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PATH INTEGRAL APPROACH TO QUANTUM BROWNIAN MOTION*

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We apply the influence-functional method of Feynman and Vernon to the study of Brownian motion at arbitrary temperature. By choosing a specific model for the dissipative interaction of the system of interest with its environment, we are able to evaluate the influence functional in closed form and express it in terms of a few parameters such as the phenomenological viscosity coefficient. We show that in the limit $\hbar \to 0$ the results obtained from the influence functional formalism reduce to the classical Fokker–Planck equation. In the case of a simple harmonic oscillator with arbitrarily strong damping and at arbitrary temperature, we obtain an explicit expression for the time evolution of the complete density matrix $\rho(x, x', t)$ when the system starts in a particular kind of pure state. We compare our results with those of other approaches to the problem of dissipation in quantum mechanics.

1. Introduction

In nature there are many systems which, in the classical regime, can adequately be described by equations of motion of the form

$$m\ddot{x} + \eta\dot{x} + v'(x) = F(t)\,. \tag{1.1}$$

This could stand, for example, for a particle of colloidal size immersed in a viscous fluid. In this case, m is the mass of the particle, η is a damping constant, $v(x)$ is the potential acting on the particle and $F(t)$ is the so-called fluctuating force. The latter obeys the relations

$$\begin{aligned} &\langle F(t)\rangle = 0\,, \\ &\langle F(t)F(t')\rangle = 2\eta kT\delta(t - t')\,, \end{aligned} \tag{1.2}$$

where $\langle\ \rangle$ represents the statistical average over the ensemble of identically prepared systems. Eq. (1.1) subject to the relations (1.2) is the well-known

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Langevin equation which has been used as the basis for the theory of Brownian motion for over half a century now[1]).

Like any other phenomenological equation, (1.1) has a restricted range of validity. It is reasonable to use Langevin equations when we are interested in the long time behaviour of the system. By long times we mean times long compared to the relaxation time of the reservoir coupled to the system in question.

In the above-mentioned example we do not need to bother about quantum effects because a macroscopic particle in a viscous medium can be well described by the classical theory. However, in many other situations, things do not work in this way. If we take, for example, a LCR circuit we know that the equation for the charge at the capacitor plates has the form (1.1). As the temperature starts to achieve very low values we expect to observe quantum effects in this system. Therefore a very natural question arises: how can one reconcile damped equations of motion with the processes of quantization?

The origin of this question lies in the fact that the standard procedures of quantization are based on the existence of either a Hamiltonian or a Lagrangian function for the system in which we are interested. On the other hand it is well known that we cannot obtain (1.1) from the application of the classical Lagrange's or Hamilton's equations to any Lagrangian or Hamiltonian which has no explicit time dependence. The employment of time-dependent functions would allow us to use the standard procedures of quantization directly[2]). However, this approach would inevitably lead us to face some problems with the uncertainty principle[3]).

Over the last two or three decades, many people have tried to answer this question. In spite of the variety of methods used, all these attempts fall into two main categories: They either look for new schemes of quantization or use the system-plus-reservoir approach. We shall list some of the more important works in each category in what follows.

In the beginning of the seventies, Kostin[4]) proposed a theory with a non-linear Schroedinger equation. Besides violating the superposition principle, this theory shows some highly controversial results such as stationary damped states. On the basis of Nelson's Stochastic Quantization[5]), K. Yasue[6]) deduced Kostin's equation. It is possible to do so because in Nelson's quantization what one needs to know is the equation of motion itself instead of Hamiltonians or Lagrangians. The main question here is whether Nelson's theory is correct or not.

Dekker[7]) developed a canonical quantization procedure using complex variables. Despite reproducing some interesting results, such as the Fokker–Planck equation for the Wigner transform of the density operator, his theory seems obscure in some points. For example, he introduces an explicit noise source for the equation of the position, $x(t)$, and another one for the momentum equation. We see no physical reason to do so. We shall return to some points in Dekker's work later on.

The most successful approach we are aware of so far was pioneered by the work of Senitzky[8]). There, he takes explicitly into account the interaction of the system of interest with a reservoir. In his work he was particularly involved with the damping of electromagnetic field modes in a cavity. His strategy is carried out in the Heisenberg picture with the elimination of the reservoir operators. This theory was generalized later by Mori[9]). Still along these lines, Zwanzig[10]) and Nakajima[11]) worked in the Schroedinger picture to get generalized master equations for the density operator. Excellent reviews of this sort of approach can be found in[12]) and [13]).

One further approach to this problem consists of attempting to generalize the classical Langevin equation (1.1) to the quantum case. The simplest way to do this is to leave equation (1.1) itself unchanged, but to replace the classical force correlation expressed by (1.2) by the equation

$$\langle F(t)F(t')\rangle = \frac{1}{2\pi}\int e^{-i\omega(t-t')}\eta\hbar\omega\coth\left(\frac{\hbar\omega}{2kT}\right)d\omega\,, \tag{1.2'}$$

with some suitable cutoff on ω, say Ω. If we are interested in time intervals $|t-t'| \gg \Omega^{-1}$, then eq. (1.2') is effectively equivalent to (1.2) at high temperatures ($kT \gg \hbar|t-t'|^{-1}$) but diverges from it at low temperatures. Very recently, this approach has been used by Koch et al.[14]) to analyze the low-temperature behaviour of Josephson junctions; its theoretical foundation has also been recently discussed by Benguria and Kac[15]). It will be clear from the latter discussion that the general question of the validity of the "quantum Langevin equation" outside the especial case of the harmonic oscillator is a very open one.

