Generalized Fick's law for new exact solutions of the Galilean Kramers' equation.

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Abstract

An attractive approach to study free particle diffusion consists in modeling the microscopic motion of the particle by stochastic processes, such as the Galilean Ornstein-Uhlenbeck process. The resulting phase-space probability distribution function for the aforementioned process is known to obey the Kramers' equation.

We present a procedure to solve analytically the Galilean Kramers' equation in the general case of an arbitrary sufficiently regular initial condition. We then apply this technique to a wide class of physically relevant initial conditions, and provide an integral form for the solution at any positive time. It turns out that these solutions obey an 'extended Fick's law', with a time-dependent diffusion coefficient and a rapidly damping drift.

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1 Introduction

The past twenty years or so have witnessed a new interest in modeling correctly the irreversible behavior of both Galilean and Relativistic macroscopic

systems [1, 2, 3]. More precisely, starting from a rather consensual statistical description of the system under consideration, usually a transport equation, the key question investigated by various authors is how to derive from that description sufficiently general constitutive relations which involve macroscopic quantities only but nevertheless describe properly the evolution of the system. The traditional method for obtaining such constitutive relations is the Chapman-Enskog expansion [4]. It restricts the study *ab initio* to cases for which the system is in a near-equilibrium situation where the characteristic length and time-scales of its behavior are much larger than some microscopic scales, typically a mean free path and a collision time. The desired constitutive relations are then obtained rigorously, but only in the afore-mentioned limit, which seems to be far too restrictive for many interesting physical situations. An alternative can be found in the Grad- or moment-method [5, 2], which delivers apparently more general constitutive relations, but whose validity range cannot be ascertained in any precise way since the expansion it requires does not involve any small-parameter.

The aim of the present article is to contribute to this debate by producing new results about one of the simplest irreversible phenomenon, free (Galilean) particle diffusion, investigated through what is arguably its simplest statistical description, the (Galilean) Ornstein-Uhlenbeck process [6]. The relevant transport equation in phase-space is sometimes called Kramers' equation [7] and delivers, when treated by the Chapman-Enskog method, the usual Fick's law for diffusion [7, 8]. On the other hand, a method originally introduced by Lax [9] to solve the rather similar Fokker-Planck equation can be generalized in a straightforward manner and furnishes the exact solution of Kramers' equation in unbounded space-phase at any time in terms of an integral transform of its initial condition. Even if some authors seem to have already been aware of this extension [7], the procedure is reviewed in Section 3 of this paper, if only to make the present article self-contained and fix various notations. We then prove in Section 4 that, for a large class of physically relevant initial conditions, the exact solution to Kramers' equation satisfies a strikingly simple generalization of Fick's law and that the usual Fick's law can then be exactly recovered, for these solutions, in the long-time limit. In a final section, we review rapidly our results and address their possible relevance for the general problematics discussed at the beginning of this introduction.

2 The Galilean Ornstein-Uhlenbeck Process

2.1 Definition

We define the Galilean Ornstein-Uhlenbeck Process for the variables $\mathbf{x}$ and $\mathbf{v}$ in $\mathbb{R}^3$ as the solution of the following stochastic differential system :

$$\left\{ \begin{array}{rcl} \frac{d}{dt}\mathbf{x} & = & \mathbf{v} \\ \\ \frac{d}{dt}\mathbf{v} & = & -\alpha\mathbf{v} + \frac{1}{m}\mathbf{F} \end{array} \right. , \tag{1}$$

where $\mathbf{F}$ is a random vector whose components are "centered Gaussian white noises" such that :

$$< \mathbf{F}(t) > \quad = \quad \mathbf{0}, \tag{2}$$

$$< F_i(t_1)F_j(t_2) > \quad = \quad 2D\delta(t_2 - t_1)\delta^i_j, \quad D > 0. \tag{3}$$

The system (1) can be interpreted as the Galilean equations of motion of a particle with mass m, under the action of a deterministic force $-\alpha\mathbf{v}$ and a stochastic Gaussian force $\mathbf{F}$. These forces can be thought of as mathematical models of the deterministic and stochastic parts of the force experienced by a Brownian (big) particle from the small particles of the surrounding fluid with which it interacts. The coefficients α, m and D are three constant parameters of the model. This physical mental image of a Brownian particle interacting with a surrounding fluid will be used throughout this article to clarify the physical discussions of the results.

