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Time Behavior of the Correlation Functions in a Simple Dissipative Quantum Model

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The force and velocity correlation functions for a particle interacting with a bath are calculated within a model allowing for finite memory effects. The relevance of a Brownian picture is delineated in view of the respective behavior of these functions and appears fully inadequate below some cross-over temperature; then, the interplay between quantum and thermal fluctuations yields some long time tails on the same time scale for both correlation functions. The real space transient diffusion coefficient is found to exceed its asymptotic Einstein value for most times in that regime. The limiting case of an infinitely short memory time is also investigated and is seen to produce weak divergences on a time scale which is small as compared to the other characteristic times.

KEY WORDS: Quantum noise; correlation functions; long time tails; Brownian motion.

1. INTRODUCTION

The behavior of a quantum system coupled to a thermal bath has been for years a much studied problem. A celebrated paper is due to Ford, Kac, and Mazur,[1] in which these authors show how to make a heat bath with a set of harmonic oscillators coupled in a prescribed manner. More recently, contradictory conclusions by Caldeira and Leggett[2] and by Widom and Clark[3] on the influence of dissipation on quantum tunneling have reactivated the interest in this problem.

Connections with the quantum Brownian motion are obvious and a general discussion can be found in Ref. 4. In the present paper, we analyze the time behavior of various correlation functions and we show that well-

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separated time scales—which are required for the interpretation in terms of a standard Brownian motion—only emerge in the high-temperature limit. In the opposite low-temperature limit, the interplay between quantum and thermal fluctuations becomes effective, leading to long time tails in the correlation functions varying like $-t^{-2}$ and, consequently, to a non-classical behavior of the diffusion coefficient as a function of time. Our analysis also illustrates, within a particular model, part of the statements or results appearing in the paper by Iche and Nozières.[5]

2. MODEL AND BASIC NOTATIONS

In the present paper we are essentially interested in specific aspects introduced by quantum effects. It is best to start from the simplest model in order to exemplify the expected differences between classical and quantum situations. This is the reason why we shall study the damped free particle.

In obvious notations, the model Hamiltonian for a free particle (mass M) linearly coupled to a set of oscillators (m_n, ω_n, b_n, $b_n^\dagger$) can be written[2]

$$H=\frac{P^2}{2M}+\sum_n M\Omega_n^2 X x_n+\sum_n \frac{p_n^2}{2m_n}+\sum_n \frac{1}{2} m_n\omega_n^2 x_n^2+\sum_n \frac{1}{2}\frac{M^2\Omega_n^4}{m_n\omega_n^2} X^2 \tag{1}$$

where the last term has been added in order to cancel spurious unphysical divergences.[2c] In the Hamiltonian (1), the interaction is taken as bilinear.[2c] Clearly, this implicitly contains a weak coupling assumption; this is reminiscent of the great M/m_n ratio characteristic of classical Brownian motion, since then the exchange of energy during an elastic collision is indeed small.

It is easy to derive from Eq. (1) the equations of motion for the coordinate $X(t)$ and the momentum $P(t)$ of the particle in the Heisenberg picture. Note that this picture is defined through the total Hamiltonian H, so that $X(t)$ and $P(t)$ act in the full space, i.e., not only in the restricted space associated with the degrees of freedom of the bare particle. Once $P(t)$ is eliminated, the dynamical equation for $X(t)$ reads as follows:

$$\ddot{X}(t)= -A(t)-\int_{t_0}^{t} dt'\, K(t-t')\, \dot{X}(t') \tag{2}$$

$A(t)$ is an instantaneous force per unit mass which only depends on the particle and bath coordinates at time $t=t_0$, namely,

$$A(t)=\sum_n \left(\left\{ \frac{M}{m_n}\frac{\Omega_n^4}{\omega_n^2}\cos[\omega_n(t-t_0)]\, X(t_0) + \Omega_n^2\left(\frac{\hbar}{2m_n\omega_n}\right)^{1/2} [e^{-i\omega_n(t-t_0)}b_n(t_0)+\text{h.c.}] \right\} \right) \tag{3}$$

and $K(t)$ is a memory kernel equal to

$$K(t) = \sum_n \Omega_n^2 \frac{M}{m_n} \frac{\Omega_n^2}{\omega_n^2} \cos \omega_n t \tag{4}$$

Equation (2), which has been established without any approximation, contains the exact dynamics of the particle, and constitutes for this particular model the expression of the Mori's theorem.[6] Note that it does not *per se* introduce any irreversible effects.

In order to induce a relaxation, the oscillators of the bath must be spread over a quasicontinuum of frequencies, and the distribution laws for the Ω_n's, the m_n's and the ω_n's must be some smooth functions; $K(t)$ is then a peaked function near $t = 0^+$, on an interval defining the memory time of the system. As is well known, this amounts to assume that the Poincaré times are so long that they can be rejected to infinity. In order to allow a detailed analysis, $K(t)$ has to be modeled along these lines; a simple choice consists in setting from now on:

$$K(t) = \frac{\gamma}{\tau_R} e^{-\gamma t} \Theta(t) \tag{5}$$

where $\Theta(t)$ is the step function. Turning back to Eq. (4), one sees that γ is linked to the bandwidth of the effectively coupled oscillators; the ratio γ/τ_R can be viewed as a measure of the average coupling strength; as for τ_R, its meaning is best found by considering Eq. (2) and taking $\gamma \to \infty$ (the so-called infinitely short memory time limit): in this limit, τ_R appears to be simply the relaxation time of the particle velocity. Note that γ and τ_R have quite different physical meanings and cannot be amalgamated in a single parameter.

The statement of the problem is now completed by specifying the initial state. Note that $A(t)$ contains $X(t_0)$ and $b_n(t_0)$, i.e., information about the initial preparation of the system (particle plus bath). The term depending on the initial position $X(t_0)$ of the particle contains a factor $K(t - t_0)$; since $K(t)$ is supposed to have a memory time of the order of γ^{-1}, we shall study the behavior of the system for times t such that $t - t_0 \gg \gamma^{-1}$. Then $K(t - t_0)$ is negligible and the initial position of the particle becomes irrelevant. We shall also assume that at time $t = t_0$ the bath is in thermodynamical equilibrium at temperature T, namely,

$$\langle b_n^\dagger(t_0)\, b_{n'}(t_0) \rangle = \delta_{nn'} (e^{\beta \hbar \omega_n} - 1)^{-1}, \qquad \beta = \frac{1}{k_B T} \tag{6}$$

We shall be interested in correlation functions of the form $\langle f(t)\, g(t') \rangle$. When $t - t_0$ and $t' - t_0$ are greater than γ^{-1}, the correlation functions only depend on the difference $t-t'$. In order to simplify the mathematical notations and computations, the best way is to set $t_0 = -\infty$. This insures that all one-time averages are time independent and that all two-time correlation functions are time translationally invariant, so that they can be viewed as corresponding to stationary stochastic processes. Moreover we can now use the Fourier integral in the ordinary sense:

$$\int_{-\infty}^{+\infty} dt\, f(t)\, e^{i\omega t} = f(\omega) \tag{7}$$

We can now obtain the symmetrized autocorrelation function of the fluctuating force per unit mass $\Phi_T(t) = \frac{1}{2}\langle A(t+t')\, A(t') + A(t')\, A(t+t')\rangle$ in the integral form:

$$\Phi_T(t) = \frac{\hbar\gamma^2}{M\tau_R} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\omega}{\omega^2+\gamma^2} \coth\frac{\beta\hbar\omega}{2}\, e^{i\omega t} \tag{8}$$

