Brownian motion in phase space

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In most treatments Brownian motion is considered either in position or in velocity space. While the description of Brownian motion as a Markov process via a master equation in phase space can, in principle, deal with the full problem, assumptions are usually introduced which lead to the formulation of the generalized Fokker-Planck equation. In the following we want to show how, in the field-free one-dimensional case, the transport equation for a time-dependent conditional average of an arbitrary physical quantity (depending on position and velocity coordinates) of a tagged particle in phase space can be derived and solved successively if the time- and position-independent moments of the transition probability can be expanded in terms of a parameter Ω^{-1}. The transport equation can then be transformed into a set of l linear partial differential equations, whose solutions provide the lth approximation in the expansion parameter Ω^{-1} to the full solution of the transport equation. The system of linear partial differential equations is closed in the sense that the solution of the lth partial differential equation is determined by the solutions of the $l-1$ partial differential equations. It turns out that the $l=0$ partial differential equation describes the macroscopic (nonfluctuating) motion of the tagged particle. It is discussed in which sense a bivariate Gaussian distribution describes the full Markov process and how the full phase-space treatment provides more insight into Brownian motion. It is shown how the special cases described by the Langevin equation and the Fokker-Planck equation are contained in the new method presented.

INTRODUCTION

Modern treatments[1] start from the N-particle Liouville equation using projection operator techniques in order to derive a generalized master equation for the time distribution function of a tagged particle. This generalized master equation is a non-Markovian equation and all the problems are hidden in the memory kernel. Neglecting these memory effects one can derive the Boltzmann equation, which appears to be a Markovian master equation. In this paper we are interested in the solution of the Markovian master equation for the motion of a particle in one dimension leading to nonlinear transport laws, rather than taking into account the memory effects entering in the generalized master equation.

The random motion of a tagged particle in the presence of a field of particles is commonly treated, e.g., either as the continuous limit of a discrete step process on a suitable chosen lattice in position space or directly in velocity space assuming uniformity in position space. A full description of the Brownian motion as a Markov process in phase space is given by a special case of the master equation namely the linear Boltzmann equation. Since the solution of this equation is not known for general interaction potentials, one usually makes assumptions about the moments of the transition probability, to obtain the linear Fokker-Planck equation, where the fundamental solution is well known.

The natural question to ask is how the process of transport of, e.g., particles, momentum, energy, or the average change of an arbitrary physical quantity can be described starting from a phase-space description. The most general method to address this problem is to calculate the tagged-particle time-dependent phase-space distribution $h(X,V,t\mid X_0,V_0)$ describing the probability to find the tagged particle in the phase-space element around (X,V) at time t, given it was at (X_0,V_0) at time $t=0$.

There are two approaches in use, which we will briefly outline, following Chandrasekhar[2] and Rice and Gray.[3] The first approach, the statistical equation of motion approach, starts by using the Langevin equation for calculating the time-dependent average velocity (in fact the first and higher velocity moments). The change in the average velocity is caused by the assumption of a velocity proportional macroscopic friction force and a fluctuating force of microscopic origin with special properties—see Uhlenbeck and Ornstein.[4] From the time-dependent average velocity, obtained by solving the Langevin equation, the time-dependent mean displacement and higher moments of the displacement and correlations of these quantities are calculated. Using the time-dependent first and second moments of the velocity, the position variable, and the cross correlation between those two, a bivariate Gaussian distribution for $h(X,V,t\mid X_0,V_0)$ is derived. In the second approach, the distribution-function approach, one tries to find a partial differential equation for the time-dependent phase-space distribution function itself, which then has to be solved subject to the initial and boundary conditions.

A convenient starting point for describing fluctuations in a system is the Markov equation or the Chapman-Kolmogorov master equation. For the terminology we use, see Van Kampen.[5] The master equation approach has been used previously to derive the velocity-space and phase-space Fokker-Planck equation[2,3] and leads in various contractions and under special assumptions to results obtained from the Langevin equation.

In this paper we start with the master equation in phase space in its integral form using the special initial condition $\delta(X-X_0)\delta(V-V_0)$. We then formulate the master equation in two equivalent forms, called forward and backward master equations, and derive from these equations the two corresponding forward and backward integro-differential equations. The central physical quantity of these master equations is the transition probability $W_\Omega(V_0 \to V_1)$. As in our previous treatment of the master equation for a single variable—see Eder and Lackner[6]—we again assume the state space of the Markov process to be unbounded, the collisional transitions to occur instantaneously (causing an impulsive change of the velocities of the two collision partners) meaning that changes on the microscopic scale can be separated from changes on the macroscopic scale, and are independent of position and time variables. It is assumed that the moments of the transition probability exist and can be expanded in a properly chosen parameter.

While the forward master equation is suited for the calculation of the time-dependent phase-space distribution function (TDF), it is the backward master equation which is especially useful for the calculation of time-dependent conditional average values (Hänggi and Thomas[7]). We develop a new method for calculating time-dependent conditional average values as functions of both position and velocity coordinates to arbitrary order in the expansion parameter Ω^{-1} by solving a corresponding set of first-order linear partial differential equations. This becomes feasible by noting that the backward form of the master equation provides an integro-differential equation for the time evolution of the conditional average of an arbitrary function. While the general method described in our earlier paper remains the same, there is a higher degree of mathematical complexity involved in finding the solutions of the set of linear partial differential equations, since we are now dealing not only with time and velocity as variables but include also the position variable. For this reason we restrict the present treatment to one dimension. From the general approximation scheme one can deduce under which approximations the time-dependent bivariate Gaussian distribution function emerges and is now in the position to assess the limitations of this approach quantitatively.

I. MASTER EQUATION IN PHASE SPACE

Let us consider the motion of a labeled Brownian particle in phase space. Owing to collisions the velocity of this particle will change instantaneously and stochastically. We assume that this process can be described by a homogeneous Markov process, using a time- and space-independent transition probability which leaves the position of the colliding particles unaltered during collisions and allows the particles to move according to free flight in between collisions. Furthermore, we assume that successive binary collision events are statistically uncorrelated.

With these assumptions in mind we formulate now a master equation for a one-dimensional motion in its forward and backward form in phase space, first as an integral equation and then as an integro-differential equation. Let us introduce the following quantities: $h(X,V,t \mid X_0,V_0)$, which is the probability to find the particle at time t in a phase-space element around (X,V) when at time $t=0$ it was at (X_0,V_0); $h(X,V,t=0 \mid X_0,V_0) = \delta(V-V_0)\delta(X-X_0)$, the initial condition; $W_\Omega(V_0 \to V_1)$, the time- and position-independent transition probability from $V_0 \to V_1$ (the subscript Ω refers to an explicit dependence on a given parameter Ω—see Appendix B); $\exp[-P_\Omega(V_0)t]$, the probability that in a time interval $(0,t)$ no transition takes place, where $P_\Omega(V_0)$ is defined by $P_\Omega(V_0)=\int W_\Omega(V_0 \to V_1)dV_1$; $\delta(X-X_0-V_0t)$, the free-flight propagator for a particle starting from (X_0,V_0) at time $t=0$.

In order to obtain an equation for the TDF $h(X,V,t \mid X_0,V_0)$ in the form of a balanced equation, we consider the following two possibilities for a change. (1) *No stochastic transitions in phase space take place.* The system is at time $t=0$ in the state (X_0,V_0) and has the probability

$$\exp[-P_\Omega(V_0)t]\delta(V-V_0)\delta(X-X_0-V_0t) \tag{1}$$

to evolve in time without stochastic transitions. (2) *There are transitions in phase space.* As in our earlier paper[5] we note that for this process two physically equivalent descriptions, which are called in agreement with the Chapman-Kolmogorov terminology the forward and backward form of the master equation, are possible.