2.2 The statistical approach

The stochastic system (1) defines a stochastic trajectory in the phase-space of the particle. This trajectory can be studied statistically by introducing a distribution function $\Pi(t, \mathbf{x}, \mathbf{v})$ in phase space, associated to the usual measure d^3xd^3v so that :

$$\int_{\mathbb{R}^6} \Pi(t, \mathbf{x}, \mathbf{v}) d^3xd^3v = 1. \tag{4}$$

This distribution function is known to obey the so-called Kramers' equation

$$\partial_t\Pi + \nabla_{\mathbf{x}}(\mathbf{v}\Pi) + \nabla_{\mathbf{v}}(-\alpha\mathbf{v}\Pi) = \frac{D}{m^2}\Delta_{\mathbf{v}}\Pi. \tag{5}$$

Several proofs of this can be found, for example in [10] or in [11] for the relativistic version of the Ornstein-Uhlenbeck process. Kramers' equation is also known as the forward Chapman-Kolmogorov equation for the Ornstein-Uhlenbeck process [12].

At least if the problem is restricted to a finite volume $\mathcal{V}$ in physical space, the Kramers' equation (10) is known to have the following uniform (global) equilibrium solutions :

$$\Pi_e(t, \mathbf{x}, \mathbf{v}) = \frac{1}{\mathcal{V}} \left(\frac{2\pi D}{m^2 \alpha} \right)^{-\frac{3}{2}} e^{-\frac{m^2 \alpha}{2D} \mathbf{v}^2}. \tag{6}$$

This leads to a natural definition of the equilibrium temperature T_e through the identification of (6) with the usual Maxwell-Boltzmann distribution at temperature T_e. This temperature is related to the fundamental parameters of the model α, m and D by the so-called 'fluctuation-dissipation theorem' :

$$k_{\mathrm{B}} T_e = \frac{D}{m\alpha}, \tag{7}$$

where k_{B} is the Boltzmann constant. With the mental image of a Brownian particle, this temperature T_e can be interpreted as the temperature of the surrounding fluid in which the particle is immersed.

It can be shown, for example by a Chapman-Enskog expansion around local equilibrium distributions (see [7] and [8] in the relativistic case), that the particle density and particle current

$$n(t, \mathbf{x}) \equiv \int_{\mathbb{R}^3} \Pi(t, \mathbf{x}, \mathbf{v}) d^3 v, \qquad \text{and} \qquad \mathbf{j}(t, \mathbf{x}) \equiv \int_{\mathbb{R}^3} \Pi(t, \mathbf{x}, \mathbf{v}) \mathbf{v} d^3 v, \tag{8}$$

are linked by a Fick's law

$$\mathbf{j}(t, \mathbf{x}) = -\chi \nabla_{\mathbf{x}} n(t, \mathbf{x}) \tag{9}$$

with a constant diffusion coefficient $\chi = D/(m\alpha)^2 = k_{\mathrm{B}} T_e/(m\alpha)$, at least in the (long time) hydrodynamic regime.

Our purpose is to investigate whether and under which form this Fick's law can be generalized to short time non-hydrodynamic regimes, for which no scale separation hypothesis is valid. We thus present a procedure to solve Kramers' equation for an arbitrary initial distribution function under the hypothesis that the Fourier transform of the solution is non-vanishing at any time and position in phase space.