Using the commutation relation for the fluctuating force per unit mass

$$[A(\omega), A(\omega')] = -4\pi \frac{\hbar\gamma^2}{M\tau_R} \frac{\omega}{\omega^2+\gamma^2}\, \delta(\omega+\omega') \tag{9}$$

one can easily show that the commutator $[X(t), P(t)]$ for the particle is equal to $i\hbar$ at all times, as it should.[7]

The autocorrelation function of the particle velocity $C_{vv}(t) = \frac{1}{2}\langle \dot{X}(t+t')\, \dot{X}(t') + \dot{X}(t')\, \dot{X}(t+t')\rangle$ can be found as follows. First, define the susceptibility $\chi(\omega)$ so that the Fourier transforms of $X(t)$ and $A(t)$, $X(\omega)$ and $A(\omega)$, are related via Eq. (2) through $X(\omega) = \chi(\omega)\, MA(\omega)$; then $C_{vv}(t)$ is easily seen to be

$$C_{vv}(t) = \frac{\hbar\gamma^2}{M\tau_R} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\omega^3}{\omega^2+\gamma^2} M^2\, |\chi(\omega)|^2 \coth\frac{\beta\hbar\omega}{2}\, e^{i\omega t} \tag{10}$$

where $\chi(\omega)$ is given by

$$\chi(\omega) = M^{-1}[\omega^2 + i\omega K(\omega)]^{-1} = \frac{1}{M} \frac{1}{\omega^2 + (\gamma/\tau_R)[i\omega/(\gamma - i\omega)]} \tag{11}$$

Clearly, the subsequent results will depend on the modeling (5); but, since most of the specific behaviors to be found essentially originate from the coth term (which brings in the quantum effects), we would expect that the basic features should be grossly independent of the modeling, especially for low temperatures. Moreover, it is obvious that in particular, for all memory kernels $K(t)$ which possess an infinitely short memory time limit, the results are effectively independent of the modeling in that limit.

3. TIME BEHAVIOR OF THE CORRELATION FUNCTIONS

We shall first examine the spectral density of the fluctuating force because, as we shall see, two different noise regimes exist according to the temperature of the bath. Then we shall proceed to the discussion of the behavior of the autocorrelation function of the fluctuating force per unit mass, $\Phi_T(t)$ [Eq. (8)] and of the autocorrelation function of the velocity, $C_{vv}(t)$ [Eq. (10)].

3.1. The Spectral Density of the Fluctuating Force

It can be seen from Eq. (8) that the spectral density of the fluctuating force per unit mass is given by

$$\langle |A(\omega)|^2 \rangle = \frac{\hbar\gamma^2}{M\tau_R} \frac{\omega}{\omega^2+\gamma^2} \coth\frac{\beta\hbar\omega}{2} \tag{12}$$

At high temperatures, this expression can be written as

$$\langle |A(\omega)|^2 \rangle \simeq 2\frac{k_B T}{M\tau_R} \frac{\gamma^2}{\omega^2+\gamma^2} \tag{13}$$

For times much longer than the memory time γ^{-1} of the system, one gets, in the relevant frequency range $\omega \ll \gamma$,

$$\langle |A(\omega)|^2 \rangle \simeq 2\frac{k_B T}{M\tau_R} \tag{14}$$

The noise is then a standard white noise.

But, if the temperature is sufficiently low, the spectral density of the fluctuating force becomes nearly equal to

$$\langle |A(\omega)|^2 \rangle \simeq \frac{\hbar\gamma^2}{M\tau_R} \frac{\omega}{\omega^2+\gamma^2} \tag{15}$$

One can remark that, in these temperature conditions, the bandwidth γ plays the role of a frequency cutoff. Indeed, for $\gamma \to \infty$, $\langle |A(\omega)|^2 \rangle$ behaves like ω and diverges when $\omega \to \infty$, which is clearly unphysical. One can equally note that this cutoff is built in from the beginning in the model, as soon as one assumes that K has a finite memory, and therefore has not been introduced in any *ad hoc* fashion to get rid of unwanted divergencies. In the frequency range $\omega \ll \gamma$ the spectral density of the fluctuating force behaves like $\hbar\omega/M\tau_R$. Such a behavior is fundamentally very different from the white noise type which prevails at high temperature in this frequency range.

Therefore, one can expect that a crossover between two noise regimes, roughly speaking classical and quantal, should occur for a temperature T_c^f such that

$$2\frac{k_B T_c^f}{M\tau_R}\frac{\gamma^2}{\omega^2+\gamma^2} \sim \frac{\hbar\gamma^2}{M\tau_R}\frac{\omega}{\omega^2+\gamma^2} \qquad \text{with } \omega \sim \gamma$$

that is,

$$\frac{\hbar}{2k_B T_c^f} \sim \gamma^{-1} \tag{16}$$

3.2. The Reservoir Correlation Time

Let us consider once again the spectral density of the fluctuating force per unit mass given by expression (12). On this expression, one easily sees that, for any given temperature T, the noise can be considered as white on the frequency range

$$\omega \ll \min\left(\gamma, \frac{k_B T}{\hbar}\right) \tag{17}$$

When the temperature is higher than the cross-over temperature T_c^f defined above, the condition for white noise is simply $\omega \ll \gamma$. This means that the force correlation function $\Phi_T(t)$ will essentially have decayed on a time scale of the order of γ^{-1}. In this temperature range, γ^{-1} thus appears as a correlation time of the reservoir.[8]

In the opposite case, when the temperature is lower than the cross-over temperature T_c^f, the condition for white noise is completely different, since it becomes $\omega \ll k_B T/\hbar$. One therefore can expect that the force correlation function $\Phi_T(t)$ will decay on a time scale of the order of $\hbar/k_B T$; let us more precisely set

$$\tau = (2\pi)^{-1}\frac{\hbar}{k_B T} \tag{18}$$

So, a new characteristic time, τ, appears to be involved in the analysis; its signification is clearly apparent is the low-temperature case (i.e., when $T < T_c^f$): it then plays the role of a reservoir correlation time.

This analysis is completely qualitative; it will nevertheless be confirmed by the detailed calculation of the force correlation function, which will be carried out in the following paragraphs, in both cases of finite memory and of the infinitely short memory time limit.

