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Approach to Field-Induced Stationary State in a Gas of Hard Rods

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The Boltzmann equation describing one-dimensional motion of a charged hard rod in a neutral hard rod gas at temperature $T = 0$ is solved. Under the action of a constant and uniform field the charged particle attains a stationary state. In the long time limit the velocity autocorrelation function decays via damped oscillations. In the reference system moving with the mean particle velocity the decay of fluctuations in the position space is governed (in the hydrodynamic limit) by the diffusion equation. Both the stationary current and the diffusion coefficient are proportional to the square root of the field. It is conjectured that this result also holds for $T > 0$ in a strong field limit.

KEY WORDS: Hard rod gas; Boltzmann's equation; diffusion; stationary state.

1. INTRODUCTION

In his 1978 paper,[1] P. Resibois solved and analyzed the self-diffusion problem for a hard rod gas at the level of Boltzmann's description. The probability density $f(r, v, t)$ for finding the test particle at time t with velocity v and position r satisfies then the linear kinetic equation

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial r}\right)f(r,v,t) = \rho\int dc\,|v-c|\left[f(r,c,t)\varphi(v) - f(r,v,t)\varphi(c)\right] \quad (1.1)$$

in which $\rho\varphi(v)$ represents the stationary uniform phase space density of the host hard rod fluid.

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Assuming $\varphi(v)$ to be Maxwell's distribution

$$\varphi^M(v) = \left(\frac{m}{2\pi k_B T}\right)^{1/2} \exp\left(-\frac{mv^2}{2k_B T}\right) \tag{1.2}$$

(m is the particle mass, T the temperature of the fluid, and k_B Boltzmann's constant) Resibois solved the initial-value problem for Eq. (1.1). He found in particular the solution $f_s(r, v, t)$ corresponding to the initial condition

$$f_s(r, v, 0) = \delta(r)\varphi^M(v) \tag{1.3}$$

where $\delta(r)$ denotes Dirac's distribution. The spatial density

$$n_s(r, t) = \int dv\, f_s(r, v, t) \tag{1.4}$$

represents the conditional probability density for finding the test particle at point r and time t, provided it was initially at the origin with equilibrium velocity distribution $\varphi^M(v)$ (the so-called van Hove self-correlation function). It has been proved that for long times (in the hydrodynamic limit) the evolution of density $n_s(r, t)$ is governed by the diffusion equation.

One can, however, expect a qualitative change at zero temperature, where

$$\varphi(v) = \lim_{T \searrow 0} \varphi^M(v) = \delta(v) \tag{1.5}$$

Indeed, in this case the test particle suffers collisions with particles at rest. When an encounter takes place its velocity instantaneously vanishes. The particle gets stopped and it cannot move anymore (not true for $T > 0$). The cooling effect of the medium is so strong that it rules out the diffusive behavior. To see this, let us insert (1.5) into (1.1). The kinetic equation now reads

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial r} + \rho|v|\right) f(r, v, t) = \rho\delta(v) \int dc\, |c| f(r, c, t) \tag{1.6}$$

Any distribution of the form

$$n(r)\delta(v) \tag{1.7}$$

yields a stationary state. The fundamental solution of (1.6) corresponding to the initial condition

$$f(r, v, 0) = \delta(r - r_0)\delta(v - v_0), \qquad v_0 \neq 0 \tag{1.8}$$

has the form

$$\begin{aligned} f(r, v, t \mid r_0, v_0) = {} & \delta(v - v_0)\delta(r - r_0 - v_0 t)\exp(-\rho|v_0|t) \\ & + \rho\Theta[v_0(r - r_0)]\Theta(|v_0|t - |r - r_0|)\exp(-\rho|r - r_0|)\delta(v) \end{aligned} \tag{1.9}$$

where Θ is the Heaviside step function

$$\Theta(x) = \begin{cases} 1, & x \geqslant 0 \\ 0, & x < 0 \end{cases} \tag{1.10}$$

Hence, in the limit $t \to \infty$, the spatial density gets frozen in the shape

$$n(r, \infty \mid r_0, v_0) = \rho\Theta[v_0(r - r_0)]\exp(-\rho|r - r_0|) \tag{1.11}$$

A uniform distribution cannot be attained. The diffusion process disappears.