(i) *Forward master equation.* Up to $t_1 \le t$ the system evolves in phase space according to the probability $h(X_1,V_1;t_1 \mid X_0,V_0)$, changes its velocity from $V_1 \to V$ in the time interval (t_1,t_1+dt_1) according to the transition probability $W_\Omega(V_1 \to V)$ (causing no change in the position coordinate during the collision), and has no stochastic transition in the remaining time interval (t_1,t)

$$\int_0^t dt_1 \int dX_1 \int dV_1 h_f(X_1,V_1,t_1 \mid X_0,V_0) W_\Omega(V_1 \to V) \exp[-P_\Omega(V)(t-t_1)]\delta(X-X_1-V(t-t_1)) \ . \tag{2a}$$

Since any process can be described by a sum of a subprocess and its complement, the TDF $h(X,V,t \mid X_0,V_0)$ is simply given by the sum of Eqs. (1) and (2a), yielding

$$\begin{aligned} h_f(X,V,t \mid X_0,V_0) = {} & \exp[-P_\Omega(V_0)t]\delta(V-V_0)\delta(X-X_0-V_0t) \\ & + \int_0^t dt_1 \int dX_1 \int dV_1 h_f(X_1,V_1,t_1 \mid X_0,V_0) W_\Omega(V_1 \to V) \\ & \times \exp[-P_\Omega(V)(t-t_1)]\delta(X-X_1-V(t-t_1)) \ . \end{aligned} \tag{2b}$$

(ii) *Backward master equation.* The succession of events for the backward master equation is obtained by interchanging the two processes in Eq. (2a) which occur before and after the collision process described,

$$\int_0^t dt_1 \int dX_1 \int dV_1 \exp[-P_\Omega(V_0)t_1]\delta(X_1-X_0-V_0t_1)W_\Omega(V_0\to V_1)h_b(X,V,t-t_1\,|\,X_1,V_1)\ . \tag{3a}$$

The TDF $h_b(X,V,t\,|\,X_0,V_0)$ is then the sum of Eqs. (1) and (3a)

$$\begin{aligned} h_b(X,V,t\,|\,X_0,V_0)=&\exp[-P_\Omega(V_0)t]\delta(V-V_0)\delta(X-X_0-V_0t)\\ &+\int_0^t dt_1 \int dX_1 \int dV_1 \exp[-P_\Omega(V_0)t_1]\delta(X_1-X_0-V_0t_1)W_\Omega(V_0\to V_1)\\ &\times h_b(X,V,t-t_1\,|\,X_1,V_1)\ . \end{aligned} \tag{3b}$$

Both equations can be transformed to the usual form of integro-differential equations yielding, respectively,

$$\begin{aligned} \frac{\partial h_f(X,V,t\,|\,X_0,V_0)}{\partial t}+V\frac{\partial h_f(X,V,t\,|\,X_0,V_0)}{\partial X} &= -P_\Omega(V)h_f(X,V,t\,|\,X_0,V_0)\\ &+\int dV_1 W_\Omega(V_1\to V)h_f(X,V_1,t\,|\,X_0,V_0) \end{aligned} \tag{4a}$$

and

$$\begin{aligned} \frac{\partial h_b(X,V,t\,|\,X_0,V_0)}{\partial t}-V_0\frac{\partial h_b(X,V,t\,|\,X_0,V_0)}{\partial X_0} &= -P_\Omega(V_0)h_b(X,V,t\,|\,X_0,V_0)\\ &+\int dV_1 W_\Omega(V_0\to V_1)h_b(X,V,t\,|\,X_0,V_1)\ , \end{aligned} \tag{4b}$$

where both equations have to be solved subject to the initial condition

$$h_{f,b}(X,V,t=0\,|\,X_0,V_0)=\delta(V-V_0)\delta(X-X_0)\ . \tag{5}$$

Note that Eq. (4a) represents the usual form of the linear Boltzmann equation which is not suited for calculating time-dependent conditional averages directly, whereas the backward form [Eq. (4b)] can be used to find an integro-differential equation for the conditional average of a time-dependent physical quantity, since the variables (X,V) enter through the distribution function $h(X,V,t\,|\,X_0,V_0)$ only. This was first pointed out by Hänggi and Thomas.[7] With the definition

$$\begin{aligned} \langle f(X,V)\,|\,X_0,V_0\rangle_t &= \chi(X_0,V_0,t)\\ &= \int f(X,V)h(X,V,t\,|\,X_0,V_0)dX\,dV \end{aligned} \tag{6}$$

we find from Eq. (4b)

$$\begin{aligned} \frac{\partial \chi(X_0,V_0,t)}{\partial t}-V_0\frac{\partial \chi(X_0,V_0,t)}{\partial X_0} &= -P_\Omega(V_0)\chi(X_0,V_0,t)\\ &+\int dV_1 W_\Omega(V_0\to V_1)\chi(X_0,V_1,t)\ , \end{aligned} \tag{7a}$$

which has to be solved subject to the initial condition

$$\chi(X_0,V_0,\ t=0)=f(X_0,V_0)\ . \tag{7b}$$

In the next sections the transport equations (7a) and (7b) will be our starting point.

II. METHOD OF SOLUTION FOR THE TRANSPORT EQUATION

In this section we focus our attention to the solution of the transport Eq. (7a) which is an integro-differential equation for an arbitrary time-dependent conditional average $\chi(X_0,V_0,t)\equiv\langle f(X,V)\,|\,X_0,V_0\rangle_t$. Our aim will be a separation of the conditional average $\chi(X_0,V_0,t)$ into a deterministic, nonfluctuating part χ_0 and fluctuating parts χ_l, $l=1,2,\ldots$. While the fluctuating parts satisfy nonhomogeneous first-order linear partial differential equations, the nonfluctuating part χ_0 is given by the solution of the following homogeneous first-order linear partial differential equation

$$\frac{\partial\chi_0}{\partial t}-V_0\frac{\partial\chi_0}{\partial X_0}-K_1(V_0)\frac{\partial\chi_0}{\partial V_0}=0 \tag{8a}$$

subject to the initial condition

$$\chi_0(X_0,V_0,t=0)=f(X_0,V_0)\ . \tag{8b}$$

We will show below that in the limit

$$\Omega^{-1}=m_B/(m_A+m_B)\to 0$$

the motion of the heavy particle A is completely determined by Eq. (8a) and the contributions of the fluctuating parts become negligible. Since the general solution of the homogeneous first-order linear partial differential equation (8a) is simply given by a functional $F[\chi_0(X_0,V_0,t)]$ we obtain in the limit $\Omega^{-1}\to 0$

$$\langle f^n(X,V)\,|\,X_0,V_0\rangle_t=[\chi_0(X_0,V_0,t)]^n \tag{8c}$$

and, e.g.,

$$\langle f^2(X,V)\,|\,X_0,V_0\rangle_t-\langle f(X,V)\,|\,X_0,V_0\rangle_t^2=0\ , \tag{8d}$$

which is characteristic for a deterministic nonfluctuating motion of a particle.

Let us first assume that the transition probability $W_\Omega(V_0\to V_1)$ can be written in a series of the form (see Van Kampen[5,8])

$$W_\Omega(V_0\to V_1)=F(\Omega)\sum_{k=0}^{\infty}\frac{1}{\Omega^k}W_k[V_0,\Omega(V_1-V_0)] \tag{9a}$$

and define the jump moments of the transition probability by

$$\begin{aligned} K_n(V_0) &= \int W_\Omega(V_0\to V_1)(V_1-V_0)^n dV_1\\ &= \frac{F(\Omega)}{\Omega^n}\sum_{k=0}^{\infty}\frac{\alpha_{n,k}(V_0)}{\Omega^{k+1}}\ , \end{aligned} \tag{9b}$$

where

$$\alpha_{n,k}(V_0)=\int W_k(V_0,Y)Y^n dY\ , \tag{10a}$$

$$K_0(V_0)=P_\Omega(V_0)\ . \tag{10b}$$

If we expand $\chi(X_0,V_0,t)$ in a Taylor series around V_0

$$\chi(X_0,V_1,t)=\sum_{n=0}^{\infty}\frac{(V_1-V_0)^n}{n!}\frac{\partial^n\chi(X_0,V_0,t)}{\partial V_0^n}\ , \tag{11}$$

we obtain by inserting Eq. (11) into Eq. (7a)

$$\frac{\partial\chi(X_0,V_0,t)}{\partial t}-V_0\frac{\partial\chi(X_0,V_0,t)}{\partial X_0}=\sum_{n=1}^{\infty}\frac{K_n(V_0)}{n!}\frac{\partial^n\chi(X_0,V_0,t)}{\partial V_0^n}\ . \tag{12}$$

