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Dynamics of a Charged Test Particle in a Hard Rod Fluid

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The motion of a charged hard rod, accelerated by a constant and uniform external field, in a fluid of mechanically identical neutral particles is studied. The system, initially at rest, is excited through collisions with the accelerated particle. A class of initial configurations is found for which recollisions between the charged rod and the excitation caused by it (a moving particle) never occur. The evolution of the velocity distribution of the test particle is analyzed in this case. The possibility of obtaining from microscopic dynamics a kinetic equation is discussed. The dependence of the current on the external field is shown to agree with that predicted by the Boltzmann equation.

KEY WORDS: Hard rod fluid; probability density; Boltzmann's equation.

1. INTRODUCTION

The one-dimensional hard rod fluid has been the object of numerous studies and is until now used to analyze problems of kinetic theory. Following the early papers concerned with mechanisms of irreversibility[1,2] efficient methods were elaborated to calculate exactly dynamical properties of the fluid.[3–5] Among variety of questions which have been discussed in great detail one finds investigations of the density expansion of kinetic equations,[4] calculation of the dynamical structure factor,[5] analysis of the behavior of kinetic equations with respect to the time reversal,[6] solution of Boltzmann's equation,[7] and relation between time correlation functions and transport coefficients.[8] Papers dealing with problems of Markovian limits and ergodic properties have been reviewed by H. Spohn.[9]

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Despite these extensive studies there is, however, relatively little known as yet about the dynamics of hard rod fluids in the presence of an external field. Apart from the discussion of conductivity based on the Kubo formula[3] and linear response calculations[4] one can hardly find any results. It has been shown recently that the propagation of a charged hard rod in a neutral hard rod gas at temperature $T = 0$ creates a stationary current proportional to the square root of the external field, when Boltzmann's equation is used.[10] This is, however, an approximate description. The purpose of the present note is to make a step toward a rigorous analysis of the stochastic process followed by the charged rod. This is achieved here only for a special class of initial conditions characterized in Section 2. In Section 3 the corresponding dynamical evolution and asymptotic steady states are discussed. Final comments are presented in Section 4.

2. INITIAL CONDITIONS: ELIMINATING RECOLLISIONS

The system considered here is a one-dimensional fluid composed of mechanically identical hard rods of diameter d, distributed on a line. One of the rods, playing the role of a test particle, has a charge which couples to a uniform, constant external field, giving rise to acceleration a. All the remaining particles are neutral and move freely between collisions, unaffected by the field. The dynamics of binary encounters reduces to instantaneous exchanges of velocities between colliding rods.

We shall study dynamical effects entirely due to the field by assuming the fluid particles to be initially at rest. The charged rod begins then to move under the action of the field with acceleration $a > 0$. In the course of time more and more particles acquire a nonzero velocity through collisions, and this excitation propagates through the system. Our aim in this section is to characterize the class of initial conditions which rule out the possibility of interaction between the test particle and the excitation caused by it. In other words, we want to investigate under what conditions recollisions do not occur so that the charged rod always collides with a particle at rest and its propagation develops as if the host fluid was not excited, leading to a great simplification in the mathematical description. It should be mentioned here that the possibility of having dynamical evolution without recollisions has been already remarked by P. Résibois[7] in the special case of a gas of hard points moving with two allowed velocities (no external field). The distribution of the tagged particle satisfies in this case rigorously the Boltzmann equation, provided molecular chaos is valid at the initial moment.

Going back to our problem let us suppose that the charged rod begins its motion at time $t = 0$ from point $x_0 = 0$. As $a > 0$, it is accelerated along the positive x axis. Neutral rods, numbered $1, 2, 3, \ldots,$ are distributed there at points $x_1, x_2, x_3, \ldots,$ respectively. The labeling is such that $x_1 < x_2 < x_3 \ldots$ As the linear ordering of particles is preserved by the dynamics the charged rod will always encounter the same neighboring rod 1.