3 Exact resolution of the Kramers' equation

We start from the Kramers' equation (5), that we rewrite in terms of the equilibrium temperature T_e, to ease further physical discussions :

$$\partial_t \Pi + \nabla_{\mathbf{x}}(\mathbf{v}\Pi) = \alpha\Big(\nabla_{\mathbf{v}}(\mathbf{v}\Pi) + \frac{k_{\mathrm{B}}T_e}{m}\Delta_{\mathbf{v}}\Pi\Big). \tag{10}$$

The development hereafter is inspired by Laxes solutions to the Fokker-Planck equation [9, 7]. We introduce the Fourier transform $\hat{\Pi}(t,\mathbf{k},\mathbf{u})$ of the distribution function $\Pi(t,\mathbf{x},\mathbf{v})$:

$$\hat{\Pi}(t,\mathbf{k},\mathbf{u}) = \frac{1}{\sqrt{2\pi}^{\,6}}\int_{\mathbb{R}^6}\Pi(t,\mathbf{x},\mathbf{v})e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{u}\cdot\mathbf{v})}d^3xd^3v. \tag{11}$$

Since the distribution function $\Pi(t,\mathbf{x},\mathbf{v})$ has to satisfy (10), its Fourier transform $\hat{\Pi}(t,\mathbf{k},\mathbf{u})$ satisfies :

$$\partial_t\hat{\Pi} = (\mathbf{k}-\alpha\mathbf{u})\cdot\nabla_{\mathbf{u}}\hat{\Pi} - \frac{k_{\mathrm{B}}T_e\alpha}{m}\mathbf{u}^2\hat{\Pi}. \tag{12}$$

If the Fourier transform does not vanish anywhere, Equation (12) leads to :

$$\partial_t(log\hat{\Pi}) = (\mathbf{k}-\alpha\mathbf{u})\cdot\nabla_{\mathbf{u}}(log\hat{\Pi}) - \frac{k_{\mathrm{B}}T_e\alpha}{m}\mathbf{u}^2. \tag{13}$$

We now introduce the new function $\lambda(t,\mathbf{k},\mathbf{u}) \equiv \partial_t(log\hat{\Pi})$, so that :

$$log\hat{\Pi}(t,\mathbf{k},\mathbf{u}) = log\hat{\Pi}_0(\mathbf{k},\mathbf{u}) + \int_0^t \lambda(\tau,\mathbf{k},\mathbf{u})d\tau, \tag{14}$$

where $\hat{\Pi}_0(\mathbf{k},\mathbf{u})$ stands for $\hat{\Pi}(0,\mathbf{k},\mathbf{u})$. Equation (13) imposes that $\lambda(t,\mathbf{k},\mathbf{u})$ verify :

$$\lambda(t,\mathbf{k},\mathbf{u}) = (\mathbf{k}-\alpha\mathbf{u})\cdot\left(\nabla_{\mathbf{u}}(log\hat{\Pi}_0) + \int_0^t\nabla_{\mathbf{u}}\lambda(\tau,\mathbf{k},\mathbf{u})d\tau\right) - \frac{k_{\mathrm{B}}T_e\alpha}{m}\mathbf{u}^2, \tag{15}$$

which, for $t=0$, leads to :

$$\lambda(0,\mathbf{k},\mathbf{u}) = (\mathbf{k}-\alpha\mathbf{u})\cdot\left(\nabla_{\mathbf{u}}(log\hat{\Pi}_0)\right) - \frac{k_{\mathrm{B}}T_e\alpha}{m}\mathbf{u}^2. \tag{16}$$

Deriving (15) with respect to t yields the following partial differential equation for λ :

$$\partial_t\lambda(t,\mathbf{k},\mathbf{u}) = (\mathbf{k}-\alpha\mathbf{u})\cdot\nabla_{\mathbf{u}}\lambda(t,\mathbf{k},\mathbf{u}). \tag{17}$$

Let us introduce the new variable $\mathbf{p} \equiv \mathbf{k} - \alpha\mathbf{u}$ and the new function $\tilde{\lambda}(t, \mathbf{k}, \mathbf{p}) \equiv \lambda(t, \mathbf{k}, (\mathbf{k} - \mathbf{p})/\alpha)$. This new function must satisfy :

$$\partial_t \tilde{\lambda} = -\alpha \mathbf{p} \cdot \nabla_{\mathbf{p}} \tilde{\lambda}, \tag{18}$$