In order to separate Eq. (12) into a deterministic part and a fluctuating one, we introduce a new time and space scale using the Ω dependence of the jump moments [see Eq. (9b)]

$$\frac{F(\Omega)}{\Omega^2}t=\tau,\quad \frac{F(\Omega)}{\Omega^2}X_0=x_0,\quad V_0=v_0\ , \tag{13a}$$

$$\chi(X_0,V_0,t)=\tilde{\chi}(x_0,v_0,\ \tau)\ , \tag{13b}$$

$$\tilde{\chi}(x_0,v_0,\ \tau=0)=\tilde{f}(x_0,v_0)\ . \tag{13c}$$

With this transformation we find the following by inserting Eqs. (13) and (9b) into Eq. (12) and dropping the tilde:

$$\frac{\partial\chi(x_0,v_0,\tau)}{\partial\tau}-v_0\frac{\partial\chi(x_0,v_0,\tau)}{\partial x_0}=\sum_{n=1}^{\infty}\sum_{k=0}^{\infty}\frac{1}{\Omega^{n+k-1}}\frac{\alpha_{n,k}(v_0)}{n!}\frac{\partial^n\chi(x_0,v_0,\tau)}{\partial v_0^n}\ . \tag{14}$$

Next we expand the conditional average $\chi(x_0,v_0,\tau)$ in powers of $1/\Omega$

$$\chi(x_0,v_0,\tau)=\sum_{l=0}^{\infty}\frac{1}{\Omega^l}\chi_l(x_0,v_0,\tau) \tag{15}$$

and find after an index transformation by comparing equal powers in $1/\Omega$ for $l=0$

$$\frac{\partial\chi_0(x_0,v_0,\tau)}{\partial\tau}-v_0\frac{\partial\chi_0(x_0,v_0,\tau)}{\partial x_0}-\alpha_{1,0}(v_0)\frac{\partial\chi_0(x_0,v_0,\tau)}{\partial v_0}=0\ , \tag{16a}$$

and for $l\geq 1$

$$\frac{\partial\chi_l(x_0,v_0,\tau)}{\partial\tau}-v_0\frac{\partial\chi_l(x_0,v_0,\tau)}{\partial x_0}-\alpha_{1,0}(v_0)\frac{\partial\chi_l(x_0,v_0,\tau)}{\partial v_0}=H_l(x_0,v_0,\tau) \tag{16b}$$

with

$$H_l(x_0,v_0,\tau)=\sum_{s=2}^{l+1}\sum_{k=1}^{s}\frac{\alpha_{k,s-k}(v_0)}{k!}\frac{\partial^k\chi_{l+1-s}(x_0,v_0,\tau)}{\partial v_0^k}\ . \tag{16c}$$

Equations (16a) and (16b) have to be solved subject to the following initial conditions:

$$\chi_0(x_0,v_0,\ \tau=0)=f(x_0,v_0)\ , \tag{17a}$$

$$\chi_l(x_0,v_0,\ \tau=0)=0\quad\text{for } l\geq 1\ . \tag{17b}$$

Since the functions $H_l(x_0,v_0,\tau)$ contain derivatives of $\chi_k(x_0,v_0,\tau)$ with $k<l$ only, the system of the Eqs. (16a) and (16b) can be solved in a successive way, meaning that higher approximations do not alter lower ones.

Equations (16a) and (16b) can be solved either using the standard method of characteristics or, more simply, with the aid of a theorem, formulated in Appendix A. In our special case this theorem states that the solutions of the system of ordinary differential equations

$$\frac{d\bar{x}}{d\tau}=\bar{v},\quad \frac{d\bar{v}}{d\tau}=\alpha_{1,0}(\bar{v})\ , \tag{18a}$$

with the initial conditions

$$\bar{x}(\tau=0)=x_0,\quad \bar{v}(\tau=0)=v_0\ , \tag{18b}$$

satisfy the corresponding set of linear first-order partial differential equations

$$\frac{\partial\bar{x}}{\partial\tau}-v_0\frac{\partial\bar{x}}{\partial x_0}-\alpha_{1,0}(v_0)\frac{\partial\bar{x}}{\partial v_0}=0\ , \tag{19a}$$

$$\frac{\partial\bar{v}}{\partial\tau}-v_0\frac{\partial\bar{v}}{\partial x_0}-\alpha_{1,0}(v_0)\frac{\partial\bar{v}}{\partial v_0}=0\ , \tag{19b}$$

where now the dependence of $\bar{x}$ and $\bar{v}$ on the initial conditions x_0 and v_0 is considered. Thus with the aid of Eqs. (19a) and (19b) the general solutions of Eqs. (16a) and (16b) subject to the initial conditions [Eqs. (17a) and (17b)] are given by

$$\chi_0(x_0,v_0,\tau)=f(\bar{x},\bar{v})\ , \tag{20}$$

$$\chi_l(x_0,v_0,\tau)=\int_0^\tau H_l(\bar{x}(\tau-s),\bar{v}(\tau-s),s)ds\ , \tag{21}$$

where $\bar{x},\bar{v}$ are the solutions of Eqs. (18a) and (18b).

Equations (18a) and (18b), which are called the macroscopic equations, determine via Eqs. (20) and (15) the nonfluctuating part of a conditional average $\chi(x_0,v_0,\tau)$, since in the limit $\Omega\to\infty$ one obtains

$$\langle f^2(x,v)\,|\,x_0,v_0\rangle_\tau-\langle f(x,v)\,|\,x_0,v_0\rangle_\tau^2=0\ . \tag{22}$$

The functions $\chi_l(x_0,v_0,\tau)$ with $l\geq 1$, however, describe the fluctuations around the deterministic motion of the particle up to arbitrary order in the expansion parameter Ω^{-1}. Combining Eqs. (18a) and (18b) and Eqs. (19a) and (19b) we obtain the following relations:

$$\frac{d\bar{x}}{dx_0}=1,\quad \frac{d\bar{x}}{dv_0}=\frac{\bar{v}-v_0}{\alpha_{1,0}(v_0)}\ , \tag{23a}$$

$$\frac{d\bar{v}}{dx_0}=0,\quad \frac{d\bar{v}}{dv_0}=\frac{\alpha_{1,0}(\bar{v})}{\alpha_{1,0}(v_0)}\ , \tag{23b}$$

which we need in the following sections.

III. GENERAL STRUCTURE OF χ_l

Equation (21) is still quite formidable to use and we fortunately find that it can be simplified considerably. To show this we first consider the case for $l=1$ and note that

$$H_1(x_0,v_0,\tau)=\alpha_{1,1}(v_0)\frac{\partial\chi_0(x_0,v_0,\tau)}{\partial v_0}+\frac{\alpha_{2,0}(v_0)}{2}\frac{\partial^2\chi_0(x_0,v_0,\tau)}{\partial v_0^2}\ , \tag{24}$$

where we have shown in the preceding section that $\chi_0(x_0,v_0,\tau)$ depends on τ through $\bar{x}$ and $\bar{v}$ only

$$\chi_0(x_0,v_0,\tau)=f(\bar{x},\bar{v})\ . \tag{25}$$

Next we calculate the first and second derivative of $\chi_0(x_0,v_0,\tau)$ with respect to v_0, using Eqs. (23a) and (23b),

$$\frac{\partial\chi_0(x_0,v_0,\tau)}{\partial v_0}=\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{x}}\frac{(\bar{v}-v_0)}{\alpha_{1,0}(v_0)}+\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{v}}\frac{\alpha_{1,0}(\bar{v})}{\alpha_{1,0}(v_0)}\ , \tag{26a}$$

$$\begin{aligned}\frac{\partial^2\chi_0(x_0,v_0,\tau)}{\partial v_0^2}=&\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{x}^2}\left[\frac{\bar{v}-v_0}{\alpha_{1,0}(v_0)}\right]^2+\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{v}^2}\left[\frac{\alpha_{1,0}(\bar{v})}{\alpha_{1,0}(v_0)}\right]^2+2\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{x}\partial\bar{v}}\frac{\alpha_{1,0}(\bar{v})}{\alpha_{1,0}(v_0)}\left[\frac{\bar{v}-v_0}{\alpha_{1,0}(v_0)}\right]\\&+\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{x}}\frac{[\alpha_{1,0}(\bar{v})-\alpha_{1,0}(v_0)]-(\bar{v}-v_0)\alpha'_{1,0}(v_0)}{\alpha_{1,0}^2(v_0)}+\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{v}}\frac{\alpha_{1,0}(\bar{v})}{\alpha_{1,0}^2(v_0)}[\alpha'_{1,0}(\bar{v})-\alpha'_{1,0}(v_0)]\ .\end{aligned} \tag{26b}$$