The first collision occurs at time τ_1 satisfying the equation

$$a\tau_1^2/2 = x_1 - d \tag{2.1}$$

The test particle gets stopped at point $(x_1 - d)$, from which it starts again its accelerated motion. Simultaneously rod 1 begins a uniform motion with velocity $a\tau_1$. It has to cover the distance $(x_2 - x_1 - d)$ to reach rod 2, and needs time $[(x_2 - x_1 - d)/a\tau_1]$ for it. Therefore, only if the inequality

$$x_2 - x_1 - d > \frac{a}{2}\left(\frac{x_2 - x_1 - d}{a\tau_1}\right)^2 \tag{2.2}$$

is satisfied the charged rod will not collide with its neighbor before the latter is immobilized by a collision with rod 2. Using equation (2.1) one can conveniently rewrite condition (2.2) in the form

$$x_2 - x_1 - d < 4(x_1 - x_0 - d), \qquad x_0 = 0 \tag{2.3}$$

When inequality (2.3) holds the second collision suffered by the test particle follows the first one after time τ_2 satisfying the equation

$$a\tau_2^2/2 = x_2 - x_1 - d \tag{2.4}$$

The charged rod is stopped now at the point $(x_2 - 2d)$, and rod 1 starts a uniform motion with velocity $a\tau_2$ from point $(x_2 - d)$. There is also a particle which carries the excitation caused by the first collision and moves with velocity $a\tau_1$. One can repeat now the same reasoning which led to inequality (2.3), considering, however, the possibility of particle 1 getting back velocity $a\tau_1$ through a collision with particle 2. This results in a set of two inequalities

$$x_3 - x_2 - d < 4(x_a - x_{a-1} - d), \qquad a = 1, 2 \tag{2.5}$$

which represent a sufficient condition for the occurrence of the third collision between the charged rod and rod 1 only when the latter is immobile.

Clearly this analysis can be continued along the same lines yielding the following general conclusion: The class of initial spatial configurations of the neutral fluid particles characterized by sets of inequalities

$$\left.\begin{array}{r} x_j - x_{j-1} - d < 4(x_a - x_{a-1} - d) \\ a = 1, 2, \ldots, j-1 \end{array}\right\}, \qquad j = 2, 3, \ldots \tag{2.6}$$

do not lead at any time $t > 0$ to an interaction between the test particle and the excitation caused by it. In the course of the dynamical evolution starting from any of such configurations consecutive collisions of the charged rod with its neighbor will occur at the moments when the latter is at rest. Denoting by τ_j the time interval between consecutive collisions $(j-1)$ and j

$$\tau_j = \left[2(x_j - x_{j-1} - d)/a\right]^{1/2} \tag{2.7}$$

one can rewrite inequalities (2.6) in a compact form

$$\left.\begin{array}{r} \tau_j < 2\tau_a \\ a = 1, 2, \ldots, j-1 \end{array}\right\} \quad j = 2, 3, \ldots \tag{2.8}$$

3. DYNAMICS OF THE CHARGED PARTICLE

For a given microscopic configuration of the host fluid, satisfying conditions (2.6), the phase space trajectory of the charged rod can be described in a simple way. Indeed, its velocity $v(t)$ and position $x(t)$ between collisions j and $(j+1)$

$$\sum_{i=1}^{j} \tau_i < t < \sum_{i=1}^{j+1} \tau_i \tag{3.1}$$

are given by equations

$$\begin{aligned} v(t) &= a\left(t - \sum_{i=1}^{j} \tau_i\right) \\ x(t) &= \frac{a}{2} \sum_{i=1}^{j} \tau_i^2 + \frac{1}{2a}\left[v(t)\right]^2 \end{aligned} \tag{3.2}$$

