Journal of Statistical Physics, Vol. 7, No. 4, 1973

One-Dimensional Time-Dependent Distributions

David G. Levitt[1]

Received August 7, 1972

A new derivation of two important one-dimensional time-dependent distributions for an infinite system of hard rods is presented. This derivation is simpler than previous derivations and it provides a direct physical interpretation of the individual terms in the final expressions. A new, more unusual distribution is also presented and discussed. Finally, an exact expression for the diffusion of a Brownian particle is obtained and compared with the exact expression for the self-diffusion coefficient.

KEY WORDS: One-dimensional; diffusion; conditional self-distribution; hard spheres; Brownian motion.

Jepson[1] has derived several interesting exact expressions describing the time-dependent behavior of a one-dimensional system of hard rods. One of his most interesting results is a relatively simple expression for $p(y, t)$, the probability of finding a rod at y at time t if it was at the origin at $t = 0$. At long time $p(y, t)$ becomes Gaussian with a diffusion coefficient equal to

$$D = (1/\rho) \int_0^\infty v g(v)\, dv \tag{1}$$

where ρ is the density and $g(v)$ is the initial velocity distribution. Lebowitz and Percus[2] elaborated on these results in a later paper. The basis of their discussion was the conditional self-distribution $f_s(y, v, t/v')$ which is the

[1] Department of Physiology, University of Minnesota, Medical School, Minneapolis, Minnesota.

probability of finding a rod at y with velocity v at time t that was at the origin with velocity v' at $t = 0$. These exact solutions are not only useful as tests of the validity of the approximate methods that have been developed for three dimensions, but they also have an intrinsic appeal of their own. In this paper a new derivation of these distributions will be presented. This derivation is not only much simpler, but since it is based almost entirely on physical arguments, the significance of the various terms in the final expressions are self-evident, whereas in the previous, more mathematical derivations the physical significance of the individual terms was obscured.

An infinite one-dimensional system of hard points will be considered. The results derived in this paper can be carried over directly to a system of rods with a finite length a simply by substituting for the point density ρ the expression $\rho/(1 - \rho a)$. For this system the rods simply exchange their velocities upon colliding so that a trajectory with a particular velocity is not affected by the collision. The only effect of the collision is to change the label of the rod on the trajectory. Thus the system can be described (as was done by Jepsen) by drawing the lines of the trajectories and labeling them by the number of the rod that is on them at $t = 0$ (Fig. 1). The slope of the line is determined by the velocity of the trajectory.

An ensemble of systems will be considered with the rods initially distributed with a probability distribution $\rho\, dy$ with each rod having a velocity distribution $g(v)\, dv$. This spatial and velocity distribution will persist for all times as can be easily seen by considering any interval dy at time t and tracing the trajectories that pass through it back to $t = 0$. As is shown in Fig. 1, a rod (labeled "0") is assumed to be at the origin at $t = 0$. Also shown in

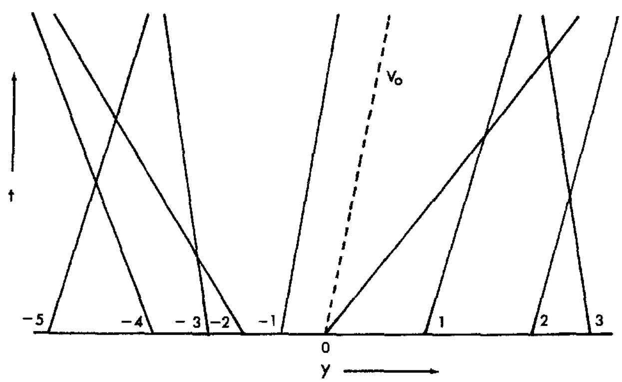

Fig. 1. Diagram showing how the "trajectories" simply pass through one another when the one-dimensional rods collide. The dashed line is a "test" trajectory with a velocity v_0. It is not related to the actual velocity of the rod initially at the origin.

Fig. 1 is a dashed line which represents a "test" trajectory with a volocity v_0 which will be used in the following derivation. Since the rods are impenetrable, everytime a trajectory crosses the "test" trajectory from the right the particle number of the rods immediately to the left and immediately to the right of the "test" trajectory will be raised by one (assuming the rods are originally numbered consecutively and increasing to the right). Similarly, if a trajectory crosses the "test" trajectory from the left the number of the nearest rods on each side of the test trajectory will be lowered by one. Thus, as was first pointed out by Jepsen, the number of the rod immediately to the right (or left) of the trajectory at time t will be changed by an (integer) amount α (positive, negative, or zero) if the test trajectory is crossed α more times from the right than from the left in time t. Then, define $A_\alpha(v_0, t)$ as equal to the probability that the number of the rod immediately adjacent to the test trajectory with a velocity v_0 has been changed by an amount α in time t. If $P_R(v_0, n, t)$ and $P_L(v_0, n, t)$ are the probabilities that the test trajectory is crossed n times from the right or left, respectively, in time t, then

$$A_\alpha(v_0, t) = \sum_{n=0}^{\infty} P_R(v_0, n, t)\, P_L(v_0, n - \alpha, t) \tag{2}$$

