, many-body system is just equal to zero, since the mean square displacement of a particle in a box cannot grow indefinitely. In particular,[(1)] this prevents one from defining the self-diffusion coefficient of an infinite system as the limit of the coefficient of sets of larger and larger systems. Thus, it is of some interest to look at a model where the

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behavior of the velocity time correlation could be studied in detail near the thermodynamic limit.

Some years ago, Jepsen[2] and Lebowitz *et al.*[3,4] found the exact velocity time correlation of a one-dimensional system of hard points. In particular, they found that, for a Maxwell velocity distribution, the asymptotic behavior of this function is given by

$$\langle v_i(0)v_i(t)\rangle \simeq [(5/2\pi) - 1](2\pi)^{-1/2}(\rho t)^{-3} \tag{1}$$

where ρ denotes the number density of the hard-point system and the units are chosen so that $kT/m = 1$. Most of these results remain true for a system of hard rods of length b, provided that ρ is replaced by $\rho(1 - \rho b)^{-1}$.

In this paper, we use the methods developed in Ref. 3 to study another one-dimensional model which at first sight does look rather similar to the Jepsen model but actually behaves in a very different manner: We consider an infinite gas which is the limit of a system of N hard points on a *half-line* of length L ($N, L \to \infty$, $\rho = N/L$ finite). At the origin of the axis, there is by assumption, a purely reflective wall or "mirror" (see Fig. 1).

If there was diffusion in the usual sense, a given particle should go away from the mirror and, since no particle comes from behind the mirror, the number density in the space between the wall and the particle should decrease indefinitely; such a situation looks very unlikely, and this explains why the self-diffusion coefficient is zero in this system. Thus, in this half-infinite system, the behavior of the velocity autocorrelation function must differ from that in a system infinite in both directions. However, one may expect that, when the particle is very far from the mirror on the average, the short-time behavior of the velocity time correlation does not change too much with respect to the case of the full infinite line. Actually, the perturbation becomes important only at times of the order of the mean distance of the particle to the wall. In some sense, this distance plays a role more or less similar to the

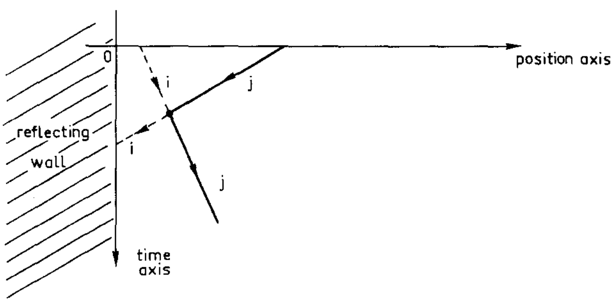

Fig. 1. Trajectories of some particles on a semiinfinite line. Particles are considered as hard points.

one of the size of a bounded system; in fact, when it grows indefinitely, the correlation at finite times keeps its value for an infinite system, although its integral remains equal to zero, as for a bounded system. Accordingly, one may hope to get some insight into the behavior of the time correlation near the thermodynamic limit from a study of this half-infinite system.

In this paper, we derive first the mean value of the pth power of

$$\Delta_n(t) = R_n(\tau) - R_n(0)$$

where $R_n(\tau)$ is the position of the particle of rank n on the line at time τ (this means that $n - 1$ particles lie between this particle and the mirror). Then, we can derive the correlations of its velocity as they are related to each other in an elementary way. The final expressions of these correlations depend on the equilibrium velocity distribution. For a system of hard points on a line, the collisions do not change this velocity distribution, and it may be chosen almost freely. Actually, it does not depend on time, provided that the ensemble of initial conditions is such that the positions of the particles are uncorrelated and their number density is space independent. In the case of a Maxwellian distribution, we show that for finite times and large n (i.e., when the particle is far from the mirror), the velocity correlation function for infinite and half-infinite systems are nearly equal; on the contrary, their asymptotic behaviors strongly differ from each other for long times of the order of n/ρ.

2. FORMULATION OF THE PROBLEM

The self-diffusion coefficient of the nth particle on the line is related to the velocity self-correlation by the Einstein formula:

$$D_n = \int_0^\infty dt \, \langle V_n(0) V_n(t) \rangle$$

where $V_n(\tau)$ is the velocity at time τ of the particle of rank n on the half-line.

In order to compute the time correlation functions of the hard-point system, we shall use the method of Jepsen and of Lebowitz *et al.*, which allows one to replace the time correlation function of the hard-point system by some other correlation of a free point system with the same initial conditions. We shall denote by capital letters the dynamical variables of the hard-point system [$R_n(t')$, $V_n(t')$,..., are position, velocity,..., of the nth particle at time t'] and by lower case letters the variables of the free point system [$r(t)$, $v(t)$,...].

Our objective is to prove that D_n is just equal to zero for any value of n in the case of a half-infinite line. Actually, we have found that it is slightly easier to study the long-time behavior of

$$\overline{\Delta_n^2(t)} = \langle [R_n(t) - R_n(0)]^2 \rangle \tag{2}$$

which is the mean square displacement of the nth particle between times 0 and t. It is easy to show from the Einstein relation

$$D_n = \tfrac{1}{2} \lim_{t\to\infty} (d/dt)\overline{\Delta_n^2(t)} \tag{3a}$$

that there is no diffusion (i.e., $D_n = 0$) if $\overline{\Delta_n^2(t)}$ tends smoothly to a constant value at $t \to \infty$. Furthermore, the asymptotic behavior of $\langle V_n(0)V_n(t)\rangle$ may be deduced at once from that of $\overline{\Delta_n^2(t)}$ by using the formula

$$\langle V_n(0)V_n(t)\rangle = \tfrac{1}{2}(d^2/dt^2)\overline{\Delta_n^2(t)} \tag{3b}$$

Now we have to calculate the average. Following Lebowitz and Percus,[3] we replace the complicated problem of averaging for hard points by a simpler problem of averaging for *free* points: In a collision between two particles i and j, it is equivalent to saying that they have exchanged their velocities or that they have permuted their indices. At time t, the particle i is then represented by a free particle k which has at time t the same rank on the line as particle i at time 0. The reflections on the wall at the origin may be accounted for by replacing the system of points on the half-line by a system of $2N$ hard points on a line of length $2L$, symmetric with respect to the origin and without the wall at the origin. A collision of a particle against the wall is then replaced by an exchange of index with its "mirror" particle (see Fig. 2). We do not care about the boundary conditions at the other end of the line, since we suppose in any calculation that the limit of an infinite line is taken before any other limiting process, so that our results do not depend on these boundary conditions. In particular, the mean square