Consequently, the probability density $f(x, v, t \mid \{\tau_j\})$ for finding the test particle with velocity v at point x at time t when it follows the trajectory characterized by the sequence $(\tau_1, \tau_2, \ldots)$ reads

$$\begin{aligned} &f(x, v, t \mid \{\tau_j\}) \\ &\quad = \theta(v) \sum_{j=0}^{\infty} \theta(a\tau_{j+1} - v)\delta\left[x - \frac{a}{2}\sum_{i=1}^{j} \tau_i^2 - \frac{v^2}{2a}\right]\delta\left[v - a\left(t - \sum_{i=1}^{j} \tau_i\right)\right] \end{aligned} \tag{3.3}$$

where

$$\theta(v) = \begin{cases} 1, & \text{for} \quad v \geqslant 0 \\ 0, & \text{for} \quad v < 0 \end{cases}$$

In statistical mechanics we are led to consider various possible microscopic trajectories, as the initial state of the fluid is described in a probabilistic way. This induces a stochastic process for the velocity and position of the charged rod. The probability density $f(x, v, t)$ for finding the test particle at time t in point x with velocity v takes the form

$$f(x,v,t) = \theta(v) \sum_{j=0}^{\infty} \int d\tau_1 \cdots \int d\tau_{j+1} \rho_{j+1}(\tau_1, \ldots, \tau_{j+1}) \theta(a\tau_{j+1} - v) \\ \times \delta\left[x - \frac{a}{2} \sum_{i=1}^{j} \tau_i^2 - \frac{v^2}{2a}\right] \delta\left[v - a\left(t - \sum_{i=1}^{j} \tau_i\right)\right] \tag{3.4}$$

where $\rho_n(\tau_1, \ldots, \tau_n)$ is the joint probability density for the time intervals between collisions $(\tau_1, \ldots, \tau_n)$, compatible with inequalities (2.8).

Two quite different cases will be studied in this note. First, the case of factorized distributions

$$\rho_n(\tau_1, \ldots, \tau_n) = \prod_{i=1}^{n} \rho(\tau_i), \qquad n = 1, 2, \ldots \tag{3.5}$$

where the density $\rho_1(\tau) = \rho(\tau)$ is supposed to vanish outside an interval $(\tau_{\min}, \tau_{\max})$, such that $0 < \tau_{\min} < \tau_{\max} < 2\tau_{\min}$. As for any two points τ, τ' lying between $\tau_{\min}$ and $\tau_{\max}$ the inequalities $(\tau < 2\tau')$ and $(\tau' < 2\tau)$ simultaneously hold, the initial state (3.5) gives a nonzero weight only for sequences $(\tau_1, \tau_2, \ldots)$ satisfying conditions (2.8).

The second case will correspond to the dynamical effect of periodic initial configurations, weighted by a probability density $\rho(\tau)$

$$\rho_n(\tau_1, \ldots, \tau_n) = \int d\tau \, \rho(\tau) \prod_{i=1}^{n} \delta(\tau_i - \tau), \qquad n = 1, 2, \ldots \tag{3.6}$$

Clearly, when all intervals between collisions are equal inequalities (2.8) are satisfied. So (3.6) is also an admissible state. In order to exclude the possibility of an accumulation of an infinite number of collisions in a finite time it will be assumed that $\rho(\tau)$ in Eq. (3.6) vanishes for $\tau < \tau_{\min}$, $\tau_{\min} > 0$. The initial state (3.6) is different from that described by Eq. (3.5) in that it introduces correlations between time intervals separating collisions, whereas the latter does not.

The main object of our study will be the evolution of the velocity distribution $\phi(v, t)$ of the charged rod. When the initial state of the host fluid has the form (3.5) we get from Eq. (3.4)

$$\varphi(v,t) = \frac{1}{a}\theta(v)\int_{v/a}^{\infty} d\tau\, \rho(\tau) \times \sum_{j=0}^{\infty} \int d\tau_1 \cdots \int d\tau_j\, \rho(\tau_1) \cdots \rho(\tau_j)\delta\left(t - \frac{v}{a} - \tau_1 - \cdots - \tau_j\right) \tag{3.7}$$

