

Velocity correlations, diffusion, and stochasticity in a one-dimensional system

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We consider the motion of a test particle in a one-dimensional system of equal-mass point particles. The test particle plays the role of a microscopic “piston” that separates two hard-point gases with different concentrations and arbitrary initial velocity distributions. In the homogeneous case when the gases on either side of the piston are in the same macroscopic state, we compute and analyze the stationary velocity autocorrelation function $C(t)$. Explicit expressions are obtained for certain typical velocity distributions, serving to elucidate in particular the asymptotic behavior of $C(t)$. It is shown that the occurrence of a nonvanishing probability mass at zero velocity is necessary for the occurrence of a long-time tail in $C(t)$. The conditions under which this is a t^{-3} tail are determined. Turning to the inhomogeneous system with different macroscopic states on either side of the piston, we determine its effective diffusion coefficient from the asymptotic behavior of the variance of its position, as well as the leading behavior of the other moments about the mean. Finally, we present an interpretation of the effective noise arising from the dynamics of the two gases, and thence that of the stochastic process to which the position of any particle in the system reduces in the thermodynamic limit.

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I. INTRODUCTION

Exactly solvable “toy” models are important in understanding the dynamic behavior of complex systems made up of a large number of particles. They also allow us to establish and understand the limitations of the approximations used in general to deal with systems of interacting particles, such as the Boltzmann equation. One such model, consisting of identical hard-point particles moving on a line and interacting through elastic collisions, was introduced several decades ago [1]. Based on the observation that the particles merely exchange velocities in a collision, Jepsen [2] was able to calculate explicitly several properties of a gas of such particles. Subsequently, Lebowitz and co-workers [3–5] refined and extended these calculations to include, among other aspects, a comparison with the results of the Boltzmann approximation. Very recently, this model system has been revisited by Piasecki and Gruber [6,7], their main motivation being the construction of a one-dimensional analog of the “adiabatic piston” [8], with a central particle playing the role of a piston separating gases at different temperatures and densities to its left and right. Attention has also been focused on several related models from the point of view of the applicability of the Fourier law for heat flux in one-dimensional systems [9]. Although the main interest in these specific contexts is in the case of an arbitrary ratio of the masses of the piston and a gas particle, the equal-mass case being a singular one in some sense, the analytical tractability of the latter makes it a valuable “theoretical laboratory” from which much can be learned. In particular, it offers a model in which

(i) one can pass to the thermodynamic limit in a rigorous manner, and (ii) the effect of recollisions can be *completely and exactly* taken into account.

The renewed interest in the model prompts us to revisit it and extend its analysis. We focus on the motion of the central particle (which we shall refer to as the “piston” for brevity). A brief recapitulation of the relevant results from earlier work is given in Sec. II. In Sec. III we compute and study the stationary velocity autocorrelation function $C(t)$ of the piston in the homogeneous case, when the gases on either side of the piston are in the same macroscopic state (i.e., equal densities and arbitrary but identical velocity distributions), to amend and extend earlier results. The explicit expressions obtained for certain archetypical velocity distributions help us analyze the asymptotic behavior of $C(t)$ to determine exactly when a power-law decay may be expected, and when the latter is a t^{-3} tail. Turning to the inhomogeneous system with different macroscopic states on either side of the piston, in Sec. IV we determine its effective diffusion coefficient from the asymptotic behavior of the variance of its position, as well as the leading behavior of the other moments about the mean. Finally, in Sec. V we show that there is an appealing and direct interpretation of the effective noise to which the many-particle interactions reduce in the thermodynamic limit as far as one-particle dynamics is concerned, and thus of the stochastic process represented by the position of any particle in the system.

II. RECAPITULATION OF EARLIER WORK

For ready reference, we record briefly the relevant results of earlier work that are needed for what follows, using the convenient notation employed by Piasecki [7]. One starts with a system of a finite number of particles, located in the

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interval $[-L, L]$ of the x axis, with free boundary conditions. The piston is initially located (without loss of generality) at $X_0=0$ and has an arbitrary initial velocity V_0 . The N^- particles to its left and N^+ particles to its right are initially at uniformly distributed random positions X_j ($j = -N^-, \dots, 0, \dots, N^+$), with independent, identically distributed velocities V_j drawn from normalized velocity distributions $\phi^\pm(V)$, respectively. As the particles merely exchange velocities upon collision, at any instant of time the piston is on one of the “free” trajectories $X_j + V_j t$. This, together with

the fact that the particles cannot move across each other, suffices to solve [2] the problem of determining, among other quantities, the phase space distribution function of the piston (or that of any of the other particles) at any time $t > 0$ by averaging over the initial positions and velocities of the gas particles on both sides of the piston [2,3]. In the thermodynamic limit $L \rightarrow \infty$ and $N^\pm \rightarrow \infty$ such that one has finite densities $\lim N^\pm / L = n^\pm$ on the left and right of the piston, the conditional one-particle distribution function of the piston is found to be

$$P(X, V, t | 0, V_0, 0) = \exp\{-t[n^-\alpha(V_0) + n^+\beta(V_0)]\} I_0(2t[n^-\alpha(V_0)n^+\beta(V_0)]^{1/2}) \delta(X - V_0 t) \delta(V - V_0) + \exp\{-t[n^-\alpha(X/t) + n^+\beta(X/t)]\} \{ [n^-\phi^-(V)\theta(Vt - X)\theta(X - V_0 t) + n^+\phi^+(V)\theta(X - Vt)\theta(V_0 t - X)] \times I_0(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2}) + [n^-\phi^-(V)\theta(Vt - X)\theta(V_0 t - X)(n^+\beta(X/t)/n^-\alpha(X/t))^{1/2} + n^+\phi^+(V)\theta(X - Vt)\theta(X - V_0 t)(n^-\alpha(X/t)/n^+\beta(X/t))^{1/2}] I_1(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2}) \}, \quad (1)$$

where

$$\alpha(W) = \int_W^\infty dU \phi^-(U)(U - W), \quad \beta(W) = \int_{-\infty}^W dU \phi^+(U)(W - U), \quad (2)$$

and I_n is the modified Bessel function of order n . For $V_0=0$, this is the result recorded in Ref. [7].

