Brownian type of motion of a randomly kicked particle far from and close to the diffusion limit

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The motion of a classical test particle, which evolves deterministically in a potential field and where at a given rate its velocity is randomized, is investigated. A path integral approach is used to find exact solutions for the free and harmonically bound particles. Both the exact solution and numerical solution for a nonlinear case show large deviations from the diffusion limit.

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I. INTRODUCTION

This paper discusses the model proposed by Il'in and Khasminskii (IK) [1] for a Brownian type of motion and presents some exact solutions for it. The model considers a one-dimensional (1D) classical test particle of a mass M which evolves deterministically in a potential field $V(x)$. At a given rate α the velocity of the particle is randomized. The change in the velocity is due to an elastic impact with gas particles of the mass m whose velocities are Maxwell distributed with a given temperature T.

Much work has been done for two special cases. The first case is when the mass ratio $\varepsilon \equiv m/M = 1$. In this case the test particle velocity is resampled according to the Maxwell distribution after each collision. Such a model was used to calculate reaction rates [4–6] by considering a particle moving in a metastable background potential and relating the collision rate α to the pressure of the surrounding gas. A comparison was made between the reaction rates computed from this model and other reaction rate theories [5,6]. A similar approach for the case $\varepsilon = 1$ was used in the field of the plasma physics [2,3].

This approach is also commonly used for numerical simulations of systems with many degrees of freedom [7–9]. In some cases the collisions follow one after the other separated by constant time intervals [10–12]. This regime was addressed in our paper [13] where a possibility of slowing down the relaxation was indicated.

Another limit investigated thoroughly is the limit of weak and frequent collisions. Under certain conditions this limit produces diffusion approximation [1,14] which may be treated also by means of a Langevin or equivalent Fokker-Planck equation (see, e.g., Refs. [15–19]). A widespread use of these two limits encourages us to try and find a unifying approach and to look for exact solutions for some simple cases but for arbitrary mass ratios ε.

This sort of a model for a free particle, called the Rayleigh piston, may incorporate also (see, e.g., [20] and references therein) a dependence of collision frequency on the reference particle velocity which may appear to be of importance at high enough velocity. However, Il'in and Khasminskii [1] deduced a master equation for the particle in a potential using the standard Kolmogorov approach and assuming a velocity independent rate of collisions. The main result of [1] is a derivation of a backward Kolmogorov equation from the master equation for the collision process.

It is understood [16,17,19] that systems which experience rare and strong fluctuations are described by integro-differential equations. These equations are rarely solved. In fact, Kramers in his seminal work [21] dwells on the validity of the diffusion approximation in order to describe chemical reaction rates. He claims that an approach in which the collisions with the surrounding medium particles are rare and strong might be more appropriate. Chemical collisions may serve as a microscopic mechanism for such noise [22]. The IK mechanical model to be considered here may serve as a simple model for such a process.

Knessel *et al.* [14] have used the same model to describe chemical reaction rates, and derived a backward Kramers-Moyal equation for this process. They then looked for asymptotic solutions of this equation, comparing these with the results of the diffusion approximation and questioning their validity.

In the fields of chemistry and physics considerable efforts have been devoted to the connection between master equations describing Markov processes and their approximate diffusion type descriptions, i.e., by means of a Fokker-Planck equation [16]. The master equation is often expanded using some small parameter and truncated after two terms. This procedure yields the Fokker-Planck equation when using, for example, van Kampen's Ω expansion [16]. Grabert, Hänggi, and collaborators [23,24] and Knessel *et al.* [14] compared the relaxation times computed by means of the master equation and the Fokker-Planck equation, pointing out that the diffusion approximation does not necessarily hold. Instead, it was suggested in Refs. [23,24] to make use of an effective Fokker-Planck equation which led to a solution similar to that of the master equation. Additional work on approximate solutions of the master equation can be found in Refs. [17,25].

In order to study the validity of the diffusion approximation, it is of interest to solve simple forms of the master equation. Then it is possible to compare between the

exact solutions and those given by the diffusion approximation. Considering a Poisson process we apply here an integration over all possible sets of collision times and all values of the momenta of colliding particles. This technique allows us to derive integro-differential equations for the moments of the coordinate and momentum describing the motion of the test particle.

A forward master equation for an evolution of the joint probability density function of the particle trajectory in the phase space is derived. In addition, low order moments are explicitly computed describing the motion of a free particle and a particle situated in a harmonic force field. This is done for all values of the masses, the mean free time between the collisions, and initial conditions.

We find the relaxation times, describing the low moments of the mechanical state of the particle. The Einstein fluctuation-dissipation relation holds for all values of the mentioned parameters, if one identifies correctly the damping coefficient. However, the evolutions of the mean square displacement and the kinetic energy are controlled by two different times which coincide only in the diffusion limit. It will also be shown that deviations from the diffusion limit are not necessarily small even when the ratio of masses of the gas and reference particles is small.

In the last section we present some numerical results for the motion in a nonlinear background potential field. We show that the damping coefficient which appears in the Einstein relation cannot serve as the only variable controlling the dynamic correlation time. Rather both the collision rate and the mass ratio must be considered.

II. MODEL

Here we consider a simple model for a system coupled with a bath. Let us assume that there is a particle with the mass M moving in the potential $V(x)$. Its motion is described by the Newton equation of motion. The particle may interact with a bath which is a one dimensional gas of other particles with the mass m. The reference particle is elastically kicked by the gas particles whose momenta $\tilde{p}$ are distributed according to the Maxwell function. Here and below, T is the temperature of the gas particles, measured in energy units ($k_B = 1$). The collisions occur at random times $\{t_1, \ldots, t_i, \ldots\}$ according to the Poisson distribution. Each elastic collision causes a change of the momentum of the reference particle according to the equation

$$p^+ = \mu_1 p^- + \mu_2 \tilde{p} \,, \tag{1}$$

where

$$\mu_1 = \frac{M-m}{M+m}, \quad \mu_2 = \frac{2M}{M+m}.$$

Here the signs $-$ and $+$ mark the values of the momentum just before and after the collision. The coordinate of the reference particle does not change. Here the duration of the collision events is assumed to be much shorter than any other time appearing in the problem.

Now a sequence $\{\tilde{p}_i\}$ and $\{t_i\}$ describing k collisions is considered. The deterministic equation of motion and rule (1) give a principal possibility to find the coordinate $x_k(t)$ and the momentum $p_k(t)$ of the test particle at a time $t > t_k$. It is clear that these two quantities depend on their initial values, x_0 and p_0, and the particular choice of the sequences $\{\tilde{p}_i\}$ and $\{\tilde{t}_i\}$.

$$x_k(t)\,(\{\tilde{p}_i\},\{t_i\};x_0,p_0)\,, \quad p_k(t)\,(\{\tilde{p}_i\},\{t_i\};x_0,p_0)\,. \tag{2}$$

The mechanical state of the reference particle is characterized by the coordinate and the mechanical momentum (x,p). In addition one may consider the number n of collisions the particle has encountered. In the usual situations this number is not measurable at a time t. An example where this number may be easily recorded is by numerical simulation of this model. After the system has been evolving for a time t and the reference particle has been kicked many times by the gas particles, these quantities can be predicted only statistically. Generally x, p, and n are of physical interest, especially their low moments and correlations between them.

Definitions

In the model described above the collision events appear as dots on the time axis. These together make the so called [16] "random set of points" or "events" or a "point process." At each dot the momentum of the incident particle is specified. The total time the reference particle has been evolving is t. The dots and the momenta of the incident particles are random numbers and one has to study the following combination of stochastic variables.

The sample space is formed by the states which are formed in the following way: (i) a non-negative integer $s = 0, 1, \ldots$ describes the number of collisions during the time t; (ii) for each s there exists an ordered set, $0 < t_1 < \cdots t_i < t_{i+1} < \cdots < t_s$, of s real numbers corresponding to the times at which the collisions occur; (iii) a real number, $-\infty < \tilde{p}_i < \infty$, is assigned to each collision event, which is the momentum of the incident gas particle.