The general approach we shall adopt in this paper has much in common with the work of refs. 8–13. That is, we shall not even attempt to quantize the dissipative system itself, but will instead treat it from the beginning as interacting with a complex environment; it is precisely this interaction which will give rise to dissipation. Since the complete "universe" formed by the system plus environment may be treated as closed, there is of course no objection to applying to it the standard quantization procedures. Having done this, we will then eliminate the environment coordinates so as to obtain closed equation for the dissipative system alone. To achieve this elimination we must of course choose a sufficiently simple model for the system–environment interaction. Moreover, the model must be so constructed as to reproduce the results for classical Brownian motion in the classical (high-temperature) limit.

A number of papers in the literature have studied related questions. Ford et al.[16]) studied an array of identical particles interacting with each other through quadratic potentials. Fixing one of them, they investigated the form the inter-particle potential would have to have to make it a Brownian particle in the classical regime. Iche and Nozières[17]) constructed a general adiabatic expansion

for heavy particles in an environment but the results they obtain are mainly formal. Davies[18]) has proved some nice rigorous results concerning the diffusive behaviour of the particles of the system, Markoffian Fokker–Planck equations and so on. However, they hold only for extremely underdamped cases. Schwinger[19]) applied his action principle to the motion of a quantum oscillator weakly coupled to a bath and studied carefully the problems of the frequency shift and constant damping.

What we aim to do in the present paper is to explore how far it is possible to obtain closed equations for a dissipative quantum-mechanical system which involve only phenomenological parameters (in principle experimentally accessible) such as mass, friction coefficient etc. To this end we set up a specific model of the system–environment interaction and fit the parameters of the model from the condition that it reproduce the classical equations of Brownian motion in the appropriate limit[20]). We then explore its consequences in the more general, e.g. quantum, case. We show that a general formal expression (in the form of a functional integral) for the propagator of the density matrix can be written down which is only slightly more complicated than that which already occurs in the noninteracting case, and that in the special case of the harmonic oscillator it can be evaluated explicitly for all degrees of damping and all temperatures. As an application we study explicitly the time development of a damped harmonic oscillator which starts out in a certain kind of pure state. The technique used throughout is the functional integral formulation of quantum mechanics, and more specifically the "influence functional" technique of Feynman and Vernon.

The original motivation of this work was our desire to understand the effect of dissipation on the phenomenon of quantum mechanical tunnelling through a potential barrier. It turns out that while the functional integral method itself is very well suited to this problem, the particular approach developed in the present paper is not; conversely, the method most appropriate to the tunneling problem (which involves the "imaginary-time" representation and the consideration of two rather than four-point functions) is not well suited to the discussion of the time evolution of a system in the classically accessible region. For this reason we feel it is logical to separate the present discussion from our treatment of the tunnelling problem, which is given in ref. 21. Nevertheless a number of questions are common to the two discussions, in particular the question of the generality and degree of realism of our model of the dissipative mechanism and the modifications introduced by velocity-dependent coupling, and some of these questions are discussed in greater detail in[21]). We will therefore cross-reference this work at various points in the present paper.

In section 2, we review the Feynman–Vernon theory of the influence functional[22,23]). In sections 3 and 4 we evaluate the influence functional for specific models of the reservoir. This gives us the propagator for the reduced density

operator of the Brownian particle under appropriate circumstances. Section 5 deals with the recovery of the classical equations of Brownian motion when we study the limit $\hbar \to 0$ of our quantal expressions. Applications of the results of sections 3 and 4 are presented in section 6; in particular, we consider a damped harmonic oscillator which is described at time zero by a Gaussian (not necessarily minimum-uncertainty) pure state wave packet, and calculate its density matrix explicitly for all subsequent times. Finally, in section 7 we draw our conclusions.

2. Feynman–Vernon theory

Let us consider a system A interacting with a second system B (the reservoir) described by the following Hamiltonian:

$$H = H_{\mathrm{A}} + H_{\mathrm{I}} + H_{\mathrm{B}}, \tag{2.1}$$

where

$$H_{\mathrm{A}} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + v(x), \tag{2.2}$$

is the Hamiltonian of the system represented by a particle of mass M and coordinate x,

$$H_{\mathrm{B}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \boldsymbol{R}^2} + \tfrac{1}{2}\sum_{i\neq j} v_{\mathrm{B}}(R_i, R_j) \tag{2.3}$$

is the Hamiltonian of the reservoir consisting of N particles of coordinates R_i and masses m. The N-component vector $\boldsymbol{R}$ stands for $\boldsymbol{R} = (R_1, \ldots, R_N)$. Finally, H_{I} is the interaction Hamiltonian given by