Inserting Eqs. (26a) and (26b) into Eq. (24) we see that $H_1(x_0,v_0,\tau)$ depends on τ through $\bar{x},\bar{v}$ only and we write

$$H_1(x_0,v_0,\tau)=H_1[\bar{x},v_0,\bar{v}] \tag{27}$$

using square brackets if H_1 (or any other function) is expressed by the independent variables $\bar{x},v_0,\bar{v}$ instead of x_0,v_0,τ. Since Eqs. (23a) and (23b) are an autonomous system we can make use of the property described in Appendix A [Eq. (A14)]: Setting $x_0=\bar{x}(\tau-s)$, $v_0=\bar{v}(\tau-s)$, and $\tau=s$ in Eq. (27), we get immediately

$$H_1(\bar{x}(\tau-s),\bar{v}(\tau-s),s)=H_1[\bar{x}(\tau),\bar{v}(\tau-s),\bar{v}(\tau)] \tag{28}$$

and, furthermore,

$$\begin{aligned}\chi_1(x_0,v_0,\tau)&=\int_0^\tau H_1(\bar{x}(\tau-s),\bar{v}(\tau-s),s)ds\\&=\int_0^\tau H_1[\bar{x}(\tau),\bar{v}(\tau-s),\bar{v}(\tau)]ds\ .\end{aligned} \tag{29}$$

Substituting on the rhs of Eq. (29)

$$y=\bar{v}(\tau-s)\ , \tag{30a}$$

$$dy=-\frac{d\bar{v}}{d\tau}ds=-\alpha_{1,0}(y)ds\ , \tag{30b}$$

and inserting $\bar{v}(0)=v_0$ we arrive at the following simple expression for χ_1:

$$\chi_1(x_0,v_0,\tau)=\chi_1[\bar{x},v_0,\bar{v}]=\int_{v_0}^{\bar{v}}\frac{H_1[\bar{x},y,\bar{v}]}{\alpha_{1,0}(y)}dy\ . \tag{31}$$

We have shown that both H_1 and χ_1 depend on τ through $\bar{x}$ and $\bar{v}$ only. The proof for $l>1$ is simply given by induction keeping in mind that according to Eq. (16c) H_l depends on the derivatives of $\chi_0,\dots,\chi_{l-1}$ only and not on χ_l. One finally arrives at the expression

$$\chi_l(x_0,v_0,\tau)=\chi_l[\bar{x},v_0,\bar{v}]=\int_{v_0}^{\bar{v}}\frac{H_l[\bar{x},y,\bar{v}]}{\alpha_{1,0}(y)}dy \tag{32}$$

which we wanted to prove. With the aid of Eq. (32) we derive in the next section a rather simple expression for the expansion of an arbitrary conditional average up to order Ω^{-1}.

It is worthwhile to note that in principle no problems occur when extending the one-dimensional Brownian motion to three dimensions. While Eqs. (18)–(21) are simply replaced by their three-dimensional versions, the calculation of the jump moments becomes much more involved. This was the reason for restricting ourselves in the present paper to the one-dimensional case.

IV. EXPLICIT EXPRESSION FOR χ_1

In the preceding section we separated an arbitrary conditional average $\langle f(x,v)\,|\,x_0,v_0\rangle_\tau$ into its deterministic part χ_0 and the fluctuating parts $\chi_l(l\geq 1)$, yielding

$$\begin{aligned}\langle f(x,v)\,|\,x_0,v_0\rangle_\tau&=\chi(x_0,v_0,\tau)\\&=\sum_{l=0}^{\infty}\frac{1}{\Omega^l}\chi_l(x_0,v_0,\tau)\ .\end{aligned} \tag{33}$$

To lowest order in Ω^{-1} the fluctuations in the system are described by $\chi_1(x_0,v_0,\tau)$, which we now want to calculate explicitly. Using Eqs. (24), (26a) and (26b), and Eq. (32) we obtain

$$\begin{aligned}\chi_1[\bar{x},v_0,\bar{v}]=&\frac{\sigma^2_{x,\mathrm{scal}}}{2}\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{x}^2}+\frac{\sigma^2_{v,\mathrm{scal}}}{2}\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{v}^2}\\&+\Phi_{1,xv}\frac{\partial^2 f(\bar{x},\bar{v})}{\partial\bar{x}\partial\bar{v}}+\Phi_{1,x}\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{x}}\\&+\Phi_{1,v}\frac{\partial f(\bar{x},\bar{v})}{\partial\bar{v}}\ ,\end{aligned} \tag{34}$$

where $\bar{x},\bar{v}$ are the solutions of the macroscopic equation and the other quantities are defined as follows:

$$\sigma^2_{x,\mathrm{scal}} = \int_{v_0}^{\bar v} \frac{\alpha_{2,0}(y)(\bar v - y)^2}{\alpha^3_{1,0}(y)} dy \ , \tag{35a}$$

$$\sigma^2_{v,\mathrm{scal}} = \alpha^2_{1,0}(\bar v) \int_{v_0}^{\bar v} \frac{\alpha_{2,0}(y)}{\alpha^3_{1,0}(y)} dy \ , \tag{35b}$$

$$\Phi_{1,xv} = \alpha_{1,0}(\bar v) \int_{v_0}^{\bar v} \frac{\alpha_{2,0}(y)}{\alpha^3_{1,0}(y)} (\bar v - y) dy \ , \tag{35c}$$

$$\Phi_{1,x} = \int_{v_0}^{\bar v} dy \left[\frac{\alpha_{1,1}(y)}{\alpha^2_{1,0}(y)} (\bar v - y) + \frac{\alpha_{2,0}(v_0)}{2\alpha^3_{1,0}(y)} \{ [\alpha_{1,0}(\bar v) - \alpha_{1,0}(y)] - (\bar v - y)\alpha'_{1,0}(y) \} \right] , \tag{35d}$$

$$\Phi_{1,v} = \int_{v_0}^{\bar v} dy \left[\frac{\alpha_{1,1}(y)\alpha_{1,0}(\bar v)}{\alpha^2_{1,0}(y)} + \frac{\alpha_{1,0}(\bar v)\alpha_{2,0}(y)}{2\alpha^3_{1,0}(y)} [\alpha'_{1,0}(\bar v) - \alpha'_{1,0}(y)] \right] . \tag{35e}$$

Note that the quantities defined in Eqs. (35a)—(35e) depend on v_0 and $\bar v$ only and not on $\bar x$. It is interesting to ask which differential equations are satisfied by the quantities entering Eq. (34).

(i) Macroscopic equations (deterministic path) for velocity and position coordinate of the tagged particle are as follows:

$$\frac{d\bar v}{d\tau} = \alpha_{1,0}(\bar v) \ \text{ with } \bar v(\tau=0) = v_0 \ , \tag{36a}$$

$$\frac{d\bar x}{d\tau} = \bar v \ \text{ with } \bar x(\tau=0) = x_0 \ . \tag{36b}$$

(ii) Mean-square deviation for velocity $\sigma^2_{v,\mathrm{scal}}$ and position $\sigma^2_{x,\mathrm{scal}}$ is shown in the following:

$$\frac{d\sigma^2_{v,\mathrm{scal}}}{d\tau} - 2\alpha'_{1,0}(\bar v)\sigma^2_{v,\mathrm{scal}} = \alpha_{2,0}(\bar v) \ \text{ with } \sigma^2_{v,\mathrm{scal}}(0) = 0 \ , \tag{37a}$$

$$\frac{d^2\sigma^2_{x,\mathrm{scal}}}{d\tau^2} - \alpha'_{1,0}(\bar v)\frac{d\sigma^2_{x,\mathrm{scal}}}{d\tau} = 2\sigma^2_{v,\mathrm{scal}} \quad \text{with } \sigma^2_{x,\mathrm{scal}}(\tau=0) = 0, \ \left.\frac{d\sigma^2_{x,\mathrm{scal}}}{d\tau}\right|_{\tau=0} = 0 \ . \tag{37b}$$

(iii) The coupling term between velocity and position coordinate is displayed in the following:

$$\frac{d\Phi_{1,xv}}{d\tau} - \alpha'_{1,0}(\bar v)\Phi_{1,xv} = \sigma^2_{v,\mathrm{scal}} \ \text{ with } \Phi_{1,xv}(\tau=0) = 0 \ . \tag{38a}$$

There exists an interesting interrelation between the mean-square deviation of the position and the coupling term

$$\frac{d\sigma^2_{x,\mathrm{scal}}}{d\tau} = 2\Phi_{1,xv} \ . \tag{38b}$$

(iv) The deviation from the macroscopic equations up to order Ω^{-1}, described by $\Phi_{1,x}$ and $\Phi_{1,v}$, respectively, is shown in the following:

$$\frac{d\Phi_{1,v}}{d\tau} - \alpha'_{1,0}(\bar v)\Phi_{1,v} = \tfrac{1}{2}\alpha''_{1,0}(\bar v)\sigma^2_{v,\mathrm{scal}} + \alpha_{1,1}(\bar v) \quad \text{with } \Phi_{1,v}(\tau=0) = 0 \ , \tag{39a}$$

$$\frac{d\Phi_{1,x}}{d\tau} = \Phi_{1,v} \ \text{ with } \Phi_{1,x}(\tau=0) = 0 \ . \tag{39b}$$