These probabilities are ensemble averages over the initial conditions. To obtain $P_R(v_0, n, t)$ consider the probability that the test trajectory is crossed from the right during the time interval between t and $t + dt$ by a trajectory of velocity v. If a trajectory of velocity v crosses the test trajectory in this time interval it must have originated initially from a position between x and $x + dx$, where $x = (v_0 - v)\, t$ and $dx = (v_0 - v)\, dt$. Since the distribution of the rod positions is uniform, the probability of finding a rod with velocity v in the region dx is $\rho g(v)\, dx\, dv$. Finally, the probability that a trajectory of any velocity crosses the test trajectory in this time interval dt is

$$\rho\, dt \int_{-\infty}^{v_0} (v_0 - v)\, g(v)\, dv \tag{3}$$

where v must be less than v_0 if the trajectory crosses from the right. Equation (3) can be written in the form $B_R\, dt$, where

$$B_R = \rho \int_{-\infty}^{v_0} (v_0 - v)\, g(v)\, dv$$

Since B_R is independent of time, the number of crossings follows a Poisson distribution and

$$P_R(v_0, n, t) = e^{-B_R t}\, (B_R t)^n / n! \tag{4}$$

Similarly,

$$P_L(v_0, n, t) = e^{-B_L t} (B_L t)^n / n! \tag{5}$$

where

$$B_L = \rho \int_{v_0}^{\infty} (v - v_0)\, g(v)\, dv$$

Substituting Eqs. (4) and (5) into Eq. (2), we have

$$\begin{aligned} A_\alpha(v_0, t) &= \sum_{n=0}^{\infty} e^{-B_R t} \frac{(B_R t)^n}{n!} e^{-B_L t} \frac{(B_L t)^{n-\alpha}}{(n-\alpha)!} \\ &= e^{-(B_R + B_L)t} (B_L t)^{-\alpha} [(B_L B_R)^{1/2} t]^\alpha \sum_{n=0}^{\infty} \frac{[(B_L B_R)^{1/2} t]^{2n-\alpha}}{n!\,(n-\alpha)!} \\ &= e^{-(B_R + B_L)t} \left(\frac{B_R}{B_L}\right)^{\alpha/2} I_{-\alpha}[2(B_L B_R)^{1/2} t] \end{aligned} \tag{6}$$

where $I_{-\alpha}$ is the imaginary Bessel function of order $-\alpha$ and for integer α, $I_\alpha(x) = I_{-\alpha}(x)$. Although A_α is equivalent to the function $J^{(\alpha)}$ in Jepsen's paper and $A_{-\alpha}$ in Percus and Lebowitz's paper, the physical significance of this expression has not been pointed out previously.

The following argument allows one to write down the distribution $f_s(y, v, t/v')$ directly in terms of the above A's. Suppose that at time t there have been no net crossings of the test trajectory v_0. That means that the particle initially at the origin will be the nearest neighbor on the left at time t if it started initially to the left of v_0 ($v' < v_0$). Now consider an interval Δy about v_0 at a time Δt later, where Δt is small enough to allow one to assume that if a rod is in Δy it has not suffered a collision between t and $t + \Delta t$. Now the knowledge that there have been no net crossings of v_0 at time t restricts the trajectories that can cross v_0 for $\tau < t$. However, if Δy is made small enough ($\Delta y \ll \bar{v}\, \Delta t$), the probability that any of the trajectories which cross v_0 for $\tau < t$ enter Δy can be made arbitrarily small. Thus the spatial and velocity distributions in Δy at time $t + \Delta t$ are undisturbed by the knowledge that there have been no net crossings at time t and the probability of finding a particle in Δy is $\rho\, \Delta y$ and its velocity distribution is $g(v)\, dv$. This probability is based on the initial distribution, neglecting the fact that it is known that there was a trajectory at the origin. This single trajectory will be included later. Note also that the probability that there are no net crossings at time t (A_0) is not correlated with the trajectory that originates at the origin because this trajectory cannot cross the test trajectory. If the particle in Δy at time $t + \Delta t$ has a velocity greater than v_0 it must have been to the left of v_0 at time t (assuming the condition that $\Delta y \ll \bar{v}\, \Delta t$) and would have been the nearest left neighbor if Δt is small enough. Thus we have the result that the particle initially at the origin with velocity v' will be in the interval Δy about the point $y = v_0(t + \Delta t)$ at time $t + \Delta t$ if: (a) it initially started to the left ($v' < v_0$); (b) there are no net crossings at time t [with a probability $A_0(y/t, t)$]; (c) its velocity at time $t + \Delta t$ [which has a probability $g(v)\,dv$] is greater than v_0, and (*d*) there is a trajectory in Δy (with a probability $\rho\,\Delta y$). All of these events are uncorrelated. Taking the limit allowing $\Delta y \to 0$ and then $\Delta t \to 0$, one arrives at one of the terms which contribute to $f_s(y, v, t/v')$:

