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Drift Velocity Induced by Collisions

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Stochastic motion of a hard point separating two semi-infinite subvolumes of a hard point gas in R^1 is studied. The partitionning particle is identical to the particles of the gas and can be looked upon as a tagged particle playing the role of a (microscopic) piston. At the initial moment it is at rest having to the right and to the left of it gases in thermodynamic equilibrium. Its further motion is entirely induced by collisions. The stochastic motion of the piston is determined rigorously. The form of the stationary velocity distribution is calculated. It turns out that at equal initial pressures the piston acquires asymptotically a drift velocity oriented towards the higher temperature region. There is no drift if the temperatures and densities combine to produce on both sides equal particle fluxes. Although the qualitative agreement with Boltzmann's theory is found, the Boltzmann equation does not predict correctly the thermodynamic conditions under which the drift vanishes.

KEY WORDS: Hard point fluid; microscopic piston; drift velocity.

1. INTRODUCTION

Consider a system composed of hard points (hard rods of vanishing diameter) of mass m moving in R^1. The motion between collisions is free. At elastic binary collisions the particles exchange instantaneously their velocities, which completes the definition of the dynamics.

The initial state considered in this paper has been suggested by the *adiabatic piston problem* (see ref. 1 and references given therein). Up to the initial moment $t=0$, the system remains separated into two semi-infinite volumes by a particle clamped at the origin $X=0$. The immobile particle plays the role of an isolating, elastically reflecting wall of infinite mass. The subvolume to the left of the wall is supposed to be in thermal equilibrium at temperature T^-, with number density n^-, and perfect gas pressure

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$p^- = n^- k_B T^-$, where k_B is Boltzmann's constant. Similarly, the initial equilibrium state to the right of the wall is characterized by temperature T^+, number density n^+, and pressure $p^+ = n^+ k_B T^+$.

It is thus supposed that at $t = 0$ the velocities of the gas particles are uncorrelated. Each particle on the negative semi-axis has the velocity distributed according to Maxwell's probability density

$$\phi^-(v) = \sqrt{\frac{m}{2\pi k_B T^-}} \exp\left(-\frac{mv^2}{2k_B T^-}\right) \tag{1}$$

The velocities of the particles filling the positive semi-axis are distributed with probability density $\phi^+(v)$, obtained from (1) by replacing T^- by T^+.

As far as the space distribution is concerned, in any interval of finite length to the left and to the right of the origin the particles have the Poisson distribution with constant density n^-, and n^+, respectively.

Then, at the moment $t = 0$, the partitioning wall is released, and becomes thus a moving microscopic piston, mechanically identical to the particles of the surrounding gas. Its mass equals m, and owing to elastic collisions the tagged particle called here a piston (for the reasons explained above) starts following a stochastic process.

Our object here is to derive rigorously the dynamical law governing the evolution of the probability density $f(X, V; t)$ for finding the piston at time $t > 0$ at point X with velocity V. The present work is a natural continuation of article[2] in which the same problem has been solved within the framework of Boltzmann's kinetic theory. In ref. 2 particular attention has been paid to the case of equal initial pressures. It has been demonstrated that even if the macroscopic mechanical equlibrium condition $p^- = p^+$ was satisfied at $t = 0$, the stationary state of the piston was characterized by a non-zero average velocity oriented towards the higher temperature region. It turns out that a rigorous study confirms this most interesting manifestation of fluctuations showing the qualitative correctness in this respect of Boltzmann's approximate theory. However, according to the rigorous solution of the Boltzmann equation found in ref. 2, the drift velocity vanishes when the condition

$$\int_0^\infty dv \frac{p^-\phi^-(v)}{I^2(v)} = \int_{-\infty}^0 dv \frac{p^+\phi^+(v)}{I^2(v)} \tag{2}$$

is satisfied, with

$$I(v) = \frac{1}{m}[p^-\phi^-(v) + p^+\phi^+(v)] + v\left[\int_{-\infty}^v dw n^+\phi^+(w) - \int_v^\infty dw n^-\phi^-(w)\right] \tag{3}$$

(In fact, (2) is an extension of the result obtained in ref. 2 to the case of different initial pressures.) As it will be shown here, equation (2) does not predict correctly the relation between the thermodynamic parameters p^-, p^+, T_-, T^+ for which the drift vanishes.

The ideas used in this paper follow closely the method invented by D. W. Jepsen[3] to solve the N-body problem for hard rods. More precisely, we use the elegant generalization of Jepsen's approach developed by J. L. Lebowitz and J. K. Percus.[4] Similar ideas have been also applied in a recent work[5] in which the stochastic process followed by the piston moving in a finite volume was shown to approach in an appropriate scaling limit a deterministic trajectory, the whole system tending to a uniform equilibrium state.