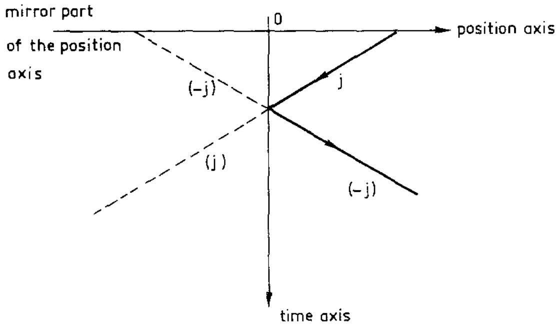

Fig. 2. Exchange of the indices of the real and mirror particles at $r = 0$ (reflection). Particles are considered as free points. The trajectory given by the solid line is that of the real, hard-point particle.

displacement is allowed to grow like the time provided that this displacement is assumed to be much smaller than the length of the line, as we should do.

We come now to the formulation of the problem. We denote by r_i, v_i ($i \neq 0$, $i = -N,..., -1, +1,..., +N$) the position and velocity of particle i at time $t = 0$. We shall call particles with positive indices *real* particles ($0 < i \leqslant N$) and those with negative indices, *mirror* particles; the particles are numbered in such a way that

$$r_{-i} = -r_i, \qquad v_{-i} = -v_i$$

To one unit, the rank of particle k on the line at time t can be defined as the integer function

$$\sigma_k(t) = \sum_{j \neq k} \epsilon[r_k(t) - r_j(t)] \tag{4}$$

where $\epsilon(x)$ is the Heaviside step function

$$\begin{aligned} \epsilon(x) &= 1 \qquad \text{when} \quad x > 0 \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{5}$$

and, of course, $0 \leqslant \sigma_k(t) \leqslant 2N - 1$.

The average value $\overline{\Delta_n{}^p(t)}$ of the pth power of the distance $\Delta_n(t) = R_n(t) - R_n(0)$ of the nth *real* particle from its original position is

$$\begin{aligned} \overline{\Delta_n{}^p(t)} &= \sum_{i=1,\cdots N} \langle [R_i(t) - R_i(0)]^p \, \delta_{\sigma_i(0),N+n-1} \rangle \\ &= \sum_{\substack{j=N,\cdots,N;\, j \neq 0 \\ i=1,\cdots,N}} \langle [r_j(t) - r_i(0)]^p \, \delta_{\sigma_i(0),N+n-1} \, \delta_{\sigma_j(t),\sigma_i(0)} \rangle \end{aligned}$$

or

$$\Delta_n{}^p(t) = \sum_{\substack{j \neq 0 = -N,\cdots,N \\ i=1,\cdots,N}} \langle [r_j + v_j t - r_i]^p \, \delta_{\sigma_i(0),N+n-1} \, \delta_{\sigma_j(t),\sigma_i(0)} \rangle \tag{6}$$

In the above expressions, $\delta_{\alpha,\beta}$ denotes the Kronecker symbol

$$\begin{aligned} \delta_{\alpha,\beta} &= 0 \qquad \text{if} \quad \alpha \neq \beta \\ \delta_{\alpha,\beta} &= 1 \qquad \text{if} \quad \alpha = \beta \end{aligned} \tag{7}$$

and the averages are now taken with the equilibrium weight for free points on a line of length L:

$$\prod_{l=1}^{N} \frac{dr_l}{L} \, dv_l \, h_0(v_l) \epsilon(r_l) \tag{8}$$

where $h_0(x)$ is the velocity distribution function, which is quite arbitrary, but which we shall choose as a Maxwellian

$$h_0(x) = (2\pi)^{-1/2} \exp(-x^2/2) \tag{9a}$$

Notice that in the above relation, units are such that $kT/m = 1$. In the following sections, we shall need also the related functions $\operatorname{Erf} x$ (error function) and $\Phi(x)$ (half collision frequency) defined by

$$\operatorname{Erf} x = \int_0^x h_0(v)\, dv \tag{9b}$$

and

$$\Phi(x) = \int_0^x \operatorname{Erf} v\, dv = h_0(x) + x \operatorname{Erf} x \tag{9c}$$

Starting now from Eq. (6), we are led to split $\overline{\Delta_n{}^p(t)}$ into four terms

$$\overline{\Delta_n{}^p(t)} = A_1 + A_1' + A_2 + A_2' \tag{10}$$

with

$$A_1 = Nt^p \langle v_i^p\, \delta_{\sigma_i(t),\sigma_i(0)} \delta_{\sigma_i(0),N+n-1} \rangle \tag{11a}$$

$$A_1' = (-1)^p t^p \left\langle \left(\frac{2r_i}{t} + v_i\right)^p \delta_{\sigma_{-i}(t),\sigma_i(0)}\, \delta_{\sigma_i(0),N+n-1} \right\rangle \tag{11b}$$

$$A_2 = N(N-1)t^p \left\langle \left[\frac{r_j - r_i}{t} + v_j\right]^p \delta_{\sigma_j(t),\sigma_i(0)}\, \delta_{\sigma_i(0),N+n-1} \right\rangle \tag{11c}$$

$$A_2' = (-1)^p N(N-1)t^p \left\langle \left[\frac{r_j + r_i}{t} + v_j\right]^p \delta_{\sigma_{-j}(t),\sigma_i(0)}\, \delta_{\sigma_i(0),N+n-1} \right\rangle \tag{11d}$$

where indices i and j denote real particles ($r_i, r_j \geqslant 0$) and indices $-i$ and $-j$ the corresponding mirror particles. It is important to realize that the indices i and j are no longer an indication of a rank on a line but represent any one of the real free particles.

The contributions A_1 and A_2 are very similar to those of the full infinite line, while A_1' and A_2' appear in the case of the half-infinite line only, since they account for the case when particles initially behind the mirror have at time t the same rank as particle n at time zero. At large n, the contributions A_1' and A_2' will be important for times of order n, which are required for the arrival of a mirror particle at a distance $n\rho^{-1}$ from the mirror on the positive axis. The four contributions listed in (11) are calculated in Appendix A and are given by Eqs. (A.3) and (A.5), respectively. However, they are complicated even for $n = 1$ and we need the help of a computer to get many of them. However, we can perform the calculations in two limiting cases, which are actually the cases of interest: (i) long-time behavior for arbitrary n [see Eq. (A.6)] and (ii) finite time and large n [Eqs. (A.4), (B.3), and (B.4)].