$$\rho\,dy\,g(v)\,dv\,u(y - v't)\,u(vt - y)\,A_0(y/t, t)$$

where u is the unit step function. One will also find this particle which was was at the origin at $t = 0$ in Δy for the additional three sets of conditions:

1. It started to the right of v_0; there are no net crossings, and it is now going to the left.
2. It started to the right; there has been one net crossing from the right (with probability A_1), and it is now going to the left.
3. It started to the left; there has been one net crossing from the left (with a probability A_{-1}), and it is now going to the right.

These conditions have neglected the fact that it was known that there was a trajectory at the origin. If this trajectory passes through Δy, then the particle on it will be the particle that started at the origin if there have been no set crossings at time t (because then the initial particle will be the nearest neighbor on the same side of v_0 that it started off on, which will be the same side that the initial trajectory is on). Thus, adding up these five terms, one gets the final expression for f_s:

$$\begin{aligned} f_s(y, v, t/v') = {} & \rho g(v)[u(y - v't)\,u(vt - y)\,A_0 + u(vt - y)\,u(y - vt)\,A_0 \\ & + u(v't - y)\,u(vt - y)\,A_1 + u(y - v't)\,u(y - vt)\,A_{-1}] \\ & + A_0\,\delta(y - v't)\,\delta(v - v') \end{aligned} \tag{7}$$

where δ is the Dirac δ-function and where the A's are given by Eq. (6) with $v_0 = y/t$. This expression is identical to the result of Lebowitz and Percus. One can go immediately from this expression to the distribution $p(y, t)$ simply by averaging over the distribution of the initial and final velocities. For the last term in Eq. (7) the probability that the initial trajectory is in dy at time t is equal to $g(y/t)\,dy/t$. Thus the expression for p becomes

$$p(y, t) = 2\rho G(1 - G)\,A_0 + \rho G^2 A_1 + \rho(1 - G)^2\,A_{-1} + (1/t)\,g(y/t)\,A_0 \tag{8}$$

where G is the probability that $v > v_0 = y/t$:

$$G(y/t) = \int_{y/t}^{\infty} g(v)\, dv \tag{9}$$

It can be easily shown that this result is identical to that of Jepsen.

Some other, more unusual, distributions can also be written down directly in terms of the A's. For example, suppose that instead of the "test" trajectory originating from a point where a rod is initially, it starts at a random position, i.e., between two neighboring rods. Now consider the short line segment that joins these two neighboring rods, and determine the distribution $s_2(y, t)\, dy$ that the point y lies on this line segment at time t. This distribution is obviously just $A_0(y/t, t)$ since if there have been no net crossings of the "test" trajectory at time t, then the point $y = v_0 t$ must lie between the two rods that were on opposite sides of the point $y = 0$ at $t = 0$. A_0 is the ensemble average of the function ∇_0, which is equal to one if y lies on this line segment at time t and zero otherwise for each of ensembles. Integrating ∇_0 over y yields the length of the line segment at time t for that ensemble. Thus, interchanging the order of the integration and the ensemble average, it is clear that the integral over y of A_0 yields the average length of this line segment at time t. It is easy to show that as $t \to 0$, A_0 approaches $\exp(-\rho \mid y \mid)$. This is the initial probability that there is no particle in the region $(-y < \omega < y)$ and therefore the probability of still being on the line segment, as expected. Integrating A_0 in this limit over y yields a value of $2/\rho$. In the limit as $t \to \infty$, A_0 approaches a Gaussian (as do all the A_j) whose integral over y is equal to $1/\rho$. This illustrates the classic paradox that when a random position is picked on a line with uniformly distributed points the average separation of the neighboring points is twice the average for the whole line. After a long time these neighbors forget their unique initial condition and now have the average separation $1/\rho$.