In Section 2 the formula for the state of the piston $f(X, V; t)$ for $t > 0$ is derived in a systematic way. Section 3 contains the analysis of physical implications of analytical results.

2. DYNAMICAL EVOLUTION OF THE PISTON

At the initial moment the piston is found at point $X_0 = 0$ with velocity $V_0 = 0$. So, the initial condition for the density $f(X, V; t)$ reads

$$f(X, V; 0) = \delta(X)\,\delta(V) \tag{4}$$

where δ is the Dirac distribution. We suppose that to the left of the piston there are N^- particles distributed within the interval $(-L, 0)$. Their initial states are (X_j, V_j), $j = -1, -2, \ldots, -N^-$, were X_j and, V_j denote the position and the velocity of particle j, respectively. Similarly, within the interval $(0, +L)$ on positive semi-axis there are N^+ particles occupying the states (X_j, V_j), $j = 1, 2, \ldots, N^+$.

The hard point dynamics with free boundary conditions implies that the piston at any moment follows one of the free trajectories $(X_a + V_a t)$ with velocity V^a, where $a \in \{-N^-, \ldots, -1, 0, +1, \ldots, N^+\}$.

As the number of particles on the left-hand side of the piston is a conserved quantity we can identify the free trajectory $(X_a + V_a t)$ followed by the piston at time t by imposing the requirement

$$\sum_{j=-N^-, j\neq a}^{N^+} \theta(X_a + V_a t - X_j - V_j t) = N^- \tag{5}$$

where θ is the unit Heaviside step function.

Therefore, the state of the piston at time $t > 0$ is given by the formula

$$f^L(X, V; t) = \left\langle \sum_{a=-N^-}^{N^+} \delta(X - X_a - V_a t)\, \delta(V - V_a) \right.$$
$$\left. \times\, \delta^{Kr}\left(N_-, \sum_{j=-N^-, j\neq a}^{N^+} \theta(X_a + V_a t - X_j - V_j t)\right)\right\rangle \tag{6}$$

where the brackets $\langle \ldots \rangle$ denote averaging over the initial statistical ensemble.

In order to pursue the calculation it is convenient to use the integral representation of the Kronecker delta $\delta^{Kr}(a, b)$ in the form

$$\delta^{Kr}(a, b) = \int_C \frac{dz}{2\pi i z}\, z^{(a-b)}, \qquad a, b \text{ integers} \tag{7}$$

where the contour C in the complex z-plane is a unit circle centered at the origin.

A straightforward calculation, analogous to that described in detail in ref. 4, leads then to the formula

$$f^L(X, V; t) = \int_C \frac{dz}{2\pi i z}\, [A(z, X/t \mid L/t)]^{N^-}\, [B(z, X/t \mid L/t)]^{N^+}$$
$$\times \{n^- \phi^-(V)\, \theta(Vt - X)\, \theta(X - Vt + L) [A(z, X/t|L/t)]^{-1}$$
$$\times [1 + (z-1)\, \theta(-X)] + \delta(X)\, \delta(V)$$
$$+ n^+ \phi^+(V)\, \theta(X - Vt)\, \theta(L - X + Vt) [1 + (z^{-1} - 1)\, \theta(X)]$$
$$\times [B(z, X/t|L/t)]^{-1}\} \tag{8}$$

Here

$$A(z, X/t \mid L/t)$$
$$= 1 + (z-1)\left[\int_{(L+X)/t}^{\infty} dU\, \phi^-(U) + \frac{1}{L}\int_{X/t}^{(X+L)/t} dU\, (Ut - X)\, \phi^-(U)\right] \tag{9}$$

$$B(z, X/t \mid L/t)$$
$$= 1 + (z^{-1}-1)\left[\int_{-\infty}^{(X-L)/t} dU\, \phi^+(U) + \frac{1}{L}\int_{(X-L)/t}^{X/t} dU\, (X - Ut)\, \phi^+(U)\right] \tag{10}$$

Equations (8), (9), (10) define the statistical state of the piston for any initial volume $[-L, +L]$ with free boundary conditions. In order to determine the evolution of the piston in an infinite space R^1 we have thus to take the limit $L \to \infty$, at fixed X, V, t and at fixed number densities $n^{\pm}$. We consider in this way a purely intrinsic dynamics of the system, with no influence of the boundaries. This situation is quite different from that studied in ref. 5 where recollisions with the boundaries played an essential role.