which implies that $\tilde{\lambda}(t, \mathbf{k}, \mathbf{p})$ is to depend on t and $\mathbf{p}$ only through the combination $\mathbf{p}e^{-\alpha t}$. According to (16), the initial value of $\tilde{\lambda}$ is :

$$\tilde{\lambda}(0, \mathbf{k}, \mathbf{p}) = \mathbf{p} \cdot \left(\nabla_{\mathbf{u}} \Big(log \hat{\Pi}_0(\mathbf{k}, \mathbf{u}) \Big) \right) \Big|_{(\mathbf{k}, (\mathbf{k}-\mathbf{p})/\alpha)} - \frac{k_{\mathrm{B}} T_e}{m\alpha} (\mathbf{k} - \mathbf{p})^2, \tag{19}$$

where the subscript $(\mathbf{k}, (\mathbf{k} - \mathbf{p})/\alpha)$ means that the expression between parentheses is to be taken for $(\mathbf{k}, \mathbf{u})$ equal to $(\mathbf{k}, (\mathbf{k} - \mathbf{p})/\alpha)$. Since the dependence of $\tilde{\lambda}$ on t and $\mathbf{p}$ must only involve $\mathbf{p}e^{-\alpha t}$, the expression (19) yields the expression for $\tilde{\lambda}(t, \mathbf{k}, \mathbf{p})$ by changing all occurrences of $\mathbf{p}$ into $\mathbf{p}e^{-\alpha t}$:

$$\tilde{\lambda}(t, \mathbf{k}, \mathbf{p}) = \mathbf{p}e^{-\alpha t} \cdot \left(\nabla_{\mathbf{u}} \Big(log \hat{\Pi}_0(\mathbf{k}, \mathbf{u}) \Big) \right) \Big|_{(\mathbf{k}, (\mathbf{k}-\mathbf{p}e^{-\alpha t})/\alpha)} - \frac{k_{\mathrm{B}} T_e}{m\alpha} (\mathbf{k} - \mathbf{p}e^{-\alpha t})^2. \tag{20}$$

It is now straightforward to use (14) to get an exact expression for $\hat{\Pi}(t, \mathbf{k}, \mathbf{u})$ in terms of $\hat{\Pi}_0$:

$$\hat{\Pi}\Big(t, \mathbf{k}, \mathbf{u}\Big) = \hat{\Pi}_0\Big(\mathbf{k}, \mathbf{u}e^{-\alpha t} + \frac{\mathbf{k}}{\alpha}(1 - e^{-\alpha t})\Big) e^{-\frac{k_{\mathrm{B}} T_e}{m\alpha} \int_0^t \left(\mathbf{k} - (\mathbf{k} - \alpha\mathbf{u})e^{-\alpha\tau}\right)^2 d\tau}. \tag{21}$$

It is convenient for further discussions to introduce the following time-dependent quantities :

$$\begin{aligned} \eta(t) &= \frac{k_{\mathrm{B}} T_e}{m\alpha^2} (\alpha t - \frac{3}{2} + 2e^{-\alpha t} - \frac{1}{2} e^{-2\alpha t}), \\ \mu(t) &= \frac{k_{\mathrm{B}} T_e}{m\alpha} (1 - e^{-\alpha t})^2, \\ \nu(t) &= \frac{k_{\mathrm{B}} T_e}{m} (1 - e^{-2\alpha t}). \end{aligned} \tag{22}$$

The expression for $\hat{\Pi}$ now takes the simpler form :

$$\hat{\Pi}\Big(t, \mathbf{k}, \mathbf{u}\Big) = \hat{\Pi}_0\Big(\mathbf{k}, \mathbf{u}e^{-\alpha t} + \frac{\mathbf{k}}{\alpha}(1 - e^{-\alpha t})\Big) e^{-\frac{1}{2}\mathbf{k}^2 \eta(t) - \mathbf{k}\cdot\mathbf{u}\mu(t) - \frac{1}{2}\mathbf{u}^2 \nu(t)}, \tag{23}$$

which leads to the complete solution in terms of Π:

$$\begin{aligned}\Pi(t,\mathbf{x},\mathbf{v}) &= \frac{1}{\sqrt{2\pi}^{\,6}}\int_{\mathbb{R}^6}\hat{\Pi}_0\Big(\mathbf{k},\mathbf{u}e^{-\alpha t}+\frac{\mathbf{k}}{\alpha}(1-e^{-\alpha t})\Big)\\ &\quad\times e^{-\frac{1}{2}\mathbf{k}^2\eta(t)-\mathbf{k}\cdot\mathbf{u}\mu(t)-\frac{1}{2}\mathbf{u}^2\nu(t)}\;e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{u}\cdot\mathbf{v})}\;d^3k d^3u.\end{aligned} \tag{24}$$

Without specifying any more the initial distribution function, we can obtain from (24) an integral expression for the particle density $n(t,\mathbf{x}) \equiv \int \Pi d^3v$:

$$n(t,\mathbf{x}) = \int_{\mathbb{R}^3}\hat{\Pi}_0\Big(\mathbf{k},\frac{\mathbf{k}}{\alpha}(1-e^{-\alpha t})\Big)e^{-\frac{1}{2}\mathbf{k}^2\eta(t)}e^{i\mathbf{k}\cdot\mathbf{x}}\;d^3k. \tag{25}$$

The gradient of the particle density follows immediately:

$$\nabla_{\mathbf{x}}n(t,\mathbf{x}) = \int_{\mathbb{R}^3} i\mathbf{k}\hat{\Pi}_0\Big(\mathbf{k},\frac{\mathbf{k}}{\alpha}(1-e^{-\alpha t})\Big)e^{-\frac{1}{2}\mathbf{k}^2\eta(t)}e^{i\mathbf{k}\cdot\mathbf{x}}\;d^3k. \tag{26}$$

Still as a consequence of (24), the particle current $\mathbf{j}(t,\mathbf{x}) \equiv \int \Pi\mathbf{v}d^3v$ reads:

$$\begin{aligned}\mathbf{j}(t,\mathbf{x}) &= \int_{\mathbb{R}^3} i\nabla_{\mathbf{u}}\left[\hat{\Pi}_0\Big(\mathbf{k},\mathbf{u}e^{-\alpha t}+\frac{\mathbf{k}}{\alpha}(1-e^{-\alpha t})\Big)e^{-\mathbf{k}\cdot\mathbf{u}\mu(t)-\frac{1}{2}\mathbf{u}^2\nu(t))}\right]\Bigg|_{\mathbf{u}=0}\\ &\quad\times e^{-\frac{1}{2}\mathbf{k}^2\eta(t)}e^{i\mathbf{k}\cdot\mathbf{x}}\;d^3k.\end{aligned} \tag{27}$$

Arbitrary order moments of $\Pi(t,\mathbf{x},\mathbf{v})$ can be expressed in a similar manner.

4 Application to a wide class of initial conditions

To proceed further, we restrict the study to initial conditions that can be factorized into an arbitrary function of the position $\mathbf{x}$, and a Maxwell-Boltzmann distribution with temperature T_0, centered around a mean velocity vector $\mathbf{v}_0$:

$$\Pi_0(\mathbf{x},\mathbf{v}) = n_0(\mathbf{x})\Big(\frac{m}{2\pi k_{\mathrm{B}}T_0}\Big)^{\frac{3}{2}}e^{-\frac{m(\mathbf{v}-\mathbf{v}_0)^2}{2k_{\mathrm{B}}T_0}}. \tag{28}$$

The Fourier transform is

$$\hat{\Pi}_0(\mathbf{k},\mathbf{u}) = \hat{n_0}(\mathbf{k})\;\frac{1}{\sqrt{2\pi}^{\,3}}e^{-i\mathbf{u}\cdot\mathbf{v}_0}e^{-\frac{1}{2}\mathbf{u}^2\frac{k_{\mathrm{B}}T_0}{m}}, \tag{29}$$

where $\hat{n_0}(\mathbf{k})$ is the Fourier transform of $f(\mathbf{x})$. The phase-space distribution function $\Pi(t, \mathbf{x}, \mathbf{v})$ at any positive time is then, according to (24) :

