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The Exact Velocity Autocorrelation Function of a Model System

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The velocity autocorrelation function of a particle in a model system with realistic diffusion is calculated exactly and compared with the corresponding result in the one-dimensional case. The method employed yields the result of Lebowitz and Sykes in one dimension in a very simple manner.

KEY WORDS: Velocity autocorrelation function; Poisson process; internal degree of freedom.

In general the exact calculation of the velocity autocorrelation function, which is of interest in an analysis of nonequilibrium problems, is prohibitively difficult. The only known such calculations deal with one-dimensional systems studied, for example, in the papers by Jepsen[(1)] and Lebowitz and Percus.[(2)] Although these one-dimensional models admit exact calculation, they lack a certain measure of realism in contrast with actual physical situations in three dimensions. For example, although one finds an exact diffusive behavior, the physical interpretation of this diffusion is quite unlike that occurring in systems of physical interest. This is because in a one-dimensional world no particle can go around its neighbors; and yet this is precisely the characteristic of the one-dimensional world which makes the exact solution possible.

We calculate below the exact velocity autocorrelation function of a simplest possible model in which the interpretation of diffusion has a more

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physical character, in that the one distinguished particle is able to go around others. The model we consider is an infinite system of very thin, hard rods (needles) of length d moving in a two-dimensional strip infinite in one of the directions, the x direction. Initially the x coordinates are randomly distributed. The y coordinates of all the rods except the one distinguished rod are equal. This exceptional rod is further distinguished by having a nonzero y component of the velocity, while all the other rods have their $v_y = 0$. The distribution of the x component of the velocities is chosen to be the same as in Ref. 3 (studied also in Ref. 2), namely that each rod is equally likely to have $v_x = +c$ or $v_x = -c$ independently of all the other rods. Initially all rods are chosen to be parallel and pointing in the y direction. The effect of the interactions is merely the exchange of their x velocities whenever two rods come into contact. Thus the distinguished rod keeps its y velocity, which is a constant of the motion assuming periodic boundary conditions in the y direction. It is assumed that all the rods are constrained against rotations (infinite moment of inertia).

Without the one distinguished rod this problem would be a purely one-dimensional problem identical with that studied in Ref. 3, where a rather lengthy calculation leads to the following expression for the velocity autocorrelation function:

$$\psi(t) = \langle v(t)\, v(0)\rangle = c^2 e^{-2\rho c t} \tag{1}$$

where ρ is the constant density of particles. This same correlation function follows much more directly from the observation that the process $\mathcal{N}(t)$, the number of collisions a chosen particle has undergone up to time t, is a Poisson process with density ρc. This statement follows from the fact (see Ref. 4, p. 405) that the initial distribution of the particles along the line is a Poisson process, i.e.,

$$P^{(\rho)}[N(\lambda) = k] = [(\rho\lambda)^k/k!]\, e^{-\rho\lambda}$$

where $N(\lambda)$ is the number of particles in an interval of length λ, and a result due to Spitzer[5] which states that such a process along the line is invariant in time when the interactions among the particles are as we have described above. Such a simple correspondence between the two processes $\mathcal{N}(t)$ and $N(\lambda)$ is of course only due to the especially simple choice of the velocity distribution, which has the property of assigning equal speeds to all the particles. Exploiting this simplicity, one directly obtains the expression (1) for $\psi(t)$ as follows: Let the particle start with velocity $+c$ at time $t = 0$; then

$$\psi_+(t) \equiv \langle v_+(t)\, v_+(0)\rangle = c^2[P(+, t, +, 0) - P(-, t, +, 0)]$$

where $P(\pm, t, +, 0)$ is the probability of the particle having velocity $\pm c$ at time t and $+c$ at time $t = 0$, and $v_+(t)$ is the random variable corresponding to the velocity of the particle at time t given that the particle started with velocity $+c$ at time zero, i.e., $v_+(0) = +c$ with probability one:

$$\begin{aligned}\psi_+(t) &= c^2[P(\mathcal{N}(t) = \text{even}) - (P(\mathcal{N}(t) = \text{odd})] \\ &= c^2 \Big[\sum_{k \text{ even}} \frac{(\rho ct)^k}{k!} e^{-\rho ct} - \sum_{k \text{ odd}} \frac{(\rho ct)^k}{k!} e^{-\rho ct} \Big] \\ &= c^2 e^{-\rho ct}[\cosh \rho ct - \sinh \rho ct] = c^2 e^{-2\rho ct}\end{aligned}$$