Now the probability density over these states $Q_s(t_1, \tilde{p}_1, t_2, \ldots, t_s, \tilde{p}_s)$ is introduced which is defined in the domain given by (ii) and (iii). We consider here the situation when each collision is an independent event and the corresponding momenta $\tilde{p}$ are distributed according to the Maxwell function. Now we need a function $q(t)dt$ which gives us the average number of collisions in the time interval $(t, t+dt)$. Then the probability density of the states with s collisions can be presented as

$$Q_s = Q_0 P(\tilde{p}_1) \cdots P(\tilde{p}_s) \cdots q(t_1) \ldots q(t_s) \,.$$

Here Q_0 is, on one hand, a factor which can be found from the normalization condition

$$\sum_{s=1}^{\infty} \prod_{i=1}^{s} \int_0^t dt_1 \int_{-\infty}^{\infty} d\tilde{p}_1 \cdots \int_0^{t_{s-1}} dt_s \int_{-\infty}^{\infty} d\tilde{p}_s$$

$$\times Q_s(t_1, \tilde{p}_1, t_2, \ldots, t_s, \tilde{p}_s) + Q_0 = 1 \tag{3}$$

and, on the other hand, it is obviously the probability of the state with zero collisions.

Here we consider the processes in which the rate α of the collisions does not change with time, i.e., $q(t) = \alpha$. Then, carrying out the integrations over the momenta $\tilde{p}_i$ in Eq. (3), the normalization condition reads

$$Q_0\left(1+\alpha\int_0^t dt_1+\alpha^2\int_0^t dt_2\int_0^{t_2} dt_1+\cdots\right)=1, \quad (4)$$

which allows one to find that $Q_0 = e^{-\alpha t}$. The terms in the left hand side of Eq. (4) are readily recognized as a Poisson distribution so that the ith term gives the probability that i collisions take place during the time t.

Now a quantity $A(x,p,n)_t$ characterizing the reference particle and depending on its coordinate x and momentum p is considered. This quantity may or may not depend on the time t explicitly. As for the values of the coordinate and the momentum they must be found at the time t. The model allows one also to consider the dependence of this function on the number n of collisions which has occurred during the time t.

In order to calculate the average value of the quantity A one has to consider its values over states defined above. These can be found by means of Eq. (2) so that one obtains the set

$$\{A_0, A_1(t_1,\tilde{p}_1,1)_t,\ldots,A_s(t_1,\ldots,\tilde{p}_i,\ldots,t_s,\tilde{p}_s,s)_t,\ldots\}$$

and as a result arrives at the average in the form

$$\langle A(x,p,n)_t\rangle = A_0Q_0+\sum_{s=1}^{\infty}\alpha^s e^{-\alpha t}\int_0^t dt_s\int_0^{t_s} dt_{s-1}\cdots\int_{-\infty}^{\infty} d\tilde{p}_s\cdots P(\tilde{p}_s)A_s(t_1,\ldots,t_s,\tilde{p}_s,s)_t. \quad (5)$$

Equation (5) represents a sum over the histories where each history is defined by a set of times when the collisions occurred and by the corresponding momenta of the incident particles. This is a generalization of the procedure considered in our paper [13] where contrary to (5) the intervals between the collision events were assumed to be constant.

III. EQUATION OF MOTION

The sum over the histories (5) allows one to analyze the time evolution of the average value of the quantity A. One can use an approach similar to that used by Feynman when deriving the Schrödinger equation from the path integral representation of quantum mechanics [26]. We have also used this technique to derive the Kramers equation [13] in the case of constant intervals between the collisions. To do this one has to consider the function $\langle A(x,p,n)_t\rangle$ at two neighboring times t and $t+\Delta t$ and calculate its derivative over time

$$\frac{d\langle A(x,p,n)_t\rangle}{dt}=\lim_{\Delta t\to 0}\frac{\langle A(x,p,n)_{t+\Delta t}\rangle-\langle A(x,p,n)_t\rangle}{\Delta t}. \quad (6)$$

Using the definition (5) of the averaging procedure one can write that

$$\begin{aligned}\langle A(x,p,n)_{t+\Delta t}\rangle &= A(x,p,0)_{t+\Delta t}Q_0(t+\Delta t)\\ &+\sum_{s=1}^{\infty}e^{-\alpha(t+\Delta t)}\int_0^{t+\Delta t}dt_s\cdots\int_0^{t_1}dt_1\int_{-\infty}^{\infty}d\tilde{p}_s\cdots\int_{\infty}^{\infty}d\tilde{p}_1P(\tilde{p}_s)\cdots P(\tilde{p}_1)\\ &\times A(t_1,\tilde{p}_1\cdots,t_s,\tilde{p}_s)_{t+\Delta t}\\ &=\langle A(x,p,n)_t\rangle+\left\langle\frac{\partial A(x,p,n)_t}{\partial t}\right\rangle\Delta t-\alpha\langle A(x,p,n)_t\rangle\Delta t\\ &+\alpha\int_{\infty}^{\infty}d\tilde{p}P(\tilde{p})\langle\hat{O}A(x,p,n)_t\rangle\Delta t+o(\Delta t)^2\ . \end{aligned} \quad (7)$$

If one looks at the typical term of the expansion (7) as it appears in the second and the third lines one can see that Δt appears in three places. That is why the linear in Δt expansion of $\langle A(x,p,n)_{t+\Delta t}\rangle$ contains four terms. The first one is just the zeroth order term. There are also three first order terms. The second term is due to explicit dependence of $A(x,p,n)$ on time t. This appears due to the evolution of the coordinate x and the mechanical momentum p with time according to the Newton second law, after the sth collision event. This means that no collision occurs at the time t. The third term is due to the time dependence of the normalization factor $e^{-\alpha t}$. As for the fourth term, it formally appears due to the variation of the upper limit of the integral over the time t_s. These two last terms appear due to the collisions which may occur just at the time t and as we will see below they lead to the collision integral in the master equation.

The fourth term contains the integration over the momentum $\tilde{p}$ of the particle incident at the time t. The operator $\hat{O}$ arranges the averaging of the quantity A in such a way that the sth collision occurs just at the time t. It is defined

as

$$\langle \hat{O}A(x,p,n)\rangle \equiv \exp(-\alpha t)A(t_1=t,\tilde{p},1)_t + \exp(-\alpha t)\sum_{s=2}^{\infty}\alpha^{s-1}\int_0^t dt_{s-1}\int_{-\infty}^{\infty}d\tilde{p}_{s-1}P(\tilde{p}_{s-1})\cdots A(t_1,\ldots,t_s=t,\tilde{p},s)_t. \quad (8)$$

In other words, one may say that the operator $\hat{O}$ adds a collision at the time t.

Collecting the first order terms in Δt, one reaches the equation

$$\frac{d\langle A(x,p,n)\rangle}{dt} = \left\langle \frac{\partial A(x,p,n)}{\partial t}\right\rangle - \alpha\langle A(x,p,n)\rangle + \alpha\int_{-\infty}^{\infty}d\tilde{p}P(\tilde{p})\langle \hat{O}A(x,p,n)\rangle\ . \quad (9)$$

The last two terms in the right hand side of Eq. (9) cancel each other, if the quantity A does not depend on the momentum and the number of collisions explicitly. In order to verify this one can first integrate over $\tilde{p}$ in the last term of Eq. (9) and then check that

$$\langle \hat{O}A(x)_t\rangle = \langle A(x)_t\rangle. \quad (10)$$

This cancellation comes from the fact that the reference particle coordinate is not changed by the last collision and the value of the momentum $\tilde{p}$ at the time t, corresponding to the last collision, is in this case irrelevant.

A simple example, $A(x,p,n)=n$, is now considered. According to the definition of the operator $\hat{O}$ one has $\langle \hat{O}n\rangle = \langle n+1\rangle$. Then Eq. (9) reads

$$\frac{d\langle n\rangle}{dt} = -\alpha\langle n\rangle + \alpha\langle n+1\rangle = \alpha\ , \quad (11)$$

whose solution is $\langle n\rangle = \alpha t$. Similar simple calculations yield $\langle n^2\rangle = (\alpha t)^2 + \alpha t$. These are the well known solutions for the Poisson process which is considered here.