The velocity distribution of the piston is obtained by integrating $P(X, V, t | 0, V_0, 0)$ over X , and is given by

$$P(V, t | 0, V_0, 0) = \exp\{-t[n^-\alpha(V_0) + n^+\beta(V_0)]\} I_0(2t[n^-\alpha(V_0)n^+\beta(V_0)]^{1/2}) \delta(V - V_0) + t \int_{-\infty}^\infty dW \exp\{-t[n^-\alpha(W) + n^+\beta(W)]\} \{ [n^-\phi^-(V)\theta(V - W)\theta(W - V_0) + n^+\phi^+(V)\theta(W - V)\theta(V_0 - W)] I_0(2t[n^-\alpha(W)n^+\beta(W)]^{1/2}) + [n^-\phi^-(V)\theta(V - W)\theta(V_0 - W)(n^+\beta(W)/n^-\alpha(W))^{1/2} + n^+\phi^+(V)\theta(W - V)\theta(W - V_0) \times (n^-\alpha(W)/n^+\beta(W))^{1/2}] I_1(2t[n^-\alpha(W)n^+\beta(W)]^{1/2}) \}. \quad (3)$$

The stationary velocity distribution to which this tends as $t \rightarrow \infty$ is found [7] by using the leading term in the asymptotic expansion of $I_n(z)$ for large argument, and carrying out the integral over the resulting Gaussian peaked at $W = \bar{W}$, where \bar{W} is the (unique) root of the equation

$$n^-\alpha(\bar{W}) = n^+\beta(\bar{W}). \quad (4)$$

The normalized asymptotic velocity distribution of the piston is then found to be

$$P_\infty(V) = \frac{n^-\phi^-(V)\theta(V - \bar{W}) + n^+\phi^+(V)\theta(\bar{W} - V)}{\Xi(\bar{W})}, \quad (5)$$

where

$$\Xi(\bar{W}) = -n^-\alpha'(\bar{W}) + n^+\beta'(\bar{W}) = n^-|\alpha'(\bar{W})| + n^+\beta'(\bar{W}) \quad (6)$$

is the normalization factor. In general, therefore, $P_\infty(V)$ has a finite discontinuity at $V = \bar{W}$. The asymptotic drift velocity of the piston, defined as $\langle V(\infty) \rangle = \int_{-\infty}^\infty dV V P_\infty(V)$, is then trivially seen to be equal to \bar{W} itself, on rewriting the definition of the latter in Eq. (4) as

$$\bar{W} = \frac{n^-\int_{\bar{W}}^\infty dU U \phi^-(U) + n^+\int_{-\infty}^{\bar{W}} dU U \phi^+(U)}{n^-\int_{\bar{W}}^\infty dU \phi^-(U) + n^+\int_{-\infty}^{\bar{W}} dU \phi^+(U)}. \quad (7)$$

In particular, for Maxwellian distributions $\phi^\pm(V)$ at temperatures T^\pm , one has $\bar{W} \geq 0$ according as $n^-\sqrt{T^-} \geq n^+\sqrt{T^+}$. Since $n(k_B T^\pm)^{1/2}$ is essentially the linear friction coefficient of the corresponding gas, it is this *dynamic* property, rather than the pressure, that determines the direction of

the drift of the central particle. The equality $n^-\sqrt{T^-} = n^+\sqrt{T^+}$ as the condition necessary for the piston to have a drift-free, purely diffusive motion asymptotically, has already been pointed out by Jepsen [2].

We can proceed to show that, in the limit $t \rightarrow \infty$, every particle attains the new stationary velocity distribution $P_\infty(V)$ (in the thermodynamic limit, of course). This remains true even if $\phi^- = \phi^+ = \phi$, but $n^- \neq n^+$. Thus, although the system under study does not have strong mixing properties, in the sense that the set of “free” trajectories $\{X_j + V_j t\}$ is fixed for all time once the initial values $\{X_j\}$ and $\{V_j\}$ are specified, the effect of the collisions of the particles with the piston and among themselves is to mix the initial velocity distributions on the right and left of the piston. This happens by a “diffusion” of the “interaction front” of the piston with the other particles, through successive collisions. Only in the special case in which

$$n^- = n^+ = n, \quad \phi^- = \phi^+ = \phi, \quad (8)$$

i.e., when the gases on both sides of the piston are initially in the same macroscopic state, does $P_\infty(V)$ reduce to $\phi(V)$ itself. We refer to this as the “homogeneous system” in what follows, in contrast to the more general inhomogeneous case. For simplicity, we shall also assume that $\phi(V) = \phi(-V)$ throughout this paper.

III. VELOCITY AUTOCORRELATION IN THE HOMOGENEOUS SYSTEM

We now study the *stationary* velocity autocorrelation function of the piston, which requires that the initial distribution be a stationary one. As mentioned above, this only happens in the homogeneous case, to which we therefore restrict ourselves in the rest of this section. The results to be obtained are in fact valid for *any* particle in the system.

Since $\bar{W} = 0$ in this case, the autocorrelation function is given by

$$C(t) = \langle V(t_0)V(t+t_0) \rangle \\ = \int_{-\infty}^{\infty} dV \int_{-\infty}^{\infty} dV_0 V_0 V P(V, t | 0, V_0, 0) \phi(V_0). \quad (9)$$

This quantity has been considered in earlier work both for a Maxwellian $\phi(V)$ [2] and in more general terms [3], and been found to exhibit a t^{-3} power-law tail. However, the conclusions regarding the conditions under which this happens require modification; nor is the exponent of the power law invariably equal to -3 . We therefore analyze the question afresh, extending and amending some of these earlier results. We also give a physical interpretation of the circumstances leading to a power-law decay of $C(t)$.