3.3. Finite Memory Case

Let us first introduce the dimensionless function $f_T(t; \gamma)$ defined as

$$f_T(t; \gamma) = \int_{-\infty}^{+\infty} dx \frac{x}{x^2+1} \coth\left(\frac{\beta\hbar\gamma}{2} x\right) e^{i\gamma t x} \tag{19}$$

The force and velocity correlation functions Φ_T and C_{vv} can be expressed as

$$\Phi_T(t) = \frac{\hbar\gamma^2}{2\pi M\tau_R} f_T(t; \gamma) \tag{20}$$

and

$$C_{vv}(t) = \frac{\hbar}{2\pi M\tau_R}\left(1 - \frac{4}{\gamma\tau_R}\right)^{-1/2} [f_T(t; \gamma\alpha_-) - f_T(t; \gamma\alpha_+)] \tag{21}$$

where

$$\alpha_\pm = \frac{1}{2}\left[1 \pm \left(1 - \frac{4}{\gamma\tau_R}\right)^{1/2}\right]$$

Before going into details, let us note that all the above expressions remain valid when $\gamma\tau_R < 4$, provided that the appropriate analytical continuations are done; we shall nevertheless essentially discuss the case $\gamma\tau_R > 4$, which corresponds to a weak coupling between the particle and the bath, an assumption already contained in the Hamiltonian (1); at the end, a few words will be said for completeness on the opposite case.

It is interesting to note that for $\gamma\tau_R \gg 1$, C_{vv} can be rewritten in the approximate form

$$C_{vv}(t) \simeq \frac{\hbar}{2\pi M\tau_R} [f_T(t; \tau_R^{-1}) - f_T(t; \gamma)] \tag{22}$$

So, C_{vv} simply appears as the difference of two similar functions with two quite distinct time scales, namely, τ_R and γ^{-1}.

For further reference, we give the value of C_{vv} for $t=0$, directly obtained from Eq. (10); for $T>0$, we find

$$C_{vv}(t=0)=\frac{\hbar}{2\pi M\tau_R}(1-4/\gamma\tau_R)^{-1/2} \times\left[2\psi(\gamma\tau\alpha_+)-2\psi(\gamma\tau\alpha_-)+\frac{1}{\gamma\tau\alpha_+}-\frac{1}{\gamma\tau\alpha_-}\right] \tag{23}$$

where ψ denotes the Euler psi function. For $T\to\infty$ it is seen by using the expression for the ψ function close to the value zero of its argument that $C_{vv}(t=0)\to k_BT/M$ (see Fig. 1), as required by the equipartition of energy. For $T=0$, $C_{vv}(t=0)$ reduces to

$$C_{vv,T=0}(t=0)=\frac{\hbar}{\pi M\tau_R}(1-4/\gamma\tau_R)^{-1/2}\ln\frac{1+(1-4/\gamma\tau_R)^{1/2}}{1-(1-4/\gamma\tau_R)^{1/2}} \tag{24}$$

independently of the order of the limits $T\to 0$, $t\to 0$.

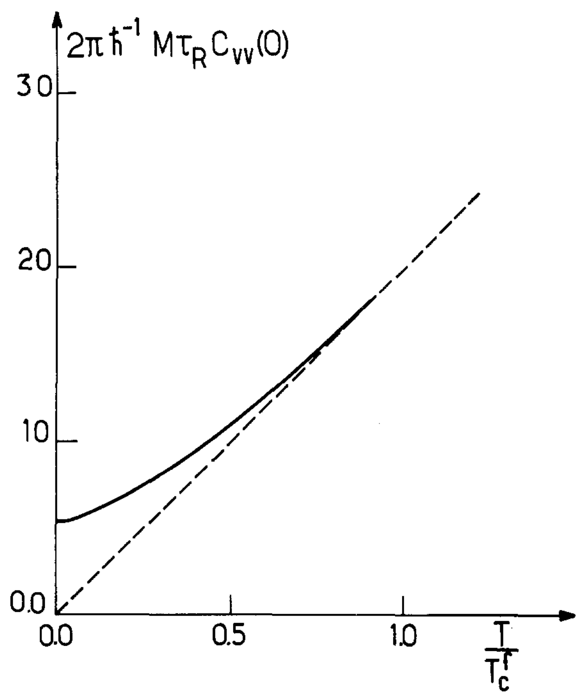

Fig. 1. Variation of the mean-squared velocity as a function of temperature. At high temperature, the classical equipartition theorem is recovered.

Since the force correlation function—directly related to the noise—clearly plays a central role, it deserves a scrutinized study, which will be the subject of the following paragraph.

3.3.1. Discussion of the Force Correlation Function. As noted before, two different behaviors of $\Phi_T(t)$ are to be expected on physical grounds according to the magnitude of the product $\gamma\tau$.

At high temperature, τ is much smaller than the other relevant time γ^{-1} so that the quantum effects are in some way averaged out except for small corrections. On the contrary, at low temperature, τ becomes larger than γ^{-1} so that the full quantum nature of the spectral density of the fluctuating force (i.e., of the noise) does have enough time to become apparent.

(a) *High Temperature Case* ($\gamma\tau \ll 1$). In this case, the most convenient expression for f_T is obtained by a contour integration; starting with Eq. (19), one straightforwardly obtains

$$f_T(t;\gamma)=\frac{1}{\gamma\tau}e^{-\gamma t}-2\ln(1-e^{-2\pi\hbar^{-1}k_BTt})+O(\gamma\tau) \tag{25}$$

This expression displays two interesting features. First, f_T essentially undergoes an exponential decay, directly reflecting the memory kernel $K(t)$. Secondly, the quantum correction (which is indeed exponentially small) exhibits an essential singularity of the form $e^{-Cste/\hbar}$ which precludes any $\hbar$-power series expansion. These quantum effects die out on a time scale τ which is quite minute at high temperature (see Fig. 2).

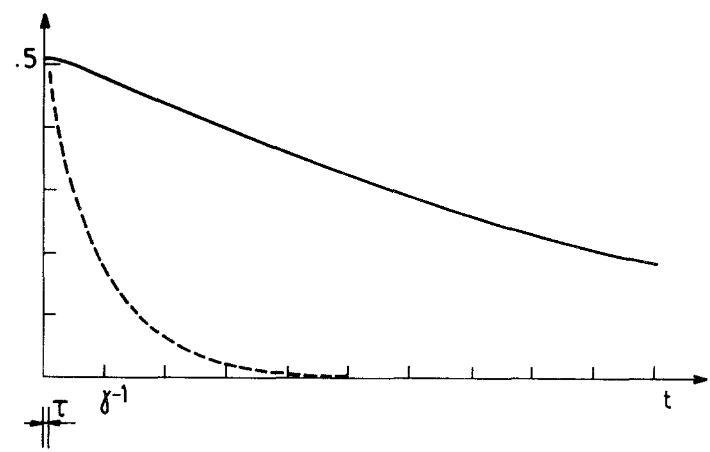

Fig. 2. Variations of $C_{vv}/\bar{C}_{vv}$ (solid line) and of $\Phi_T/\bar{\Phi}_T$ (dashed line) as functions of t for $\gamma\tau=0.1$ and $\gamma\tau_R=10$. The bar denotes the mean value defined as $\bar{f}=\int_{-\infty}^{+\infty} d\gamma t\, f(t)$. The noise is in its classical regime; the force as well as the velocity correlation functions decay quasi-exponentially.