Master equation

As a specific and important example the characteristic function defined as $C(h,l;t|x_0,p_0) = \langle e^{ihx+ilp}\rangle$ is considered. The operator $\hat{O}$ (8) acts at the time t and changes the momentum of the reference particle according to (1). As a result one has

$$\langle \hat{O}e^{ihx+ilp}\rangle = \langle e^{ihx+il\mu_1 p+il\mu_2\tilde{p}}\rangle.$$

Now using the equation of motion (9) the time derivative of the characteristic function reads

$$\frac{d\langle e^{ihx+ilp}\rangle}{dt} = ih\left\langle \frac{p}{M}e^{ihx+ilp}\right\rangle + il\langle f(x)e^{ihx+ilp}\rangle - \alpha\langle e^{ihx+ilp}\rangle + \alpha\int_{-\infty}^{\infty}\frac{d\tilde{p}}{\sqrt{2\pi mT}}e^{-\frac{\tilde{p}^2}{2mT}} \times e^{il\mu_2\tilde{p}}\langle e^{ihx+il\mu_1 p}\rangle, \quad (12)$$

where $f(x)$ is the external force acting on the reference particle.

It is convenient to introduce the Fourier transform of the characteristic function

$$u(x,p,t|x_0,p_0) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dhdl}{(2\pi)^2}C(h,l;t|x_0,p_0) \times e^{-ilx-ihp}\ , \quad (13)$$

which as we see below has a meaning of the probability density. The derivative over time in the left hand side of Eq. (12) does not act on the parameters h and l of the characteristic function. It must not also act on x and p in the Fourier transformed characteristic function (13). Therefore the Fourier transformed equation (12) reads

$$\frac{\partial u(x,p,t)}{\partial t} = -\frac{p}{M}\frac{\partial u(x,p,t)}{\partial x} - f(x)\frac{\partial u(x,p,t)}{\partial p} - \alpha\int_{-\infty}^{\infty}\left[u(x,p,t) - u\left(x,\frac{p-\mu_2\tilde{p}}{\mu_1},t\right)\frac{1}{\mu_1}\right] \times P(\tilde{p})d\tilde{p}\ , \quad (14)$$

with the partial time derivative in the left hand side.

This equation contains the integral term which can be interpreted as a collision integral typical for master equations. Really the first term in the integrand is proportional to $u(x,p,t)$, i.e., to the probability that at the time t the reference particle occupies the point (x,p) of the phase space. It is multiplied by the function $P(\tilde{p})$ so that this product gives the probability that this particle is kicked by a gas particle with the momentum $\tilde{p}$ and as a result the reference particle leaves the point (x,p) in the phase space. The second term of the subintegrand describes the reversed process at which the reference particle with a momentum p_f is kicked in such a way that its momentum converts into p.

To see this let us omit the x dependence which is not of importance here and present the rate of the reversed process in the form of the integral

$$\alpha\int_{-\infty}^{\infty}dp_f\int_{-\infty}^{\infty}d\tilde{p}_f u(p_f)P(\tilde{p}_f)\delta(p-\mu_1 p_f-\mu_2\tilde{p}_f)\ , \quad (15)$$

where $\tilde{p}_f$ is the momentum of the gas particle before the collision in the reversed process. The δ function in the integral (15) reflects the fact that the variables p_f and $\tilde{p}_f$ are not independent. They are connected by the conditions of type (1), since we demand that the momentum of the reference particle is p after this reversed process. Integrating over p_f the integral (15) is in the form as it appears in Eq. (14).

It can also be checked by direct substitution that the Maxwell-Boltzmann distribution is a stationary solution

of Eq. (14). Equation (14) is a forward master equation and differs in this respect from that of Il'in and Khasminskii [1], who considered a backward equation.

In the special case when the mass of the reference particle is equal to the mass of the gas particle (i.e., $\mu_1 = 0$, $\mu_2 = 1$) one can suspect a divergence in Eq. (14). However, this divergence does not show up in Eq. (12). Assuming in it $\mu_1 = 0$ and carrying out the Fourier transformation (13) one arrives at the equation

$$\frac{\partial u(x,p,t)}{\partial t} = -\frac{p}{M}\frac{\partial u(x,p,t)}{\partial x} - f(x)\frac{\partial U(X,P,t)}{\partial p} - \alpha u(x,p,t) + \frac{\alpha}{\sqrt{2\pi MT}} \times \exp\left[-\frac{p^2}{2MT}\right]\bar{u}(x,t)\ , \tag{16}$$

in which

$$\bar{u}(x,t) = \int_{-\infty}^{\infty}\frac{dh}{2\pi}e^{-ihx}C(h,l=0;t|x_0,p_0)$$

is just the probability density of the coordinate of the particle. The last term in Eq. (16) appears in such a form due to the fact that due to equal masses, the particles exchange momenta at each collision and, hence, one collision is enough to yield the Maxwell distribution for the reference particle momentum.

Equation (14) is written for a finite rate α of the collisions so that the average interval between the collisions is also finite. Now we are going to consider the diffusion limit when the collisions increase and $\alpha \to \infty$. In order to avoid a highly overdamped motion, the limit $\varepsilon \to 0$ must be simultaneously taken under the condition that $\alpha\varepsilon$ remains constant. This means that the number of collisions per unit time increases while each collision becomes weaker. This limit corresponds to the Langevin limit considered in our paper [13] for a constant interval between the collisions.

Now the equalities $\mu_1 \simeq 1 - 2\varepsilon$, $\mu_2 \simeq 2(1-\varepsilon)$ are used and Eq. (14) becomes

$$\frac{\partial u}{\partial t} \approx -\frac{p}{M}\frac{\partial u}{\partial x} - f(x)\frac{\partial u}{\partial p} + \alpha\int_{-\infty}^{\infty}[(1+2\varepsilon)u(x,p+y,t) - u(x,p,t)] \times P(\tilde{p})d\tilde{p}\ . \tag{17}$$

Here $y = 2\varepsilon p - 2(1+\varepsilon)\tilde{p}$ may be taken as a small parameter in the integral, due to the fact that the Gaussian integration has a width $M\varepsilon T \to 0$. Expanding over y and integrating over $\tilde{p}$ one arrives at the Kramers equation

$$\frac{\partial u}{\partial t} = -\frac{p}{M}\frac{\partial u}{\partial x} - f(x)\frac{\partial u}{\partial p} + \beta_{dif}\frac{\partial(pu)}{\partial p} + \beta_{dif}TM\frac{\partial^2 u}{\partial p^2}\ , \tag{18}$$

in which the friction coefficient, for this diffusion limit,

$$\beta_{dif} = \lim_{\varepsilon,\alpha^{-1}\to 0} 2\varepsilon\alpha\ , \tag{19}$$

is explicitly connected with the microscopic parameters of the model.

IV. FREE PARTICLE

This section will consider the problem of motion of a reference particle in the absence of any external field so that it experiences only the collisions with gas particles. Such a reference particle will be called free. Equation of motion (9) allows one to obtain the following set of equations, for the first and second order moments of the coordinate x and momentum p of the reference particle:

$$\frac{d}{dt}\begin{pmatrix}\langle x\rangle\\ \langle p\rangle\\ \langle xp\rangle\\ \langle x^2\rangle\\ \langle p^2\rangle\end{pmatrix} = \begin{pmatrix}0 & \frac{1}{M} & 0 & 0 & 0\\ 0 & -\beta & 0 & 0 & 0\\ 0 & 0 & -\beta & 0 & \frac{1}{M}\\ 0 & 0 & \frac{2}{M} & 0 & 0\\ 0 & 0 & 0 & 0 & -2\gamma\end{pmatrix}\begin{pmatrix}\langle x\rangle\\ \langle p\rangle\\ \langle xp\rangle\\ \langle x^2\rangle\\ \langle p^2\rangle\end{pmatrix} + \begin{pmatrix}0\\ 0\\ 0\\ 0\\ 2\gamma MT\end{pmatrix}. \tag{20}$$

Here

$$2\gamma = (1-\mu_1^2)\alpha, \qquad \beta = (1-\mu_1)\alpha. \tag{21}$$

These equations are obtained in the following way. Considering, for example, the equation of motion for $\langle x\rangle$ one has to take into account the cancellation (10) and the trivial fact that

$$\left\langle\frac{dx}{dt}\right\rangle = \frac{1}{M}\langle p\rangle.$$

In order to get the equation of motion for $\langle p\rangle$ one has to make use of Eq. (1) and obtain that

$$\langle\hat{O}p\rangle = \mu_1\langle p\rangle.$$

The equations of motion for second order moments are obtained in a similar way.