3. THE RESULTS

As explained in the introduction, we are mainly interested in the properties of the time correlations near the thermodynamic limit. From this point of view it is enough to consider the behavior of $\overline{\Delta_n{}^p(t)}$ first when the time increases indefinitely for an arbitrary n, and then when n increases, the time remaining fixed. In this section, we shall briefly list the results.

3.1. Long-Time Behavior

The only important contributions arise from A_2 and A_2'. Taking only the dominant part, we get

$$\overline{\Delta_n{}^p(t)} \sim A_2 + A_2' = 2A_2$$
$$= \frac{1}{\rho^p}\int_0^\infty d\omega' \int_0^\infty dx[\exp(-\omega' - x)](\omega' - x)^p \frac{x^{n-1}}{(n-1)!}\frac{\omega'^{n-1}}{(n-1)!}$$

For $p = 1$, we recover $\overline{\Delta_n(t)} = 0$, i.e., $\langle R_n(t)\rangle \sim \langle R_n(0)\rangle = n/\rho$, since the gas is invariant with respect to time translation. The nth particle oscillates around its position with a width given by

$$\overline{\Delta_n{}^2(t)} = 2n/\rho^2 \tag{12}$$

and then the self-diffusion coefficient D_n is zero; as a supplementary result, we get the factorization property[5]

$$\langle R_n(t)R_n(0)\rangle \underset{t\to\infty}{\sim} \langle R_n(t)\rangle\langle R_n(0)\rangle$$

and more generally

$$\langle \exp[ikR_n(t)]\exp[-ikR_n(0)]\rangle \underset{t\to\infty}{\sim} \langle\exp[ikR_n(t)]\rangle\langle\exp[-ikR_n(0)]\rangle \tag{13}$$

For $p > 2$, all the calculations are tractable but it seems to be more interesting to study directly the distribution law $p_n(Z)$ of the displacement $Z = \rho\,\Delta_n(t)$ around its *initial* position; we get

$$p_n(Z) = (\exp -|Z|)\int_0^\infty d\omega'[\exp(-2\omega')]\frac{\omega'^{n-1}}{(n-1)!}\frac{(\omega' + |Z|)^{n-1}}{(n-1)!} \tag{14a}$$

which is an even function of Z because of the time reversal symmetry. Notice that $|Z|/\rho$ may become larger than the mean distance $\langle R_n(0)\rangle = n/\rho$ (for example, $Z < -n$), since there is a nonzero probability that $R_n(0)$ takes very large, positive values. The function p_n is plotted in Fig. 3 for $n = 2, 8$. When $n \to \infty$, for finite Z, $p_n(Z)$ is a small constant, $-1/2(\pi n)^{1/2}$; for $|Z| \sim n$ it decreases exponentially to zero.

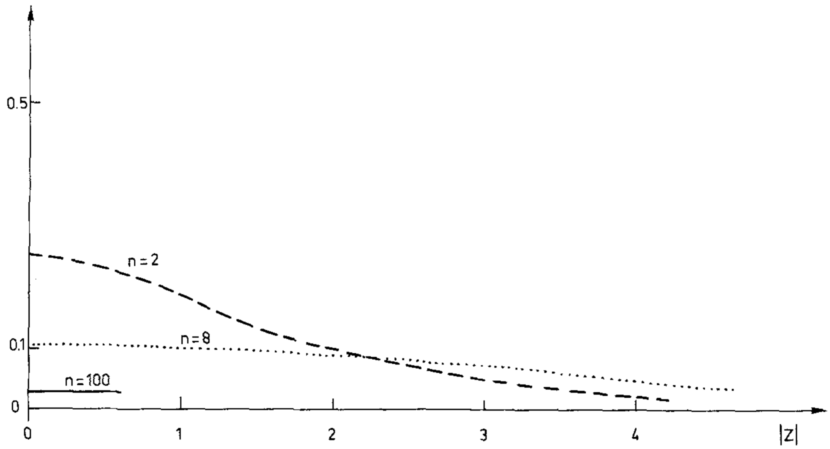

Fig. 3. Plot of $p_n(Z)$ vs. $|Z|$ for $n = 2$(dashed curve) and $n = 8$ (dotted line). We have indicated the beginning of $p_n(|Z|)$ when $n = 100$ (solid line); the function is nearly a constant for $|Z| < 5$.

The behavior of the displacement $Y = \rho[R_n(t) - (n/\rho)]$ around the *average* position is quite different; the distribution law $q_n(Y)$ reads

$$q_n(Y) = \epsilon(Y + n)\frac{(Y + n)^{n-1}}{(n - 1)!}e^{-(Y+n)} \tag{14b}$$

and $\epsilon(x)$ is again the Heaviside step function, which takes into account the fact that a particle cannot go behind the mirror. This distribution law $q_n(Y)$ is, of course, the same as the distribution law of the static fluctuations (i.e., the fluctuations at a given time with the equilibrium ensemble) of the position of the nth particle around its average position. When $n > 2$, $q_n(Y)$ varies slowly near the reflecting wall; for large n, $q_n(Y)$ is maximum around $Y = 0$, with a width of the order of $\sqrt{n}$ and a value which decreases like $1/(2\pi n)^{1/2}$.

We can now investigate the higher order terms. For rather large n ($n \gg 1$ but $n \ll N$), A_1 is quite negligible and so is A_1'. All the largest contributions at every order in t^{-1} arise from terms A_2, A_2'. From expressions (A.9) for A_2 and A_2' and for $p = 2$ we get

$$\begin{aligned} A_2 &= (n/\rho^2) + (0/\rho^3 t) + O(t^{-2}) \\ A_2' &= (n/\rho^2) - [4n(n + 1)/\rho^3 t] + O(t^{-2}) \end{aligned}$$

whence from (3b)

$$\langle V_n(t)V_n(0)\rangle \underset{t\to\infty}{\sim} -\frac{4n(n + 1)}{\rho^3 t^3} + O(t^{-4}) \tag{15}$$

Because of their complexity we have not calculated the higher order terms in the long-time expansion of $\langle V_n(0)V_n(t)\rangle$ but presumably they are of order $n^{k+1}/\rho^{k+2}t^k$ since no cancellation seems to occur for $k > 1$. Then, the expansion of the velocity autocorrelation function $\langle V_n(t)V_n(0)\rangle$ has a general term of order $(n/t)^{k+2}$; a characteristic "cutoff" time t^* appears, which is of the order of $2n/\rho$; it is the time necessary for the mirror particle to come in the vicinity of the studied particle and for large n, the tail of the velocity correlation function keeps the same t^{-3} behavior as for the infinite system, except that the coefficient in front of t^{-3} is changed and grows larger and larger when the particle goes farther and farther from the mirror.