Using Eqs. (33), (34), and (20) we can calculate the fluctuations of an arbitrary conditional average $\langle f(x,v)g(x,v) \mid x_0,v_0 \rangle_\tau$ up to order Ω^{-1}, yielding

$$\langle f(x,v)g(x,v) \mid x_0,v_0 \rangle_\tau - \langle f(x,v) \mid x_0,v_0 \rangle_\tau \langle g(x,v) \mid x_0,v_0 \rangle_\tau = \frac{1}{\Omega} \left[\sigma^2_{x,\mathrm{scal}} \frac{\partial f}{\partial \bar x}\frac{\partial g}{\partial \bar x} + \sigma^2_{v,\mathrm{scal}} \frac{\partial f}{\partial \bar v}\frac{\partial g}{\partial \bar v} + \Phi_{1,xv} \left[\frac{\partial f}{\partial \bar x}\frac{\partial g}{\partial \bar v} + \frac{\partial f}{\partial \bar v}\frac{\partial g}{\partial \bar x} \right] \right] + O\left[\frac{1}{\Omega^2}\right] . \tag{40}$$

Equation (40) shows most clearly that the function $\chi_1[\bar x, v_0, \bar v]$ [see Eq. (34)] describes both the fluctuations of the system and the deviation from the deterministic path [see Eqs. (36a) and (36b)] up to order Ω^{-1}, since one has the following relations:

$$\langle x \mid x_0 v_0 \rangle_\tau = \bar x + \frac{1}{\Omega}\Phi_{1,x} + O\left[\frac{1}{\Omega^2}\right] , \tag{41a}$$

$$\langle v \mid x_0 v_0 \rangle_\tau = \bar v + \frac{1}{\Omega}\Phi_{1,v} + O\left[\frac{1}{\Omega^2}\right] , \tag{41b}$$

$$\langle x^2 \mid x_0 v_0 \rangle_\tau - \langle x \mid x_0 v_0 \rangle^2_\tau = \frac{1}{\Omega}\sigma^2_{x,\mathrm{scal}} + O\left[\frac{1}{\Omega^2}\right] , \tag{41c}$$

$$\langle v^2 \mid x_0 v_0 \rangle_\tau - \langle v \mid x_0 v_0 \rangle^2_\tau = \frac{1}{\Omega}\sigma^2_{v,\mathrm{scal}} + O\left[\frac{1}{\Omega^2}\right] , \tag{41d}$$

$$\langle xv \mid x_0 v_0 \rangle_\tau - \langle x \mid x_0 v_0 \rangle_\tau \langle v \mid x_0 v_0 \rangle_\tau = \frac{1}{\Omega}\Phi_{1,xv} + O\left[\frac{1}{\Omega^2}\right] . \tag{41e}$$

Next we consider the short- and long-time behavior of the scaled variance $\sigma^2_{x,\mathrm{scal}}$ and $\sigma^2_{v,\mathrm{scal}}$, respectively, and of the coupling term $\Phi_{1,xv}$, since they determine the bivariate Gaussian distribution in the linear noise approximation (see Sec. V). Using Eqs. (37a) and (37b) and Eq. (38b), we obtain for the short-time behavior

$$\sigma^2_{x,\mathrm{scal}}=\tfrac{1}{3}\alpha_{2,0}(v_0)\tau^3+O(\tau^4)\ , \tag{42a}$$

$$\sigma^2_{v,\mathrm{scal}}=\alpha_{2,0}(v_0)\tau+O(\tau^2)\ , \tag{42b}$$

$$\Phi_{1,xv}=\tfrac{1}{2}\alpha_{2,0}(v_0)\tau^2+O(\tau^3)\ . \tag{42c}$$

The short-time behavior of the scaled variance $\sigma^2_{x,\mathrm{scal}}$ must not be confused with the short-time behavior of the mean-square displacement $\langle(\Delta x)^2\rangle_\tau$ of a Brownian particle, which is given by

$$\begin{aligned}\langle(\Delta x)^2\rangle_\tau&=\langle(x-x_0)^2\,|\,x_0v_0\rangle_\tau\\&=\left[\int_0^\tau \bar{v}(s)ds\right]^2+\frac{\sigma^2_{x,\mathrm{scal}}}{\Omega}\\&\quad+\frac{2}{\Omega}\Phi_{1,x}\int_0^\tau\bar{v}(s)ds+O\left[\frac{1}{\Omega^2}\right]\ ,\end{aligned} \tag{43a}$$

and has the short-time behavior up to order Ω^{-2}

$$\langle\Delta x^2\rangle_\tau=v_0^2\tau^2+O(\tau^3)\ . \tag{43b}$$

In order to evaluate the long-time behavior of the quantities given in Eqs. (35a)—(35c) we have to consider the Taylor expansion of the jump moments. According to Eq. (B8) two completely different Taylor expansions are possible depending on whether the temperature (or v_{T_B}) of the heat bath has a finite positive value ($v_{T_B}>0$) or is identical to zero ($v_{T_B}=0$).

(i) $v_{T_B}>0$. The Taylor expansion for the jump moments yields

$$\alpha_{1,0}(v_0)=-\frac{4n_Bv_{T_B}}{\sqrt{\pi}}v_0\left[1+O\left[\frac{v_0^2}{v_{T_B}^2}\right]\right]\ , \tag{44a}$$

$$\alpha_{2,0}(v_0)=\frac{4n_Bv_{T_B}^3}{\sqrt{\pi}}\left[1+O\left[\frac{v_0^2}{v_{T_B}^2}\right]\right]\ . \tag{44b}$$

Equation (44a) implies that the solution of the macroscopic equation is stable and has the limiting property

$$\lim_{\tau\to\infty}\bar{v}(\tau)=0\ . \tag{45}$$

For the long-time behavior of the quantities defined in Eqs. (35a)—(35c) we obtain

$$\lim_{\tau\to\infty}\sigma^2_{x,\mathrm{scal}}\approx\frac{\alpha_{2,0}(0)}{[\alpha'_{1,0}(0)]^2}\tau=\frac{v_{T_B}\sqrt{\pi}}{4n_B}\tau\ , \tag{46a}$$

$$\lim_{\tau\to\infty}\sigma^2_{v,\mathrm{scal}}=-\frac{\alpha_{2,0}(0)}{2\alpha'_{1,0}(0)}=\frac{v_{T_B}^2}{2}\ , \tag{46b}$$

$$\lim_{\tau\to\infty}\Phi_{1,xv}=\frac{\alpha_{2,0}(0)}{2[\alpha'_{1,0}(0)]^2}=\frac{v_{T_B}\sqrt{\pi}}{8n_B}\ . \tag{46c}$$

Combining Eq. (43a) and Eq. (46a) we obtain the well-known long-time behavior of the mean-square displacement of a Brownian particle.

(ii) $v_{T_B}=0$. In this limit the jump moments are given by the simple expression [see Eq. (B10)]

$$\alpha_{n,0}(v_0)=(-2)^n n_B\,|\,v_0\,|\,v_0^n\ . \tag{47a}$$

While in this case the solution of the macroscopic equation remains stable, its decay is slow, which is a sort of critical slowing down. The macroscopic equation can now be solved explicitly, yielding

$$\bar{v}=\frac{v_0}{1+2n_B\,|\,v_0\,|\,\tau}\ , \tag{47b}$$

which is identical to the result by Miller and Stein.[9]

For the long-time behavior of the scaled variances $\sigma^2_{x,\mathrm{scal}}$ and $\sigma^2_{v,\mathrm{scal}}$, respectively, and of the coupling term $\Phi_{1,xv}$, we obtain

$$\lim_{\tau\to\infty}\sigma^2_{x,\mathrm{scal}}\approx\frac{1}{2n_B^2}\ln(1+2n_B\,|\,v_0\,|\,\tau)\ , \tag{48a}$$

$$\lim_{\tau\to\infty}\sigma^2_{v,\mathrm{scal}}=0\ , \tag{48b}$$

$$\lim_{\tau\to\infty}\Phi_{1,xv}=0\ . \tag{48c}$$

Equations (48a)—(48c) indicate that the energy of the Rayleigh piston tends to zero with increasing time, and the mean-square displacement grows logarithmically. This result, which is in contradiction to the well-known Einstein formula, is an immediate consequence of the nonlinearity of the first and higher jump moments.