It is interesting to note that two relaxation parameters connected by the condition

$$2\gamma = (1+\mu_1)\beta \tag{22}$$

appear in the equations of motion (20). These two constants appear in the solutions of Eqs. (20) which read

$$\langle p\rangle = p_0 e^{-\beta t} , \tag{23a}$$

$$\langle x\rangle = \frac{p_0}{M\beta}(1-e^{-\beta t}) , \tag{23b}$$

$$\langle p^2\rangle = p_0^2 e^{-2\gamma t} + MT\left(1-e^{-2\gamma t}\right) , \tag{23c}$$

$$\langle xp\rangle = \frac{T}{\beta}(1-e^{-\beta t}) + \left(\frac{p_0^2 - MT}{M(2\gamma-\beta)}\right)(e^{-\beta t}-e^{-2\gamma t}) , \tag{23d}$$

$$\langle x^2\rangle = \frac{2Tt}{M\beta} + \frac{2T}{M\beta^2}(e^{-\beta t}-1) + 2\frac{p_0^2 - MT}{M^2(2\gamma-\beta)}\left[\frac{1}{2\gamma}(e^{-2\gamma t}-1) + \frac{1}{\beta}(1-e^{-\beta t})\right] . \tag{23e}$$

Here $x_0 = 0$.

Equations (23a) and (23b) can be formally interpreted as solutions of the equation

$$\dot{v} = -\beta v \tag{24}$$

for the average velocity of the reference particle assuming initial coordinate $x_0 = 0$ and momentum p_0. This means that the parameter β must be treated as the friction coefficient. The same parameter β determines the limiting behavior at $t \to \infty$ of Eq. (23e) for the mean square displacement which allows one to find the diffusion coefficient

$$D = \frac{T}{M\beta} \tag{25}$$

satisfying the Einstein relation. This relation holds for all mass ratios ε. Here we see an important difference from the result of our paper [13] where deviations from the Einstein relations are found for finite ratios of masses. It is clearly connected with the fact that contrary to the Poisson process studied here the paper [13] considers strong time correlation between the collision events.

Equation (23c) shows that the mean square momentum (proportional to the kinetic energy of the reference particle) tends at $t \to \infty$, as expected, to its equilibrium value MT. It is emphasized that this statement appears as a result of the calculations rather than as an *ad hoc* assumption. However, considering the relaxation of the mean square momentum one surprisingly finds that it is characterized by another constant γ. According to Eq. (22) $\gamma \le \beta$ since $\mu_1 \le 1$. The equality $\gamma = \beta$ holds in the Langevin limit (19). Only then do the solutions (23a)–(23e) become identical to the solutions of the Langevin equation of a free particle which can be found in various textbooks (see, e.g., [16–18]).

It is often assumed (see, e.g., [15]) that we deal with an ensemble of the test particles whose initial states are characterized by equilibrium distribution. In this case averaging of Eqs. (23a)–(23e) produces the standard results of the Langevin equation. However, one can easily imagine a situation when the initial distribution of the test particle is rather far from equilibrium and deviations of the relaxation kinetics from that of the Langevin type must be observed.

The solution presented here does not contain any restriction on the mass ratio $\varepsilon = m/M$. We may, for example, consider the case of equal masses $M = m$. Then

$$\mu_1 = 0, \quad 2\gamma = \beta = \alpha.$$

This means that the relaxation times are extremely rapid and close to the microscopic time scale α^{-1}. This rapid relaxation is obviously connected with the fact that colliding particles exchange momenta and the reference particle "forgets" its initial momentum after the first collision. Such a strong condition is certainly due to our one dimensional model. Considering a multidimensional problem will result in slower relaxation.

One may consider also the extreme situation when the mass of the gas particles becomes large, $\varepsilon \gg 1$. This case is very far from conventional theories of Brownian motion, where this ratio is usually assumed to be small. The motion resembles now random flights [15]. One has in this case

$$\mu_1 \to -1, \quad \beta \to 2\alpha, \quad \gamma \to 0.$$

In this limit each collision changes the direction of the reference particle flight keeping the absolute value of the momentum constant. Therefore the average momentum relaxes to its equilibrium zero value rather rapidly with the characteristic time α^{-1} the averaged squared momentum and, hence, kinetic energy of the reference particle relaxes extremely slowly.

For a large but finite value of the mass ratio ε one can find a time period when $\gamma t \ll 1$ while $\beta t \gg 1$. Then the mean square displacement takes the form

$$\langle x^2\rangle = \frac{2p_0^2 t}{M^2\beta},$$

meaning a strong violation of the Einstein relation. The effective diffusion coefficient measured in this time period,

$$D = \frac{p_0^2}{M^2\beta} ,$$

depends on the initial momentum of the particle rather than on the temperature. The conventional Einstein relation recovers only after a long time $t \gg \gamma^{-1}$. Only then is the information on the initial conditions lost and the equilibrium achieved.

Characteristic function of the mechanical momentum

This subsection considers the characteristic function of the mechanical momentum defined as

$$C(l,t;p_0) = \langle \exp(ilp)\rangle.$$

The equation of motion for this function can be obtained from Eq. (12) by assuming that $f(x) = 0$ and $h = 0$,

$$\frac{dC(l,t;p_0)}{dt} = -\alpha C(l,t;p_0) + \alpha \exp\left(-\frac{l^2\mu_2^2 mT}{2}\right) \times C(l\mu_1,t;p_0) \ . \quad (26)$$

On the other hand, Eq. (5) allows one to represent the characteristic function as a sum

$$C(p,t;p_0) = \sum_{s=0}^{\infty} C(p,t;p_0)_s \ , \quad (27)$$

where the partial characteristic function

$$C(p,t;p_0)_s = \langle (\exp ilp | n = s) \rangle \quad (28)$$

assumes that exactly s collisions have occurred during the time t.

Using the properties of the operator $\hat{O}$ in Eq. (9) the equations of motion for these partial characteristic functions become

$$\frac{dC(l,t;p_0)_s}{dt} = -\alpha C(l,t;p_0)_s + \alpha \exp\left(\frac{-l\mu_2^2 mT}{2}\right) C(\mu_1 l,t;p_0)_{s-1}. \quad (29)$$

Solutions of Eqs. (29) are looked for in the factorized form

$$C(l,t;p_0)_s = f_s(t) g_s(l) \exp(-\alpha t) \ , \quad (30)$$

which on substituting into Eq. (29) produces

$$\dot{f}_s = f_{s-1}. \quad (31)$$

Keeping in mind the obvious initial condition $f_s(t=0) = \delta_{s0}$ the solution of Eq. (29) is

$$f_s(t) = \frac{(\alpha t)^s}{s!}. \quad (32)$$

The problem now is to find the function $g_s(l)$. One can do it by comparing Eq. (27) with the solution of the similar problem found in our paper [13]. First, notice that the time dependent part of (30)

$$f_s(t) \exp(-\alpha t) \quad (33)$$

is just the Poisson distribution function describing the probability that s collisions have occurred by the time t. In the case of the constant intervals, τ_0, between the collisions this function should be substituted by the probability of a process with s collisions. This is given by the Kronecker function δ_{ss_t} where $s_t = [t/\tau_0]$ ([] is the integer part). Then one expects that Eq. (27) will convert into the corresponding part of Eq. (13) of the Ref. [13]. For this to be true the equation

$$g_s(l) = \exp\left[ilp_0\mu_1^s - \frac{MTl^2}{2}(1-\mu_1^{2s})\right] \quad (34)$$

must hold.