With the use of the Laplace transformation

$$\tilde{F}(z) = \int_0^{\infty} dt\, e^{-zt} F(t) \tag{3.8}$$

Eq. (3.7) can be rewritten

$$\tilde{\varphi}(v,z) = \left[\frac{1}{a}\theta(v)\int_{v/a}^{\infty} d\tau\, \rho(\tau)\right] \frac{e^{-zv/a}}{1-\tilde{\rho}(z)} \tag{3.9}$$

Using the fact that $\varphi(v,0) = \delta(v)$ one finds

$$z\tilde{\varphi}(v,z) - \varphi(v,0) + a\frac{\partial}{\partial v}\tilde{\varphi}(v,z) = \delta(v)\frac{\tilde{\rho}(z)}{[1-\tilde{\rho}(z)]} - \theta(v)\rho\left(\frac{v}{a}\right)\frac{e^{-zv/a}}{a[1-\tilde{\rho}(z)]} \tag{3.10}$$

The second term in the right-hand side of Eq. (3.10) can be written in the form

$$-\mu(v)\tilde{\varphi}(v,z) \tag{3.11}$$

where

$$\mu(v) = \rho(v/a)\left[\int_{v/a}^{\infty} d\tau\, \rho(\tau)\right]^{-1}$$

Hence, by applying to Eq. (3.10) the inverse Laplace transformation the following linear, local in time kinetic equation is obtained:

$$\left(\frac{\partial}{\partial t} + a\frac{\partial}{\partial v}\right)\varphi(v,t) = \delta(v)\left[\int dv'\, \mu(v')\varphi(v',t)\right] - \mu(v)\varphi(v,t) \tag{3.12}$$

As in the Boltzmann equation the effect of collisions is represented here by the difference between the gain and the loss term. The gain term is proportional to the Dirac distribution $\delta(v)$, because the postcollisional velocity of the charged rod is always equal to zero. The steady state velocity distribution is found by calculating the limit $\lim_{z\to 0} z\tilde{\phi}(v,z) = \phi^{st}(v)$. As

$\tilde{\rho}(0) = 1$, one obtains from Eq. (3.9)

$$\phi^{\text{st}}(v) = \left[a^{-1}\theta(v) \int_{v/a}^{\infty} d\tau\, \rho(\tau) \right] M_1^{-1} \tag{3.13}$$

with

$$M_1 = -\tilde{\rho}'(0) = \int_0^{\infty} d\tau\, \tau \rho(\tau)$$

(the prime denotes the derivative with respect to z). It can be readily verified that the distribution $\phi^{\text{st}}(v)$ is a stationary solution of the kinetic equation (3.12). It is interesting to remark that the current $j(t) = \int dv\, v\phi(v, t)$, associated with the motion of the charged rod (the charge is put equal to 1) is a linear function of the field at any time $t > 0$. Indeed, its Laplace transform, calculated from Eq. (3.9), has the form

$$\tilde{j}(z) = a\left[\frac{\tilde{\rho}'(z)}{z[1 - \tilde{\rho}(z)]} + \frac{1}{z^2} \right] \tag{3.14}$$

The steady state current reads

$$j^{\text{st}} = \lim_{z \to 0} z\tilde{j}(z) = -a\tilde{\rho}''(0)/2\tilde{\rho}'(0) = aM_2/2M_1 \tag{3.15}$$

where

$$M_n = \int_0^{\infty} d\tau\, \tau^n \rho(\tau), \qquad n = 1, 2$$

One remarkable property of the kinetic equation (3.12) is its locality in time. In the collision term the distribution $\varphi(v, t)$ is multiplied by a function of velocity only, which is related to the fact that the collision frequency of the charged rod is entirely defined by the initial configurations of the neutral fluid.