Notice that for the first term of the expansion (of order t^{-1}) A_2 gives no contribution at all and that the correction arises because of the mirror term A_2'. It is possible that the predominance of the A_2' term survives for higher terms in the large-t expansion, but we have not been able to prove it.

3.2. Large-n Behavior

For finite times (or rather $\rho t \ll n$), the only contributing terms, A_1 and A_2, are given by Eqs. (B.3) and (B.4), which are the same as the terms giving the mean square displacement for a hard point on an infinite line (see Appendix B).

3.3. Finite-n Behavior

In order to illustrate the difference between $\langle [R_n(t) - R_n(0)]^2\rangle$ for a semiinfinite and for an infinite line, we have studied the cases $n = 1$ and $n = 8$. For $n = 1$, formulas (A.3) and (A.5) become

$$\begin{aligned}
A_1 &= t^p(\rho t)\int_{-\infty}^{+\infty} v_1{}^p\, dv_1\, h_0(v_1)\\
&\quad\times \int_{v_1}^{\infty} d\omega\, \epsilon(\omega)\exp\{-\rho t[(2\omega - v_1) - \Phi(2\omega - v_1) + \Phi(v_1)]\}\\
A_1' &= (-1)^p t^p(\rho t)\int_{-\infty}^{0} dv_1\, h_0(v_1)\\
&\quad\times \int_{v_1}^{0} d\omega\, \epsilon(-\omega)(2\omega - v_1)^p \exp\{\rho t v_1 - \Phi(2\omega - v_1) + \Phi(v_1)\}\\
A_2 &= t^p(\rho t)^2\int_0^{\infty} d\omega' \int_0^{\infty} (\omega - x)^p\, dx\\
&\quad\times [\tfrac{1}{2} + \mathrm{Erf}(\omega' - x)][1 - \mathrm{Erf}(\omega' + x) - \mathrm{Erf}(\omega' - x)]\\
&\quad\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\}\\
A_2' &= t^p(\rho t)^2\int_0^{\infty} d\omega' \int_0^{\infty} (\omega' - x)^p\, dx\\
&\quad\times [\tfrac{1}{2} - \mathrm{Erf}(\omega' + x)][1 - \mathrm{Erf}(\omega' + x) - \mathrm{Erf}(\omega' - x)]\\
&\quad\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\}
\end{aligned}$$

After some manipulations we get for $n = 1$

$$
\begin{aligned}
A_1 &+ A_1' + A_2 + A_2' \\
&= \rho t \int_0^\infty d\omega\, (t\omega)^p[1 + (-1)^p] \exp\{-\rho t\Phi(\omega)\} \int_\omega^\infty dy \exp\{-\rho t y + \rho t \Phi(y)\} \\
&\quad \times \{h_0(\omega) + h_0(y) + \rho t[1 - 2\,\mathrm{Erf}\, y + \mathrm{Erf}^2 y - \mathrm{Erf}^2 \omega]\} \qquad (16a)
\end{aligned}
$$

and for $n > 1$, we get the general formula

$$
\begin{aligned}
A_1 &+ A_1' + A_2 + A_2' \\
&= (\rho t)^n \int_0^\infty d\omega \{\exp[-\rho t \Phi(\omega)]\}(t\omega)^p[1 + (-1)^p] \\
&\quad \times \int_\omega^\infty dy \exp\{-\rho t y + \rho t \Phi(y)\} \\
&\quad \times \left\{ \sum_{l=0}^{n-1} \frac{(\rho t)^l}{l!\, l!\, (n-1-l)!} \left[\frac{\omega + y}{2} - \Phi(y) + \Phi(\omega)\right]^l \right. \\
&\quad \times \left[\frac{y - \omega}{2} - \Phi(y) + \Phi(\omega)\right]^l [\Phi(y) - \Phi(\omega)]^{n-1-l} \\
&\quad \times [h_0(y) + h_0(\omega) + \rho t(1 - 2\,\mathrm{Erf}\, y + \mathrm{Erf}^2 y - \mathrm{Erf}^2 \omega)] \\
&\quad + \sum_{l=0}^{n-2} \frac{(\rho t)^l}{l!\, l!\, (n-2-l)!} \left[\frac{\omega + y}{2} - \Phi(y) + \Phi(\omega)\right]^l \\
&\quad \times \left[\frac{y - \omega}{2} - \Phi(y) + \Phi(\omega)\right]^l [\Phi(y) - \Phi(\omega)]^{n-2-l} \\
&\quad \times \left[\mathrm{Erf}^2 y - \mathrm{Erf}^2 \omega + \frac{2\rho t}{l+1}\left(\frac{y}{2} - \Phi(y) + \Phi(\omega)\right) \right. \\
&\quad \left.\left. \times (\mathrm{Erf}\, y - \mathrm{Erf}^2 y + \mathrm{Erf}^2 \omega) - \frac{\rho t}{l+1}\, \omega\, \mathrm{Erf}\, \omega \right] \right\} \qquad (16b)
\end{aligned}
$$

Functions (16a) and (16b) for $n = 1, 8$ are plotted on Fig. 4 for $p = 2$ (mean square displacement of the first and eighth particles) after computation by a double Gauss integration method. The corresponding average for an infinite line also has been represented and its linear ($\propto Dt$) asymptotic behavior is quite clear. The curve for $n = 1$ departs very quickly from the curve $n = \infty$ and then tends slowly to its limit value of 2. For $n = 8$, the departure from the curve $n = 8$ begins at $\rho t \simeq 5$, and then it goes very slowly to its limit value 16 (for $\rho t = 40$, it has not yet reached the value 14).