On inserting Eq. (3) in Eq. (9) and simplifying, we obtain the expression

$$C(t) = \int_{-\infty}^{\infty} dW \exp\{-nt[\alpha(W) + \beta(W)]\} \\ \times \left\{ I_0(2nt[\alpha(W)\beta(W)]^{1/2}) W^2 \phi(W) \right. \\ \left. + nt[\alpha(W) - W\alpha'(W)]^2 \left[\frac{\alpha(W) + \beta(W)}{[\alpha(W)\beta(W)]^{1/2}} \right] \right. \\ \left. \times I_1(2nt[\alpha(W)\beta(W)]^{1/2}) \right. \\ \left. - 2I_0(2nt[\alpha(W)\beta(W)]^{1/2}) \right\}, \quad (10)$$

where the functions $\alpha(W)$ and $\beta(W)$ have been defined in Eqs. (2). It is readily verified that in the special case of a dichotomic velocity distribution

$$\phi^+(V) = \phi^-(V) = \phi(V) = \frac{1}{2}[\delta(V+c) + \delta(V-c)], \quad (11)$$

one obtains from Eq. (10) the exponential decay

$$C(t) = c^2 e^{-2nct}. \quad (12)$$

Similarly, the known result for a Maxwellian $\phi(V)$ is also recovered.

$C(0)$ is of course $\int dW W^2 \phi(W)$, and $C(t)$ initially decreases linearly with t , with a slope that works out to

$$(dC/dt)_{t=0} = -2n \int_{-\infty}^{\infty} dW \{ W^2 \phi(W) \alpha(W) + [\alpha(W) \\ - W\alpha'(W)]^2 \}. \quad (13)$$

In particular, for a Maxwellian $\phi(V)$ one can evaluate the integral involved to obtain $(dC/dt)_{t=0} = -4n(k_B T / \pi m)^{1/2}$. In the general case, $C(t)$ is a nonmonotonic function of t , that becomes negative beyond a certain point and eventually approaches zero from below as $t \rightarrow \infty$. The long-time behavior of the velocity autocorrelation yields valuable information on the mixing properties and memory effects in the system. The extraction of this behavior from Eq. (10) is nontrivial. It is helpful to note that $\alpha(W)$ is a nonincreasing function of W , with $\alpha(W) \sim -W$ as $W \rightarrow -\infty$ and $\alpha(\infty) = 0$; whereas $\beta(W)$ is a nondecreasing function of W , with $\beta(-\infty) = 0$ and $\beta(W) \sim W$ as $W \rightarrow \infty$. Further, whenever $\phi^-(V) = \phi^+(V) = \phi(V)$, we have $\beta(W) = \alpha(-W) = W + \alpha(W)$. An adequate number of terms in the asymptotic expansions of the Bessel functions and the other terms in the integrand in Eq. (10) must be retained, consistent with the fact that nonvanishing contributions to the integral come from the region $W^2 t \lesssim O(1)$. As already mentioned, it has been shown [2,3] that $C(t)$ has a leading asymptotic behavior $\sim t^{-3}$ for a Maxwellian $\phi(V)$ [10]. We have corroborated this, and also extended the result to the next term in the asymptotic expansion: after a very lengthy calculation, we find

$$C(t) \sim -\frac{1}{(nt)^3} \left(\frac{m}{2\pi k_B T} \right)^{1/2} \left(1 - \frac{5}{2\pi} \right) - \frac{1}{8(nt)^4} \left(\frac{m}{2\pi k_B T} \right) \\ \times \left(177 - \frac{315\pi}{16} - \frac{367}{\pi} \right) - \dots \quad (14)$$

Based on the emergence of a t^{-3} tail in the Maxwellian case (and also for another extended distribution $\phi(V)$ that falls off like $|V|^{-3}$), as opposed to an exponential decay [Eq. (12)] for the dichotomic distribution, it has been concluded [3] that $C(t)$ decays exponentially if $\phi(V)$ is a compact (“finite”) distribution, and has a power-law tail whenever the support of $\phi(V)$ is noncompact. However, as we now proceed to show, the actual criterion for the emergence of a power-law tail in $C(t)$ turns out to be the *existence of a nonzero probability mass at $V=0$ in $\phi(V)$* . (The physical reason for this will be described subsequently.) The issue is most clearly elucidated with the help of two simple yet archetypical distributions $\phi(V)$ for which $C(t)$ can be determined analytically, and exact asymptotic expansions obtained. These are, respectively, (i) a uniform distribution in the finite interval $-c \leq V \leq +c$, and (ii) a discrete distribution consisting of δ -functions at $V = \pm c$ and an additional one at $V=0$. The former has a compact support, and yet $C(t)$ turns out to have a t^{-3} tail; while the latter, in contrast to the dichotomic distribution of Eq. (11), leads in fact to an even heavier tail ($\sim t^{-3/2}$) for any nonvanishing weight of the central δ -function. We also extend the result in Eq. (14) to the case of a general $\phi(V)$ that is sufficiently smooth at the origin.

(i) Accordingly, let us consider the uniform distribution

$$\phi(V) = \frac{1}{2c} \theta(V+c) \theta(c-V). \quad (15)$$

For this distribution, $\alpha(W)$ is respectively equal to $-W$ for $W \leq -c$, and $(c-W)^2/4c$ for $-c \leq W \leq +c$; it vanishes identically for $W > c$. Recall also that $\beta(W) = W + \alpha(W)$. Inserting these in Eq. (10) and carrying out the necessary calculations, we finally obtain a closed-form expression for $C(t)$. In terms of the dimensionless time $\tau = nct$, this reads

$$C(\tau) = \frac{c^2}{4} \left[\frac{1}{2} - \frac{1}{4\tau} + \left(\frac{1}{4\tau} + 1 - \tau \right) e^{-\tau} {}_1F_1 \left(\frac{1}{2}; \frac{3}{2}; \tau \right) \right], \quad (16)$$

where ${}_1F_1$ is the usual confluent hypergeometric function. The slope at the origin is $[dC(\tau)/d\tau]_{\tau=0} = -\frac{2}{5}c^2$. The analytic form of $C(\tau)$ enables us to write down its exact asymptotic expansion for large τ ,

$$C(\tau) \sim -c^2 \sum_{n=3}^{\infty} \frac{(n-1)(n-2)(2n-5)!!}{\tau^n}. \quad (17)$$

As mentioned earlier, this starts with an $O(\tau^{-3})$ term, although the support of $\phi(V)$ is compact. Figure 1 depicts the long-time behavior of the correlation function.