V. THE BIVARIATE GAUSSIAN DISTRIBUTION FUNCTION

In the preceding sections we calculated the functions χ_0 and χ_1 explicitly. It showed that χ_0 describes the deterministic path, whereas χ_1 determines the fluctuations around the macroscopic motion up to order Ω^{-1}. When going beyond the first order in the Ω expansion the calculations remain straightforward, although they are rather long and tedious. For this reason we restrict ourselves to the explicit expressions χ_0 and χ_1, respectively, and show in this section, how one can arrive at a bivariate Gaussian distribution function, neglecting certain terms in the general expression for χ_l ($l\geq 1$).

Let us first introduce the following differential operator:

$$\begin{aligned}D(a,b)=&\frac{\sigma^2_{x,\mathrm{scal}}[a,b]}{2}\frac{\partial^2}{\partial\bar{x}^2}+\frac{\sigma^2_{v,\mathrm{scal}}[a,b]}{2}\frac{\partial^2}{\partial\bar{v}^2}\\&+\Phi_{1,xv}[a,b]\frac{\partial}{\partial\bar{x}}\frac{\partial}{\partial\bar{v}}\ .\end{aligned} \tag{49}$$

With the aid of this differential operator D we rewrite the expressions for χ_0 and χ_1, respectively [see Eqs. (20) and

(34)],

$$\chi_0[\bar{x},v_0,\bar{v}]=f(\bar{x},\bar{v})\ , \tag{50a}$$

$$\chi_1[\bar{x},v_0,\bar{v}]=D(v_0,\bar{v})f(\bar{x},\bar{v})+O(f^{(1)})\ , \tag{50b}$$

where the symbol $O(f^{(l)})$ stands for all terms containing derivatives of $f(\bar{x},\bar{v})$ with respect to $\bar{x}$ and $\bar{v}$ up to order l only.

Next we will prove by induction that the general structure of $\chi_k[\bar{x},v_0,\bar{v}]$ is given by

$$\chi_k[\bar{x},v_0,\bar{v}]=\frac{1}{k!}[D^k(a,b)f(\bar{x},\bar{v})]_{a=v_0,b=\bar{v}}+O(f^{(2k-1)})\ . \tag{51}$$

Assuming that Eq. (51) is valid, we obtain using Eq. (16c) and Eq. (32)

$$\chi_{k+1}[\bar{x},v_0,\bar{v}]=\int_{v_0}^{\bar{v}}dy\frac{\alpha_{2,0}(y)}{2\alpha_{1,0}(y)}\left.\frac{d^2\chi_k[\bar{x},v_0,\bar{v}]}{dv_0^2}\right|_{v_0=y}+O(f^{(2k+1)})\ . \tag{52}$$

With the aid of Eq. (51) we get for the second derivative of χ_k with respect to v_0

$$\frac{d^2\chi_k[\bar{x},v_0,\bar{v}]}{dv_0^2}=\frac{1}{k!}\left[D^k(a,b)\frac{d^2f(\bar{x},\bar{v})}{dv_0^2}\right]_{a=v_0,b=\bar{v}}+O(f^{(2k+1)})\ . \tag{53}$$

The derivatives of $D^k(v_0,\bar{v})$ and of the terms indicated in Eq. (51) by the symbol $O(f^{(2k-1)})$ yield contributions which are collected in Eq. (53) by the symbol $O(f^{(2k+1)})$. The second derivative of $f(\bar{x},\bar{v})$ with respect to v_0 has been yet calculated in Eq. (23b) and can be cast into a more convenient form using the partial derivatives of Eqs. (35a)–(35c) with respect to v_0. With the aid of Eq. (49) we finally obtain

$$\frac{d^2f(\bar{x},\bar{v})}{dv_0^2}=-\frac{2\alpha_{1,0}(v_0)}{\alpha_{2,0}(v_0)}\left[\frac{\partial D(a,b)}{\partial a}f(\bar{x},\bar{v})\right]_{a=v_0,b=\bar{v}}+O(f^{(1)})\ . \tag{54}$$

If we now insert Eq. (54) into Eq. (53) we can simplify Eq. (52), yielding

$$\chi_{k+1}[\bar{x},v_0,\bar{v}]=-\int_{v_0}^{\bar{v}}dy\frac{1}{k!}\left[D^k(y,b)\frac{\partial D(y,b)}{\partial y}\right]_{b=\bar{v}}\times f(\bar{x},\bar{v})+O(f^{(2k+1)})\ . \tag{55a}$$

Keeping in mind that according to Eqs. (49) and (35a) and (35c),

$$D(a,a)=0\ , \tag{55b}$$

we obtain

$$\chi_{k+1}[\bar{x},v_0,\bar{v}]=\frac{1}{(k+1)!}[D^{k+1}(a,b)f(\bar{x},\bar{v})]_{a=v_0,b=\bar{v}}+O(f^{(2k+1)})\ , \tag{56}$$

which proves Eq. (51).

If we now "neglect" in Eq. (51) all terms indicated by the symbol $O(f^{(2k-1)})$ we obtain, in connection with Eq. (15) for the expansion of an arbitrary conditional average χ in powers of $1/\Omega$, the following "approximation" formula:

$$\chi(x_0,v_0,\tau)=\langle f(x,v)\,|\,x_0,v_0\rangle_\tau\approx f(\bar{x},\bar{v})+\sum_{k=1}^{\infty}\frac{1}{k!}\left[\frac{\sigma_{x,\mathrm{scal}}^2}{2\Omega}\frac{\partial^2}{\partial\bar{x}^2}+\frac{\sigma_{v,\mathrm{scal}}^2}{2\Omega}\frac{\partial^2}{\partial\bar{v}^2}+\frac{\Phi_{1,xv}}{\Omega}\frac{\partial}{\partial\bar{x}}\frac{\partial}{\partial\bar{v}}\right]^k f(\bar{x},\bar{v})\ . \tag{57}$$

Equation (57) can be obtained in an alternative way, using in Eq. (6) a bivariate Gaussian distribution function

$$h(x,v,\tau\,|\,x_0,v_0)=h^G(x-\bar{x},v-\bar{v}) \tag{58a}$$

with

$$h^G(x,v)=\frac{1}{2\pi(FG-H^2)^{1/2}}\exp\left[-\frac{(Gx^2-2Hxv+Fv^2)}{2(FG-H^2)}\right]\ . \tag{58b}$$

In order to see this we expand in Eq. (6) $f(x,v)$ in a Taylor series around $\bar{x},\bar{v}$

$$\langle f(x,v)\,|\,x_0,v_0\rangle_\tau=f(\bar{x},\bar{v})+\sum_{k=1}^{\infty}\frac{1}{k!}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dv\,h^G(x-\bar{x},v-\bar{v})\left[(x-\bar{x})\frac{\partial}{\partial\bar{x}}+(v-\bar{v})\frac{\partial}{\partial\bar{v}}\right]^k f(\bar{x},\bar{v})\ . \tag{59}$$

The integration can be performed using the following relations for the moments of a bivariate Gaussian distribution function:

$$\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dv(ax+bv)^{2n+1}h^G(x,v)=0\ , \tag{60a}$$

$$\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dv(ax+bv)^{2n}h^G(x,v)=\frac{(2n)!}{n!}\left[\frac{F}{2}a^2+\frac{G}{2}b^2+Hab\right]^n\ , \tag{60b}$$

where a,b are arbitrary constants. With the aid of Eqs. (60a) and (60b) we finally get instead of Eq. (59)

$$\langle f(x,v)\,|\,x_0,v_0\rangle_\tau=f(\bar{x},\bar{v})+\sum_{k=1}^{\infty}\frac{1}{k!}\left[\frac{F}{2}\frac{\partial^2}{\partial\bar{x}^2}+\frac{G}{2}\frac{\partial^2}{\partial\bar{v}^2}+H\frac{\partial}{\partial\bar{x}}\frac{\partial}{\partial\bar{v}}\right]^k f(\bar{x},\bar{v})\;, \tag{61a}$$

where the functions F,G,H are determined by a comparison of Eqs. (57) and (61a), respectively, yielding

$$F=\frac{\sigma^2_{x,\text{scal}}}{\Omega},\quad G=\frac{\sigma^2_{v,\text{scal}}}{\Omega},\quad H=\frac{\Phi_{1,xv}}{\Omega}\;. \tag{61b}$$

It is easy to prove that

$$F\geq 0,\quad G\geq 0,\quad H\geq 0\;, \tag{62a}$$

and

$$FG-H^2\geq 0\;, \tag{62b}$$

where the latter relation can be immediately derived using the Cauchy-Schwarz inequality. So we have shown that the assumptions of a bivariate Gaussian distribution function [see Eqs. (58a) and (58b)] with time-dependent mean $\bar{x},\bar{v}$ and variance F,G,H [see Eqs. (35a)–(35c) and Eq. (61b)] suffices to obtain Eq. (57). This approximation is usually called the linear-noise approximation.[5,8] From a mathematical point of view there is, of course, no reason for neglecting the second term on the rhs of Eq. (51), since in general it is of the same order as the first term.