The main problem which we want to discuss in this paper is what happens when the test particle has a charge which couples to a constant and uniform external field. Brief comments on the effect of the field at finite temperature T can be found in the rigorous study of self-diffusion in a hard rod fluid by Lebowitz and Percus.[2] The discussion is, however, restricted there to the linear response term. Here we solve exactly the Boltzmann equation

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial r} + a\frac{\partial}{\partial v} + \rho|v|\right)f(r, v, t) = \rho\delta(v)\int dc\,|c|\,f(r, c, t) \tag{1.12}$$

describing the propagation of the test particle through zero temperature fluid under the action of the field giving rise to a constant acceleration a (term $a\partial/\partial v$).

One can ask the following physically relevant questions: (i) Will the system be driven to a stationary state? It has been established that for the Lorentz model in which the charged particle ("electron") conserves its energy at collisions with infinitely heavy scatterers ("ions") no stationary state (in an infinite space) is possible.[3] The situation considered here is quite different, as the scatterers are mechanically identical to the charged test particle. (ii) What is the dynamics of the fluctuations around the stationary state? Will the diffusive mode be restored by the field? (iii) Can one apply to Eq. (1.12) the linear response theory? Answers to these questions are given in the following two sections. The paper ends with some comments on what one can learn from the results obtained here about the behavior of the system at finite temperature.

2. STATIONARY STATE

The stochastic motion of the test particle corresponding to Eq. (1.12) consists of periods of time in which it moves with a constant acceleration and of collisions which instantaneously break the motion and stop the particle. Then the field makes it move again, and so on. It is thus clear that in a stationary state only velocities in the direction of the field can be observed. Consequently, assuming that $a > 0$, we look for the stationary velocity distribution in the form

$$\varphi^{st}(v) = \Theta(v)\, g(v) \tag{2.1}$$

Inserting (2.1) into (1.12) one finds

$$\Theta(v)\left[a\frac{\partial}{\partial v} + \rho v\right] g(v) + \left[a - \rho\int_0^\infty dc\, cg(c)\right]\delta(v) = 0 \tag{2.2}$$

The general solution of (2.2): $g(v) = \text{const}\exp(-\rho v^2/2a)$ leads to the normalized stationary distribution

$$\varphi^{st}(v) = \Theta(v)\left(\frac{2\rho}{a\pi}\right)^{1/2} \exp\left(-\frac{\rho v^2}{2a}\right) \tag{2.3}$$

Distribution φ^{st} is one-half of Maxwell's distribution with "temperature" proportional to the acceleration a and inversely proportional to the density ρ. The charged particle moves under the action of the field with mean velocity

$$u = \left(\frac{2a}{\pi\rho}\right)^{1/2} \tag{2.4}$$

and mean kinetic energy (ma/ρ). The result (2.4) indicates that the linear response theory cannot be applied to Eq. (1.12) (we come back to this point in the last section).

In order to investigate how the system is actually driven to the stationary state, one has to solve the initial value problem for Eq. (1.12). Clearly, the solution must have the form

$$f(r,v,t) = \exp\left(-\frac{\rho v|v|}{2a}\right)\left\{\Theta(v)\chi^+\left(v - at, \frac{v^2}{2} - ar\right) + \Theta(-v)\chi^-\left(v - at, \frac{v^2}{2} - ar\right)\right\} \tag{2.5}$$

and satisfy the condition

$$\lim_{v\to 0^+} f(r,v,t) - \lim_{v\to 0^-} f(r,v,t) = \chi^+(-at, -ar) - \chi^-(-at, -ar) = a^{-1}\rho\int dc\,|c|f(r,c,t) \tag{2.6}$$