It is easy to extend this derivation to a line segment connecting n contiguous rods. If n is odd, one can avoid the problem of the peculiar initial length. For example, let the test trajectory originate from a rod and consider the line segment that connects the two rods which lie on either side of the central rod. The point $y = v_0 t$ will lie on this line segment if (a) there have been no net crossings at time t, or (b) there has been one net crossing from the left and the rod at the origin started off to the left of the test trajectory, or (c) there has been one net crossing from the right and the rod started off to the right. Since there is now nothing special about the initial distribution around the "test" trajectory, the integral over y of the sum of these three conditions is equal to $2/\rho$ at all times and the normalized distribution $s_3(y, t)$ is equal to

$$s_3(y, t) = (\rho/2)[A_0 + A_{-1}(1 - G) + A_1(G)] \tag{10}$$

This can be generalized to the line segment that connects the end points of a sequence that consists of n (odd) adjacent points:

$$s_n(y, t) = \frac{\rho}{n-1}\left[\sum_{j=-K}^{K} A_j + A_{-(K+1)}(1-G) + A_{(K+1)}G\right] \tag{11}$$

where $K = (n-3)/2$ and where $s_n(y, t)$ is the normalized probability that the point y lies on this line segment at time t, and at $t = 0$ the line segment is centered about $y = 0$. As $t \to \infty$ all the A_j become Gaussian with the same diffusion coefficient [Eq. (1)] so that s_n also becomes Gaussian with this diffusion coefficient. That is, after a long enough time, the line segment which is n particles long has exactly the same distribution about the origin as does a single particle. This is not unexpected since n particles which are initially adjacent must remain adjacent at all times and when the displacement becomes long with respect to the length of the line segment, any one of the particles on the line segment is representative of the position of the whole segment.

This observation may explain the computer (molecular dynamics) results of Bishop and Berne.[3] They had obtained the dynamics of 1000 particles interacting with a Lennard-Jones potential in a periodic one-dimensional system. They then attempted to study the behavior of a Brownian particle by observing the movement of a contiguous cluster of n particles (the mass of the "Brownian" particle was n times that of a single particle). Although the above results for hard spheres are not exactly applicable to these computer experiments, the general behavior should be the same. Thus one would expect that after a long enough time the diffusion of the cluster should be the same as the diffusion of a single particle. This would explain the observation of Bishop and Berne that the diffusion coefficient of the "Brownian" particle was mass independent.

An exact expression for the one-dimensional diffusion coefficient of a Brownian (B) particle is already available in the hard-sphere case. Green[4] has derived the friction coefficient ξ for a B particle in a (three-dimensional) gas of noninteracting hard spheres. For this gas Green's result becomes exact in the limit where $\gamma = m_B/m$ becomes large (where m_B and m are the masses of the Brownian and fluid particle, respectively). Since in a one-dimensional system of hard rods the trajectories simply pass through each other (Fig. 1), the fluid behaves exactly as if it were noninteracting. A deviation from the noninteracting assumption could occur only if the B particle collided with a fluid trajectory (which would then have its velocity changed or "bent") and then collided again with that "bent" trajectory at a later time. However, if γ is large, the "bent" trajectory will move away from the B particle with a relatively high velocity and the probability that the B particle will collide with it again will be negligible. Thus Green's result is exact for a one-dimensional B particle in the limit of large γ.

Modifying Green's derivation for the one-dimensional case, one finds an expression for the diffusion coefficient of the B particle:

$$D_B = kT/m_B\xi = kT/8\rho\bar{v}m \tag{12}$$

where $\bar{v} = \int_0^\infty vg(v)\,dv$. It can be seen that D_B is independent of the mass of the B particle (if γ is large enough). Comparing Eq. (12) with Eq. (1), it can be seen that if $g(v)$ is Maxwellian, the ratio of D_B to D (self-diffusion coefficient) is $\pi/4$. These results are consistent with the molecular dynamic results of Bishop and Berne[3] although, as was mentioned above, their results may also be explained by the fact that they did not study a real Brownian particle.

ACKNOWLEDGMENTS

I wish to thank Drs. T. A. Wilson and S. Prager for their helpful comments and discussions.

REFERENCES

1. D. W. Jepsen, *J. Math. Phys.* **6**:405 (1965).
2. J. L. Lebowitz and J. K. Percus, *Phys. Rev.* **155**:122 (1967); J. L. Lebowitz, J. K. Percus, and J. Sykes, *Phys. Rev.* **171**:224 (1968).
3. M. Bishop and B. J. Berne, *J. Chem. Phys.* **56**:2850 (1972).
4. M. S. Green, *J. Chem. Phys.* **19**:1036 (1951).