We shall now show that in the second case, characterized by the initial distribution (3.6), the possibility of obtaining a kinetic equation of this type is lost. The distribution (3.6), when put into Eq. (3.4), yields

$$\varphi(v, t) = \theta(v) \int d\tau\, \rho(\tau) \theta(a\tau - v) \sum_{j=0}^{\infty} \delta[v - a(t - j\tau)] \tag{3.16}$$

Using again the Laplace transformation we find

$$\tilde{\varphi}(v, z) = \frac{1}{a}\theta(v) e^{-zv/a} \int_{v/a}^{\infty} d\tau\, \rho(\tau) [1 - e^{-z\tau}]^{-1} \tag{3.17}$$

The analog of Eq. (3.10) has thus the form

$$z\tilde{\varphi}(v,z) - \varphi(v,0) + a\frac{\partial}{\partial v}\tilde{\varphi}(v,z)$$

$$= \delta(v)\left[\int_0^\infty d\tau \frac{e^{-z\tau}\rho(\tau)}{1-e^{-z\tau}}\right] - \frac{1}{a}\theta(v)\left[\frac{\rho(v/a)e^{-zv/a}}{1-e^{-zv/a}}\right] \quad (3.18)$$

Analyzing the loss term here we find that in contradistinction to the analogous term in Eq. (3.10) it cannot be written as a product of a z-independent function and the distribution $\tilde{\varphi}(v,z)$. It is thus impossible in this case to obtain a kinetic equation whose structure would correspond to that of the Boltzmann equation. In fact there is a qualitative difference between the initial distributions (3.5) and (3.6). There are no correlations between time intervals separating collisions in the former, whereas they are present in the latter. Loosely speaking one could say that there is not enough randomness in the initial state (3.6) to make the kinetic description of the type represented by Eq. (3.12) possible.

The steady state velocity distribution calculated from Eq. (3.17) is given by

$$\phi^{st}(v) = \lim_{z\to 0} z\tilde{\phi}(v,z) = \frac{1}{a}\theta(v)\int_{v/a}^\infty d\tau \frac{\rho(\tau)}{\tau} \quad (3.19)$$

The mean velocity of the charged rod is proportional to the field at any moment $t > 0$. In the steady state

$$j^{st} = \int dv\, v\phi^{st}(v) = \frac{a}{2}\int_0^\infty d\tau\, \tau\rho(\tau) \quad (3.20)$$

4. DISCUSSION

The results of this note permit to make some comments on the realtionship between the microscopic dynamics and kinetic equations. Résibois' paper[7] shows (in an example) that if initially molecular chaos exists and recollisions are impossible the further evolution is rigorously governed by the Boltzmann equation. Here, we characterized the class of initial states which ruled out recollision processes [notice that conditions (2.6) do not depend on the external field]. However, elimination of recollisions is not enough for the Boltzmann equation to be valid. In fact this elimination implied in our case necessarily the existence of correlations between positions of the fluid particles. No such correlations occurred in the initial state considered by Résibois. Our analysis shows that a closed, linear, local in time evolution equation can be obtained only if the initial state is sufficiently chaotic. In the case studied here this means that the distances between neighboring particles are independent stochastic variables, with an appropriate distribution, compatible with inequalities (2.8). However, even in such a chaotic case, the initial state of the fluid contains spatial correlations. And this influences substantially the velocity distribution of the test particle [see, for example Eqs. (3.13) and (3.19)].

We have emphasized in our analysis that Eqs. (3.14) and (3.20) showed a linear dependence of the current on the field. This is, however, a correct statement provided the distributions $\rho_n(\tau_1, \tau_2, \ldots, \tau_n)$ for the time intervals between collisions are field independent. From the physical point of view this is very artificial indeed. We should rather consider the class of initial conditions in which the distributions of positions of the neutral fluid particles are field independent. Then, because of relations (2.7), the currents turn out to be proportional to the square root of the field, in qualitative accordance with the result found by solving the Boltzmann equation.[10]

In conclusion let us recall again that eliminating recollisions one can obtain a Boltzmann-like equation [our Eq. (3.12)] if the system is random enough, despite the presence of spatial correlations.

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