$$H_{\mathrm{I}} = \sum_i v_i(x, R_i) \tag{2.4}$$

Our starting point in presenting the Feynman–Vernon theory[22,23]) is the integral form of the density operator of the system plus reservoir at a time t,

$$\rho(t) = \exp -\frac{\mathrm{i}Ht}{\hbar}\,\rho(0)\exp\frac{\mathrm{i}Ht}{\hbar}, \tag{2.5}$$

which in the coordinate representation can be written as

$$\langle x\boldsymbol{R}|\rho(t)|y\boldsymbol{Q}\rangle = \int \mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}\boldsymbol{R}'\,\mathrm{d}\boldsymbol{Q}' \left\langle x, \boldsymbol{R}\left|\exp -\frac{\mathrm{i}Ht}{\hbar}\right|x'\boldsymbol{R}'\right\rangle \times \langle x'\boldsymbol{R}'|\rho(0)|y'\boldsymbol{Q}'\rangle \left\langle y'\boldsymbol{Q}'\left|\exp\frac{\mathrm{i}Ht}{\hbar}\right|yQ\right\rangle. \tag{2.6}$$

Those terms containing H in (2.6) are easily recognized as[22])

$$\left\langle x\boldsymbol{R}\left|\exp-\frac{\mathrm{i}Ht}{\hbar}\right|x'\boldsymbol{R}'\right\rangle \equiv K(x,\boldsymbol{R},t;x',\boldsymbol{R}',0)=\int\int \mathrm{D}x\,\mathrm{D}\boldsymbol{R}\exp\frac{\mathrm{i}}{\hbar}S[x,\boldsymbol{R}] \tag{2.7}$$

and

$$\left\langle y'\boldsymbol{Q}'\left|\exp\frac{\mathrm{i}Ht}{\hbar}\right|y\boldsymbol{Q}\right\rangle \equiv K^*(y,\boldsymbol{Q},t;y',\boldsymbol{Q}',0)=\int\int \mathrm{D}y\,\mathrm{D}\boldsymbol{Q}\exp-\frac{\mathrm{i}}{\hbar}S[y,\boldsymbol{Q}], \tag{2.8}$$

where all the functional integrations are evaluated over paths $x(t')$, $y(t')$, $\boldsymbol{R}(t')$ and $\boldsymbol{Q}(t')$ with endpoints $x(t)=x$, $x(0)=x'$, $y(t)=y$, $y(0)=y'$, $\boldsymbol{R}(t)=\boldsymbol{R}$, $\boldsymbol{R}(0)=\boldsymbol{R}'$, $\boldsymbol{Q}(t)=\boldsymbol{Q}$ and $\boldsymbol{Q}(0)=\boldsymbol{Q}'$. In (2.7) and (2.8) the action S is given by

$$S=S_{\mathrm{A}}+S_{\mathrm{I}}+S_{\mathrm{B}}=\int_0^t L\,\mathrm{d}t', \tag{2.9}$$

where

$$L=L_{\mathrm{A}}+L_{\mathrm{I}}+L_{\mathrm{B}}=\tfrac{1}{2}Mx^2-v(x)-\sum_i v_i(x,R_i)+\sum_i \tfrac{1}{2}m\dot{R}_i^2-\tfrac{1}{2}\sum_{i\neq j}v_{\mathrm{B}}(R_i,R_j). \tag{2.10}$$

In this way we can write (2.6) as

$$\langle x\boldsymbol{R}|\rho(t)|y\boldsymbol{Q}\rangle=\int \mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}\boldsymbol{Q}'\,\mathrm{d}\boldsymbol{R}'K(x,\boldsymbol{R},t;x',\boldsymbol{R}',0)K^*(y,\boldsymbol{Q},t;y',\boldsymbol{Q}',0)\times\langle x'\boldsymbol{R}'|\rho(0)|y'\boldsymbol{Q}'\rangle. \tag{2.11}$$

This expression for the density operator describes the behaviour of the system plus reservoir as a whole. However, we do not wish to have all that information. We want access to the properties of the system A regardless of the specific behaviour of the reservoir. All we need is its influence on the system A. Then the quantity we are really looking for is not the total density operator but the so-called reduced density operator[3,12,13]). This is easily obtained by tracing out all the environment coordinates in (2.11). So,

$$\tilde{\rho}(x,y,t)\equiv\int \mathrm{d}\boldsymbol{R}\langle x\boldsymbol{R}|\rho(t)|y\boldsymbol{R}\rangle=\int \mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}\boldsymbol{R}'\,\mathrm{d}\boldsymbol{Q}'\,\mathrm{d}\boldsymbol{R}K(x,\boldsymbol{R},t;x',\boldsymbol{R}',0)\times K^*(y,\boldsymbol{R},t;y'\boldsymbol{Q}',0)\langle x'\boldsymbol{R}'|\rho(0)|y'\boldsymbol{Q}'\rangle. \tag{2.12}$$