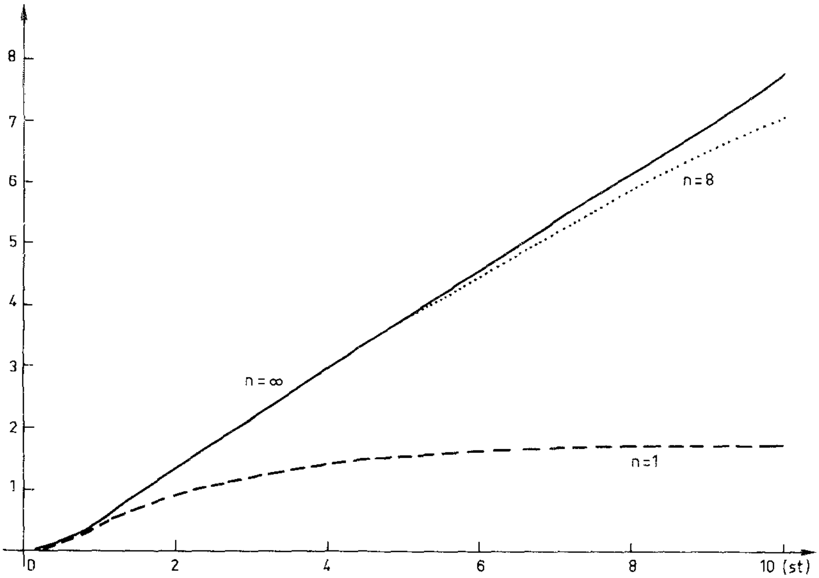

Fig. 4. Plot of $\langle[R_n(t) - R_n(0)]^2\rangle$ vs. time ρt for an infinite line (solid curve) and for a semiinfinite line when $n = 1$ (dashed curve) and $n = 8$ (dotted curve).

APPENDIX A. CALCULATION OF A_1, A_1', A_2, A_2'

We shall detail the calculation of the "direct" term A_1 only and give some indications for A_1', A_2, and A_2'.

A.1. Calculation of A_1 and A_1'

We start from (11a) and use for the Kronecker symbols the representation of Ref. 3. We have

$$\begin{aligned}
\delta_{\sigma_i(t),\sigma_i(0)} &= \int_0^{2\pi} \frac{d\theta}{2\pi} \exp\{i\theta[\sigma_i(t) - \sigma_i(0)]\} \\
&= \int_0^{2\pi} \frac{d\theta}{2\pi} \exp\{i\theta[\epsilon(r_i + v_i t) - \epsilon(r_i)]\} \\
&\quad \times \prod_{l \neq i} \exp\{-i\theta[\epsilon(r_i - r_l) + \epsilon(r_i + r_l)]\} \\
&\quad \times \exp\{i\theta[\epsilon(r_i - r_l + v_i t - v_l t) + \epsilon(r_i + r_l + v_i t + v_l t)]\}
\end{aligned}$$

and

$$\delta_{\sigma_i(0),N+n-1} = \int_0^{2\pi} \frac{d\varphi}{2\pi} \exp[i\varphi\epsilon(r_i)] \exp[-i\varphi(N + n - 1)] \times \prod_{l \neq i} \exp\{i\varphi[\epsilon(r_i - r_l) + \epsilon(r_i + r_l)]\}$$

A first integration gives for $l \geqslant 2$

$$\begin{aligned}\int_{-\infty}^{\infty} & dv_l\, h_0(v_l) \exp\{i\theta[\epsilon(r_i - r_l + v_i t - v_l t) + \epsilon(r_i + r_l + v_i t + v_l t)]\} \\ &= e^{i\theta}\left\{1 - [(1 - \cos\theta)\operatorname{sg}\omega - i\sin\theta]\left[\operatorname{Erf}\left(\omega + \frac{r_l}{t}\right) + \operatorname{Erf}\left(\omega - \frac{r_l}{t}\right)\right]\right\} \\ &= e^{i\theta}F(\omega, \theta, r_l/t) \qquad \text{(A.1)}\end{aligned}$$

which defines the function F. We have set

$$\omega = v_i + r_i/t \qquad \text{(A.2)}$$

and sg x is the sign function (sg $x = x/|x|$). The integration over r_l is straightforward. We now perform the integration over φ; doing so, we select the term as $e^{i(n-1)\varphi}$. For $n \ll N$, we get

$$\begin{aligned}A_1 = t^p \frac{(\rho t)^n}{(n-1)!} & \int_{-\infty}^{+\infty} dv_1\, v_1{}^p h_0(v_1) \int_{v_1}^{\infty} d\omega \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta\epsilon(\omega)} e^{-in\theta} \\ & \times \left\{\frac{r_1}{t} - [(1 - \cos\theta)\operatorname{sg}\omega - i\sin\theta]\Delta\left(\omega, \frac{r_1}{t}\right)\right\}^{n-1} \\ & \times \exp\left\{-\rho t\left(\frac{r_1}{t} - [(1 - \cos\theta)\operatorname{sg}\omega - i\sin\theta]\left[\Delta\left(\omega, \frac{r_1}{t}\right) - \omega\right]\right\}\end{aligned}$$

where $\Delta(\omega, x) = \Phi(\omega + x) - \Phi(\omega - x)$.

Now, when $\omega < 0$, the variable θ appears through the combination $e^{-i\theta}$ only and the integration for $0 \leqslant \theta \leqslant 2\pi$ gives zero. When $\omega > 0$, both combinations $e^{-i\theta}$ and $e^{i\theta}$ appear and the integration over θ selects the term as $e^{i(n-1)\theta}$ of the last two products in the integrand; this simply means that the mirror particle has not yet crossed the wall. The final result is

$$\begin{aligned}A_1 = t^p \frac{(\rho t)^n}{(n-1)!} & \int_{-\infty}^{+\infty} dv_1\, v_1{}^p h_0(v_1) \int_{v_1}^{\infty} d\omega\, \epsilon(\omega) \\ & \times \exp\left\{-\rho t\left[\frac{r_1}{t} + \omega - \Delta\left(\omega, \frac{r_1}{t}\right)\right]\right\} \\ & \times \sum_{l=0}^{n-1} \frac{(n-1)!\,(\rho t)^l}{l!\,l!\,(n-1-l)!}\left[\frac{r_1}{t} - \Delta\left(\omega, \frac{r_1}{t}\right)\right]^l\end{aligned}$$

$$\times \left[\omega - \Delta\left(\omega, \frac{r_1}{t}\right)\right]^l \left[\Delta\left(\omega, \frac{r_1}{t}\right)\right]^{n-1-l} \tag{A.3a}$$

where $r_1/t = \omega - v_1$.