From Eq. (20), Φ_T is seen to have exactly the same properties and thus the characteristic correlation time of the fluctuating force appears to be simply the inverse of the bandwidth of the bath, a standard result.[8]

(b) *Low-Temperature Case* ($\gamma^{-1} \ll \tau$). Now, the contour integration which led to expression (25) is of no use. A direct asymptotic evaluation of the integral (19) allows to write

$$f_T(t;\gamma) = f_0(t;\gamma) + \frac{1}{2}(\gamma\tau)^{-2}\left[\frac{1}{(t/2\tau)^2} - \frac{1}{\sinh^2(t/2\tau)}\right] + O(\gamma\tau)^{-4} \qquad (26)$$

where f_0, the $T=0$ part, is expressed in terms of exponential integral functions[9]

$$f_0(t;\gamma) = -e^{-\gamma t}Ei(\gamma t) + e^{\gamma t}E_1(\gamma t) \qquad (27)$$

The net time behavior of $f_T(t;\gamma)$ is rather subtle. As long as $t \lesssim \tau$, the two terms of the $(\gamma\tau)^{-2}$ correction nearly cancel one another and f_T deviates from f_0 in terms of the order of $(\gamma\tau)^{-4}$. In other words, f_0 is representative of all the low-temperature functions within the large interval $t \lesssim \tau$.

When $t \lesssim \gamma^{-1}$, f_0 behaves as $-2(C + \ln \gamma t)$, where C denotes the Euler constant.

For $\gamma^{-1} \ll t$, the asymptotic expansion of f_0 can be used and is found to start with $-2/(\gamma t)^2$. So, in the interval $\gamma^{-1} \lesssim t \lesssim \tau$, f_0 displays a long time tail $\sim -Cste/t^2$. As contrasted to the high-temperature case, this power-law behavior does not depend on the precise form of the kernel $K(t)$ [for instance, it can be shown that the same long time tail of f_0 exists when $K(t)$ is Gaussian].

When t approaches τ, the first correction to f_0 becomes significant; its first contribution cancels the t^{-2} term originating from f_0; it essentially remains the second contribution, which behaves as $-2^{-1}(\gamma\tau)^{-2} \sinh^{-2}(t/2\tau)$ and ultimately gives the exponential decay $e^{-t/\tau}$ with the very small negative amplitude $-2/(\gamma\tau)^2$.

So, in the quantum regime, the basic function $f_T(t;\gamma)$ displays a long time tail in the large interval $\gamma^{-1} \lesssim t \lesssim \tau$ and only recovers an exponential decay (with a negative and minute amplitude) for times greater than $\hbar/k_B T$.

Turning back to the full expression (20) for the force correlation function $\Phi_T(t)$ and taking into account the preceding analysis, we can consider three time intervals. Within each of them, an approximate expression for the force correlation function can be written, namely,

$$\Phi_T(t) \simeq \frac{\hbar\gamma^2}{2\pi M\tau_R} \times \begin{cases} -2(C+\ln\gamma t), & 0<t\lesssim\gamma^{-1} \\ -2/(\gamma t)^2, & \gamma^{-1}\lesssim t\lesssim\tau \\ -2(\gamma\tau)^{-2}\,e^{-t/\tau}, & \tau\lesssim t \end{cases} \tag{28}$$

Thus $\Phi_T(t)$ displays a long time tail up to $t\lesssim\tau$ (see Fig. 3).

(c) *Intermediate-Temperature Range* $(\gamma^{-1}\sim\tau)$. In the intermediate-temperature range, a convenient finite expression for f_T is hard to find, if it exists. Nevertheless it is possible to obtain an exact closed

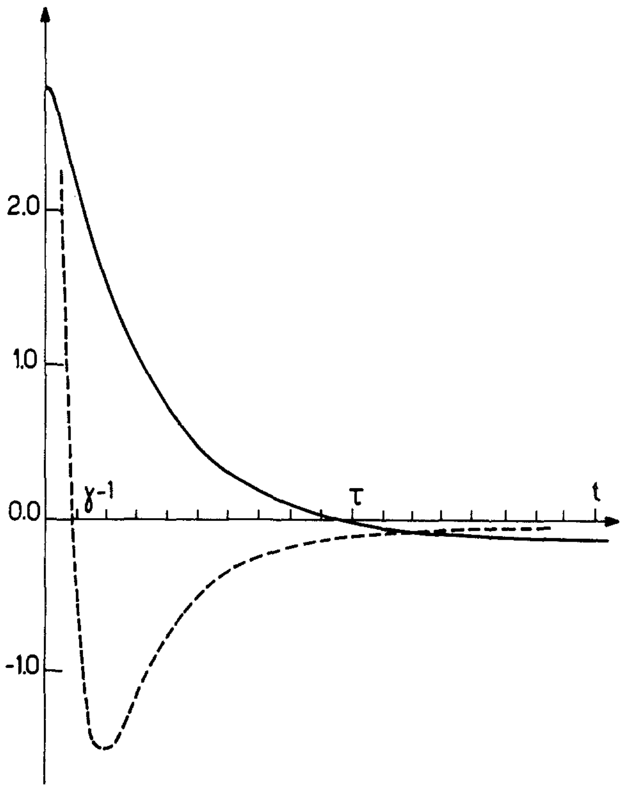

Fig. 3. Variations of $C_{vv}/\bar{C}_{vv}$ (solid line) and of $\Phi_T/\bar{\Phi}_T$ (dashed line) as functions of t for $\gamma\tau=10$ and $\gamma\tau_R=10$. The noise is in its quantum regime; the force correlation function exhibits a long time tail up to $t\simeq\tau$; the velocity correlation function displays an intermediate behavior $(\tau_R=\tau)$.

expression valid for all half-integer values of the parameter $\gamma\tau$; namely, for $\gamma\tau = n_0 - 1/2 (n_0 = 1, 2, \ldots)$, one has

$$f_T(t; \gamma) = 2 \cosh \gamma t \ln \left| \coth \frac{t}{4\tau} \right| - \frac{1}{\gamma\tau} - \sum_{n=0}^{n_0-2} \frac{\cosh[\gamma - (n+1/2)/\tau]\, t}{n+1/2} \tag{29}$$

This formula evidently shows that, in the intermediate-temperature range, f_T does not have a simple behavior and that a clear-cut time scale defined in function of the other times γ^{-1} and τ does not exist (see Fig. 4).

(d) *Cross-Over Temperature.* The above analysis confirms that the existence of two different noise regimes leads, as expected, to different

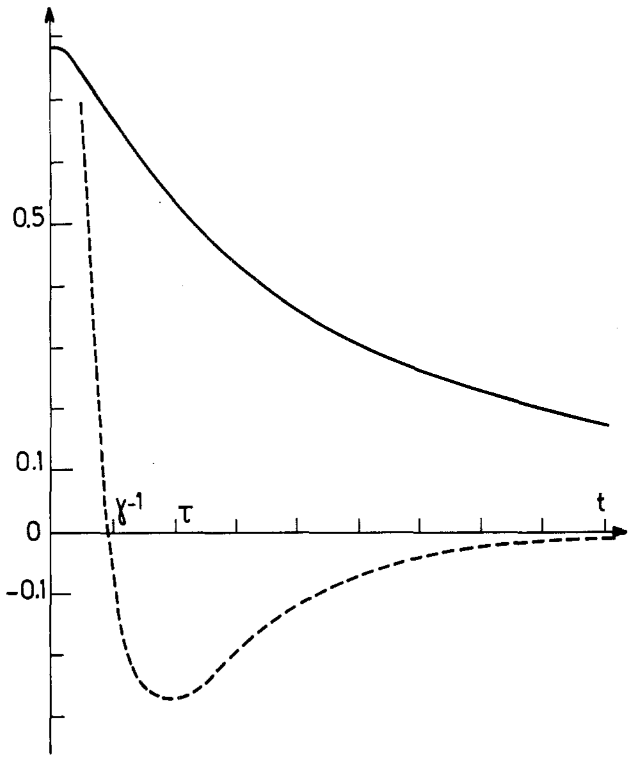

Fig. 4. Variations of $C_{vv}/\bar{C}_{vv}$ (solid line) and of $\Phi_T/\bar{\Phi}_T$ (dashed line) as functions of t for $\gamma\tau = 2$ and $\gamma\tau_R = 10$. The noise and the force correlation function are in an intermediate regime; the velocity correlation function has still a classical behavior.