Now, suppose we initially have the total density operator given by

$$\rho(0)=\rho_{\mathrm{A}}(0)\rho_{\mathrm{B}}(0), \tag{2.13}$$

where $\rho_B(0)$ and $\rho_A(0)$ are the density operators of the reservoir and the system respectively, when they are not interacting with each other. After $t = 0$ they may both change with time. Inserting (2.13) in (2.12) and using (2.7) to (2.10) we get

$$\tilde{\rho}(x, y, t) = \int dx' \, dy' J(x, y, t; x', y', 0) \rho_A(x', y', 0), \tag{2.14}$$

where

$$J(x, y, t; x', y', 0) = \int\int \mathrm{D}x \, \mathrm{D}y \exp i \frac{S_A[x]}{\hbar} \exp - i \frac{S_A[y]}{\hbar} \mathscr{F}[x, y] \tag{2.15}$$

and

$$\mathscr{F}[x, y] = \int d\boldsymbol{R}' \, d\boldsymbol{Q}' \, d\boldsymbol{R} \rho_B(\boldsymbol{R}', \boldsymbol{Q}', 0) \int\int \mathrm{D}\boldsymbol{R} \, \mathrm{D}\boldsymbol{Q} \exp \frac{i}{\hbar}$$
$$\times (S_I[x, \boldsymbol{R}] - S_I[y, \boldsymbol{Q}] + S_B[\boldsymbol{R}] - S_B[\mathbf{Q}]) \tag{2.16}$$

is the so-called influence functional[22,23]).

When there is no interaction between the system of interest and the environment the influence functional is equal to one. Then our expression (2.15) reduces to a product of two propagators, one forward and the other one backward in time. This happens because for a closed system the density operator can be written as the product of the wave function with its complex conjugate. When the interaction is switched on we do not have these two propagations taking place freely. Instead, the influence functional couples them.

Expression (2.15) is the central formula in our development of the quantum theory of Brownian motion.

3. The model

In principle our problem is solved. Once we know the interparticle potentials $v_i(x, R_i)$ and $v_B(R_i, R_j)$ in equations (2.3) and (2.4) and the initial state of the reservoir, described by $\rho_B(0)$, we can find the influence functional in (2.16). However, our experience tells us that life is not that simple. We know that very few problems can be solved exactly in the field of many body systems. It is hopeless to think we can solve the problem exactly in its full generality. What we need to do is to employ a specific model, soluble by construction, from which we expect to draw some general conclusions we believe can be extended to many other systems.

Let us assume our reservoir is composed of particles interacting through a general potential $v(R_1, \ldots, R_N)$ which has an absolute minimum $\boldsymbol{R}_0 = (R_{10}, R_{20}, \ldots, R_{N0})$. Now, suppose we couple to it the system A described by the general

Hamiltonian (2.2) and that the coupling is weak in the sense that we have to consider just the linear response of the reservoir to the system. In this way, the reservoir is very weakly perturbed by the system and we are allowed to describe the former in the harmonic approximation*. The interaction between the two systems is linear by hypothesis and the system is subject to a general potential $v(x)$. The only thing we must be sure of is that we shall not have to consider very drastic deviations from equilibrium in the system; this is necessary in order to preserve all the approximations we have already started to make. In other words we want to study the whole system described by a Hamiltonian of the form

$$H = H_A + H_I + H_B = \frac{p^2}{2M} + v(x) + x\sum_k C_k R_k + \sum_k \frac{p_k^2}{2m} + \sum_k \tfrac{1}{2} m\omega_k^2 R_k^2 , \tag{3.1}$$

where the C_k's are the coupling constants of the reservoir particles to the system A and the ω_k's are the frequencies of motion of the reservoir particles. The action that appears in (2.16) can now be written as

$$S_B[\boldsymbol{R}] + S_I[x, \boldsymbol{R}] = \int_0^t L_B(\boldsymbol{R}, \dot{\boldsymbol{R}})\,\mathrm{d}t + \int_0^t L_I(x, \boldsymbol{R})\,\mathrm{d}t , \tag{3.2}$$

where

$$L_B = \sum_k \tfrac{1}{2} m\dot{R}_k^2 - \sum_k \tfrac{1}{2} m\omega_k^2 R_k^2 \tag{3.3}$$

and

$$L_I = -x\sum_k C_k R_k . \tag{3.4}$$

This problem has been solved exactly in[22,23]) and the final expression for the influence functional in (2.16) is

$$\mathscr{F}[x, y] = \exp -\frac{1}{\hbar}\int_0^t\int_0^\tau [x(\tau) - y(\tau)][\alpha(\tau - s)x(s) - \alpha^*(\tau - s)y(s)]\,\mathrm{d}\tau\,\mathrm{d}s , \tag{3.5}$$

where

$$\alpha(\tau - s) = \sum_k \frac{C_k^2}{2m\omega_k}\left[\exp -\mathrm{i}\omega_k(\tau - s) + \frac{\exp \mathrm{i}\omega_k(\tau - s)}{\exp\dfrac{\hbar\omega_k}{kT} - 1} + \frac{\exp -\mathrm{i}\omega_k(\tau - s)}{\exp\dfrac{\hbar\omega_k}{kT} - 1}\right] \tag{3.6}$$