Equation (2.6) implies that for $v < 0$

$$\chi^-\left(v - at, \frac{v^2}{2} - ar\right) = \chi^+\left(v - at, \frac{v^2}{2} - ar\right) - a^{-1}\rho\int dc\,|c| f\left(r - \frac{v^2}{2a}, c, t - \frac{v}{a}\right) \tag{2.7}$$

Inserting (2.7) into (2.5) and putting $t = 0$ one finds

$$\chi^{+}\left(v, \frac{v^2}{2} - ar\right) = \exp\left(\frac{\rho}{2a} v|v|\right) f(r, v, 0)$$
$$+ a^{-1}\rho\Theta(-v)\int dc\,|c| f\left(r - \frac{v^2}{2a}, c, -\frac{v}{a}\right) \quad (2.8)$$

Combining now Eq. (2.5), (2.7), and (2.8) one arrives at an integral equation

$$f(r, v, t) = \exp\left\{-\frac{\rho}{2a}\left[v|v| - (v - at)|v - at|\right]\right\} f\left(r - vt + \frac{at^2}{2}, v - at, 0\right)$$
$$+ u^{-1}\varphi^{\mathrm{st}}(v)\Theta(at - v)\int dc\,|c| f\left(r - \frac{v^2}{2a}, c, t - \frac{v}{a}\right) \quad (2.9)$$

where $\varphi^{\mathrm{st}}(v)$ and u are given by Eq. (2.3) and (2.4), respectively. The normalization condition has the form

$$\int dv \exp\left\{-\frac{\rho}{2a}\left[(v + at)|v + at| - v|v|\right]\right\}\varphi(v, 0)$$
$$+ a\int_0^t d\tau\, \varphi^{\mathrm{st}}(a\tau)\mu(t - \tau) = 1 \quad (2.10)$$

where

$$\mu(t) = u^{-1}\int dv\,|v|\varphi(v, t) \quad (2.11)$$

and $\varphi(v, t)$ is the velocity distribution. The second term in the right-hand side of Eq. (2.10) has the convolution structure. $\mu(t)$ can thus be calculated in a straightforward way by using the Laplace transform method. Knowing $\mu(t)$ one knows $\varphi(v, t)$ as integrating Eq. (2.9) over r yields the relation

$$\varphi(v, t) = \exp\left\{-\frac{\rho}{2a}\left[v|v| - (v - at)|v - at|\right]\right\}\varphi(v - at, 0)$$
$$+ \varphi^{\mathrm{st}}(v)\Theta(at - v)\,\mu\left(t - \frac{v}{a}\right) \quad (2.12)$$

From (2.10) one finds

$$\mu(t) = \int \frac{dz}{2\pi i}\,\frac{\exp(zt - z^2/2\rho a)}{\operatorname{erfc}\left[z(2\rho a)^{-1/2}\right]}$$
$$\times\left[\frac{1}{z} - \int_0^\infty dt \int dv \exp\left\{-z\tau - \frac{\rho}{2a}\left[(v + a\tau)|v + a\tau| - v|v|\right]\right\}\right.$$
$$\left.\times\,\varphi(v, 0)\right] \quad (2.13)$$

where

$$\operatorname{erfc} z = 2\pi^{-1/2}\int_z^\infty dt \exp(-t^2) \tag{2.14}$$

and the integral over the complex variable z represents the inverse Laplace transformation.

The complementary error function $\operatorname{erfc} z$ is an entire function with no zeros in the half-plane $\operatorname{Re} z > -1$. Its first zeros (closest to the origin) $z_0^{\pm} = x_0 \pm iy_0$ have coordinates[4]

$$x_0 \simeq -1.35, \qquad y_0 \simeq 1.99 \tag{2.15}$$

Hence, when $t \to \infty$ only the pole at $z = 0$ contributes to the right-hand side of (2.13), and we find

$$\lim_{t\to\infty} \mu(t) = 1 \tag{2.16}$$

This means that Eq. (2.12) does describe the approach to the stationary state (2.3). In the next section we discuss in more detail this point by studying the temporal behavior of fluctuations.