If the particle starts with either $+c$ or $-c$ at $t = 0$, then $\psi(t)$ is the correlation function of the random variable $v(t) = av_+(t)$, where a is the random variable with $P(a = +1) = \frac{1}{2}$ and $P(a = -1) = \frac{1}{2}$, so that

$$\begin{aligned}\psi(t) = \langle v(t)\, v(0)\rangle &= \langle a^2 v_+(t)\, v_+(0)\rangle = \langle a^2\rangle\langle v_+(t)\, v_+(0)\rangle \\ &= c^2 e^{-2\rho ct}\end{aligned}$$

which is the same as the problem of the random telegraph signal in Ref. 6, p. 288.

Now these same observations allow us to write down

$$\psi(t) = \langle v_x(t)\, v_x(0))\rangle$$

for the distinguished rod in the more general problem in the strip mentioned above. Again let the initial $v_x = +c$. For convenience we can arrange the width of the strip such that the time intervals t_1 and t_2 during which time the distinguished rod is within the interaction region and outside that region, respectively, are equal, i.e., $t_1 = t_2 = \tau$. This gives maximum simplicity without sacrificing the essential features of the problem we want to study. In terms of the geometric cross section of the rods $\tau = 2d/v_y$ and the strip has width $4d$. Clearly the two-dimensionality of the problem is illusory since this can still be regarded as a one-dimensional problem where one particle has an internal degree of freedom whose value at a given time determines whether that particle is or is not available for interaction at that time. Nevertheless, in the following we speak of this internal degree of freedom as the y position.

Let $\alpha = y_0/v_y$, with y_0 the initial y position of the distinguished rod. This is randomly distributed between zero and 2τ, where $\alpha = 0$ corresponds to the initial y position such that the rod is just emerging from the interaction region. Then for all initial positions such that $0 \leqslant \alpha \leqslant \tau$

$$\psi_\alpha(t) = \begin{cases} c^2 & \text{for} \quad 0 \leqslant t \leqslant \tau - \alpha \\ c^2 e^{-2\rho c(t-\tau+\alpha)} & \text{for} \quad \tau - \alpha \leqslant t \leqslant 2\tau - \alpha \\ c^2 e^{-2\rho c\tau} & \text{for} \quad 2\tau - \alpha \leqslant t \leqslant 3\tau - \alpha \end{cases}$$

given that the initial $v_x = +c$.

In general for $(2n + 1)\tau - \alpha \leqslant t \leqslant (2n + 2)\tau - \alpha$, $n = 0, 1, \ldots$, we have

$$\begin{aligned}\psi_\alpha(t) = c^2\{&P[\mathcal{N}(n\tau) = \text{even}]\, P[\mathcal{N}(t - (2n + 1)\tau + \alpha) = \text{even}]\\ &+ P[\mathcal{N}(n\tau) = \text{odd}]\, P[\mathcal{N}(t - (2n + 1)\tau + \alpha) = \text{odd}]\\ &- P[\mathcal{N}(n\tau) = \text{even}]\, P[\mathcal{N}(t - (2n + 1)\tau + \alpha) = \text{odd}]\\ &- P[\mathcal{N}(n\tau) = \text{odd}]\, P[\mathcal{N}(t - (2n + 1)\tau + \alpha) = \text{even}]\\ = c^2\{&e^{-n\rho c\tau}\cosh(n\rho c\tau)\, e^{-\rho c[t-(2n+1)\tau+\alpha]}\cosh[t - (2n + 1)\tau + \alpha]\\ &+ e^{-n\rho c\tau}\sinh(n\rho c\tau)\, e^{-\rho c[t-(2n+1)\tau+\alpha]}\sinh[t - (2n + 1)\tau + \alpha]\\ &- e^{-n\rho c\tau}\cosh(n\rho c\tau)\, e^{-\rho c[t-(2n+1)\tau+\alpha]}\sinh[t - (2n + 1)\tau + \alpha]\\ &- e^{-n\rho c\tau}\sinh(n\rho c\tau)\, e^{-\rho c[t-(2n+1)\tau+\alpha]}\cosh[t - (2n + 1)\tau + \alpha]\}\\ = c^2&e^{-2n\rho c\tau}e^{-2\rho c[t-(2n+1)\tau+\alpha]}\end{aligned}$$