As a result the solution of Eq. (26) becomes

$$C(l,t;p_0) = \sum_{s=0}^{\infty} \exp\left[il\mu_1^s p_0 - \frac{MT}{2} l^2 (1-\mu_1^{2s})\right] \times \frac{(\alpha t)^s e^{-\alpha t}}{s!}. \quad (35)$$

One can easily find the behavior of the function (35) in the large time limit $\alpha t \to \infty$. Really the Poisson distribution (33) as a function of the number of collisions s for a large value of αt has a sharp maximum around $s_0 = \alpha t/e \gg 1$. Then one can use the fact that $\mu_1^s \to 0$ for large values of s and obtain that Eq. (35) becomes

$$C(l,t;p_0) = \exp\left[-\frac{MT}{2} l^2\right] \quad (36)$$

in the limit of large times. One can easily understand (see, e.g., [13]) that this limit means that the system arrives at equilibrium.

V. HARMONIC OSCILLATOR

Equations of motion for a particle situated in the harmonic potential are obtained in a fashion similar to that used for the free particle. The only difference is that now the force term

$$f(x) = -M\omega^2 x$$

must be taken into account.

$$\frac{\partial}{\partial t}\begin{pmatrix} \langle\tilde{x}\rangle \\ \langle p\rangle \\ \langle\tilde{x}p\rangle \\ \langle\tilde{x}^2\rangle \\ \langle p^2\rangle \end{pmatrix} = \begin{pmatrix} 0 & \omega & 0 & 0 & 0 \\ -\omega & -\beta & 0 & 0 & 0 \\ 0 & 0 & -\beta & -\omega & \omega \\ 0 & 0 & 2\omega & 0 & 0 \\ 0 & 0 & -2\omega & 0 & -2\gamma \end{pmatrix} \begin{pmatrix} \langle\tilde{x}\rangle \\ \langle p\rangle \\ \langle\tilde{x}p\rangle \\ \langle\tilde{x}^2\rangle \\ \langle p^2\rangle \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2\gamma MT \end{pmatrix}, \quad (37)$$

where $\tilde{x} = M\omega x$. It is important for the analysis presented in this section that the force $f(x)$ is linear in x. Only in this case are the equations for the moments of different orders decoupled.

To begin with the stationary solutions of Eqs. (37) are readily found in the form

$$\langle\tilde{x}^2\rangle_{st} = \langle p^2\rangle_{st} = MT, \quad \langle x\rangle_{st} = \langle p\rangle_{st} = \langle xp\rangle_{st} = 0. \quad (38)$$

We notice that the relaxation coefficients which enter the solution for the free particle, also determine the relaxation in the harmonic field. When the diffusion limit is approached, the equations for the five moments are identical to the equations for the moments, which can be derived directly from Kramers equation (18). Solutions for this case can be found in [15]. For $\langle x \rangle$ and $\langle p \rangle$, the equations of motion are identical to those of the diffusion limit, for all mass ratios and mean times between the collision events. Only one friction parameter, β, is important for these moments. As usual, one arrives at the standard condition that for $\beta < 2\omega$ the relaxation of these moments is underdamped and it is overdamped in the opposite case.

Time dependence of the three second order moments generally differs from that in the diffusion limit. The motion is characterized by two parameters β and γ which produce three relaxation rates which are the eigenvalues of the 3×3 matrix in the lower right corner of the matrix (37). These eigenvalues are solutions of the third order equation

$$\lambda^3 + a_1\lambda^2 + a_2\lambda + a_3 = 0 \ , \tag{39}$$

where

$$a_1 = 2\gamma + \beta, \quad a_2 = 2\beta\gamma + 4\omega^2, \quad a_3 = 4\omega^2\gamma \ . \tag{40}$$

Using the standard equations (see, e.g., [27]) for solutions of cubic equations three quantities, Q, R, and G, are defined as

$$Q = \frac{3a_2 - a_1^2}{9}, \quad R = \frac{9a_1a_2 - 27a_3 - 2a_1^3}{54}, \tag{41}$$

$$G = Q^3 + R^2.$$

Then three types of solutions can be found: (i) if $G > 0$, then one root is real, two are complex conjugate; (ii) if $G = 0$ all roots are real, and at least two of them are equal; and (iii) if $G < 0$ all roots are real and unequal. They correspond to an underdamped motion (i) when oscillations of the solution exist and to an overdamped motion (iii) when only pure attenuation can be observed. The transition between these two regimes is determined by the condition (ii) and in the general case differs from the similar condition obtained for the first order moments. Using definitions (40) the quantity G becomes

$$G = \frac{(-4\gamma^2 + 2\gamma\beta - \beta^2 + 12\omega^2)^3}{729} + \frac{(\beta - \gamma)^2(8\gamma^2 + 2\gamma\beta - \beta^2 + 18\omega^2)^2}{729}. \tag{42}$$

In the diffusion limit, when $\gamma = \beta$, the type of motion is determined by the much simpler expression

$$G = \frac{(-\beta^2 + 4\omega^2)^3}{27} \ , \tag{43}$$

which yields the same criterion for the well known underdamped and overdamped motion of the oscillator, which experiences a linear friction force (see, e.g., [15]) as obtained above for the first order moments. However, it is important to emphasize that, contrary to the first order moments for which this criterion is of a general character, the higher order moments obey this criterion only in the diffusion limit.

One can consider also small deviations from the diffusion limit when $\varepsilon \ll 1$. Then expanding the function G with respect to this small parameter one arrives at the critical value

$$\frac{\beta_c}{\omega} \approx 2 + \frac{3}{\sqrt[3]{4}}\varepsilon^{2/3} \tag{44}$$

marking the transition from the underdamped to overdamped type of motion and increasing with increasing ε.

Two cases are considered far from the diffusion limit. First, if the masses of the reference and gas particles are identical, i.e., $\beta = 2\gamma$, one gets

$$G = \frac{\omega^2(2\beta^4 - 13\beta^2\omega^2 + 64\omega^4)}{27}. \tag{45}$$

This means that $G > 0$ for all values of β and ω and we deal only with the underdamped motions. In the limit $M \gg m$ when $\gamma = 0$

$$G = \frac{4\omega^4(-\beta^2 + 16\omega^2)}{27}.$$

Then transition from an underdamped $G > 0$ to overdamped $G < 0$ motion is again possible at $\beta_c/\omega = 4$.

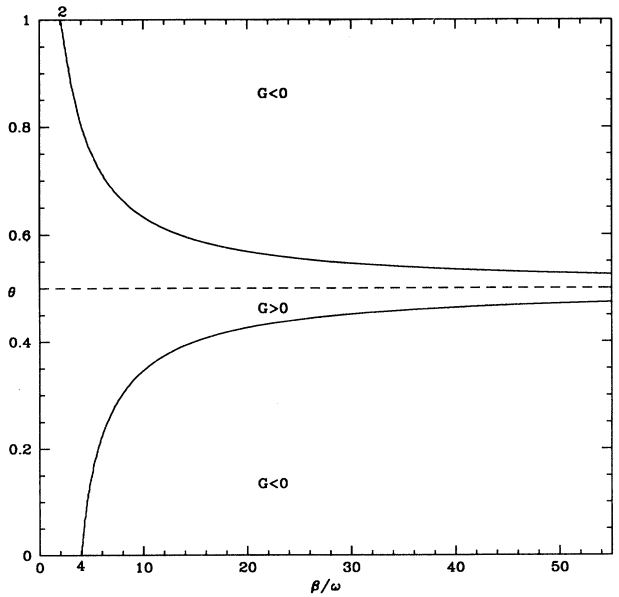

FIG. 1. Phase plane for $G(\theta, \beta/\omega)$. Areas of underdamped, $G > 0$, and overdamped, $G < 0$, motions are indicated. Two separatrices (solid lines) converge to the line $\theta = 1/2$ (dashed line) in the limit $\beta \to \infty$.