* The question of the justification for this model as general description of dissipative systems is further discussed in ref. 21.

and we have assumed that the environment is initially in equilibrium at temperature T which means that its initial density matrix can be written as

$$\rho_B(\boldsymbol{R}', \boldsymbol{Q}', 0) = \prod_k \rho_B^{(k)}(R_k', Q_k', 0), \tag{3.7}$$

with the usual

$$\rho_B^{(k)}(R_k', Q_k', 0) = \frac{m\omega_k}{2\pi\hbar \sinh(\hbar\omega_k/kT)} \exp - \left\{ \frac{m\omega_k}{2\hbar \sinh(\hbar\omega_k/kT)} \times \left[(R_k'^2 + Q_k'^2) \cosh \frac{\hbar\omega_k}{kT} - 2R_k'Q_k' \right] \right\}. \tag{3.8}$$

A much more useful way to write the influence functional is in terms of the real and imaginary parts, α_R and α_I of $\alpha(\tau - s)$. In fact we can write the propagator for the density operator as

$$J(x, y, t; x', y', 0) = \int\int \mathrm{D}x\, \mathrm{D}y \exp \frac{\mathrm{i}}{\hbar} \left\{ S_A[x] - S_A[y] - \int_0^t \int_0^\tau [x(\tau) - y(\tau)] \times \alpha_I(\tau - s)[x(s) + y(s)]\, \mathrm{d}\tau\, \mathrm{d}s \right\} \times \exp - \frac{1}{\hbar} \int_0^t \int_0^\tau [x(\tau) - y(\tau)]\alpha_R(\tau - s)[x(s) - y(s)]\, \mathrm{d}\tau\, \mathrm{d}s, \tag{3.9}$$

where α_R and α_I are given by

$$\alpha_R(\tau - s) = \sum_k \frac{C_k^2}{2m\omega_k} \coth \frac{\hbar\omega_k}{2kT} \cos \omega_k(\tau - s) \tag{3.10}$$

and

$$\alpha_I(\tau - s) = -\sum_k \frac{C_k^2}{2m\omega_k} \sin \omega_k(\tau - s). \tag{3.11}$$

Now, once we have the reduced density matrix of the system at $t = 0$, expressions (2.14) and (3.9) will give us its time development. There is no dependence on reservoir coordinates any longer. As far as the model Hamiltonian (3.1) is concerned we have solved the problem exactly. Now, our main goal in developing all this was to describe a Brownian particle in the classical limit. At this stage it is clear we have no evidence of any such thing occurring. On the contrary, we see no way we can get an irreversible process out of our exact solution.

To solve this problem we need to remember that the ensemble of oscillators must have some definite characteristics in order to behave as an actual reservoir. For example, a reservoir must have infinite size in such a way that the energy lost by the system of interest will not return to it within a finite period of time. Now, suppose that our ensemble of oscillators represents the set of normal modes of vibration of a certain physical quantity in a finite region of space. For instance, it could be the set of normal modes of the electromagnetic field in a box or the vibration of atoms from their equilibrium positions in a crystal (however, see ref. 21 for more general considerations about the ensemble of oscillators). Therefore, taking the limit of infinite volume means that we need to consider a continuum of allowed oscillator frequencies.

What we intend to do next is to give some arguments to indicate that one can manage to choose a very suitable distribution of oscillators in the continuum limit which will lead us to the Brownian motion. Later on, we shall adopt the chosen model to deduce the Fokker–Planck equation in the classical limit.

Suppose that instead of coupling the system A to a reservoir B as we have done in (3.1), we were to excite it by applying a classical external force $F(\tau)$. In that case, one can easily convince oneself that the propagator of the density matrix would be given by[22])

$$J(x, y, t; x', y', 0) = \int\int \mathrm{D}x\, \mathrm{D}y \exp \frac{\mathrm{i}}{\hbar} \left\{ S_{\mathrm{A}}[x] - S_{\mathrm{A}}[y] + \int_0^t [x(\tau) - y(\tau)] F(\tau)\, \mathrm{d}\tau \right\}. \tag{3.12}$$

If, in addition, we consider that $F(\tau)$ is not known exactly but instead we know the probability distribution functional $P[F(\tau)]$ of different histories $F(\tau)$, the averaged density matrix propagator reads

$$J(x, y, t; x', y', 0) = \int\int\int \mathrm{D}x\, \mathrm{D}y\, \mathrm{D}F P[F(\tau)] \exp \frac{\mathrm{i}}{\hbar} \left\{ S_{\mathrm{A}}[x] - S_{\mathrm{A}}[y] + \int_0^t [x(\tau) - y(\tau)] F(\tau)\, \mathrm{d}\tau \right\}. \tag{3.13}$$

The functional integration over $F(\tau)$ in the expression (3.13) is the well-known characteristic functional[22])

$$\phi\left[\frac{x(\tau) - y(\tau)}{\hbar}\right] \equiv \int \mathrm{D}F(\tau) P[F(\tau)] \exp \mathrm{i} \int_0^t \left[\frac{x(\tau) - y(\tau)}{\hbar}\right] F(\tau)\, \mathrm{d}\tau\,. \tag{3.14}$$