behaviors of the force correlation function. The cross-over can be located at the appearance of a zero for the force correlation function Φ_T at some instant t_f. A close inspection reveals that such a t_f does exist for $T < T_c^f$ given by

$$T_c^f = \frac{\hbar\gamma}{\pi k_B} \tag{30}$$

in accordance with the qualitative expression (16).

3.3.2. Discussion of the velocity correlation function. (a) *Classical Noise Regime* ($T > T_c^f$). The two first quantum corrections in $C_{vv}(t)$ as given by Eq. (21) cancel each other and one is left with

$$C_{vv}(t) = \frac{\hbar e^{-\gamma t/2}}{2\pi M\tau} \left\{ \left(1 + \frac{\pi^2\tau}{3\tau_R}\gamma\tau\right) \cosh\left[\left(1 - \frac{4}{\gamma\tau_R}\right)^{1/2} \frac{\gamma t}{2}\right] + \left(1 - \frac{\pi^2\tau}{3\tau_R}\gamma\tau\right)\left(1 - \frac{4}{\gamma\tau_R}\right)^{-1/2} \times \sinh\left[\left(1 - \frac{4}{\gamma\tau_R}\right)^{1/2} \frac{\gamma t}{2}\right] + O(\gamma\tau)^3 \right\} \tag{31}$$

For $t \ll \tau$, $C_{vv}(t) \simeq (\hbar/2\pi M\tau_R)(1 - \gamma t^2/2\tau_R)$ so that it has a parabolic variation near $t = 0$. When $\gamma\tau_R \gg 1$, expression (31) simplifies, and, for $t \gtrsim \tau$, one can write

$$C_{vv}(t) \sim \frac{\hbar}{2\pi M\tau} \left[\left(1 - \frac{1}{\gamma\tau_R}\right) e^{-t/\tau_R} - \frac{1}{\gamma\tau_R}\left(1 - \frac{\pi^2}{3}\gamma^2\tau^2\right) e^{-\gamma t} - O(\gamma\tau_R)^{-2} \right] \tag{32}$$

This expression shows that, at high temperature and when $\gamma\tau_R \gg 1$, $C_{vv}(t)$ is essentially an exponential with the decay time τ_R, which is the largest time scale of the problem; it also contains a small correction decaying on the time γ^{-1}. When the condition $\gamma\tau_R \gg 1$ is not fulfilled, $C_{vv}(t)$ is a linear combination of exponentials with time constants $2\gamma^{-1}[1 \pm (1 - 4/\gamma\tau_R)^{1/2}]^{-1}$.

Thus, at high temperature, two time scales simply emerge: γ^{-1}, which is the correlation time of the fluctuating force (fast variable) and τ_R which roughly describes the relaxation of the velocity (slow variable). In the physically interesting range $\gamma\tau_R \gg 1$, the interpretation as a standard Brownian motion is thus still meaningful. The first time scale is the inverse of the bandwith of the coupled oscillators; the second one is linked to the interaction strength between the Brownian particle and the bath. In fact, except for small (but singular) quantum corrections, we here recover the gross features of the classical Brownian motion. Figure 2 displays the exact variations of Φ_T and C_{vv} in this case.

(b) *Quantum Noise Regime* ($T < T_c^f$). In this noise regime, two different behaviours of C_{vv} can be distinguished, whether $\tau \ll \tau_R$ or $\tau \gg \tau_R$.

When $\tau \ll \tau_R$, C_{vv} displays no long time tail and therefore its behavior may be considered as quasiclassical. In other words, the quantum effects, already visible on the force correlation function, have not enough time to appear on the velocity correlation function. However, in view of the long negative time tail of the force correlation function, a description in terms of Brownian motion begins to be unappropriate (see Fig. 4).

For $\tau \gg \tau_R$, C_{vv} also exhibits a long negative time tail. Using Eq. (21), one sees that several time intervals can be considered. The variations of C_{vv} in these intervals are outlined in the following formula:

$$C_{vv}(t) \simeq \frac{\hbar}{2\pi M\tau_R}\left(1-\frac{4}{\gamma\tau_R}\right)^{-1/2} \times \begin{cases} -2\left(C+\ln\dfrac{t}{\tau_R}\right), & \gamma^{-1} \lesssim t \lesssim \tau_R \\ -2\left(\dfrac{\tau_R}{t}\right)^2, & \tau_R \lesssim t \lesssim \tau \\ -2\left(\dfrac{\tau}{\tau_R}\right)^{-2} e^{-t/\tau}, & \tau \lesssim t \end{cases} \tag{33}$$

Note that $C_{vv}(t=0)$ is finite. However, $C_{vv}(t)$, albeit continuous, has no Taylor expansion close to $t=0$, so that the precise behavior has been obtained by numerical calculation for $t \lesssim \gamma^{-1}$. Comparing formulas (28) and (33), it is seen that Φ_T and C_{vv} both display a long time tail up to $t \lesssim \tau$.

Figure 3 plots these two functions (in order to get a clear diagram for both Φ_T and C_{vv}, we chose $\tau = \tau_R$; C_{vv} is then in an intermediate temperature range and does not exhibit a clear-cut time scale[1]).

So, it is seen that the dynamical behavior of the force and velocity correlation functions now involves the three times γ^{-1}, τ_R, and τ in a rather intricate way. One could have hoped that, by keeping the inequality $\gamma^{-1} \ll \tau_R$, two different time scales (one for the force, one for the velocity) would still have emerged, corresponding to fast and slow variables. This is not the case: the force and velocity correlation functions both display a

[3] However, the long time tail $\sim -t^{-2}$ of $C_{vv}(t)$ will be clearly apparent in Fig. 6, curves c and d (see the following paragraph).

$-t^{-2}$ tail within the same time interval ($t \lesssim \tau$). It is therefore impossible to delineate two well-separated time scales characterizing slow and fast variables. Thus, at low temperature, the dynamics of the particle cannot be interpreted in terms of Brownian motion, in contradistinction to classical mechanics.