and for the interval $(2n + 2)\tau - \alpha \leqslant t \leqslant (2n + 3)\tau - \alpha$ we have

$$\psi_\alpha(t) = c^2e^{-2n\rho c\tau}e^{-2\rho c\tau}$$

since for any t in this interval $\psi_\alpha(t)$ must equal $\psi_\alpha[(2n + 2)\tau - \alpha]$ from the preceding interval.

Similarly when the initial y position is such that $\tau \leqslant \alpha \leqslant 2\tau$ it can easily be seen that

$$\psi_\alpha(t) = \begin{cases} c^2e^{-2\rho ct} & \text{for } 0 \leqslant t \leqslant 2\tau - \alpha \\ c^2e^{-2\rho c(2\tau-\alpha)} & \text{for } 2\tau - \alpha \leqslant t \leqslant 3\tau - \alpha \end{cases}$$

and in general for the following time intervals ($n = 0, 1, 2, \ldots$)

$$\psi_\alpha(t) = c^2e^{-(2n+4)\rho c\tau}e^{-2\rho c[t-(2n+3)\tau]}, \qquad (2n + 3)\tau - \alpha \leqslant t \leqslant (2n + 4)\tau - \alpha$$

and

$$\psi_\alpha(t) = c^2e^{-(2n+2)\rho c\tau}e^{-2\rho c(2\tau-\alpha)}, \qquad (2n + 4)\tau - \alpha \leqslant t \leqslant (2n + 5)\tau - \alpha$$

To obtain the final correlation function we must average $\psi_\alpha(t)$ over all α. For this purpose we need the expressions $\psi_t(\alpha)$, i.e. the values of the correlation functions for fixed time t as a function of the initial y position. These are seen to be

$$\psi_t(\alpha) = \begin{cases} c^2, & 0 \leqslant \alpha \leqslant \tau - t \\ c^2e^{-2\rho c(t-\tau+\alpha)} & \tau - t \leqslant \alpha \leqslant \tau \\ c^2e^{-2\rho ct} & \tau \leqslant \alpha \leqslant 2\tau - t \\ c^2e^{-2\rho c(2\tau-\alpha)}, & 2\tau - t \leqslant \alpha \leqslant 2\tau \end{cases}$$

for the first time interval $0 \leqslant t \leqslant \tau$. Similarly for the second time interval $\tau \leqslant t \leqslant 2\tau$ we have

$$\psi_t(\alpha) = \begin{cases} c^2 e^{-2\rho c(t-\tau+\alpha)}, & 0 \leqslant \alpha \leqslant 2\tau - t \\ c^2 e^{-2\rho c\tau} & 2\tau - t \leqslant \alpha \leqslant \tau \\ c^2 e^{-2\rho c(2\tau-\alpha)}, & \tau \leqslant \alpha \leqslant 3\tau - t \\ c^2 e^{-2\rho c(t-\tau)}, & 3\tau - t \leqslant \alpha \leqslant 2\tau \end{cases}$$

And in general for the odd time intervals $2n\tau \leqslant t \leqslant (2n+1)\,\tau$, $n = 0, 1,\ldots,$ we can write

$$\psi_t(\alpha) = \begin{cases} c^2 e^{-2n\rho c\tau}, & 0 \leqslant \alpha \leqslant \tau - [t - 2n\tau] \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c(t-2n\tau+\alpha)}, & \tau - [t-2n\tau] \leqslant \alpha \leqslant \tau \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c(t-2n\tau)} & \tau \leqslant \alpha \leqslant 2\tau - [t - 2n\tau] \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c(2\tau-\alpha)}, & 2\tau - [t-2n\tau] \leqslant \alpha \leqslant 2\tau \end{cases}$$