$$\Pi(t, \mathbf{x}, \mathbf{v}) = \frac{1}{\sqrt{2\pi}^9} \int_{\mathbb{R}^6} \hat{n_0}(\mathbf{k}) e^{-\frac{1}{2}\mathbf{k}^2\sigma^2(t) - \mathbf{k}\cdot\mathbf{u}\chi(t) - \frac{k_\mathrm{B}}{2m}\mathbf{u}^2 T(t)} \; e^{i(\mathbf{k}\cdot\mathbf{x}' + \mathbf{u}\cdot\mathbf{v}')} \; d^3k d^3u, \tag{30}$$

where the quantities σ^2, χ, T, $\mathbf{x}'$ and $\mathbf{v}'$ are defined as follows, in terms of the temperature difference $\Delta T = T_e - T_0$:

$$\begin{aligned}
\sigma^2(t) &= \frac{k_\mathrm{B}}{m\alpha^2}\left(T_e\Big(\alpha t - \frac{1}{2} + \frac{1}{2}e^{-2\alpha t}\Big) - \Delta T\Big(1 - 2e^{-\alpha t} + e^{-2\alpha t}\Big)\right), \\
\chi(t) &= \frac{k_\mathrm{B}}{m\alpha}(1 - e^{-\alpha t})\Big(T_e - \Delta T e^{-\alpha t}\Big), \\
T(t) &= T_e - \Delta T e^{-2\alpha t}, \\
\mathbf{x}' &= \mathbf{x} - \frac{\mathbf{v}_0}{\alpha}(1 - e^{-\alpha t}). \\
\mathbf{v}' &= \mathbf{v} - \mathbf{v}_0 e^{-\alpha t}.
\end{aligned} \tag{31}$$

The application of the relations (25) yields a very simple expression for the particle density :

$$n(t, \mathbf{x}) = \frac{1}{\sqrt{2\pi}^3} \int_{\mathbb{R}^3} \hat{n_0}(\mathbf{k}) e^{-\frac{1}{2}\mathbf{k}^2\sigma^2(t)} e^{i\mathbf{k}\cdot\mathbf{x}'} \; d^3k. \tag{32}$$

In other words, the particle density at time t is the convolution product :

$$n(t, \mathbf{x}) = n_0(\mathbf{x}) \star \Phi(t, \mathbf{x}), \tag{33}$$

of the particle density at time $t = 0$ with a 'propagator' $\Phi(t, \mathbf{x})$ that can be explicitly written as :

$$\Phi(t, \mathbf{x}) = \frac{1}{\sqrt{2\pi\sigma^2(t)}^{\,3}} \exp - \frac{\Big(\mathbf{x} - \frac{\mathbf{v}_0}{\alpha}(1 - e^{-\alpha t})\Big)^2}{2\sigma^2(t)} \tag{34}$$

The quantity $\frac{\mathbf{v}_0}{\alpha}(1 - e^{-\alpha t})$ can be interpreted as the position of a point, initially at $\mathbf{x} = 0$, moving with velocity $\mathbf{v}_0 e^{-\alpha t}$. Thus, the propagator Φ involves a uniform drift which is damped exponentially on a time scale α^{-1}, and a diffusive spreading with a growing typical width $\sigma(t)$.

Equations (26) and (27) show that the particle current obeys the following simple relation :

$$\mathbf{j} = -\chi(t)\nabla_{\mathbf{x}} n + e^{-\alpha t}\mathbf{v}_0 n. \tag{35}$$

We identify in the right-hand side of (35) two contributions to the particle current :

- a diffusion term proportional to the gradient of the particle density with a time-varying 'diffusion' coefficient $\chi(t)$,
- an 'advection' term that damps exponentially, and which is a remnant of the initial mean drift a velocity $\mathbf{v}_0$.