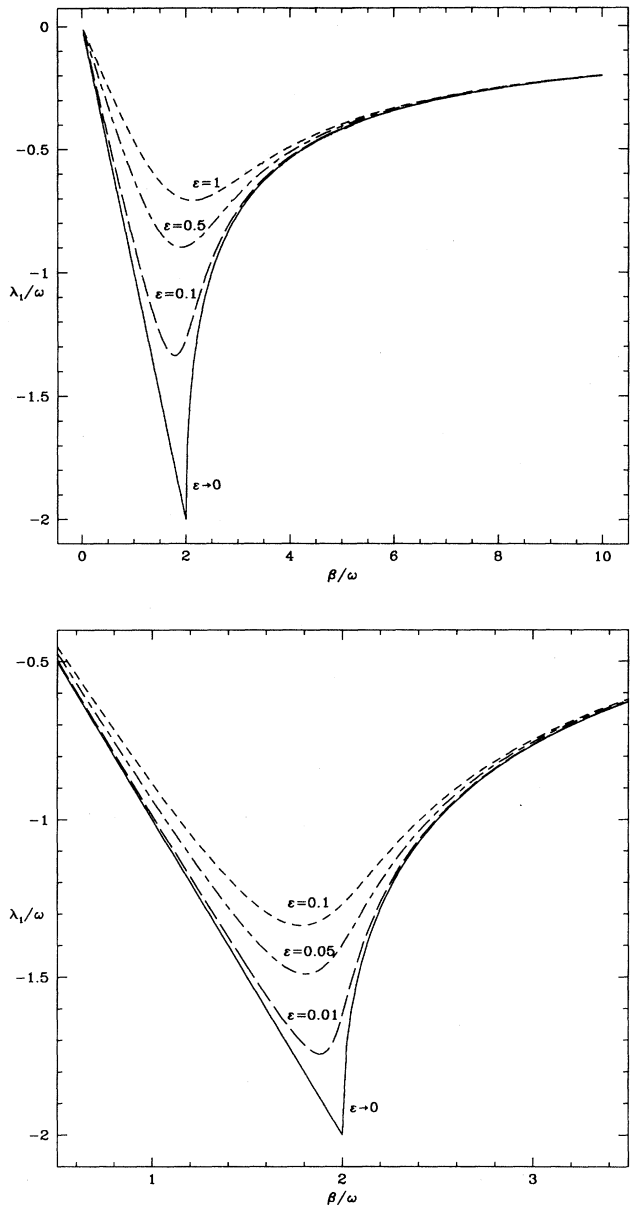

FIG. 2. λ_1/ω versus β/ω exhibited in two graphs [(a) and (b)] for different values of the mass ratio ε. The quantity λ_1 is real for all values of the parameters γ, β, ω.

A general plot of the behavior of the parameter G as the function of β and

$$\theta = \frac{\gamma}{\beta} = \frac{1}{1+\varepsilon}$$

is shown in Fig. 1. Two curves corresponding to $G(\theta,\beta) = 0$ in this plot separate the areas of the underdamped and overdamped types of motion. It is interesting to note that the dashed line $\theta = 1/2$ ($M = m$) lies completely in the underdamped domain. Two separatrices converge to this line so that at $\beta \to \infty$ there remains only one point lying on this line with the underdamped type of motion while all the other values of $\theta \neq 1/2$ yield overdamped motions.

These conclusions can be made directly from Eq. (42). At $\beta \to \infty$ its leading term in

$$G = A(\theta)\beta^6 + B(\theta)\beta^4 + O(\beta^2) \tag{46}$$

is proportional to β^6 and has the negative coefficient

$$A(\theta) = -\frac{\theta^2(2\theta-1)^2}{27}$$

for all values of θ. The only important exclusion is the point $\theta = 1/2$ where this coefficient becomes zero and the sign is determined by the term proportional to β^4 which is always positive, e.g., (45).

Now the relaxation times determined by three solutions of the cubic equation (39) are considered (see, e.g., in [27]). One of these solutions is always real while two other solutions can be, depending on the sign of G, either both real or complex conjugate. Their graphical representation can be viewed in Figs. 2–5. For mass ratio ($\varepsilon \ll 1$) the solutions can be expanded with respect to this small parameter. Considering the solution which is always real one gets

$$\lambda_1 = -\beta + \varepsilon\beta\frac{\omega^2}{4\omega^2-\beta^2} + o(\varepsilon^2) \quad \text{for} \quad 0 < 4\omega^2 - \beta^2 \tag{47a}$$

and

$$\lambda_1 = -\beta\left(1 - \varepsilon\frac{\beta^2-2\omega^2}{\beta^2-4\omega^2}\right) + \sqrt{\beta^2-4\omega^2}\left(1-\varepsilon\frac{\beta^2}{\beta^2-4\omega^2}\right) + o(\varepsilon^2) \tag{47b}$$

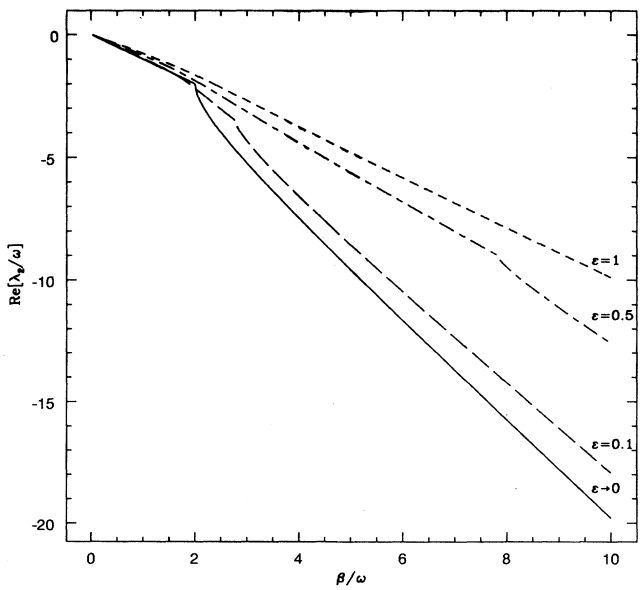

FIG. 3. $\mathrm{Re}\lambda_2/\omega$ versus β/ω for different mass ratios ε.

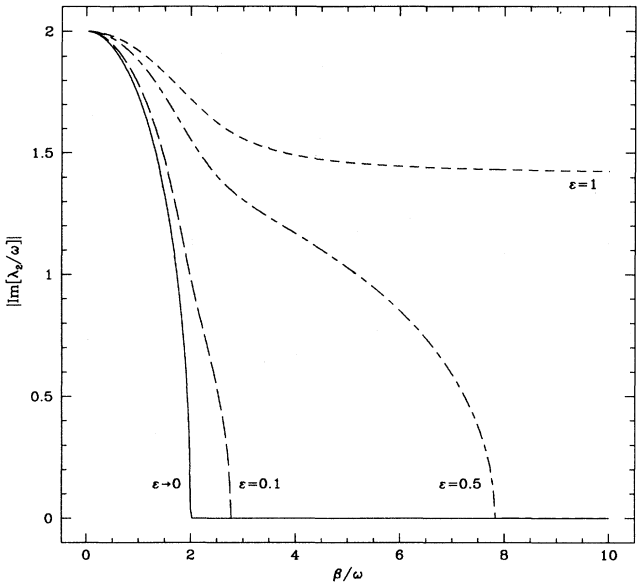

FIG. 4. $\mathrm{Im}\lambda_2/\omega$ versus β/ω for different mass ratios ε. $\mathrm{Im}\lambda_2 = -\mathrm{Im}\lambda_3$.