With the help of (3.14) we can find the correlation of forces between two different

instants as

$$\langle F(\xi)F(s)\rangle = -\frac{\delta^2\phi}{\delta\left[\dfrac{x(\xi)-y(\xi)}{\hbar}\right]\delta\left[\dfrac{x(s)-y(s)}{\hbar}\right]}\Bigg|_{x=y}, \tag{3.15}$$

where δ stands for functional differentiation (or variation). When $P[F(\tau)]$ is a Gaussian distribution, ϕ has a very simple form[22],

$$\phi\left[\frac{x(\tau)-y(\tau)}{\hbar}\right] = \exp -\frac{1}{\hbar^2}\int_0^t\int_0^\tau [x(\tau)-y(\tau)]A(\tau-s)[x(s)-y(s)]\,\mathrm{d}\tau\,\mathrm{d}s\,, \tag{3.16}$$

which with the help of (3.15) gives

$$\langle F(\xi)F(s)\rangle = A(\xi-s)\,. \tag{3.17}$$

Now, inserting (3.14) back into (3.13) and assuming $P[F(\tau)]$ is a Gaussian functional distribution, the propagator J reads

$$J(x,y,t;x',y',0) = \int\int \mathrm{D}x\,\mathrm{D}y \exp\frac{\mathrm{i}}{\hbar}\{[S_A[x]-S_A[y]\}\exp -\frac{1}{\hbar^2}\int_0^t\int_0^\tau [x(\tau) - y(\tau)]A(\tau-s)[x(s)-y(s)]\,\mathrm{d}\tau\,\mathrm{d}s\,. \tag{3.18}$$

Comparing (3.18) to (3.9) we notice that those two expressions are very similar to each other except for the additional imaginary part that appears in the exponent of (3.9). Regardless of this difference we believe that the real part of the exponents plays the same role in the two cases. The physical meaning of $A(\tau-s)$ in (3.18) or $\hbar\alpha_R(\tau-s)$ in (3.9) cannot be different. So, $\hbar\alpha_R(\tau-s)$ must give the correlation of forces in the classical regime. The question now is: under what conditions will our quantum-mechanical model reproduce the correlation between the stochastic forces acting on a classical Brownian particle? This is not hard to answer. The only thing we need to do is to investigate the behaviour of $\hbar\alpha_R(\tau-s)$ for high temperatures. When $kT \gg \hbar\omega_k$ (3.10) becomes

$$\alpha_R(\tau-s) \approx \frac{kT}{m\hbar}\sum_i \frac{C_i^2}{\omega_i^2}\cos\omega_i(\tau-s) + \frac{\hbar}{12mkT}\sum_i C_i^2\cos\omega_i(\tau-s) + \cdots, \tag{3.19}$$

As we are looking for the expansion of $\hbar\alpha_R(\tau-s)$ we see that its leading term is

$$\hbar\alpha_R(\tau-s) \approx \frac{kT}{m}\sum_i \frac{C_i^2}{\omega_i^2}\cos\omega_i(\tau-s) + \mathcal{O}(\hbar^2)\,, \tag{3.20}$$

thus, this is the classical correlation to which our quantum mechanical model led

us. We wish to compare (3.20) to the well-known correlation of forces[1]),

$$\langle F(\tau)F(s)\rangle = 2\eta kT\delta(\tau - s)\,, \tag{3.21}$$

given by the classical theory of the Brownian motion. Here, η is the damping constant. To do so, let us consider a continuum of oscillators with density $\rho_D(\omega)$. Then,

$$\hbar\alpha_R(\tau - s) \approx \frac{kT}{m}\int_0^\infty \rho_D(\omega)\frac{C^2(\omega)}{\omega^2}\cos\omega(\tau - s)\,d\omega\,. \tag{3.22}$$

If we choose[20])

$$\rho_D(\omega)C^2(\omega) = \begin{cases} \dfrac{2m\eta\omega^2}{\pi}\,, & \omega < \Omega\,, \\ 0\,, & \omega > \Omega\,, \end{cases} \tag{3.23}$$

where we have introduced a high frequency cutoff Ω in the distribution of oscillators, eq. (3.22) becomes

$$\hbar\alpha_R(\tau - s) = \langle F(\tau)F(s)\rangle = 2\eta kT\frac{1}{\pi}\frac{\sin\Omega(\tau - s)}{(\tau - s)}\,, \tag{3.24}$$

which tends to (3.21) if we let $\Omega \to \infty$. In other words, we shall recover (3.21) when we are interested in times much longer than the typical time Ω^{-1}, meaning that it is the low-frequency behaviour of (3.23) which is important in this case. This fact is in accordance with the classical theory of Brownian motion since (3.21) is valid only when we consider times longer than the typical relaxation time of the reservoir.