Coming now to the mirror term A_1', it can be seen that the θ-integration can be restricted to $\omega < 0$ (the mirror particle has crossed the wall) and one obtains

$$\begin{aligned} A_1' = {} & (-1)^p t^p \frac{(\rho t)^n}{(n-1)!} \int_{-\infty}^0 dv_1\, h_0(v_1) \int_{v_1}^0 \epsilon(-\omega)\, d\omega \\ & \times \left(\omega + \frac{r_1}{t}\right)^p \exp\left\{\rho t v_1 - \rho t \Delta\left(\omega, \frac{r_1}{t}\right)\right\} \\ & \times \sum_{l=0}^{n-1} (-1)^{n-1-l} \frac{(n-1)!\,(\rho t)^l}{l!\, l!\, (n-1-l)!} \left[\frac{r_1}{t} + \Delta\left(\omega, \frac{r_1}{t}\right)\right]^l \\ & \times \left[|\omega| + \Delta\left(\omega, \frac{r_1}{t}\right)\right]^l \left[\Delta\left(\omega, \frac{r_1}{t}\right)\right]^{n-1} \end{aligned} \tag{A.3b}$$

Expressions (A.3a) and (A.3b) are complicated even for $n = 1$ and we need the help of a computer to get numerical results. However, we can achieve the calculations in two limiting cases, which are actually the ones of interest.

(*a*) *Long-Time Behavior for Arbitrary n.* Most of the integrand is concentrated near $v_1 = 0$, $\omega = 0$ with a spread of the order of t^{-1}. It is then easy to verify that $\Delta(\omega, r_1/t)$ behaves like t^{-2}, then that A_1' behaves like t^{-2}, and A_1 like t^{-1}; the dominant contribution arises from the term $l = n - 1$ when neglecting $\Delta(\omega, r_1/t)$.

For $p = 2$ and long times, the contribution to $\overline{\Delta_n^2(t)}$ of $A_1 + A_1'$ is then of order t^{-1} and reads

$$A_1 + A_1' \underset{t\to\infty}{\sim} \frac{2h_0(0)}{\rho^3 t} \frac{1}{[(n-1)!]^2} \int_0^\infty dv_1\, v_1^2 e^{-v_1} \int_0^\infty d\omega\, e^{-2\omega} \omega^{n-1} (\omega + v_1)^{n-1}$$

The integrals are elementary but become very tedious for large n. In this latter case, a rough majoration gives

$$A_1 + A_1' \leqslant \frac{C}{\rho^3 t} \frac{n^2}{2^n}$$

where C is a constant; this contribution will become negligible in the evaluation of the asymptotic behavior of the velocity correlation function, as we shall see in the next section.

(*b*) *Finite Time and Large n.* When t is finite ($\rho t \sim 1$) and the particle is far on the line, we expect to recover the same behavior as for a double infinite line, since the particles coming from behind the mirror have not yet perturbed the region surrounding the particle of rank n. We can see this as follows.

When n is large, every term in the summation $\sum_{l=0}^{n-1}$ has the same importance but, because of the presence of the $h_0(v_1)$ factor, it gives a nonnegligible contribution only in a region of the (ω, v_1) plane where v_1 is finite and ω (or $x = r_1/t$) is large. In this region, $\Delta(\omega, r_1/t) = x + \frac{1}{2}v_1 - \Phi(v_1) +$ terms which decrease like $h_0(x)$ at large x; whence

$$A_1 \simeq t^p \int_{-\infty}^{+\infty} dv_1\, v_1{}^p h_0(v_1) \exp\left\{-\rho t\left[\frac{v_1}{2} + \Phi(v_1)\right]\right\} \int_{v_1}^{\infty} d\omega(\rho t) \exp(-\rho t x)$$
$$\times \sum_{l=0}^{n-1} \frac{[\Phi^2(v_1) - v_1{}^2/4]^l}{l!\, l!} (\rho t)^{2l} \frac{\{\rho t[x + \frac{1}{2}v_1 - \Phi(v_1)]\}^{n-1-l}}{(n-1-l)!}$$

or

$$A_1 = t^p \int_{-\infty}^{+\infty} dv_1\, h_0(v_1) v_1{}^p \{\exp[-\rho t \mu(v_1)]\} I_0(\rho t[\mu^2(v_1) - v_1{}^2]^{1/2}) \qquad \text{(A.4)}$$

where $I_0(x)$ is the modified Bessel function, $\mu(x) = 2\Phi(x)$ and is the collision frequency (we have used here the notation of Ref. 3). As briefly sketched in Appendix B, we get the same result as for a hard-point gas on a full infinite line. The remaining problem is the estimation of the error in replacing A_1 by its limiting expression (A.4).

Similar arguments hold for A_1', but since ω is limited by the condition $v_1 \leqslant \omega \leqslant 0$, A_1' is exponentially decreasing with n large, i.e., the mirror contribution does not affect the short-time behavior, as expected.

A.2. Calculation of A_2 and A_2'

The method explained above is still valid. We only give the results (for $n \ll N$)

$$A_2 = t^p \frac{(\rho t)^n}{(n-2)!} \int_0^\infty d\omega' \int_0^\infty dx\, (\omega' - x)^p$$
$$\times [\operatorname{Erf} \omega' - \operatorname{Erf}(\omega' - x)][1 - \operatorname{Erf}(\omega' + x) - \operatorname{Erf}(\omega' - x)]$$
$$\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\} \sum_{l=0}^{n-2} \frac{(n-2)!\,(\rho t)^{l+1}}{l!\,(l+1)!\,(n-2-l)!}$$
$$\times [x - \Delta(\omega', x)]^l [\omega' - \Delta(\omega', x)]^{l+1} [\Delta(\omega', x)]^{n-2-l}$$
$$+ t^p \frac{(\rho t)^n}{(n-2)!} \int_0^\infty d\omega' \int_0^\infty dx\, (\omega' - x)^p$$
$$\times [\operatorname{Erf} \omega' - \operatorname{Erf}(\omega' - x)][\operatorname{Erf}(\omega' + x) + \operatorname{Erf}(\omega' - x)]$$