Taking the $L \to \infty$ limit we find

$$\begin{aligned} f(X, V; t) \equiv \lim_{L \to \infty} f^L(X, V; t) = \int_C \frac{dz}{2\pi i z} \Big\{ \delta(X)\, \delta(V) + n^- \phi^-(V)\, \theta(Vt - X) \\ \times [1 + (z-1)\, \theta(-X)] + n^+ \phi^+(V)\, \theta(X - Vt) \Big[1 + \Big(\frac{1}{z} - 1 \Big) \theta(X) \Big] \Big\} \\ \times \exp \Big\{ n^-(z-1) \int_{X/t}^{\infty} dU\, (Ut - X)\, \phi^-(U) \\ + n^+ \Big(\frac{1}{z} - 1 \Big) \int_{-\infty}^{X/t} dU\, (X - Ut)\, \phi^+(U) \Big\} \end{aligned} \tag{11}$$

Equation (11) defines the state of the piston for any $t > 0$. The probability density $f(X, V; t)$ can be expressed in terms of the Bessel functions owing to the formula

$$\int_C \frac{dz}{2\pi i z} \exp \Big[z\alpha + \frac{1}{z} \beta \Big] = I_0(2 \sqrt{\alpha\beta}) \tag{12}$$

We shall also use the relation

$$\frac{d}{dz} I_0(z) = I_1(z) \tag{13}$$

Let us introduce the shorthand notation

$$\alpha(X/t) = \int_{X/t}^{\infty} dU \Big(U - \frac{X}{t} \Big) \phi^-(U) \tag{14}$$

$$\beta(X/t) = \int_{-\infty}^{X/t} dU \Big(\frac{X}{t} - U \Big) \phi^+(U) \tag{15}$$

Equations (12), (13) permit to rewrite the formula for the state of the piston in the form

$$
\begin{aligned}
f(X, V; t) = R(t)\, \delta(X)\, \delta(V) + \exp\{-t[n^{-}\alpha(X/t) + n^{+}\beta(X/t)]\} \\
\times \Bigg\{ [n^{-}\phi^{-}(V)\, \theta(Vt - X)\, \theta(X) + n^{+}\phi^{+}(V)\, \theta(X - Vt)\, \theta(-X)] \\
\times I_0(2t \sqrt{n^{-}n^{+}\alpha(X/t)\, \beta(X/t)}) \\
+ \Bigg[n^{-}\phi^{-}(V)\, \theta(Vt - X)\, \theta(-X) \sqrt{\frac{n^{+}\beta(X/t)}{n^{-}\alpha(X/t)}} \\
+ n^{+}\phi^{+}(V)\, \theta(X - Vt)\, \theta(X)] \sqrt{\frac{n^{-}\alpha(X/t)}{n^{+}\beta(X/t)}} \Bigg] \\
\times I_1(2t \sqrt{n^{-}n^{+}\alpha(X/t)\, \beta(X/t)}) \Bigg\}
\end{aligned}
\tag{16}
$$

The coefficient $R(t)$ of the product $\delta(X)\delta(V)$ is given by

$$
R(t) = \exp\{-t[n^{-}\alpha(0) + n^{+}\beta(0)]\}\, I_0(2t \sqrt{n^{-}n^{+}\alpha(0)\, \beta(0)}) \tag{17}
$$

where (see equations (14), (15))

$$
\alpha(0) = \sqrt{k_B T^{-}/2\pi m}, \qquad \beta(0) = \sqrt{k_B T^{+}/2\pi m}
$$

Clearly, $R(t)$ represents the probability weight for finding the piston in its initial state for $t > 0$. When $t \to \infty$, the asymptotic behaviour of the Bessel functions $I_\nu(z)$ for large $|z|$

$$
I_\nu(z) \approx \frac{e^z}{\sqrt{2\pi z}} \tag{18}
$$

implies the rapid vanishing of $R(t)$ according to the formula

$$
R(t) \sim \frac{\exp\{-t[\sqrt{n^{-}\alpha(0)} - \sqrt{n^{+}\beta(0)}]^2\}}{2\sqrt{\pi t \sqrt{n^{-}n^{+}\alpha(0)\beta(0)}}} \tag{19}
$$

Notice that this exponential decrease is significantly slowed down to a power law $\sim t^{-1/2}$ when the condition

$$
n^{-} \sqrt{k_B T^{-}} = n^{+} \sqrt{k_B T^{+}} \tag{20}
$$

is satisfied. Equation (20) expresses the equality of the initial collision frequencies (particle fluxes) on the left- and on the right-hand side of the piston.