The physical meaning of $T(t)$ is more subtle. Indeed, since the distribution function $\Pi(t, \mathbf{x}, \mathbf{v})$ for $t > 0$ cannot be an equilibrium solution when spatially non-uniform, it is not trivial to define a time-dependent temperature. The mean square velocity[1], that can give some sense to the notion of temperature, is *a priori* position-dependent in the most general case. However, the *space-averaging* of the mean square velocity is a well-defined quantity that amounts to $3k_{\mathrm{B}}T(t)/m$. The quantity $T(t)$ defined in (31) can thus be thought of as a space-averaged temperature, characteristic of the distribution Π at time t.

The physically relevant quantities $\sigma^2(t)$, $\chi(t)$ ant $T(t)$ are plotted on Figure 1, 2 and 3. The solid curves correspond to $\Delta T = 0$, that is, the initial condition is at thermal equilibrium with the surrounding fluid. The dashed curves correspond to $\Delta T = T_e$, that is, $T_0 = 0$, so that they describe situations with vanishing initial velocities.

5 Discussion

The Galilean Kramers' equation considered in this paper describes the statistical behavior of Brownian particles which diffuse freely in a given fluid according to the (Galilean) Ornstein-Uhlenbeck process. Without loss of generality, the system has been studied in the (global) proper frame of the fluid in which the particles diffuse. We have extended to Kramers' equation a method developed by Lax for solving the Fokker-Planck equation in terms of its initial condition. This has enabled us to prove that, for a very wide class of physically important initial conditions, the exact solution to Kramers' equation verifies a very simple generalization of the usual Fick's law. In particular, if the initial phase-space distribution is factorized into

[1] with uniform damped drift $\mathbf{v}_0 e^{-\alpha t}$ subtracted.

Figure 1: $\frac{m\alpha^2}{k_B T_e}\sigma^2(t)$ *versus* αt *for* $\Delta T = 0$ *(solid) and* $\Delta T = T_e$ *(dashed).*

Figure 2: $\frac{m\alpha}{k_B T_e}\chi(t)$ *versus* αt *for* $\Delta T = 0$ *(solid) and* $\Delta T = T_e$ *(dashed).*

Figure 3: $\frac{T(t)}{T_e}$ *versus* αt *for* $\Delta T = 0$ *(solid) and* $\Delta T = T_e$ *(dashed).*

an arbitrary (initial) spatial density and a position independent Maxwellian distribution (with arbitrary temperature and mean-velocity), the particle current at all times is the sum of two contributions which can be easily interpreted. The first one describes the relaxation towards zero of an initially non-vanishing contribution to the current due to an initial non-vanishing mean velocity of the diffusing particles. The characteristic time-scale of this relaxation is simply the inverse of the friction coefficient which appears in the deterministic part of the force acting on the Brownian particles. The second contribution to the current is proportional to the spatial density-gradient at all times. The involved coefficient however does depend on time and on the difference between the initial temperature T_0 and the temperature T_e of the surrounding fluid. This coefficient relaxes to its usual value predicted by the Chapman-Enskog expansion on the same time-scale, *i.e.* the inverse of the friction coefficient. We think that these striking results could, in principle, be tested experimentally and that the result of such a test would be of crucial importance for a proper evaluation of the Ornstein-Uhlenbeck process. In other words, one of the main features of the Ornstein-Uhlenbeck process is its simplicity; despite this simplicity, it is at least able to predict, in the long-time limit, the usual Fick's law, which is well confirmed experimentally. The natural question to ask is obviously : What about other, more subtle predictions of this seemingly rather crude model ? We believe that the analytical results presented in this article are particularly suited for providing the basis to a possible partial answer to this question.

We also believe these results to be of another, more methodological importance. As mentioned in the introduction, there are essentially two standard ways of deriving constitutive relations between macroscopic quantities from a given transport equation. The first one is the Chapman-Enskog method and it delivers, in the case under consideration in this article, the standard Fick's law and diffusion equation. The same method, when applied to Boltzmann equation, furnishes the usual Navier-Stokes model of dissipative fluids [4]. If one wants to describe the solutions of the transport equation beyond the regime for which the Chapman-Enskog expansion is valid, the only method really documented and developed in the literature seems to be the so-called Grad- or moments-method. The basic idea behind this method is to include also as macroscopic field variables moments of the phase-space distribution function higher than those usually retained in the Chapman-Enskog method. The best-known application of this philosophy is the thirteen-moments expansion of the solution to Boltzmann equation and the resulting 'hydrodynamical' equations actually involve 13