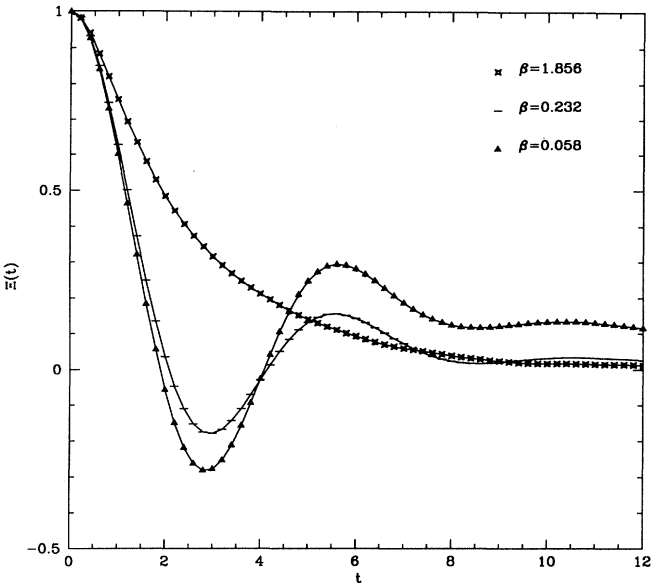

FIG. 5. The correlation function $\Xi(t)$ versus time, for different values of β. Here the mean time between collisions is (1) 9.85 for $\beta = 0.058$, (2) 2.46 for $\beta = 0.232$, and (3) 0.31 when $\beta = 1.856$.

for

$$0 < \beta^2 - 4\omega^2.$$

For λ_2 we get

$$\mathrm{Re}\lambda_2 = -\beta + \varepsilon\beta\frac{2\omega^2 - \beta^2}{4\omega^2 - \beta^2} + o(\varepsilon^2)\ ,$$

$$\mathrm{Im}\lambda_2 = \sqrt{4\omega^2 - \beta^2}\left(1 + \varepsilon\frac{\beta^2}{4\omega^2 - \beta^2}\right) + o(\varepsilon^2) \tag{47c}$$

for

$$0 < 4\omega^2 - \beta^2,$$

and

$$\lambda_2 = -\beta\left(1 + \varepsilon\frac{\beta^2 - 2\omega^2}{\beta^2 - 4\omega^2}\right) - \sqrt{\beta^2 - 4\omega^2}\left(1 + \varepsilon\frac{\beta^2}{4\omega^2 - \beta^2}\right) + o(\varepsilon^2) \tag{47d}$$

for

$$\beta^2 - 4\omega^2 > 0.$$

λ_3 is determined by

$$\lambda_3 = -\lambda_1 - \lambda_2 - \beta\,(3 - 2\varepsilon) + o(\varepsilon^2).$$

These expressions show that the expansion can hardly be carried out near the point $2\beta = \omega$ where in the Langevin limit the transition from the overdamped to underdamped motion takes place. The small parameter ε is divided by the quantity $4\omega^2 - \beta^2$ which becomes small near this point. The solution λ_1 is plotted in Fig. 2, showing that its absolute value passes the maximum near this point and is extremely sensitive even to small variations of the mass ratio ε.

As shown above, $G > 0$ for all values of the parameter β if masses of the references and gas particles are equal. The relaxation parameters in this limit are

$$\lim_{\beta\to\infty} \lambda_1(\varepsilon = 1) = 0\ , \tag{48a}$$

$$\lim_{\beta\to\infty} \lambda_{2,3}(\varepsilon = 1) = -\beta \pm i\sqrt{2}\omega\ . \tag{48b}$$

The motion is now strongly damped and does not relax — one of the eigenvalues is zero. Formally it is not overdamped since oscillations are possible, however, these can hardly be observed since their period $2\pi/\omega$ is much smaller than the characteristic relaxation time $1/\beta$ associated with the oscillations.

Finally the results of this section are compared with those of Ref. [13] where strong correlation between the kicks is assumed. They follow one after another with the time interval τ_0. A very long relaxation time is then found in [13] when the frequency of the harmonic oscillator is connected by sort of a resonance condition $\tau_0 = \pi n/\omega$ (n is an integer) with this time interval. In the case of the Poisson process considered here when the kicks are completely not correlated this effect is smeared out and does not show up in the relaxation process.

VI. NUMERICAL SIMULATIONS

Simulations of Brownian type of motion for the test particle situated in a nonharmonic background potential

field are often carried out [28–30]. In many cases it is done using the Langevin approach which is based on the equation

$$M\ddot{x} = -\beta_{dif}\dot{x} - \frac{dV(x)}{dx} + \xi(t), \tag{49}$$

where the random force satisfies the standard conditions $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2\beta_{dif} T \delta(t - t')$.

The IK model is used for numerical simulations, but, as far as we know, only for the mass ratio $\epsilon = 1$. Both methods produce the same stationary Maxwell-Boltzmann distribution in the limit of large times, but, as will be shown below, the dynamics can differ considerably.

The double well potential (DWP)

$$V(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

is chosen to stand for the background potential. The temperature of the system of the bath particles is $T = 1$. The deterministic evolution of the test particle in the DWP is obtained by solving numerically the Newton equation of motion by means of the fourth order Runge-Kutta method. The time step is chosen as $dt = 0.01$ and, as we have checked, the results are not sensitive to this particular choice. Poisson distributed times between collisions and normally distributed bath particle momenta are achieved by using algorithms [31]. To simulate the Langevin equation the algorithm given by [30] [see Eq. (7.5.5)] is applied. The potential $V(x)$ and the parameters T, dt coincide with those chosen for the IK simulation.

It is first of all checked that the two algorithms produce samples which agree well with the Maxwell-Boltzmann distribution. For example, $\langle x^2 \rangle$ is calculated by averaging over 50 000 independent sample points. This is done for all mass ratios and collision rates to be considered in what follows and in simulation of the Langevin equation as well.

Calculating the Boltzmann averaged $\langle x^2 \rangle_{th}$ the ratio

$$0.995 < \frac{\langle x^2 \rangle}{\langle x^2 \rangle_{th}} < 1.008$$

indicates an excellent equilibration of the system in the course of the simulation process. We have also produced histograms of the stationary distributions by both simulation procedures which agree well with that produced by the Boltzmann distribution.

Turning now to dynamical properties the correlation time

$$t_{cor} \equiv \int_0^\infty \Xi(t) dt \tag{50}$$

characterizing the decay of the correlation function

$$\Xi(t) \equiv \frac{\langle x(t)x(0) \rangle}{\langle x^2 \rangle_{th}}$$

is calculated. Relaxation patterns for different mass ratios ε and different rates α will be discussed below. As shown in Eqs. (18), (19) the limit $\varepsilon \to 0$ and $\alpha \to \infty$ for a constant β_{dif} should produce the same results as those obtained directly from the Langevin equation.

To calculate the correlation function 50 000 independent realizations are used. Each realization is sampled every 0.2 time units. The correlation time t_{cor} is then obtained by means of a numerical integration, the ∞ in (50) being chosen to be 60 time units, which is much larger than the relaxation time of our problem. Dealing with a harmonic oscillator, one can easily get the average coordinate $\langle x(t) \rangle$ from Eq. (37). The correlation function is obtained by multiplying this by the randomly distributed initial coordinate $x(0)$ and averaging over its values. As for the correlation time it is readily obtained in the form

$$t_{cor} = \frac{\beta}{\omega^2}, \tag{51}$$

where β is defined by Eq. (21). This result is used to check our numerical procedure. For example, when $\varepsilon = 0.2$ and $\omega = 1$ the correlation time $t_{cor,n}$ is found numerically for five values of β in the range between 0.25 and 4.0. Then the average ratio $t_{cor,n}\omega^2/\beta$ of the numerical to theoretical (51) values of the correlation times appears to be 0.998 with the variance 0.032.

The temperature is chosen to be rather high so that $\Delta E/T = 0.25$, where ΔE is the energy barrier the particle has to traverse when crossing from one local minimum to the other. This means that we are going to consider here shallow wells as in Ref. [32] rather than the usually addressed problem of deep wells or large barriers (see, e.g., [4]).

We now turn to a discussion of our numerical results. Figure 5 shows the time dependences of the correlation function for three different values of the damping coefficient β. For all cases shown the mass ratio was $\varepsilon = 0.4$ and only the rate α was varied. The correlation function approaches zero nonmonotonically when β is small enough, which may be compared with the underdamped relaxation of a harmonic oscillator. The values of β are chosen close to the averaged temperature dependent frequency of the background potential

$$\langle \omega^2 \rangle \equiv \left\langle -\frac{d^2V(x)}{dx} \right\rangle_{th},$$

which gives a rough estimate on the location of the transition from the underdamped to overdamped motion shown in Fig. 5.