These two different behaviors of $C_{vv}(t)$ inside the quantum noise regime can in turn be distinguished by a cross-over temperature $T_c^v(\gamma)$. Exactly as for the force correlation function, the cross-over can be located at the appearance of a zero for $C_{vv}(t)$ at some instant t_v. Such a t_v does exist for $T < T_c^v$ given by

$$T_c^v(\gamma) = \frac{1}{2}\left[1 - \left(1 - \frac{4}{\gamma\tau_R}\right)^{1/2}\right]\frac{\hbar\gamma}{\pi k_B} \tag{34}$$

T_c^v is a decreasing function of γ; it is plotted in Fig. 5. For $T \lesssim T_c^v$, t_v is found to be

$$t_v \simeq \gamma^{-1} \ln\left(\frac{16}{3\pi}\frac{k_B T_c}{\hbar\gamma}\frac{T}{T_c - T}\right) \tag{35}$$

and thus has a logarithmic divergence for $T = T_c - 0$; it uniformly decreases toward $0.879\,\gamma^{-1}$ when T goes to zero.

Before examining the limit $\gamma \to \infty$, let us briefly say what happens when $\gamma\tau_R < 4$. Then all previous formulas have to be analytically continued and, because $\alpha_\pm$ has now an imaginary part, oscillations in time appear

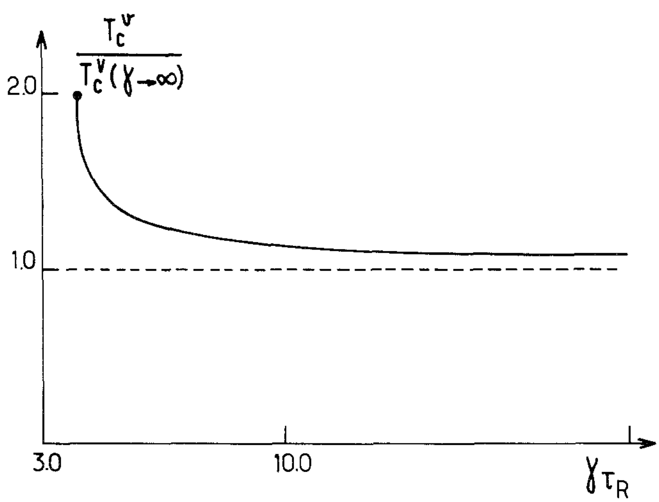

Fig. 5. Cross-over temperature T_c^v for the velocity correlation function versus $\gamma\tau_R$.

here and there, so that T_c^v cannot be defined as simply as before. The occurrence of such oscillations when the coupling constant is increased and becomes of the order of magnitude of the bandwidth of the dissipative continuum is a most general phenomenon in quantum physics.

3.4. Infinitely Short Memory Time Limit

It is interesting to study how the previous behaviors are modified when one disregards the memory effects in the equation of motion (2); by taking the limit $\gamma \to +\infty$ [see Eq. (5)], $X(t)$ is seen to obey the ordinary nonretarded differential equation

$$\ddot{X}(t) = -A(t) + \frac{1}{\tau_R} \dot{X}(t) \tag{36}$$

One can remark here that, since the cross-over temperature T_c^f delineating the two noise regimes becomes infinite in the limit $\gamma \to +\infty$ [see Eq. (30)], the quantum noise regime prevails whatever the temperature T of the bath. The force correlation function $\Phi_T(t)$ is obtained from Eq. (20) and given by

$$\Phi_T(t) = \frac{\hbar}{\pi M \tau_R} \left[\frac{d}{dt} \,\text{P.P.}\, \frac{1}{t} + 8 \left(\frac{k_B T}{\hbar} \right)^2 \sum_{n=1}^{\infty} \frac{n^2 - [(2/\hbar)\, k_B T t]^2}{\{n^2 + [(2/\hbar)\, k_B T t]^2\}^2} \right] \tag{37}$$

where P.P. denotes the principal part. At $T = 0$, this expression reduces to the Schmid's result.[10] Note that Φ_T has a long negative time tail for any temperature T, although an infinitely short time scale ($\gamma^{-1} = 0$) has been introduced by construction. Moreover, as expected, expression (37) for $\Phi_T(t)$ is independent of the choice of the modeling for the memory kernel $K(t)$.

The velocity correlation function $C_{vv}(t)$ can be obtained along the same line from Eq. (21). Since $\gamma \to +\infty$, the form (22) can be used and one has

$$C_{vv}(t) \simeq \frac{\hbar}{2\pi M \tau_R} f_T(t; \tau_R^{-1}) - [\gamma^{-2} \Phi_T(t)]_{\gamma \to +\infty} \tag{38}$$

The last term disappears in the limit $\gamma \to +\infty$ and C_{vv} reads

$$C_{vv}(t) \simeq \frac{\hbar}{2\pi M \tau_R} f_T(t; \tau_R^{-1}) \tag{39}$$

an expression which obviously could have been directly deduced from the equation of motion (36).

Thus C_{vv} in the limit $\gamma \to +\infty$ exactly behaves like Φ_T in the finite memory case, but with a time scale τ_R instead of γ^{-1}. It will present two different behaviors according to the temperature, above or below the cross-over temperature T_c^v which can be found from Eq. (34) with $\gamma \to +\infty$, i.e.,

$$T_c^v = \frac{\hbar}{\pi k_B \tau_R} \tag{40}$$

Thus, suppressing the memory tends to decrease the cross-over temperature (see Fig. 5).

$C_{vv}(t)$ is plotted in Fig. 6 for different values of the ratio τ/τ_R; note how close to one another are the two low-temperature curves corresponding to $\tau/\tau_R = 1$ and $\tau/\tau_R = +\infty$. The long time tails $\sim -t^{-2}$ of $C_{vv}(t)$ are visible on the low-temperature curves 6c and 6d.

C_{vv} is seen to diverge for $t \to 0^+$. Indeed, for $T > 0$ but finite, one has

$$C_{vv}(t=0) \underset{\gamma \to +\infty}{\sim} \frac{\hbar}{\pi M \tau_R} \ln \gamma\tau \tag{41}$$

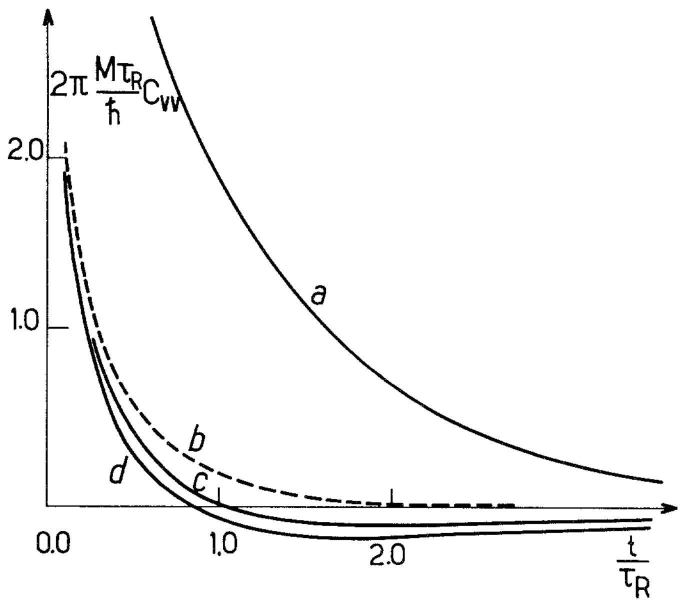

Fig. 6. Variations of C_{vv} in the limit $\gamma \to +\infty$ as a function of t for different values of the ratio τ/τ_R: curve (a), classical behavior ($\tau/\tau_R = 0.1$); curve (b), this curve corresponds to the cross-over temperature $T = T_c^v$ ($\tau/\tau_R = 0.5$); curve (c), quantum behavior ($\tau/\tau_R = 1$); curve (d), this curve corresponds to $T = 0$ ($\tau/\tau_R = +\infty$).

whereas for T strictly equal to zero

$$C_{vv}(t=0) \underset{\gamma \to +\infty}{\sim} \frac{\hbar}{\pi M \tau_R} \ln \gamma \tau_R \tag{42}$$

This divergence leads to questioning the validity of the approximation $\gamma \to +\infty$ for this model. However, we now show that the divergence of C_{vv} occurs on a small time interval.