3. DYNAMICS OF FLUCTUATIONS

Fluctuations of the velocity of the charged particle around its mean value u [see Eq. (2.4)] are described by the velocity autocorrelation function

$$\Gamma(t) = \langle v(t)v\rangle_{\mathrm{st}} - u^2$$

Here, $\langle\ \rangle_{\mathrm{st}}$ denotes the average value, with respect to the stationary distribution (2.3). Using formulas (2.12) and (2.13) with the initial condition $\varphi(v,0) = v\varphi^{\mathrm{st}}(v)$ one readily finds the Laplace transform of $\Gamma(t)$

$$\tilde{\Gamma}(z) = \int_0^\infty dt \exp(-zt)\Gamma(t) \tag{3.1}$$

$$= au\left\{\frac{1}{z^2}\left[\frac{\exp(-z^2/2\rho a)}{\operatorname{erfc}\left[z(2\rho a)^{-1/2}\right]} - 1\right] - \frac{u}{az}\right\} \tag{3.2}$$

$\Gamma(z)$ has no singularity at $z = 0$. We find

$$\lim_{z\to 0}\tilde{\Gamma}(z) = \left(\frac{4-\pi}{2\pi}\right)\frac{u}{\rho} \tag{3.3}$$

The approach to zero of $\Gamma(t)$ in the long time limit is determined by the poles of $\tilde{\Gamma}(z)$ at $z_0^{\pm} = x_0 \pm iy_0$ [see Eq. (2.15)]. For $t \to \infty$ the velocity autocorrelation function vanishes via exponentially damped oscillations with relaxation time $\tau_0 = x_0^{-1}(2\rho a)^{-1/2}$, and the period of oscillations $T_0 = |y_0|^{-1}(2\rho a)^{-1/2}$.

We shall show now that Eq. (3.3) defines the diffusion coefficient which appears in the asymptotic (hydrodynamic) evolution of fluctuations in the position space.

To this end, let us suppose that the charged particle is initially at the origin with the velocity distribution $\varphi^{st}(v)$. In order to calculate the probability density $n_s(r,t)$ for finding it at time t at point r (van Hove's self-correlation function in a stationary state) one has to solve the integral equation (2.9) with the initial condition

$$f_s(t,v,0) = \delta(r)\varphi^{st}(v) \tag{3.4}$$

Inserting (3.4) into (2.9) and applying to the resulting equation the Fourier and Laplace transformations we find

$$\hat{f}_s(k,v,z) = \left\{ \int_0^{v/a} dt \exp\left[-(z+ikv)t + ik\frac{at^2}{2} \right] + u^{-1}\exp\left[-\frac{zv}{a} - ik\frac{v^2}{2a} \right] \int_0^{\infty} dc\, c\hat{f}_s(k,c,z) \right\} \varphi^{st}(v) \tag{3.5}$$

where

$$\hat{f}_s(k,v,z) = \int dr \exp(-ikr) \int_0^{\infty} dt \exp(-zt) f(r,v,t) \tag{3.6}$$

Equation (3.5) can be readily solved for $\hat{f}_s(k,v,z)$. Integrating then over v one obtains the following result:

$$\hat{n}_s(k,z) = \hat{n}_0(k,z) + \frac{(\rho+ik)\alpha(z,k)}{ik+\rho z\alpha(z,k)} \left[\rho u\alpha(z,k) + ika\frac{\partial}{\partial z}\hat{n}_0(k,z) \right] \tag{3.7}$$

where $\hat{n}_0(k,z)$ is the Fourier–Laplace transform of the function

$$n_0(r,t) = \left\langle \Theta(v-at)\delta\left(r - vt + \frac{at^2}{2} \right) \right\rangle_{st} \tag{3.8}$$

and

$$\alpha(z,k) = \left[\frac{\pi}{2a(\rho+ik)} \right]^{1/2} \exp\left[\frac{z^2}{2a(\rho+ik)} \right] \operatorname{erfc}\left(\frac{z}{[2a(\rho+ik)]^{1/2}} \right) \tag{3.9}$$