(ii) Next, consider the discrete distribution

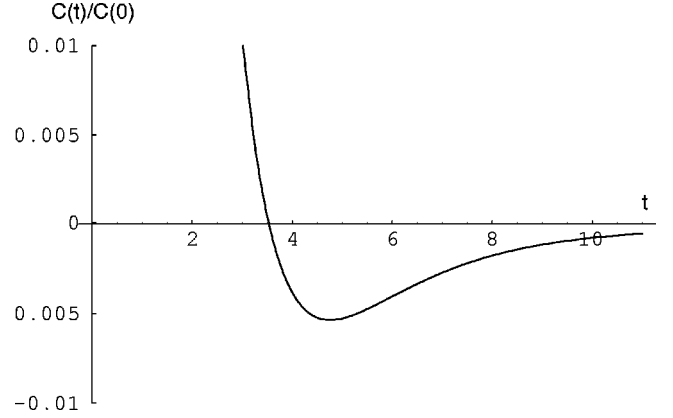


FIG. 1. Asymptotic behavior of the normalized velocity auto-correlation $C(t)/C(0)$ as a function of time (in units of $1/nc$), for a uniform distribution $\phi(V)$ [Eq. (15)].

$$\phi(V) = \mu \delta(V) + \frac{1-\mu}{2} [\delta(V+c) + \delta(V-c)], \quad 0 \leq \mu < 1, \quad (18)$$

which is an extension of the dichotomic distribution of Eq. (11) to include an additional δ -function at $V=0$ with a weight μ . Once again, $\alpha(W)$ vanishes identically for $W > c$. For $W \leq c$, it is piecewise linear, being given by

$$\alpha(W) = \begin{cases} -W, & W < -c \\ \frac{1}{2}(1-\mu)c - \frac{1}{2}(1+\mu)W, & -c \leq W < 0 \\ \frac{1}{2}(1-\mu)(c-W), & 0 \leq W \leq c. \end{cases} \quad (19)$$

We obtain in this case (with $\tau = nct$ as before)

$$C(\tau) = c^2 (1-\mu) e^{-\tau} \left\{ 1 + (1-\mu)\tau \int_0^1 du e^{\mu(1-u)\tau} \right. \\ \left. \times \left[\frac{1-\mu+\mu u}{g(u)} I_1(\tau g(u)) - I_0(\tau g(u)) \right] \right\}, \quad (20)$$

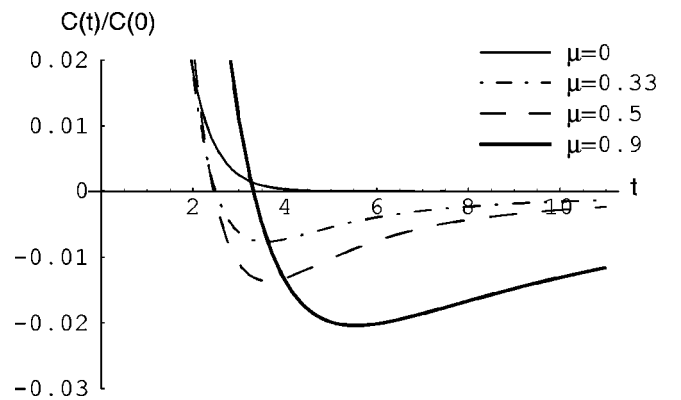


FIG. 2. Asymptotic behavior of the normalized velocity auto-correlation $C(t)/C(0)$ as a function of time (in units of $1/nc$) for different values of μ , for the discrete distribution $\phi(V)$ in Eq. (18).

where $g(u) = \{(1-\mu)(1-u)[(1-\mu) + (1+\mu)u]\}^{1/2}$. The slope at the origin is $[dC(\tau)/d\tau]_{\tau=0} = -(1-\mu)(2-\mu)c^2$. The long-time behavior in this case is, however, quite different from that found in the previous cases. Owing to the singularity in $\phi(V)$ at the origin, $\alpha'(W)$ has a jump at $W=0$. As a consequence, the integrand in Eq. (10) is now a function of $|W|$ rather than W . This leads to the occurrence of both even and odd powers of $|W|$ in the small- W expansion of the integrand, using which the asymptotic expansion of $C(t)$ is determined. For the latter, we now obtain

$$C(\tau) \sim -\frac{\mu c^2 (1-\mu)^{1/2}}{\tau^{3/2}} \frac{1}{4(2\pi)^{1/2}} - \frac{\mu c^2}{\tau^{5/2}} \frac{3(3-2\mu^2)}{32(2\pi)^{1/2}(1-\mu)^{1/2}} + \dots \quad (21)$$

Thus $C(t)$ now has an even *slower* power-law decay, starting with an $O(t^{-3/2})$ term, as long as $\mu \neq 0$, i.e., as long as there is a finite probability mass at $V=0$. When $\mu=0$, all the terms in the asymptotic expansion vanish, and $C(t)$ reverts to the exponential decay that obtains in the case of the dichotomic distribution, Eq. (12). Figure 2 shows the long-time behavior of the correlation function for different values of the weight parameter μ , including (for ready comparison) the case $\mu=0$.