We can still go a bit further if we write (3.10) as

$$\hbar\alpha_R(\tau - s) = \frac{\hbar}{\pi}\int_0^\infty d\omega\chi''_{FF}(\omega)\coth\frac{\hbar\omega}{2kT}\cos\omega(\tau - s)\,, \tag{3.25}$$

where we have defined

$$\chi''_{FF}(\omega) = \sum_i \frac{\pi C_i^2}{2m\omega_i}\delta(\omega - \omega_i)\,. \tag{3.26}$$

This induces us to regard $\hbar\alpha_R(\tau - s)$ as a time correlation function of an operator $\tilde{F}(t)$ at different instants. Thus, defining

$$\hbar\alpha_R(\tau - s) = \tfrac{1}{2}\langle\{\tilde{F}(\tau), \tilde{F}(s)\}\rangle - \langle\tilde{F}(\tau)\rangle\langle\tilde{F}(s)\rangle\,, \tag{3.27}$$

we recover (3.21) in the classical limit provided that $\tilde{F}(t)$ becomes the classical fluctuating force $F(t)$ in that limit. Expression (3.25) is the well-known

fluctuation–dissipation theorem[24]). The advantage of using (3.25) and (3.26) is that besides allowing us to find a suitable distribution of oscillators to recover (3.21) it allows us to find corrections to that distribution by employing sum rules for $\chi''_{FF}(\omega)$. Obviously, these corrections will be important only when we are interested in the short time behaviour of the system[24]).

In order to find the final form of the propagator for the reduced density operator, we still need to find the additional imaginary part in the exponent we have mentioned earlier. At this stage it is a very simple task because the distribution of oscillators is already fixed by (3.23). Inserting this expression in (3.11) one gets

$$\alpha_1(\tau - s) = \frac{\eta}{2\pi} \frac{\mathrm{d}}{\mathrm{d}(\tau - s)} \int_{-\Omega}^{\Omega} \cos \omega(\tau - s)\, \mathrm{d}\omega\,, \tag{3.28}$$

which tends to

$$\alpha_1(\tau - s) = \eta \frac{\mathrm{d}}{\mathrm{d}(\tau - s)} \delta(\tau - s) \tag{3.29}$$

as $\Omega \to \infty$. Finally, using (3.25) and (3.28) in (3.9) we have

$$\begin{aligned} J(x, y, t; x', y', 0) = \int\int \mathrm{D}x\, \mathrm{D}y \exp \frac{\mathrm{i}}{\hbar} \Big\{ S_{\mathrm{A}}[x] - S_{\mathrm{A}}[y] - \int_0^t \int_0^\tau \eta[x(\tau) - y(\tau)] \\ \times \frac{\mathrm{d}}{\mathrm{d}(\tau - s)} \delta(\tau - s)[x(s) + y(s)]\, \mathrm{d}\tau\, \mathrm{d}s \Big\} \\ \times \exp - \frac{1}{\hbar} \int_0^\Omega \frac{\eta\omega}{\pi} \coth \frac{\hbar\omega}{2kT} \int_0^t \int_0^\tau [x(\tau) - y(\tau)] \\ \times \cos \omega(\tau - s)[x(s) - y(s)] \cdot \mathrm{d}\tau\, \mathrm{d}s\, \mathrm{d}\omega\,. \end{aligned} \tag{3.30}$$

This expression can be further simplified if we integrate the term containing the derivative of the delta function by parts. The procedure is straightforward and the result is

$$\begin{aligned} \int_0^t \int_0^\tau \eta[x(\tau) - y(\tau)] \frac{\mathrm{d}}{\mathrm{d}(\tau - s)} \delta(\tau - s)[x(s) + y(s)]\, \mathrm{d}\tau\, \mathrm{d}s \\ = - \int_0^t \eta[x^2(\tau) - y^2(\tau)] \delta(0)\, \mathrm{d}\tau \\ + \frac{\eta}{2} \int_0^t [x(\tau)\dot{x}(\tau) + x(\tau)\dot{y}(\tau) - y(\tau)\dot{x}(\tau) - y(\tau)\dot{y}(\tau)]\, \mathrm{d}\tau\,. \end{aligned} \tag{3.31}$$

At first sight one would worry about the divergence due to $\delta(0)$. However, we must be careful in interpreting that term. We do better to remember that it comes from the expression (3.28) when $\Omega \to \infty$. Thus we can write

$$\delta(0) = \lim_{\Omega\to\infty} \frac{\sin \Omega(\tau - s)}{\pi(\tau - s)}\bigg|_{\tau = s} = \lim_{\Omega\to\infty} \frac{\Omega}{\pi}. \tag{3.32}$$

Now, as we can see from (3.31), $\delta(0)$ appears multiplying the damping constant η, so, the product $\eta\delta(0)$ is actually

$$\eta\delta(0) = \lim_{\Omega\to\infty} \frac{\eta\Omega}{\pi}. \tag{3.33}$$

This is a very subtle point. At first sight, one should obviously say that when $\Omega \to \infty$ this expression diverges. On the other hand, we could argue against this statement by saying that the meaning of the limit $\Omega \to \infty$ is to consider Ω much higher than the typical frequencies for the motion of the Brownian particle. Consequently, depending on how η is related to Ω, one would expect the product $\eta\Omega$ to be finite (if η is really the phenomenological damping constant). However, this argument is not free from criticism either.