Indeed for high temperatures ($\tau \ll \tau_R$) C_{vv} reads

$$C_{vv}(t) = \frac{\hbar}{2\pi M \tau_R} \left[\frac{\tau_R}{\tau} e^{-t/\tau_R} - 2 \ln(1 - e^{-t/\tau}) + O\left(\frac{\tau}{\tau_R}\right) \right] \tag{43}$$

The divergence thus occurs for

$$t \lesssim t_1 = \tau e^{-\tau_R/2\tau} \tag{44}$$

i.e., on an exponentially small interval.

For low temperatures, C_{vv} is obtained from Eq. (33) with $\gamma^{-1} \to 0$. Clearly the divergence occurs for $t \lesssim t'_1 < \tau_R$. Remind that at low temperature C_{vv} displays a $-t^{-2}$ tail on a time scale $\tau \gg \tau_R$. Here again the divergence is restricted to a narrow domain.

One can conclude that the approximation $\gamma \to +\infty$ certainly fails for $t < t_1$ or t'_1 depending on the temperature. For $t > t_1$ (respectively $t > t'_1$) the limit $\gamma \to +\infty$ corresponds to a physically sensible model as can be seen from Eqs. (31) and (33).

When $\hbar \to 0$, $t_1 \to 0$ and the approximation $\gamma \to +\infty$ can be retained for all temperatures (except T strictly equal to zero) as could be expected since the system becomes classical.

4. DIFFUSION COEFFICIENT

One can, as usual in purely classical Brownian motion theory, define for our quantum mechanical model a frequency-dependent diffusion coefficient $D(\omega)$ as

$$D(\omega) = \int_0^\infty dt\, C_{vv}(t)\, e^{i\omega t} \tag{45}$$

Using the spectral representation (10) for $C_{vv}(t)$, one obtains

$$D(\omega) = \frac{\hbar \gamma^2}{2M\tau_R} \frac{\omega}{(\omega^2 - \gamma/\tau_R)^2 + \gamma^2 \omega^2} \coth \frac{\beta \hbar \omega}{2} \tag{46}$$

in the finite memory case, and

$$D(\omega) = \frac{\hbar}{2M\tau_R} \frac{\omega}{\omega^2 + \tau_R^{-2}} \coth \frac{\beta\hbar\omega}{2} \tag{47}$$

in the infinitely short memory time limit. Let us now discuss the consequences of the presence of quantum factors in the expression for $D(\omega)$.

4.1. Static Diffusion Coefficient

The static diffusion coefficient is obtained by taking the limit $\omega \to 0$ of expression (46). One gets, whatever the temperature (provided that it is finite)

$$D_0 = \lim_{\omega \to 0} D(\omega) = \frac{k_B T \tau_R}{M} \tag{48}$$

in accordance with the Einstein relation. The behavior of the particle at long times is thus of diffusive type, as is usual in purely classical Brownian motion theory. So we see that, even in our quantum mechanical description, the diffusive motion prevails at long times. But nothing is said on the behavior of the particle at intermediate times, that is, before it begins to diffuse. In particular, the time after which the motion of the particle begins to be of the diffusive type is not precised when only D_0 is known, and depends on the temperature with respect to T_c^v. Moreover, when $T=0$, one gets $D_0 = 0$, which evidently implies that a finer analysis is necessary to describe the long time behavior of the particle.

4.2. Transient Diffusion Coefficient

In order to get a finer description, let us define a nonstationary diffusion coefficient $\mathscr{D}(t)$. Since for $t \to +\infty$, the average dispersion of the particle position $\Delta x^2(t) = \langle [x(t+t') - x(t')]^2 \rangle_s$ is expected to behave as $2D_0 t$, a convenient definition of $\mathscr{D}(t)$ is

$$\mathscr{D}(t) = \frac{1}{2} \frac{d}{dt} \langle [x(t+t') - x(t')]^2 \rangle_s \tag{49}$$

It is clear that

$$\mathscr{D}(t) = \int_0^t dt' \, C_{vv}(t') \tag{50}$$

For $t \to +\infty$, $\mathscr{D}(t) \to D_0$ [see Eq. (48)], which means that the long time limit of $\mathscr{D}(t)$ is precisely the static diffusion coefficient.

From the foregoing analysis of $C_{vv}(t)$, one sees that in the classical noise regime (i.e., when $T > T_c^f$), $\mathscr{D}(t)$ increases monotoneously in an exponential manner toward its limit value D_0; the diffusive regime is attained when $C_{vv}(t)$ has essentially decreased to zero, that is, for $t \gg \tau_R$. When $t \to +\infty$, $\Delta x^2(t) \simeq (2k_B T/M)\, \tau_R[t - (1 - 4/\gamma\tau_R)\, \tau_R]$.

In the quantal noise regime (i.e., when $T < T_c^f$), $\mathscr{D}(t)$ has still a classical behavior when $T > T_c^v$ [exactly as $C_{vv}(t)$]. However, below T_c^v, $\mathscr{D}(t)$ presents a markedly different behavior, since it first increases and then slowly ($\sim 1/t$) decreases toward D_0. Thus, when quantum effects are dominant, the nonstationary diffusion coefficient can exceed its stationary value given by the Einstein relation. In this case, the diffusive regime is only attained very slowly after times $t \gg \hbar/k_B T$. When $t \to +\infty$, one has in this case: $\Delta x^2(t) \simeq (2k_B T/M)\, \tau_R t + \hbar^2/6Mk_B T$.