$$
\begin{aligned}
&\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\} \sum_{l=0}^{n-2} \frac{(n-2)!\,(\rho t)^l}{l!\,l!\,(n-2-l)!} \\
&\times [x - \Delta(\omega', x)]^l[\omega' - \Delta(\omega', x)]^l[\Delta(\omega', x)]^{n-2-l} \\
&+ t^p \frac{(\rho t)^{n+1}}{(n-1)!} \int_0^\infty d\omega' \int_0^\infty dx\,(\omega' - x)^p \\
&\times [\tfrac{1}{2} + \mathrm{Erf}(\omega' - x)][1 - \mathrm{Erf}(\omega' + x) - \mathrm{Erf}(\omega' - x)] \\
&\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\} \sum_{l=0}^{n-1} \frac{(n-1)!\,(\rho t)^l}{l!\,l!\,(n-1-l)!} \\
&\times [x - \Delta(\omega', x)]^l[\omega' - \Delta(\omega', x)]^l[\Delta(\omega', x)]^{n-1-l} \\
&+ t^p \frac{(\rho t)^{n+1}}{(n-1)!} \int_0^\infty d\omega' \int_0^\infty dx\,(\omega' - x)^p \\
&\times [\tfrac{1}{2} + \mathrm{Erf}(\omega' - x)][\mathrm{Erf}(\omega' + x) + \mathrm{Erf}(\omega' - x)] \\
&\times \exp\{-\rho t[x + \omega' - \Delta(\omega', x)]\} \sum_{l=1}^{n-1} \frac{(n-1)!\,(\rho t)^{l-1}}{l!\,(n-1-l)!\,(l-1)!} \\
&\times [x - \Delta(\omega', x)]^l[\omega' - \Delta(\omega', x)]^{l-1}[\Delta(\omega', x)]^{n-1-l} \qquad \text{(A.5)}
\end{aligned}
$$

A very similar formula gives A_2', except that the factor $[\mathrm{Erf}\,\omega' - \mathrm{Erf}(\omega' - x)]$ which appears in the first and second integrands is replaced by $[\mathrm{Erf}(\omega' + x) - \mathrm{Erf}\,\omega']$, although the factor $[\frac{1}{2} + \mathrm{Erf}(\omega' - x)]$ which appears in the third and fourth integrands is replaced by $[\frac{1}{2} - \mathrm{Erf}(\omega' + x)]$. Again the exact formulas for A_2 and A_2' are complicated and we shall study only the two limiting cases of Section 3.

(*a*) *Long-Time Behavior for an Arbitrary n.* The integrand is concentrated around $\omega' = 0$, $x = 0$ and ω', x are of order t^{-1}, whence $\Delta(\omega', x) = O(t^{-2})$. Then the four contributions to A_2 (resp. A_2') are of order t^{-1}, t^{-2}, 1, and t^{-1}, respectively. We shall neglect $O(t^{-2})$ terms again. The dominant contribution in the first and fourth terms comes from the maximum value of l and $\Delta \sim 0$; the second term is negligible. As to the third term, a little more care is necessary, since we must keep the two largest contributions, i.e., (i) $l_{\text{maximum}} = n - 1$, with the second correction, (ii) $l = n - 2$ with $\Delta = 0$.

Collecting all these results, we get for A_2

$$
A_2 \sim \frac{h_0(0)}{\rho^{p+1}t} \int_0^\infty d\omega'\, e^{-\omega'} \int_0^\infty dx\, e^{-x}(\omega' - x)^p \frac{x^{n-1}\omega'^{n-1}}{(n-2)!\,(n-1)!} \qquad \text{(first term)}
$$

$$
+ \frac{h_0(0)}{\rho^{p+1}t} \int_0^\infty d\omega'\, e^{-\omega'} \int_0^\infty dx\, e^{-x}(\omega' - x)^p \frac{x^{n-1}\omega'^{n-1}}{(n-2)!\,(n-1)!}
$$

(fourth term)

$$\frac{1}{2}\frac{1}{\rho^p}\int_0^\infty d\omega' e^{-\omega'}\int_0^\infty dx\, e^{-x}(\omega'-x)^p \frac{x^{n-1}\omega'^{n-1}}{(n-1)!\,(n-1)!}$$

[dominant contribution (i) of the third term]

$$+\frac{h_0(0)}{\rho^{p+1}t}\int_0^\infty d\omega' e^{-\omega'}\int_0^\infty dx\, e^{-x}(\omega'-x)^p[\omega' x - x - (n-1)(\omega'+x)]$$

[rest of (i) of third term]

$$+\frac{1}{2}\frac{h_0(0)}{\rho^{p+1}t}\int_0^\infty d\omega'\, e^{-\omega'}\int_0^\infty dx\, e^{-x}(\omega'-x)^p \frac{x^{n-2}}{(n-2)!}\frac{\omega'^{n-2}}{(n-2)!}$$

[(ii) of third term] (A.6)

A very similar formula holds for A_2'. We do not write it here. The only difference appears in the fourth term of Eq. (A.6) [referred to as "rest of (i) of third term"], which must be replaced by

$$\frac{h_0(0)}{\rho^{p+1}t}\int_0^\infty d\omega'\, e^{-\omega'}\int_0^\infty dx\, e^{-x}(\omega'-x)^p[\omega' x - 2\omega' - x - (n-1)(\omega'+x)]$$
$$\times\frac{x^{n-1}}{(n-1)!}\frac{\omega'^{n-1}}{(n-1)!}$$

(*b*) *Finite Time and Large n.* The problem does not differ very much from that for A_1 and A_1'. Starting from Eqs. (A.5), we see that the dominant contribution to A_2 (resp. A_2') comes from a domain where ω' and x are both large but $\omega' - x$ remains finite. Then $\Delta(\omega', x) \simeq \frac{1}{2}(\omega' + x) - \Phi(\omega' - x)$. Setting now as new variables $v = \omega' - x$, $v' = \frac{1}{2}(\omega' + x) - \Phi(v)$, and integrating over v', we get the same expression as the result given for the infinite line in Eq. (B.4) in Appendix B.

Coming now to A_2', there is a big difference since the functions $\mathrm{Erf}(\omega'+x) - \mathrm{Erf}\,\omega'$ and $\frac{1}{2} - \mathrm{Erf}(\omega' + x)$ are replaced by $\pm(\mathrm{Erf}\,2v' - \frac{1}{2})$, which vanish as $h_0(2v')$ for large v'; the contribution of A_2' is then negligible, as expected.