The relative roles of the δ -functions in $\phi(V)$ at $V=0$ and at $V=\pm c$ may be examined a little more closely. This aspect is not so transparent in the representation of Eq. (20) for $C(t)$, but is made more manifest with the help of its Laplace transform. This enables us to write $C(t)$ in the form

$$C(t) = (1-\mu)c^2 \left\{ \frac{e^{-2nct/(1+\mu)}}{1+\mu} + \mu \mathcal{L}^{-1} \frac{s\mu + [s^2 + 2snc(1-\mu)]^{1/2}}{[(1+\mu)s + 2nc][s + \mu[s^2 + 2snc(1-\mu)]^{1/2} + 2nc(1-\mu)]} \right\}, \quad (22)$$

where \mathcal{L}^{-1} denotes the inverse Laplace transform. Comparing this with the pure exponential decay $c^2 e^{-2nct}$ that obtains for the dichotomic velocity distribution, we see that the δ -function in $\phi(V)$ at $V=0$ is entirely responsible for the second term (which vanishes when $\mu=0$). Further, the time scale in the exponential part is itself modified from the usual correlation time for a dichotomic process, which is $(2nc)^{-1}$ in the present context, to $(1+\mu)(2nc)^{-1}$, as one might expect on physical grounds.

We are now in a position to understand the physical origin of the power-law tail in $C(t)$. The particles of the system do not undergo any systematic drift in the homogeneous case. Going back to an inspection of the manner in which the particle under consideration skips from one free trajectory to another through collisions, we see that, if the stationary velocity distribution $\phi(V)$ of the gas particles has a *finite probability mass at $V=0$* , the particle will repeatedly find itself on a trajectory with zero slope, i.e., revert to the zero (equal to average) velocity state. This persistence is like a memory effect, and it shows up as a slow (power-law) decay of $C(t)$. The compactness or otherwise of the support of $\phi(V)$ does not play a role as far as this aspect is concerned.

It is also possible to find the precise conditions under which the leading asymptotic behavior of $C(t)$ starts with a t^{-3} term: this is so if $\phi(V)$ is at least twice differentiable at the origin, and, moreover, both $\phi(0)$ and $\phi''(0)$ do not happen to be zero. [We recall that $\phi(V)$ has been taken to be a symmetric function, so that all its derivatives of odd order vanish at the origin.] The general asymptotic expansion of $C(t)$, for a distribution $\phi(V)$ that is differentiable a sufficient number of times at $V=0$, reads

$$\begin{aligned} C(t) \sim & -\frac{1}{(nt)^3} [\phi(0) - 6\alpha(0)\phi^2(0) - \alpha^2(0)\phi''(0)] \\ & - \frac{1}{256\alpha(0)(nt)^4} [-315\phi(0) + 3456\alpha(0)\phi^2(0) \\ & - 2880\alpha^2(0)\phi^3(0) + 19840\alpha^3(0)\phi(0)\phi''(0) \\ & - 2208\alpha^2(0)\phi''(0) - 256\alpha(0)\phi^{(iv)}(0)] - \dots \end{aligned} \quad (23)$$

This extends the result presented in Eq. (14) for a Maxwellian. Thus, for a distribution $\phi(V)$ that is *regular* at the origin and has a nonvanishing derivative of some finite order at that point, implying that there is a nonzero probability mass at $V=0$, $C(t)$ will certainly have a power-law decay: If $\phi(0) \neq 0$, the leading term is generically $\sim t^{-3}$; on the other hand, if $\phi(0)=0$ and its first nonvanishing derivative at the origin is its $(2r)$ th derivative, the leading term in $C(t)$ is $\sim t^{-r-2}$.

IV. THE INHOMOGENEOUS SYSTEM

We turn now to the inhomogeneous system, in which the particles to the left and right of the piston are initially in different macroscopic states specified by (n^-, ϕ^-) and (n^+, ϕ^+) , respectively. The piston now has, in general, a nonvanishing mean drift velocity that asymptotically approaches \bar{W} . However, as we shall see, the variance of its

position indeed increases linearly with time. The quantity of interest is therefore the effective diffusion coefficient D , which we shall determine. We also find the leading asymptotic behavior of the other moments of the position (about its mean value).

In the homogeneous system, D is of course equal to $\int_0^\infty C(t)dt$ (this integral being absolutely convergent for the system at hand). However, owing to the nonstationarity of the velocity autocorrelation in the inhomogeneous case, D must now be computed directly from the long-time behavior of the mean square displacement of the piston. The asymptotic behavior of the position does not depend on its initial state. We can therefore set $V_0=0$ in $P(X, V, t|0, V_0, 0)$

[Eq. (1)] and integrate it over V to calculate the position distribution function $p(X, t)$ of the piston. Using the fact that the derivatives of the functions α and β are given by

$$\alpha'(W) = - \int_W^\infty dU \phi^-(U)$$

and

$$\beta'(W) = \int_{-\infty}^W dU \phi^+(U), \quad (24)$$

we find

$$\begin{aligned} p(X, t) = & \exp\{-t[n^-\alpha(0) + n^+\beta(0)]\} I_0(2t[n^-\alpha(0)n^+\beta(0)]^{1/2}) \delta(X) + \exp\{-t[n^-\alpha(X/t) + n^+\beta(X/t)]\} \\ & \times \{[n^-\theta(X)|\alpha'(X/t)| + n^+\theta(-X)\beta'(X/t)] I_0(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2}) \\ & + [n^-\theta(-X)|\alpha'(X/t)|[n^+\beta(X/t)/n^-\alpha(X/t)]^{1/2} + n^+\theta(X)\beta'(X/t) \\ & \times [n^-\alpha(X/t)/n^+\beta(X/t)]^{1/2}\} I_1(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2}). \end{aligned} \quad (25)$$