4.3. The Zero-Temperature Case

As we said previously, D_0 is then equal to zero, and, in that case, $\mathscr{D}(t) \sim 1/t$ as long as $t \gg \tau_R$. This is easily seen to yield a $\ln t$ behavior for the average dispersion of the position of the particle with respect to its initial position. This means in particular that the diffusive regime, which is attained after a time of the order of $\hbar/k_B T$ at low but finite temperature, can never be reached at zero temperature. This fact has to be associated with the $1/\omega$ present at low frequencies in the spectral density of the position fluctuations of the particle at zero temperature, as opposed to the

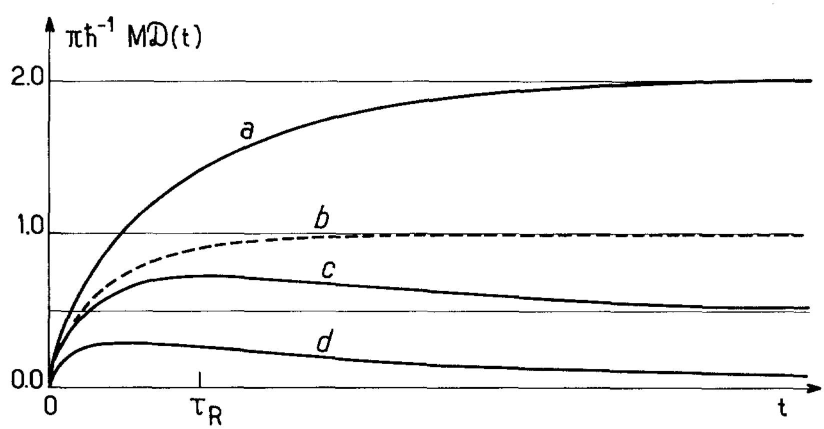

Fig. 7. Nonstationary diffusion coefficient $\mathscr{D}(t)$ in the limit $\gamma \to +\infty$ as a function of t: curve (a), classical behavior ($\tau/\tau_R = 0.25$); curve (b), this curve corresponds to the cross-over temperature $T = T_c^v$ ($\tau/\tau_R = 0.5$); curve (c), quantum behavior ($\tau/\tau_R = 1$); curve (d), this curve corresponds to $T = 0$ ($\tau/\tau_R = +\infty$).

$1/\omega^2$ factor which governs the low-frequency spectral density of the position fluctuations at any finite temperature. Indeed, one can remark that the diffusional motion which prevails at any finite temperature is accompanied with the emission and absorption of reservoir quanta; since at $T=0$ no excitations are present in the system, only emission processes are possible, which in turn profoundly modifies the time behavior of the dispersion of the particle position. When $t \to +\infty$, one has in the zero-temperature case: $\Delta x^2(t) \simeq (2\hbar\tau_R/\pi M) \ln \gamma t + C^{ste}$.

The nonstationary diffusion coefficient $\mathscr{D}(t)$ is plotted as a function of t in Fig. 7.

CONCLUSION

In this paper, we investigated a model, often considered in the past and, more recently, by Caldeira and Leggett,[2,4] in which a quantum free particle is coupled to a bath of quantum harmonic oscillators. The coupling between the particle and the bath being bilinear, it is possible to eliminate the bath degrees of freedom and to rewrite the particle equations of motion under a simple form containing a dissipative term and a fluctuating force term, for which exact microscopic expressions can be given, which is one of the main advantages of the model. When one uses for the dissipative term an exponential modeling $K(t) \sim e^{-\gamma t}$, where $\hbar\gamma$ is the bandwidth of the bath, one can compute all the correlation functions of interest. For an infinitely short memory, we recovered the basic equations of Ford, Kac, and Mazur,[1] who studied the conditions under which the particle coupled to the bath exhibits Brownian motion. However, their study is limited to the classical case. In the quantum case, they wrote the formulas for the various correlation functions involved in the problem, namely, the correlation function of the fluctuating force and the correlation function of the particle velocity, but they did not study their behavior in detail.

The question of the time behavior of the correlation functions in this model was recently raised by Lindenberg and West[11]; they asserted that, at low temperature, the characteristic time of the correlation function of the fluctuating force is $\hbar/k_B T$. However, their study remains rather qualitative and does not consider the correlation function of the particle velocity.

So, we intended to undertake a quantitative discussion of the time behavior of the various correlation functions involved in the problem, and, consequently, of the possibility of Brownian motion. We first remarked that it is possible to distinguish two noise regimes, roughly speaking classical (for $T > T_c^f$) and quantal (for $T < T_c^f$), where $2\pi\hbar k_B T_c^f = \hbar\gamma$, and, consequently, that the time behavior of the force correlation function in these two noise regimes should be very different.

We then proceeded to a detailed quantitative analysis of the time behavior of the correlation functions. This analysis revealed that these behaviors are indeed very different in the two noise regimes quoted above.

In the first case (classical noise regime), the correlation functions decrease exponentially. The correlation time of the fluctuating force appears as being of the order of γ^{-1}. One can then, as usual, separate slow and fast variables, the latter ones evolving on a time scale γ^{-1} characteristic of the bath and the former ones on a time of the order of the relaxation time τ_R of the particle velocity. This regime can therefore properly be described as a Brownian motion.

However, if the temperature becomes lower than the cross-over temperature T_c^f, one enters the quantum noise regime, in which quantum effects do manifest themselves in the following striking way: the correlation function of the fluctuating force exhibits a long time tail $\sim -1/t^2$, which appears to be essentially independent of the precise form of the memory kernel $K(t)$. The quantum fluctuations have thus a very long range, of the order of $\hbar/k_B T$. This long time tail is equally present in the correlation function of the particle velocity when T becomes lower than T_c^v (with $T_c^v < T_c^f$).

In the intermediate temperature range ($T_c^v < T < T_c^f$), the force and the velocity correlation functions have qualitatively different behaviors; the former is already in its quantum regime, whereas the latter still keeps a quasiexponential decay on the time scale τ_R.

The main consequence of this fact is that, below the cross-over temperature T_c^f, it is impossible to consider the correlation time of the fluctuating force as the short time scale of the problem. One cannot then separate slow and fast variables: in particular, at low temperature (i.e., when $T < T_c^v$), all relevant variables are slow. It is therefore impossible to speak of Brownian motion in the temperature range $T < T_c^f$, and, *a fortiori* $T < T_c^v$.

Since it is possible to define a different cross-over temperature for each relevant physical quantity, it is seen that, globally, the system enters gradually the quantum regime. In that sense, one may speak of a smooth cross-over region between the classical and the quantum behavior of the system.

We equally studied the particle diffusion coefficient, which is the transport coefficient of interest in this problem. We have shown that this coefficient always satisfies the Einstein relation, whatever the temperature. However, if one defines a transient diffusion coefficient $\mathscr{D}(t)$, its behavior as a function of time is seen to be very different depending on temperature. For instance, for $T < T_c^v$, $\mathscr{D}(t)$ can exceed its limit value given by the Einstein relation and the diffusive regime is attained very slowly ($\sim 1/t$). In particular, at zero temperature, the nonclassical behavior of $\mathscr{D}(t)$ manifests itself by a ln t dependence of the average dispersion of the particle position, corresponding to a $1/\omega$ factor in the associated spectral density.

Finally, let us point out as a matter of conclusion that one of the main advantages of the model lies in its simplicity, which allowed us to analytically calculate all the correlation functions.

Clearly, from a physical point of view, it is interesting to determine the behavior at all times of the various correlation functions in a quantum system coupled to a bath. An obvious generalization would be to consider a particle in a given potential: the harmonic potential is also exactly soluble but only leads to a more complicated algebra without gain in physical insight. The double-well potential has been analyzed by Bray and Moore[(12)] using instanton techniques; they found a symmetry breaking for a finite value of the coupling constant. It would be interesting to tackle this problem by more conventional methods.

NOTE ADDED IN PROOF

We are indebted to Drs. Grabert *et al.* for drawing our attention on formula (3.23) of their paper (*Z. Phys. B* **55**:87 (1984)) which also displays $a - t^{-2}$ tail in the position correlation function of an harmonic oscillator at $T = 0$.

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