The formula (16) is the main result of our calculation. Its physical content is discussed in the next section.

3. ASYMPTOTIC DRIFT VELOCITY

The velocity of the piston is entirely induced by collisions. We shall focus here on the study of the long time behaviour of the velocity distribution

$$
\begin{aligned}
\phi(V;t) &= \int dX\, f(X,V;t) \\
&= R(t)\,\delta(V) + t\int dW\, \exp\{-t[n^-\alpha(W)+n^+\beta(W)]\} \\
&\quad \times\Big\{[n^-\phi^-(V)\,\theta(V-W)\,\theta(W)+n^+\phi^+(V)\,\theta(W-V)\,\theta(-W)] \\
&\quad \times I_0(2t\sqrt{n^-n^+\alpha(W)\beta(W)}) \\
&\quad +\Bigg[n^-\phi^-(V)\,\theta(V-W)\,\theta(-W)\sqrt{\frac{n^+\beta(W)}{n^-\alpha(W)}} \\
&\quad +n^+\phi^+(V)\,\theta(W-V)\,\theta(W)]\sqrt{\frac{n^-\alpha(W)}{n^+\beta(W)}}\Bigg] \\
&\quad \times I_1(2t\sqrt{n^-n^+\alpha(W)\,\beta(W)})\Big\}
\end{aligned}
\tag{21}
$$

In writing equation (21) the change of the integration variable $X = Wt$ has been used.

The first term on the right hand side of (21) has been already analyzed. Using the large $|z|$ asymptotics (18) of the Bessel functions we find that when $t\to\infty$, the remaining terms take the form

$$
\begin{aligned}
&\int dW\, \frac{\sqrt{t}}{2\sqrt{\pi\sqrt{n^-n^+\alpha(W)\,\beta(W)}}}\exp\{-t[\sqrt{n^-\alpha(W)}-\sqrt{n^+\beta(W)}]^2\} \\
&\times\Bigg\{n^-\phi^-(V)\,\theta(V-W)\left[\theta(W)+\theta(-W)\sqrt{\frac{n^+\beta(W)}{n^-\alpha(W)}}\right] \\
&+n^+\phi^+(V)\theta(W-V)\left[\theta(-W)+\theta(W)\sqrt{\frac{n^-\alpha(W)}{n^+\beta(W)}}\right]\Bigg\}
\end{aligned}
\tag{22}
$$

The integrand in (22), considered as a function of variable W, vanishes for $t \to \infty$ everywhere but in one point $\bar{W}$ solving the equation

$$n^{-}\alpha(\bar{W}) = n^{+}\beta(\bar{W}) \tag{23}$$

or, (see definitions (14), (15))

$$n^{-}\int_{\bar{W}}^{\infty} dU(U-\bar{W})\,\phi^{-}(U) = n^{+}\int_{-\infty}^{\bar{W}} dU(\bar{W}-U)\,\phi^{+}(U) \tag{24}$$

When $W = \bar{W}$, the integrand diverges as $\sqrt{t}$. Considering the $t \to \infty$ limit we can thus rewrite equation (21) as

$$\begin{aligned}\phi(V;t) = {} & \frac{\sqrt{t}}{2\sqrt{\pi\sqrt{n^{-}n^{+}\alpha(\bar{W})\,\beta(\bar{W})}}}\{n^{-}\phi^{-}(V)\,\theta(V-\bar{W})\\ & +n^{+}\phi^{+}(V)\,\theta(\bar{W}-V)\}\\ & \times\int dW\,\exp\left\{-t\left[\sqrt{\frac{n^{-}}{\alpha(\bar{W})}}\,\alpha'(\bar{W})-\sqrt{\frac{n^{+}}{\beta(\bar{W})}}\,\beta'(\bar{W})\right]^{2}\left(\frac{W-\bar{W}}{2}\right)^{2}\right\}\end{aligned} \tag{25}$$

where $\alpha'(W)$, $\beta'(W)$ are first order derivatives of $\alpha(W)$ and $\beta(W)$, respectively.

$$\alpha'(W) = -\int_{W}^{\infty} dU\,\phi^{-}(U) \tag{26}$$

$$\beta'(W) = \int_{-\infty}^{W} dU\,\phi^{+}(U) \tag{27}$$

Evaluating the integral we find eventually the following asymptotic form of the velocity distribution

$$\phi^{\infty}(V) = \frac{1}{\Xi(\bar{W})}\,[n^{-}\phi^{-}(V)\,\theta(V-\bar{W})+n^{+}\phi^{+}(V)\,\theta(\bar{W}-V)] \tag{28}$$

where Ξ is the normalizing factor

$$\Xi(\bar{W}) = n^{-}\int_{\bar{W}}^{\infty} dU\,\phi^{-}(U)+n^{+}\int_{-\infty}^{\bar{W}} dU\,\phi^{+}(U)$$