The variance of the position is given by

$$\int_{-\infty}^{\infty} dX (X - \langle X(t) \rangle)^2 p(X, t). \quad (26)$$

In the long-time limit, $\langle X(t) \rangle = \bar{W}t$. Using the asymptotic behavior of the Bessel functions in $p(X, t)$, the leading behavior of the variance is given by

$$\begin{aligned} \langle (X - \bar{W}t)^2 \rangle \sim & \frac{t^{5/2}}{2(\pi n^-\alpha(\bar{W}))^{1/2}} [n^-\alpha'(\bar{W}) + n^+\beta'(\bar{W})] \\ & \times \int_{-\infty}^{\infty} dW (W - \bar{W})^2 \exp[-t(W - \bar{W})^2] \\ & \times \{[n^-/4\alpha(\bar{W})]^{1/2} |\alpha'(\bar{W})| \\ & + [n^+/4\beta(\bar{W})]^{1/2} |\beta'(\bar{W})|\}^2, \end{aligned} \quad (27)$$

which simplifies to $2Dt$, with a diffusion coefficient given by

$$\begin{aligned} D = & \frac{n^-\alpha(\bar{W})}{[n^-\alpha'(\bar{W}) + n^+\beta'(\bar{W})]^2} \\ = & \frac{1}{2} \frac{n^-\alpha(\bar{W}) + n^+\beta(\bar{W})}{[n^-\alpha'(\bar{W}) + n^+\beta'(\bar{W})]^2}. \end{aligned} \quad (28)$$

This is the general formula sought.

We first note (as a check) that in the special case of the homogeneous system, Eq. (28) reduces to

$$D = \frac{\alpha(0)}{n} = \frac{1}{n} \int_0^\infty dU U \phi(U) = \frac{\langle |U| \rangle}{2n}, \quad (29)$$

in agreement with the known result [3]. As mentioned earlier, in this case D must also be equal to the integral of the velocity autocorrelation $C(t)$. We have verified that this is indeed so.

Some interesting special cases emerge from the general formula of Eq. (28). If the densities n^- and n^+ are such that the drift velocity $\bar{W}=0$ even though one has different (but symmetric) distributions $\phi^+(V)$ and $\phi^-(V)$ on either side of the piston, the formula for D simplifies somewhat. Since $\alpha'(0) = -\beta'(0) = -1/2$, we find

$$D = \frac{n^-\alpha(0)}{(n^- + n^+)^2}. \quad (30)$$

In particular, if ϕ^\pm are Maxwellians (with $n^-\sqrt{T^-} = n^+\sqrt{T^+}$ to ensure that $\bar{W}=0$),

$$D = \frac{n^-}{(n^- + n^+)^2} \left(\frac{8k_B T^-}{\pi m} \right)^{1/2}. \quad (31)$$

On the other hand, if $\phi^-(V) = \phi^+(V) = \phi(V)$, but the system remains inhomogeneous because $n^+ \neq n^-$, then $\bar{W} \neq 0$. For the compact uniform velocity distribution of Eq. (15), we find

$$\bar{W} = c \frac{\sqrt{n^-} - \sqrt{n^+}}{\sqrt{n^-} + \sqrt{n^+}} \quad (32)$$

and

$$D = \frac{c}{(\sqrt{n^-} + \sqrt{n^+})^2}. \quad (33)$$

For the discrete distribution of Eq. (18), we have

$$\bar{W} = c \frac{(1 - \mu)(n^- - n^+)}{n_>(1 - \mu) + n_<(1 + \mu)}, \quad (34)$$

where $n_> = \max(n^-, n^+)$, $n_< = \min(n^-, n^+)$. The corresponding diffusion coefficient is found to be

$$D = \frac{4cn^-n^+(1 - \mu)}{[n_>(1 - \mu) + n_<(1 + \mu)]^3}. \quad (35)$$

It is noteworthy that the interplay of the central δ function in the velocity distribution and the inhomogeneity due to the different densities on either side of the piston affects even the *diffusion* coefficient. Setting $\mu = 0$ in the above yields the corresponding expressions for the dichotomic distribution of Eq. (11).

The leading asymptotic behavior of the higher moments $\langle (X - \bar{W}t)^r \rangle$ can also be determined. Here we merely quote the salient result obtained. For the even moments $r = 2l$, it is straightforward to show (along the same lines as in the case of the variance) that $\langle (X - \bar{W}t)^{2l} \rangle \sim O(t^l)$. The calculation is more involved for the odd moments $r = 2l + 1$, but the final result is that $\langle (X - \bar{W}t)^{2l+1} \rangle \sim O(t^l)$ as well. As the expressions obtained for the precise coefficients are lengthy, we do not write them down here.

V. INTERPRETATION AS A STOCHASTIC PROCESS

We conclude by showing that (in the thermodynamic limit) the form of the distribution of the position of the piston, in fact that of *any* of the particles in the system, is effectively that of a stochastic process driven by a noise that can be given a direct physical interpretation.

Conventionally, the stochastic approach to single-particle

dynamics in a many-body system begins with its modeling by a stochastic evolution equation involving noise terms with prescribed statistical properties. One then extracts the corresponding properties of the driven variable(s). Here, however, we have the converse situation. The exact time-dependent one-particle distributions are known, and the task is to identify the stochastic process to which the complicated dynamics effectively reduces, at least as far as the one-particle dynamics is concerned. What kind of stochastic process does the position $X(t)$ of the piston (or any other particle) represent, after the averaging over the initial states of the gas particles is done, and the thermodynamic limit taken? And in what kind of “noise” are the combined effects of the other particles in the system encapsulated?