The term $n_0(r,t)$ vanishes rapidly and plays no role in the long-time limit. The long time behavior of the spatial density $n_s(r,t)$ is determined by the solutions of the dispersion relation

$$ik + \rho z\alpha(z,k) = 0 \tag{3.10}$$

[see Eq. (3.7)]. $\alpha(z,k)$ is an entire function of the complex variable z. When

$z \to 0$, we can use its asymptotic representation

$$\alpha(z,k) \underset{z\to 0}{=} \left[\frac{\pi}{2a(\rho + ik)} \right]^{1/2} - \frac{z}{a(\rho + ik)} \tag{3.11}$$

Inserting (3.11) into (3.10) and solving for z one finds

$$z(k) = -iuk - Dk^2 + o(k^2) \tag{3.12}$$

where

$$D = \left(\frac{4-\pi}{2\pi} \right) \frac{u}{\rho} = \int_0^\infty dt\, \Gamma(t) \tag{3.13}$$

[see Eq. (3.3)].

$z(k)$ has the structure corresponding formally to the hydrodynamic sound mode frequency. The role of "sound velocity" is played here by u, whereas the damping coefficient D is determined by the time integral of the velocity autocorrelation function. The field restores thus the hydrodynamic behavior. In the long time limit and at large distances the charged particle, localized initially at $r = 0$, propagates in the direction imposed by the field according to the law

$$n_s(r,t) \underset{\substack{t\to\infty \\ r-ut \simeq t^{1/2}}}{=} \int \frac{dk}{2\pi} \int \frac{dz}{2\pi i} \frac{\exp(zt)}{\left[z - z(k)\right]} = \left[4\pi Dt\right]^{-1/2} \exp\left[-\frac{(r-ut)^2}{4Dt} \right] \tag{3.14}$$

In the reference system moving with velocity u we observe the simple diffusion process. The initial delta-fluctuation at $r = 0$ decays away at large distances [see Eq. (3.14)] only as $t^{-1/2}$.

4. DISCUSSION

The hydrodynamic frequency (3.12) is a pure effect of the external field. Both the mean velocity u and the diffusion coefficient D are proportional to $a^{1/2}$, and vanish for $a = 0$. The nonanalyticity at $a = 0$ shows that the linear response theory cannot be applied to the kinetic equation (1.12). This fact was to be expected. Indeed, at finite temperature T the medium provides a characteristic energy ($k_B T$) corresponding to the thermal motion. One can then give a meaning to the weak field limit by requiring that the energy absorbed by the charged particle on a mean free path is much smaller than its thermal energy

$$ma\rho^{-1} \ll k_B T \tag{4.1}$$

It is in region (4.1) that the linear response approach should give valuable information. For $T = 0$ inequality (4.1) cannot be satisfied. The thermal energy scale disappears and in a sense the field becomes infinitely strong at any value of a.

It seems thus reasonable to conjecture that for a system at temperature $T > 0$ our results describe correctly the properties of the stationary state and the dynamics of fluctuations for very strong fields: $ma\rho^{-1} \gg k_B T$. The fact that the current becomes then proportional to $a^{1/2}$ may even remain true in three dimensions. Indeed, putting $T = 0$ we shall be left again (as in one dimension) with only one physical parameter involving time, the acceleration a. The mean velocity in the stationary state (if there is any) must be proportional to $a^{1/2}$ for dimensional reasons.

Let us finally stress that the presence of a stationary current introduces a qualitative change in the hydrodynamic mode of motion. At zero field and $T > 0$ a purely diffusive law is found[1,2] whereas the hydrodynamic frequency (3.12) contains the imaginary part $(-iuk)$, reflecting the uniform propagation of the density fluctuation with mean velocity u. It should be expected that this important modification persists also for $T > 0$.

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