However, contrary to the harmonic oscillator or free particle motion the damping coefficient β alone is not sufficient and does not control the relaxation in a nonlinear case completely. Rather both ε and α separately must be considered as illustrated in Fig. 6. Results of four simulations are shown. The IK simulation was carried out for three different mass ratios and an additional simulation used the Langevin approach. One sees that only for the large β values (overdamped relaxation) do the results of the four simulations nearly coincide. When the motion is underdamped (small values of β) the correlation times differ dramatically for different mass ratios and decrease with them. The Langevin results corresponding to the limit $\varepsilon \to 0$ are always the lowest.

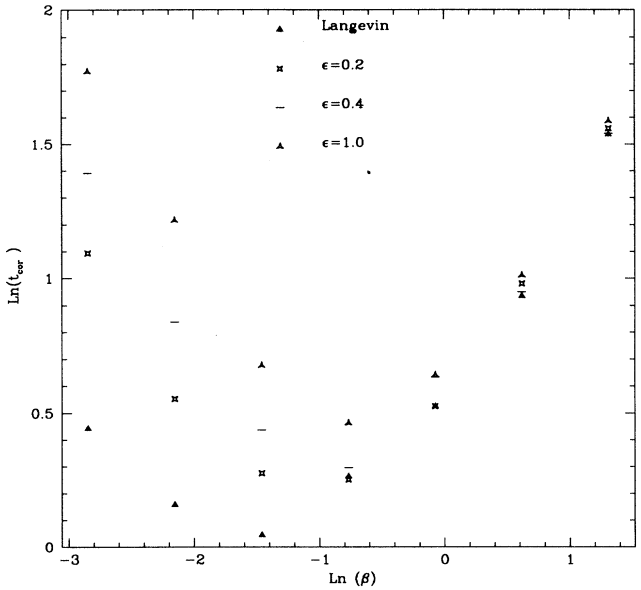

FIG. 6. A ln-ln plot of the t_{cor} as a function of β. For the data presented, the averaged time between collisions (inverse collision rate) gets its maximal value of 17.23 for the strong collision limit $\varepsilon = 1$ and for $\beta = 0.059$. The minimum of this variable is 0.09 for $\varepsilon = 0.2$ and $\beta = 3.71$.

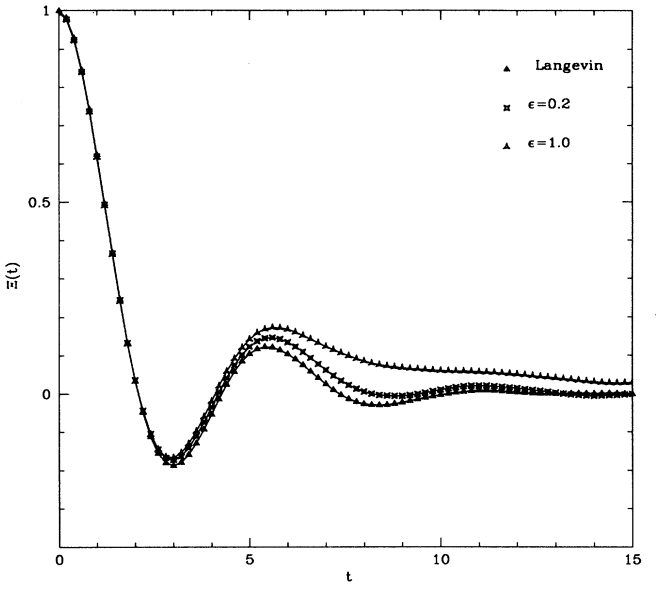

FIG. 7. The correlation function vs time. For all the cases shown $\beta = 0.232$. The correlation time calculated from these functions with (50) is (1) 1.96 for $\varepsilon = 1.0$, (2) 1.31 for $\varepsilon = 0.2$, and (3) 1.04 for the Langevin simulation. Notice that for small t the correlation functions practically coincide.

The correlation time is a nonmonotonic function of β with a minimum whose position depends on the mass ratio (see Fig. 6). Large values of the correlation times in the highly overdamped or underdamped cases are connected with the fact that the particle may be trapped at a local minimum of the background potential and stays there for a relatively long time. This behavior is found for both the IK and the Langevin simulations.

In many cases the aim of a stochastic simulation is to produce uncorrelated samples obeying the Maxwell-Boltzmann statistics. Even though the correlation time gets its minimal value for the Langevin simulation this does not mean that this approach is the most efficient. One must remember that for the Langevin algorithm a random number is generated every step dt while in the IK approach two random numbers are produced only every $1/\alpha dt$ time steps (on average). As a result the latter approach may require less computer time.

Considering a finite number of realizations (50 000) is a limitation. In order to estimate the error additional simulations were carried out. For four cases we calculated seven data points instead of one. Each data point has been computed using different random numbers. For the case of $\beta = 0.116$ and $\varepsilon = 0.2$ ($\varepsilon = 0.4$) we found the averaged correlation time $t_{cor} = 1.751$ ($t_{cor} = 2.319$) and variance 0.048 (0.059). When $\beta = 1.85$ and $\varepsilon = 0.2$ ($\varepsilon = 0.4$) we found $t_{cor} = 2.594$ ($t_{cor} = 2.646$) and the variance 0.074 (0.063).

As a final remark, Fig. 7 shows the correlation functions for $\beta = 0.232$ and different mass ratios. One sees that for short times t the correlation functions coincide. Hence the differences between the correlation times are caused by the behavior of the correlation functions at long times.

VII. CONCLUSIONS

This paper presents both exact and numerical solutions of the IK model for a Brownian type of motion. In this model the collisions with the particles constituting the surrounding gas may be characterized by an arbitrary rate and strength. Similarly to our previous paper [13] an approach based on summing over histories is applied.

Standard results of the conventional theory of the Brownian motion are obtained in the diffusion limit, when the gas particle mass tends to zero, while the frequency of the collisions tends simultaneously to infinity. For example, Kramers equation is deduced. However, we are able also to analyze the situations when these parameters are finite and deviations from the standard results can be expected. One of the interesting observations of this study is that deviations from the diffusion limit are not necessarily small even if the mass ratio ε is small. It may happen in the case of a harmonic oscillator near the point $2\beta = \omega$ where in the diffusion limit the transition from the underdamped to overdamped type of motion takes place. A nonanalytical behavior of the critical value β_c as the function of the mass ratio ε [see Eq. (44)] is also characteristic of this point.

An analysis far from the diffusion limit (the mass ratio ε of the reference to gas particles is finite) is also carried

out. It is found, for example, that the relaxation of the energy fluctuations of a free particle and its deceleration are governed by different coefficients. Considering the ratio between the relaxation coefficient β of the first order moments and the diffusion coefficient D produced from the large time limit of the mean square displacement the Einstein relation (25) is obtained which holds for any value of ε. Therefore one sees that the deviations from the Einstein relation found in [13] are smeared out by the fluctuations of the time intervals between the collisions in the Poisson process. However, the second coefficient, γ, controlling the kinetic energy relaxation, does not satisfy the Einstein relation and the deviation can be rather large if ε is not small.

For a fixed value of β the second relaxation coefficient $\gamma = \beta/(1+\varepsilon)$ gets its maximal value when $\varepsilon \to 0$. A similar phenomenon was also found for a nonlinear case investigated numerically. Our data points (when considering the underdamped case) show that the correlation time at the diffusion limit is shorter than that found far from this limit.

The results presented in this paper may be of importance for numerical simulations of a system in contact with a heat bath. When doing such simulations the collisions are sometimes chosen to follow one after the other with a constant interval of time elapsing between collision events. In [13] we demonstrated that such a choice may lead to slowing down the relaxation. As shown here, this effect does not appear when choosing the time intervals between the collisions from a Poisson distribution.

ACKNOWLEDGMENTS

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