It is evident from the rather complicated expressions for $P(X, V, t | 0, V_0, 0)$ and the reduced distributions derived from it that $X(t)$ is unlikely to satisfy any simple or standard stochastic differential equation; nor does $p(X, t)$ appear to be the solution of any simple master equation—in particular, of any obvious partial differential equation of finite order. Intricate correlations exist, that cannot be neglected. The effects of recollisions are obviously significant, a direct instance being provided by the form of the first term in Eq. (1). This term represents the probability for the piston to find itself in its initial state at time t . Now, the probability that the initial state of the piston ($X = X_0 = 0, V = V_0$) *persists* till time t (i.e., the piston suffers no collisions till time t) is easily shown to be simply $\exp[-t\{n^- \alpha(V_0) + n^+ \beta(V_0)\}]$. Thus the extra factor I_0 in the term proportional to $\delta(X - V_0 t) \delta(V - V_0)$ in $P(X, V, t | 0, V_0, 0)$ is entirely due to the effects of recollisions [3]. As the concept of an effective noise is only meaningful in the thermodynamic limit and when ergodicity obtains, we must examine for this purpose the structure of the terms in the solutions *other* than the ones arising from the returns to any specific initial state.

The occurrence of the Bessel functions I_0 and I_1 in Eqs. (1) and (25) seems to suggest some sort of link with dichotomic diffusion (i.e., the integral of a dichotomic Markov process) and the well-known telegrapher’s equation and its solution. Indeed, in the homogeneous case, with $\phi(V)$ equal to the dichotomic velocity distribution of Eq. (11) and $V_0 = \pm c$, Eq. (25) for $p(X, t)$ does reduce to the solution corresponding to dichotomic diffusion [11], once again except for the extra factor of $I_0(nct)$ in the “ballistic” term representing the probability of the occurrence of the initial state at time t . But this does not explain the origin of the Bessel functions in the general case. Nor does it really do so even in the special case referred to, other than the not-very-helpful observation that the solution of the telegrapher’s equation involves I_0 and I_1 . As the effective “noise” we seek should be essentially the same for every particle, our arguments should indeed apply to any of the particles, and not just the piston. Proceeding as in the case of the piston (i.e., averaging over the initial positions and velocities of all the particles except the piston, and with $X_0 = 0, V_0 = 0$), we find the following result for the position distribution of the b th particle at time t :

$$\begin{aligned}
p_b(X,t) = & \exp\{-t[n^-\alpha(0)+n^+\beta(0)]\}[n^+\beta(0)/n^-\alpha(0)]^{b/2}I_b(2t[n^-\alpha(0)n^+\beta(0)]^{1/2})\delta(X) \\
& + \exp\{-t[n^-\alpha(X/t)+n^+\beta(X/t)]\}[n^+\beta(X/t)/n^-\alpha(X/t)]^{b/2}\{[n^-\theta(X)|\alpha'(X/t)|+n^+\theta(-X)\beta'(X/t)] \\
& \times I_b(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2})+n^-\theta(-X)|\alpha'(X/t)|[n^+\beta(X/t)/n^-\alpha(X/t)]^{1/2}I_{b+1}(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2}) \\
& + n^+\theta(X)\beta'(X/t)[n^-\alpha(X/t)/n^+\beta(X/t)]^{1/2}I_{b-1}(2t[n^-\alpha(X/t)n^+\beta(X/t)]^{1/2})\}. \tag{36}
\end{aligned}$$

Here $b \in \mathbb{Z}$. [Setting $b=0$ one recovers the result in Eq. (25) for the piston, remembering that $I_{-1}=I_1$.] The occurrence of the Bessel functions I_{b+1} , I_b and I_{b-1} shows quite clearly that we must look for a link to Bessel functions other than one via the solution to the telegrapher's equation.

The example of the dichotomic velocity distribution in the homogeneous case does provide a valuable clue, though. Let us therefore examine this case for a moment, focusing on the piston, and taking V_0 also to be either c or $-c$, to mask the effects of any special initial conditions. The actual “free” trajectories of all the particles are then straight lines with slopes restricted to the values $\pm c$. A little thought shows that after its first collision, the piston alternately “rides” on a free trajectory belonging to the gas on its right, and one belonging to the gas on its left. For brevity, we shall refer to these as “right” and “left” trajectories. (Which of these the piston gets on to first, depends on whether its initial velocity V_0 is equal to c or $-c$.) Moreover, the piston is alternately hit by a “right” particle with velocity $-c$ and a “left” particle with velocity $+c$. The number of right collisions minus the number of left collisions can only take on the values $+1$, 0 , and -1 . The resulting zigzag path is precisely that of a particle whose position X satisfies the stochastic differential equation $\dot{X}=c\xi(t)$, where $\xi(t)$ is a stationary dichotomic Markov process (DMP) alternating between the values ± 1 with a certain mean switching rate λ . Such a DMP is generated by a stationary Poisson pulse process of intensity λ . One could also regard it as made up of two independent Poisson pulse processes, each with an intensity $\lambda/2$, alternating with each other. This would seem to be a little more closely linked to the present situation, where one might imagine the two states of $\xi(t)$ to be related in some sense to the piston being on a right trajectory and a left trajectory, respectively. But the connection is still far from obvious, and requires some more work.

Let ν^+ and ν^- be two independent stationary Poisson processes with respective intensities (i.e., mean rates) λ^+ and λ^- , so that their mean values at time t are λ^+t and λ^-t . It is easily shown that their *difference* ($\nu^+ - \nu^-$), which can take on any integer value, has a time-dependent distribution given by

$$\begin{aligned}
\Pr(\nu^+ - \nu^- = r; t) = & e^{-(\lambda^+ + \lambda^-)t} (\lambda^+ t / \lambda^- t)^{r/2} \\
& \times I_r(2\sqrt{(\lambda^+ t)(\lambda^- t)}), \quad r \in \mathbb{Z}. \tag{37}
\end{aligned}$$