We will see in the next section that only rather unrealistic assumptions concerning the jump moments imply that the second term in the rhs of Eq. (51) vanishes, and therefore lead to a Gaussian distribution function. We will show in a future paper that a correction to the bivariate Gaussian distribution function can be obtained, taking into account the second term in the rhs of Eq. (51). It will turn out that our Ω expansion provides a systematic method for expanding the distribution function in Hermite functions.

Examples

To illustrate the power of our Ω expansion, two examples are given. In our first example, which we call the Langevin approach, we assume that all jump moments except the first and second ones vanish,

$$\alpha_{1,0}(v_0)=-\gamma v_0\;, \tag{63a}$$

$$\alpha_{2,0}(v_0)=\Gamma\;, \tag{63b}$$

$$\alpha_{n,k}(v_0)=0\quad\text{otherwise}\;. \tag{63c}$$

These assumptions are identical to those which are usually made in deriving the Langevin or Fokker-Planck equation. Owing to the simple structure of the jump moments, we obtain for the solution of the macroscopic equation [see Eqs. (18a) and (18b)]

$$\bar{v}=v_0\exp(-\gamma\tau),\quad \bar{x}=x_0+\frac{v_0}{\gamma}[1-\exp(-\gamma\tau)]\;, \tag{64}$$

and for the quantities defined in Eqs. (35a)–(35e),

$$F=\frac{\sigma^2_{x,\text{scal}}}{\Omega}=\frac{\Gamma}{2\gamma^3\Omega}[2\gamma\tau-3+4\exp(-\gamma\tau)-\exp(-2\gamma\tau)]\;, \tag{65a}$$

$$G=\frac{\sigma^2_{v,\text{scal}}}{\Omega}=\frac{\Gamma}{2\gamma\Omega}[1-\exp(-2\gamma\tau)]\;, \tag{65b}$$

$$H=\frac{\Phi_{1,xv}}{\Omega}=\frac{\Gamma}{2\gamma^2\Omega}[1-\exp(-\gamma\tau)]^2\;, \tag{65c}$$

$$\Phi_{1,x}=\Phi_{1,v}=0\;. \tag{65d}$$

In order to get the correct equilibrium values, the constant Γ and the damping constant γ must be related by the fluctuation-dissipation theorem. Using Eqs. (41d) and (65) we obtain

$$\lim_{\tau\to\infty}\langle v^2\,|\,v_0\rangle_\tau=\frac{\Gamma}{2\gamma\Omega}=\frac{v^2_{T_A}}{2}=\frac{kT}{m_A}\;. \tag{66}$$

Since Eqs. (65d) and (63c) hold and since all derivatives of F,G,H with respect to v_0 are identical to zero, it is easy to show that the second term in the rhs of Eq. (56) vanishes. Therefore, we conclude that the Langevin approach is completely determined by the bivariate Gaussian distribution function [Eqs. (58a) and (58b)] and the time-dependent variances F,G,H [see Eqs. (65a)–(65c)]. This bivariate Gaussian distribution function has been derived previously by Chandrasekhar[2] using both the Langevin equation and the Fokker-Planck equation.

In our first example—the Langevin approach—*ad hoc* assumptions for the jump moments are made, which are unphysical in the sense that no realistic interaction potential would produce these moments. We choose in our second example a special limiting case for a hard-core interaction potential. We assume that the temperature of the heat bath ($v_{T_B}=2kT/m_B$) tends to zero.

With the aid of Appendix B and the special choice of the parameter Ω [see Eq. (B2)], the jump moments assume the simple form

$$\alpha_{n,k}(v)=\alpha_n(v)\delta_{k,0}\;, \tag{67a}$$

$$\alpha_n(v)=(-2)^n n_B\,|\,v\,|\,v^n\;. \tag{67b}$$

The macroscopic equation can be solved explicitly, yielding

$$\bar{v}=\frac{v_0}{1+2n_B\,|\,v_0\,|\,\tau},\quad \bar{x}=x_0+\frac{v_0}{2n_B\,|\,v_0\,|}\ln(1+2n_B\,|\,v_0\,|\,\tau)\;. \tag{68}$$

For the quantities defined in Eqs. (35a) and (35e), we obtain after some straightforward integrations

$$F=\frac{\sigma^2_{x,\mathrm{scal}}}{\Omega}=-\frac{1}{4n_B^2\Omega}\left[\left[\frac{\bar{v}}{v_0}\right]^2-4\left[\frac{\bar{v}}{v_0}\right]+3+2\ln\left[\frac{\bar{v}}{v_0}\right]\right], \quad (69a)$$

$$G=\frac{\sigma^2_{v,\mathrm{scal}}}{\Omega}=\frac{\bar{v}^2}{\Omega}\left[1-\left[\frac{\bar{v}}{v_0}\right]^2\right], \quad (69b)$$

$$H=\frac{\Phi_{1,xv}}{\Omega}=\frac{|\bar{v}|}{2n_B\Omega}\left[1-\left[\frac{\bar{v}}{v_0}\right]\right]^2, \quad (69c)$$

$$\Phi_{1,x}=\frac{1}{4n_B}\frac{v_0}{|v_0|}\left[\left[\frac{\bar{v}}{v_0}\right]^2-4\left[\frac{\bar{v}}{v_0}\right]+3+2\ln\left[\frac{\bar{v}}{v_0}\right]\right], \quad (69d)$$

$$\Phi_{1,v}=-\bar{v}\left[1-\left[\frac{\bar{v}}{v_0}\right]\right]^2. \quad (69e)$$

The Gaussian approximation, which is completely determined by the quantities F,G,H, yields in the limit $v_{T_B}\to 0$ a rough approximation for conditional averages only, since the functions $\Phi_{1,x}$ and $\Phi_{1,v}$, respectively, do not vanish. One might hope to resolve this problem by replacing in the Gaussian distribution function [see Eq. (58a)] the terms $x-\bar{x}$ and $v-\bar{v}$ by

$$x-\bar{x}-\frac{1}{\Omega}\Phi_{1,x} \quad \text{and} \quad v-\bar{v}-\frac{1}{\Omega}\Phi_{1,v}, \quad (70)$$

respectively. Indeed, such a shift in the mean values is suggested by looking at the characteristic function instead of the distribution function itself (see Kubo *et al.*[10]), which proves useful only in the limit of large Ω.

Since our Ω expansion provides a method for expanding conditional averages in powers of Ω^{-1} it can, of course, be used for calculating the characteristic function

$$Q(\xi,\eta,t)=\int dx\int dy\,\exp[i(\xi x+\eta v)]h(x,v,t\mid x_0,v_0). \quad (71a)$$

Assuming that the characteristic function has the form

$$Q(\xi,\eta,t)=\exp[q(\xi,\eta,t)], \quad (71b)$$

we can expand the exponent $q(\xi,\eta,t)$—or equivalently $\ln Q$—in a power series of Ω^{-1}

$$q(\xi,\eta,t)=\sum_{l=0}^{\infty}\frac{1}{\Omega^l}q_l(\xi,\eta,t). \quad (71c)$$

The functions $q_l(\xi,\eta,t)$ can be uniquely determined expressing Eq. (14) by $\ln\mathcal{X}$ instead of $\mathcal{X}$, and again comparing equal powers in Ω^{-1}. Neglecting in Eq. (71c) all terms higher than order Ω^{-1}, we arrive with the aid of Eq. (71b) at the characteristic function of the bivariate Gaussian distribution function [see Eq. (58b)]

$$h^G\left[x-\bar{x}-\frac{1}{\Omega}\Phi_{1,x}v-\bar{v}-\frac{1}{\Omega}\Phi_{1,v}\right], \quad (72)$$

where the functions $\Phi_{1,x}$, $\Phi_{1,v}$, and F,G,H are determined by Eqs. (35a)–(35e) and Eq. (61b), respectively. Now the mean position or the mean velocity of a particle, calculated with the aid of the Gaussian distribution function [see Eq. (72)] is identical with Eqs. (41a) and (41b) up to order Ω^{-1}. However, especially for mass ratios $m_A/m_B\approx 1$, the terms indicated in the rhs of Eqs. (41a)–(41e) by the symbol $O(\Omega^{-2})$, should not be disregarded since, in general, they are comparable with the first two terms.