field variables instead of the usual five used by the Navier-Stokes model[2]. Apart from the problematic fact already mentioned in the introduction that Grad's method is based on an expansion which does not involve any small parameter, this kind of theory has run into various problems, both experimental and theoretical [13]. As far as we know, Grad's method has never been applied to Kramers' equation[3]. If it were, it would lead to the inclusion of (at least) the particle current among the macroscopic field variables, on equal footing with the spatial density. The macroscopic equations verified by the 'extended' set of fields would be derived from the momentum hierarchy associated to Kramers' equation and would most certainly exhibit damped oscillatory behavior, which seems to be a common feature to the various evolution equations obtained so far via Grad's method. This kind of behavior is clearly absent from the exact solutions to Kramers' equation presented in this article.

In quite general a context, it is naturally tempting to try and guess from the new exact results on Kramers' equation presented in this article how one could fruitfully extend usual constitutive relations obtained from an arbitrary transport equation via a Chapman-Enskog expansion. If one ventures to do so, one gets the following picture. The addition of new macroscopic fields to the usual ones considered by Chapman and Enskog does not seem to be compulsory, even if it could help take into account, for certain initial conditions, contributions to the currents similar to the first term on the right-hand side of (35); on the other hand, one should probably let the various kinetic coefficients which appear in the Chapman-Enskog constitutive relations depend explicitly on time, having them relax in time to their constant Chapman-Enskog value.

This section would certainly not be complete without a brief discussion of Titulaer's work [14] and de Groot's and Mazur's work [15]. Indeed, Titulaer has considered a more general Kramers' equation than (10), which describes the statistical behavior of Brownian particles under the influence of a constant inhomogeneous force-field. He has proposed a systematic solution scheme to the equation, under the hypothesis that the force be weak enough. His scheme is actually of the Chapman-Enskog type and we already have discussed it at great length in a previous publication, to which we refer the interested reader [16].

[2]These equations are identical to those of the simplest non-trivial implementation for simple fluids of what is commonly called Extended Thermodynamics Theories [2].

[3]The Extended Thermodynamics of binary mixtures do not start from a transport equation for the diffusing particles alone but from the system of coupled Boltzmann-equations for both components and apply to them the Chapman-Enskog method only [2].

In their famous book [15], De Groot and Mazur also propose an apparently rather general scheme for solving Kramers' equation. Their scheme is based on the ansatz that the solution takes the form of a local equilibrium Maxwellian distribution at all time, with position- and time-dependent particle density, mean-velocity and temperature. It can easily be proven with the help of equations (138), (139), (141), (144) and (145) of their book (pages 192 and 193), or with equation (24) of this article, that the ansatz is correct only if the distribution function is Gaussian in position and velocity at all time, including therefore at the initial instant, with a time-dependent only temperature. In terms of initial particle density, their work is therefore far less general than ours. It is true that the initial mean-velocity field of their solutions is not restricted to be uniform and can be, up to an additive constant, an arbitrary linear function of the position. It is obvious however that the method presented in Section 3 of the present work also applies to a generalization of (28) with such a mean-velocity field. It just leads to more cumbersome algebra than those presented in Section 4 and did not seem to us to be of sufficient physical relevance to justify its inclusion in this article. Let us finally remark that De Groot and Mazur do derive the usual Fick's law for the solutions they consider, but in the long-time limit only, and that, contrary to us, they do not mention an extension of the result valid for arbitrary instants.

Possible extensions of this work are currently envisaged by the authors. A first one is to take into account, at least perturbatively, the effects of a small enough force field. Another, certainly not trivial one, would be to devise a suitable generalization of Laxes method to the relativistic Kramers' equation, to which one could then obtain exact solutions at all time. Finally, one should certainly investigate further if, and under which circumstances, a generalization of the usual Navier-Stokes model along the lines suggested in this section makes sense.

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