It is *this* distribution that holds the key to understanding the structure of the one-particle distributions in the problem under consideration. Let the piston be at a position $X > 0$ at

time t , on a (segment) of a free trajectory. Translating the entire system to bring the initial coordinate of this trajectory to the origin, the instantaneous velocity of the piston is X/t (recall that the trajectories are all straight lines, a direct consequence of the equal mass condition). It can be hit by a left particle provided the latter has a positive velocity ($+c$ in the case under consideration) that is greater than X/t . The mean rate at which this happens is given by the product of the concentration n of the gas, the magnitude of the *relative* velocity ($c - X/t$), and the probability $\frac{1}{2}$ that the velocity of the gas particle is c [see Eq. (11)]: in other words, $\lambda^- = \frac{1}{2}n(c - X/t)$. Similarly, the mean rate at which the piston is hit by a right particle is given by $\lambda^+ = \frac{1}{2}n(c + X/t)$. Moreover, the number of right collisions minus the number of left collisions only takes on the values $+1$, 0 , and -1 . Putting in all the foregoing facts and their obvious extension to the case $X < 0$, and transforming from the random variable ($\nu^+ - \nu^-$) to X , we are led to the expression

$$\begin{aligned}
\frac{n}{2} e^{-nct} \{ & I_0(n(c^2t^2 - X^2)^{1/2}) + ((ct+X)/(ct-X))^{1/2} I_1(n(c^2t^2 \\
& - X^2)^{1/2}) \} \theta(X+ct)\theta(ct-X). \tag{38}
\end{aligned}$$

This is precisely the solution for $p(X,t)$ to which Eq. (25) reduces in this special case, *apart* from the contribution from the initial state. The latter is $e^{-nct}\delta(X \pm ct)$ when $V_0 = \pm c$, and $e^{-nct}I_0(nct)\delta(X)$ when $V_0 = 0$. It is also worth noting how the factors of 2 [coming from the formula of Eq. (37)] and $\frac{1}{2}$ (coming from the rates λ^\pm) cancel out in the argument of the Bessel functions in Eq. (38).

These arguments are extended to the general inhomogeneous case as follows. When the piston is at position X at time t , collision with a left particle is possible provided the latter has a velocity U in the range $(X/t, \infty)$, and the magnitude of the relative velocity is $(U - X/t)$. Since the gas on the left has a concentration n^- , and the velocities of its particles are drawn from the distribution ϕ^- , the effective mean rate of left collisions of the piston is given by

$$\lambda^- = n^- \int_{X/t}^{\infty} dU \phi^-(U)(U - X/t), \tag{39}$$

which is nothing but $n^- \alpha(X/t)$. Similarly, in the same given state the piston can only be hit by a right particle with a velocity in the range $(-\infty, X/t)$, and it follows that

$$\lambda^+ = n^+ \int_{-\infty}^{X/t} dU \phi^+(U)(X/t - U) = n^+ \beta(X/t), \tag{40}$$

since it is the *magnitude* of the relative velocity that appears in the mean collision rate. This explains the genesis and form of the argument of the Bessel functions in Eq. (25). The extra factors involving $n^-|\alpha'(X/t)|$ and $n^+\beta'(X/t)$ that appear in the expression for $p(X,t)$ in Eq. (25) are just the Jacobians that arise when we transform from the distribution of $(\nu^+ - \nu^-)$ to that of X . Finally, although the piston *can* have successive left collisions or right collisions in the general case, unlike what happens in the case of the dichotomic velocity distribution, the remarkable fact is that their contribution to the probability distributions seems to vanish in the system at hand. The number of right collisions minus the number of left collisions only takes on the values $+1$, 0 , and -1 even in the general case, presumably as a consequence of the smearing out implied by the averaging and the thermodynamic limit. Likewise, for the b th particle from the piston, the difference between the number of times the particle has occupied a right trajectory and the number of times it has occupied a left trajectory up to any time t predominantly takes on the values b and $b \pm 1$ in this limit. The central value b of this difference is in fact a consequence of its initial ordering, that is not altered by the collisions. The foregoing provides an understanding of the structure of the terms (other than the contribution due to the initial state) in Eq. (36).

In conclusion, we see that the motion of any particle in the system may be regarded, in the thermodynamic limit, as being driven by two independent Poisson pulse processes representing the effects of the gases on the left and right of the central particle. The intensities (mean rates) of these processes have the direct physical interpretation given above with regard to Eqs. (39) and (40). As a Poisson process *per se* is an uncorrelated pulse process, each particle is effectively subjected to two independent noises in this precise sense. However, as the intensity of each noise is state-dependent [the driven variable X appears explicitly in the limits of integration in $\alpha(X/t)$ and $\beta(X/t)$], the flow of X is not given by any simple stochastic differential equation with additive or even multiplicative noise, which is only to be expected.

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- [1] H. L. Frisch, Phys. Rev. **104**, 1 (1956); E. Teramoto and C. Suzuki, Prog. Theor. Phys. **14**, 411 (1955).
 - [2] D. W. Jepsen, J. Math. Phys. **23**, 405 (1965).
 - [3] J. L. Lebowitz and J. K. Percus, Phys. Rev. **155**, 122 (1967).
 - [4] J. L. Lebowitz, J. K. Percus, and J. Sykes, Phys. Rev. **171**, 224 (1968).
 - [5] M. Aizenman, J. L. Lebowitz, and J. Marro, J. Stat. Phys. **18**, 179 (1978).
 - [6] J. Piasecki and Ch. Gruber, Physica A **265**, 463 (1999).
 - [7] J. Piasecki (unpublished).
 - [8] The problem of the “adiabatic piston” has a long history. For a recent critical discussion, see Ch. Gruber, Europhys. Lett. **20**, 259 (1999).
 - [9] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, e-print math-ph/0002052; A. Dhar, Phys. Rev. Lett. **86**, 3554 (2001); e-print cond-mat/0102208, and references therein.
 - [10] As one invokes the asymptotic behavior of I_n for large argument in Eq. (10) to obtain the long-time behavior of $C(t)$, the onset of the latter is given by the condition $t \gg (\pi m/2n^2 k_B T)^{1/2}$ for a Maxwellian $\phi(V)$.
 - [11] V. Balakrishnan and S. Chaturvedi, Physica A **148**, 581 (1988).