In order to show the error, which results from neglecting the terms of order Ω^{-2} in Eqs. (41a)–(41e), we calculate the mean velocity of a particle up to order Ω^{-2}. Using the special jump moments [see Eqs. (67a) and (67b)] we obtain with the aid of Eq. (32) and Eq. (16c)

$$\langle v\mid v_0\rangle_\tau=\bar{v}+\frac{1}{\Omega}\Phi_{1,v}+\frac{1}{\Omega^2}\Phi_{2,v}+O\left[\frac{1}{\Omega^3}\right], \quad (73a)$$

where $\Phi_{1,v}$ is given in Eq. (69e) and

$$\Phi_{2,v}=-\bar{v}\left[1-\frac{\bar{v}}{v_0}\right]^3\left[\tfrac{1}{3}+3\frac{\bar{v}}{v_0}\right]. \quad (73b)$$

In the limit $\tau\to\infty$ one has

$$\lim_{\tau\to\infty}\langle v\mid v_0\rangle_\tau\approx\bar{v}\left[1-\frac{1}{\Omega}-\frac{1}{3\Omega^2}\right]+O\left[\frac{1}{\Omega^3}\right]. \quad (73c)$$

This shows most clearly that, in general, the Gaussian distribution function yields only a rough approximation for conditional averages, since, e.g., it reproduces the first two terms of the rhs of Eqs. (73a) and (73c) only [for $\Omega^{-1}\approx\frac{1}{2}$ the contribution of the term $1/3\Omega^2$ in Eq. (73c) is about 16%]. Our approximation scheme, however, provides a systematic method for calculating conditional averages up to arbitrary order in the expansion parameter Ω^{-1}.

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APPENDIX A

For completeness we briefly sketch a theorem, which is essential in the theory of first-order partial differential equations.[11,12] Let $\underline{\varphi}(t,\tau,\underline{a})$ denote the solution of the system of n ordinary first-order differential equations

$$\frac{d\underline{x}}{dt}\equiv\dot{\underline{x}}=\underline{f}(\underline{x},t) \quad (A1)$$

subject to the initial condition

$$\underline{\varphi}(\tau,\tau,\underline{a})=\underline{a}. \quad (A2)$$

Then $\underline{\varphi}(t,\tau,\underline{a})$ is a solution of the partial differential equation

$$\frac{\partial\underline{\varphi}(t,\tau,\underline{a})}{\partial\tau}+\sum_{s=1}^{n}f_s(\underline{a},\tau)\frac{\partial\underline{\varphi}(t,\tau,\underline{a})}{\partial a_s}=0. \quad (A3)$$

For proving this we note that according to Eq. (A1) the solution $\underline{\varphi}$ satisfies

$$\dot{\underline{\varphi}}(t,\tau,\underline{a})=\underline{f}[\underline{\varphi}(t,\tau,\underline{a}),t] \; . \tag{A4}$$

Thus, if $\underline{\varphi}$ and $\underline{f}$ are sufficiently differentiable (see Ref. 12) we obtain, taking the derivative of Eq. (A4) with respect to τ and a_s, respectively, the following linear differential equations:

$$\dot{\underline{\varphi}}_\tau=\underline{B}\underline{\varphi}_\tau \; , \tag{A5}$$

$$\dot{\underline{\varphi}}_{a_s}=\underline{B}\varphi_{a_s} \quad \text{with } s=1,\ldots,n \tag{A6}$$

where $\underline{B}$ denotes a matrix with the elements

$$B_{i,k}=\frac{\partial f_i}{\partial \varphi_k} \; .$$

Equations (A5) and (A6) have to be solved subject to the initial conditions

$$\underline{\varphi}_\tau(t=\tau,\tau,\underline{a})=-\underline{f}(\underline{a},\tau) \; , \tag{A7}$$

$$\underline{\varphi}_{a_s}(t=\tau,\tau,\underline{a})=\underline{e}_s \quad \text{for } s=1,\ldots,n \tag{A8}$$

where $\underline{e}_s$ is a vector with all components zero except the sth which is 1. Since both Eqs. (A5) and (A6) are linear differential equations with the same matrix $\underline{B}$ but different initial conditions, we can construct the solution $\underline{\varphi}_\tau$ of Eq. (A5) as a linear combination of the solutions of Eq. (A3), yielding

$$\underline{\varphi}_\tau=-\sum_{s=1}^{n} f_s(\underline{a},\tau)\underline{\varphi}_{a_s} \; , \tag{A9}$$

which is just Eq. (A3).

For an autonomous system

$$\dot{\underline{x}}=\underline{f}(\underline{x}) \tag{A10}$$

the solution has the general form

$$\underline{x}(t)=\underline{\varphi}(t-\tau,\underline{a}) \tag{A11}$$

and because of $\partial\underline{\varphi}/\partial\tau=-\partial\underline{\varphi}/\partial t$ one has instead of Eq. (A3) (for $\tau=0$)

$$\frac{\partial\underline{\varphi}(t,\underline{a})}{\partial t}-\sum_{s=1}^{n} f_s(\underline{a})\frac{\partial\underline{\varphi}(t,\underline{a})}{\partial a_s}=0 \; . \tag{A12}$$

Another useful property can be derived from the following identity:

$$\underline{\varphi}(t,\tau,\underline{a})=\underline{\varphi}(t,\tau',\underline{\varphi}(\tau',\tau,\underline{a})) \tag{A13}$$

which holds, since by definition $\underline{\varphi}$ is a solution of Eq. (A1) and both sides are identical for $t=\tau'$. For an autonomous system we obtain in particular using Eq. (A11)

$$\underline{\varphi}(t,\underline{a})=\underline{\varphi}(t',\underline{\varphi}(t-t',\underline{a})) \tag{A14}$$

which has been used in deriving Eq. (28).

APPENDIX B

The transition probability for a one-dimensional hard-sphere gas is given by

$$W_\Omega(v_0\to v_1)=n_B\left[\frac{m_A+m_B}{2m_B}\right]^2 |v_1-v_0| \times f_B\left[\frac{m_A+m_B}{2m_B}v_1-\frac{m_A-m_B}{2m_B}v_0\right] , \tag{B1}$$

where m_A is the mass of the tagged particle (Rayleigh piston), m_B is the mass of the bath particles, n_B is the number density, and

$$f_B(v)=\frac{1}{\sqrt{\pi}v_{T_B}}\exp\left[-\frac{v^2}{v_{T_B}^2}\right], \quad v_{T_B}^2=\frac{2kT}{m_B} \; .$$

For convenience we choose as our expansion parameter

$$\frac{1}{\Omega}=\frac{m_B}{m_A+m_B} \; . \tag{B2}$$

Comparing Eqs. (B1) and (9a) we obtain

$$W_0(v_0,y)=\frac{n_B}{4}|y|f_B\left[\frac{y}{2}+v_0\right] \quad \text{with } y=\Omega(v_1-v_0) \tag{B3}$$

$$W_k(v_0,y)=0 \quad \text{for } k\geq 1 \tag{B4}$$

$$F(\Omega)=\Omega \; . \tag{B5}$$

The jump moments [see Eq. (9b)] now assume the simple form

$$K_n(v_0)=\frac{\alpha_{n,0}(v_0)}{\Omega^n} \; , \tag{B6}$$

with

$$\alpha_{n,k}(v_0)=\alpha_{n,0}(v_0)\delta_{k,0} \tag{B7}$$

and

$$\alpha_{n,0}(v_0)=\int W_0(v_0,y)y^n dy \; . \tag{B8}$$

In the limit $v_{T_B}\to 0$ one can replace in Eq. (B3) the Maxwell-Boltzmann distribution function by a δ function, yielding for $\alpha_{n,0}$

$$\alpha_{n,0}(v_0)=(-2)^n n_B |v_0| v_0^n \; . \tag{B9}$$

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