Equation (28) shows the simple structure of the asymptotic stationary velocity distribution of the piston. The stationary drift velocity $\langle V\rangle$ equals

$$\langle V\rangle_\infty = \int dV\, V\phi^\infty(V) = \frac{1}{m\Xi(\bar{W})}\,[n^- k_B T^- \phi^-(\bar{W}) - n^+ k_B T^+ \phi^+(\bar{W})] \tag{29}$$

Let us recall that in equations (28) and (29) the velocity $\bar{W}$ is the solution of equation (24), so that $\bar{W}$ is a zero of function χ defined by

$$\begin{aligned}\chi(W) &= n^- k_B T^- \phi^-(W) - n^+ k_B T^+ \phi^+(W)\\ &\quad - mW\left(n^- \int_W^\infty dU\, \phi^-(U) + n^+ \int_{-\infty}^W dU\, \phi^+(U)\right)\end{aligned} \tag{30}$$

It follows that $\langle V\rangle_\infty = \bar{W}$.

Notice that $\chi(W)$ is a monotonically decreasing function, with exactly one zero, which shows that the drift velocity is uniquely defined. When condition (20) of equal fluxes is satisfied, we find $\bar{W} = 0$ and no drift is present. Of course, $\bar{W} = 0$ when both the temperatures and the pressures are equal on both sides of the piston. In this case our general formula (16) reduces to the solution of the self-diffusion problem derived in refs. 3 and 4 and equation (29) becomes $\phi^\infty(V) = \phi^-(V) = \phi^+(V)$, reflecting the asymptotic approach to thermal equilibrium.

However, if the initial pressures are equal

$$p = n^- k_B T^- = n^+ k_B T^+$$

a nonzero drift occurs for nonzero temperature difference

$$\langle V\rangle_\infty = \frac{p}{m\Xi(\bar{W})}\,(\phi^-(\bar{W}) - \phi^+(\bar{W})) \tag{31}$$

Suppose that $p^- = p^+ = p$, and $T^+ > T^-$. Then

$$\chi(0) = p\left[\sqrt{\frac{m}{2\pi k_B T^-}} - \sqrt{\frac{m}{2\pi k_B T^+}}\right] > 0$$

As the function $\chi(W)$ is monotonically decreasing, it attains zero for $W = \bar{W} > 0$. The drift is thus oriented towards the higher temperature region.

This rigorous conclusion qualitatively coincides with the prediction based on Boltzmann's kinetic equation.[2] However, as it has been already remarked in the introduction, the Boltzmann equation does not predict the vanishing of the drift at equal fluxes, yielding rather a different, and physically less transparent condition (2). We find here the situation where neglecting the recollision processes, which create precollisional correlations, absent in Boltzmann's theory, leads to an erroneous prediction. It is only by taking into account all possible dynamic events, inculding the interaction of the piston with the perturbations it causes in the states of the surrounding medium, that we arrive at a simple equal flux condition (20).

We have mentioned in the introduction that the choice of the initial state in the present paper was suggested by the thermodynamic adiabatic piston problem.[1] This is also why our discussion was focused on the phenomenon of the drift velocity induced by collisions. Of course, one can look at the probability density (16) as describing self-diffusion in a special type of an inhomogeneous medium, composed of two semi-infinite volumes of the gas in different thermodynamic states. A general study of the motion of a tagged particle in an inhomogeneous environment presents an interesting question for future investigation (for previous works on this subject see refs. 6 and 7).

A still challenging problem is to develop a rigorous approach in the case where the mass of the piston M is different from that of the surrounding particles. The perturbative argument based on the Boltzmann equation predicts a nonzero drift at equal pressures even for $M \gg m$.[8] A quite different dynamical evolution occurs when the system fills a finite volume and boundary conditions become of great importance. In a recent work dealing with this question a scaling regime for a massive piston in an ideal gas has been studied, leading to a system of coupled autonomous equations whose physical content is still being analyzed[9].

Finally, it seems worth noting that the solution (16) contains the complete information about the modes of approach to the asymptotic stationary state for arbitrary values of the initial thermodynamic parameters. We plan to study this question thoroughly.

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