and similarly for the even time intervals $(2n+1)\,\tau \leqslant t \leqslant (2n+2)\,\tau$

$$\psi_t(\alpha) = \begin{cases} c^2 e^{-2n\rho c\tau} e^{-2\rho c[t-(2n+1)\tau+\alpha]}, & 0 \leqslant \alpha \leqslant \tau - [t-(2n+1)\,\tau] \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c\tau}, & \tau - [t-(2n+1)\,\tau] \leqslant \alpha \leqslant \tau \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c(2\tau-\alpha)}, & \tau \leqslant \alpha \leqslant 2\zeta - [t-(2n+1)\,\tau] \\ c^2 e^{-2n\rho c\tau} e^{-2\rho c[t-(2n+1)\tau]}, & 2\tau - [t-(2n+1)\,\tau] \leqslant \alpha \leqslant 2\tau \end{cases}$$

Finally, doing the required averaging, we obtain

$$\psi(t) = (1/2\tau)\int_0^{2\tau} \psi_t(\alpha)\,d\alpha$$

For the first time interval $0 \leqslant t \leqslant \tau$ we get

$$\psi(t) = (c^2/2\tau)(\tau - t)(1 + e^{-2\rho ct}) + (c/2\rho\tau)(1 - e^{-2\rho ct})$$

for the second time interval $\tau \leqslant t \leqslant 2\tau$ we get

$$\psi(t) = (c^2/2\tau)(t-\tau)(e^{-2\rho c(t-\tau)} + e^{-2\rho c\tau}) + (c/2\rho\tau)(e^{-2\rho c(t-\tau)} - e^{-2\rho c\tau})$$

and in general for $(2n\tau) \leqslant t \leqslant (2n+1)\,\tau$

$$\psi(t) = \frac{c^2}{2\tau}\,e^{-2n\rho c\tau}\left\{[(2n+1)\,\tau - t](1 + e^{-2\rho c[t-2n\tau]}) + \frac{1}{\rho c}\,(1 - e^{-2\rho c[t-2n\tau]})\right\}$$

and for $(2n+1)\,\tau \leqslant t \leqslant (2n+2)\,\tau$

$$\psi(t) = \frac{c^2}{2\tau}\,e^{-2n\rho c\tau}\left\{[t-(2n+1)\,\tau](e^{-2\rho c[t-(2n+1)\tau]} + e^{-2\rho c\tau}) + \frac{1}{\rho c}\,(e^{-2\rho c[t-(2n+1)\tau]} - e^{-2\rho c\tau})\right\}$$

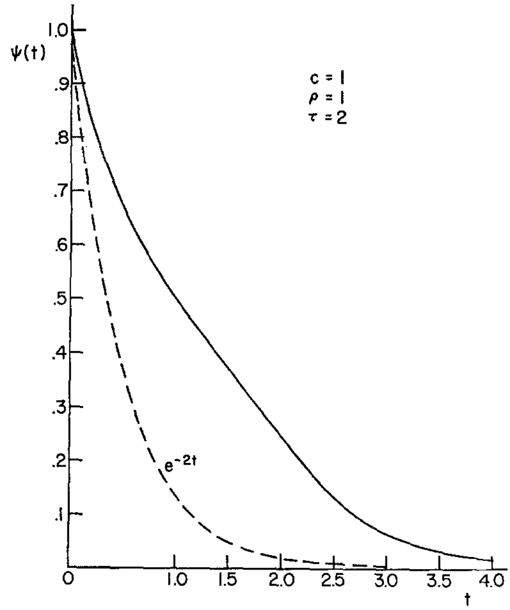

Fig. 1

A plot of this function for $0 \leqslant t \leqslant 2\tau$ is given in Fig. 1. Calculation of the diffusion coefficient yields

$$D = \tfrac{3}{4}(c/\rho) + (c^2\tau/4) \coth \rho c\tau$$

If one restricts the initial y position of the distinguished rod to lie within the interaction region, then one obtains for the diffusion coefficient $D = c/\rho$, independent of τ and precisely twice the value for the purely one-dimensional case.

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