APPENDIX B. THE VELOCITY AUTOCORRELATION FUNCTION FOR HARD POINTS ON AN INFINITE LINE

The system is considered as the limit of a gas of N points on a line of length L (for example $[-L/2, +L/2]$). Because of the translational invariance, the result does not depend on the initial rank of the particle. The mean square displacement can be rewritten, using averages for free points on an infinite line,

$$\langle[R_1(t) - R_1(0)]^2\rangle$$
$$= t^2\langle v_1^2\, \delta_{\sigma_1(t),\sigma_1(0)}\rangle + (N-1)t^2\left\langle\left[\frac{r_2 - r_1}{t} + v_2\right]^2 \delta_{\sigma_2(t),\sigma_1(0)}\right\rangle \quad \text{(B.1)}$$

with the statistical weight

$$\prod_{l=1}^{N} \frac{dr_l}{L} h_0(v_l)\, dv_l \qquad \text{and} \qquad -\frac{L}{2} \leqslant r_l \leqslant \frac{L}{2} \tag{B.2}$$

Using the integral representation of the Kronecker symbol, the first term is

$$\begin{aligned}
t\int_{-\infty}^{+\infty} & dv_1\, h_0(v_1)v_1^2 \int_0^{2\pi} \frac{d\theta}{2\pi} \prod_{l>1} \int_{-\infty}^{+\infty} dv_l\, h_0(v_l) \\
&\times \int_{-L/2}^{L/2} \frac{dr_l}{L} \exp\{i\theta[\epsilon(r_1 - r_l + v_1 t - v_l t) - \epsilon(r_1 - r_l)]\} \\
&\underset{\substack{N\to\infty \\ N/L=\rho,\ \text{finite}}}{\simeq} t^2 \int_{-\infty}^{+\infty} dv_1\, h_0(v_1)v_1^2 \\
&\qquad \times \int_0^{2\pi} \frac{d\theta}{2\pi} \exp\{it\rho \sin\theta v_1 - t\rho(1-\cos\theta)\mu(v_1)\} \\
&\qquad \text{(see Ref. 3)} \\
&= t^2 \int_{-\infty}^{+\infty} dv_1\, h_0(v_1)v_1^2 I_0(\rho t[\mu^2(v_1) - v_1^2]^{1/2}) \exp[-\rho t\mu(v_1)]
\end{aligned} \tag{B.3}$$

where $\mu(v_1)$ is the collision frequency

$$\left[=2\Phi(v_1) = 2\int_0^{v_1} \operatorname{Erf} x\, dx = \int_{-\infty}^{+\infty} |v_1 - x| h_0(x)\, dx\right]$$

We recover the limit expression (A.6) for large n and for A_1. The second term reads

$$\begin{aligned}
t^2(N-1) & \int_{-\infty}^{+\infty} dv_1\, h_0(v_1) \int_{-\infty}^{+\infty} dv_2\, h_0(v_2) \\
&\times \int_{-L/2}^{+L/2} \frac{dr_1}{L} \int_{-L/2}^{+L/2} \frac{dr_2}{L} \left(\frac{r_2 - r_1}{t} + v_2\right)^2 \\
&\times \int_0^{2\pi} \frac{d\theta}{2\pi} \exp\{i\theta\epsilon[r_2 - r_1 + v_2 t - v_1 t] - i\theta\epsilon(r_1 - r_2)\} \\
&\times \prod_{l\geq 3} \int_{-\infty}^{+\infty} dv_l\, h_0(v_l) \int_{-L/2}^{L/2} \frac{dr_l}{L} \\
&\times \exp\{i\theta[\epsilon(r_2 - r_l + v_2 t - v_l t) - \epsilon(r_1 - r_l)]\} \\
&\underset{\substack{N\to\infty \\ N/L=\rho}}{\sim} t^2 \int_{-\infty}^{+\infty} dv_1\, h_0(v_1) \int_{-\infty}^{+\infty} dv_2\, h_0(v_2) \\
&\qquad \times \int_{-\infty}^{+\infty} d\,\frac{(r_2 - r_1)}{t} \int_0^{2\pi} \frac{d\theta}{2\pi} (\rho t) \left(\frac{r_2 - r_1}{t} + v_2\right)^2
\end{aligned}$$

$$\times \exp\{i\theta[\epsilon(r_2 - r_1 + v_2 t - v_1 t) - \epsilon(r_1 - r_2)]\}$$
$$\times \exp\left\{it\rho \sin\theta\left(\frac{r_2 - r_1}{t} + v_2\right) - t\rho(1 - \cos\theta)\mu\left(\frac{r_2 - r_1}{t} + v_2\right)\right\}$$

Setting $[(r_2 - r_1)/t] + v_2 = \omega$ and integrating over v_1 and $(r_2 - r_1)/t$. we get

$$t^2 \int_{-\infty}^{+\infty} \omega^2 \, d\omega \int_0^{2\pi} \rho t \frac{d\theta}{2\pi} \exp\{it\rho \sin\theta\omega - t\rho(1 - \cos\theta)\mu(\omega)\}$$
$$\times \left[\frac{1 + e^{i\theta}}{2} - (1 - e^{i\theta}) \operatorname{Erf}\omega\right]\left[\frac{1 + e^{-i\theta}}{2} + (1 - e^{-i\theta}) \operatorname{Erf}\omega\right]$$
$$= t^2 \int_{-\infty}^{+\infty} \omega^2 \, d\omega \int_0^{2\pi} \rho t \frac{d\theta}{2\pi} \exp\{it\rho \sin\theta\omega - t\rho(1 - \cos\theta)\mu(\omega)\}$$
$$\times \left[\frac{1 + \cos\theta}{2} + 2i \sin\theta \operatorname{Erf}\omega - 2(1 - \cos\theta) \operatorname{Erf}^2\omega\right]$$
$$= t^2 \int_{-\infty}^{+\infty} \omega^2 \, d\omega \Big\{ e^{-\rho\mu t}[\rho t I_0(\rho t[\mu^2(\omega) - \omega^2]^{1/2})$$
$$- \frac{2\rho t\omega}{[\mu^2(\omega) - \omega^2]^{1/2}} I_0'(\rho t[\mu^2(\omega) - \omega^2]^{1/2}) \operatorname{Erf}\omega]$$
$$- 2(\tfrac{1}{4} + \operatorname{Erf}^2\omega) e^{-\rho\mu t}\rho t[I_0(\rho t[\mu^2(\omega) - \omega^2]^{1/2})$$
$$- \frac{\mu}{[\mu^2(\omega) - \omega^2]^{1/2}} I_0'(\rho t[\mu^2(\omega) - \omega^2]^{1/2})\Big\} \tag{B.4}$$

which is exactly the limiting expression (A.11) for large n and for A_2. Moreover, we can say that for finite time and for any smooth function F

$$\lim_{n\to\infty} \langle F[R_n(t) - R_n(0)]\rangle_{\text{half-infinite line}} = \langle F[R_i(t) - R_i(0)]\rangle_{\text{infinite line}}$$

the correction being of order $n^{-1/2}$ at most since $R_n(t) - R_n(0)$ remains finite for small t.

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