A more formal way to see what happens is by integrating both sides of (3.23). Then, assuming that we have N oscillators in the reservoir and that $C(\omega) = C$, a constant, we can express the right hand side of (3.33) as

$$\frac{\eta\Omega}{\pi} = \frac{3NC^2}{2m\Omega^2}. \tag{3.34}$$

In this expression both N and Ω tend to infinity. Therefore, $\eta\Omega$ diverges or not depending on the term $N\Omega^{-2}$. If we adopt an ensemble of oscillators where $\Omega \propto N^{1/2}$ as a model (3.34) clearly converges.

However, all these arguments can be avoided if we investigate the limit of large Ω only after evaluating those integrals which contain $\alpha_1(\tau - s)$. If we do this, the first integral on the right-hand side of (3.31) reads

$$-\frac{\eta\Omega}{\pi}\int_0^t [x^2(\tau) - y^2(\tau)]\,d\tau + \frac{\eta[x(0) + y(0)]}{\pi}\int_0^t \frac{\sin \Omega t}{\tau}\,[x(\tau) - y(\tau)]\,d\tau, \tag{3.35}$$

where we have appropriately replaced $\delta(\tau - s)$ by $(1/\pi)\sin[\Omega(\tau - s)]/(\tau - s)$. The limit of large Ω simply reflects the fact that we are interested in times $t \approx \omega^{-1} \gg \Omega^{-1}$. Consequently the second term in (3.35) becomes $\frac{1}{2}\eta[x^2(0) - y^2(0)]$ which is clearly much smaller than the first one. This result allows us to substitute $\eta\delta(0)$ by $\eta\Omega/\pi$ in (3.31) without taking the limit $\Omega \to \infty$. For further considerations about the frequency shift (see definition (3.37) below) we refer the reader to section 4 of this paper and to[21]).

Defining the relaxation constant γ as

$$\gamma \equiv \eta/2M \tag{3.36}$$

and the frequency shift $\Delta\omega$ as

$$(\Delta\omega)^2 \equiv \frac{4\gamma\Omega}{\pi}, \tag{3.37}$$

we can finally write (3.30) as

$$\begin{aligned} J(x, y, t; x', y', 0) = \int\!\!\int \mathrm{D}x\, \mathrm{D}y \exp \frac{\mathrm{i}}{\hbar} \Big\{ & S_{\mathrm{R}}[x] - S_{\mathrm{R}}[y] \\ & - M\gamma \int_0^t (x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x})\, \mathrm{d}\tau \Big\} \\ & \times \exp - \frac{1}{\hbar} \frac{2M\gamma}{\pi} \int_0^{\Omega} \omega \coth \frac{\hbar\omega}{2kT} \int_0^t \int_0^{\tau} [x(\tau) - y(\tau)] \\ & \times \cos \omega(\tau - s)[x(s) - y(s)]\, \mathrm{d}\tau\, \mathrm{d}s\, \mathrm{d}\omega, \end{aligned} \tag{3.38}$$

where we have introduced S_{R} as the renormalized action given by

$$S_{\mathrm{R}} = \int_0^t [\tfrac{1}{2}M\dot{x}^2 - v(x)]\, \mathrm{d}\tau + \int_0^t \tfrac{1}{2} M(\Delta\omega)^2 x^2\, \mathrm{d}\tau\,. \tag{3.39}$$

In other words S_{R} is the action with the potential $v(x)$ renormalized by the subtraction of a harmonic term with frequency $\Delta\omega$. From now on we shall call it the renormalized potential $v_{\mathrm{R}}(x)$. In the case $v(x) = \frac{1}{2}M\omega^2 x^2$ (simple harmonic oscillator) we define also a renormalized frequency ω_{R} by $\omega_{\mathrm{R}}^2 \equiv \omega^2 - (\Delta\omega)^2$. This effective potential felt by the particle may always result when we couple it to a reservoir[17]). Here, this assumes a very simple form because of the model we have been employing to the environment.

At this point we wish to emphasize some connections of our expression (3.38) with other previously developed ones. To start with let us notice that the imaginary exponent of that expression is very similar to a two variable action proposed by Morse and Feshbach[25]). Suppose for simplicity that $v_{\mathrm{R}}(x) = 0$, then calling the imaginary part of that exponent S_{eff} we have

$$S_{\mathrm{eff}} = \int_0^t [\tfrac{1}{2}M\dot{x}^2 - \tfrac{1}{2}M\dot{y}^2 - M\gamma(x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x})]\, \mathrm{d}\tau\,. \tag{3.40}$$

Now, defining a new set of variables $\{\bar{x}, \bar{y}\}$ obtained from the original set by a

rotation by $\pi/4$ we get

$$S_{\text{eff}} = \int_0^t \left[M\dot{\bar{x}}\dot{\bar{y}} - \frac{\eta}{2}(\bar{x}\dot{\bar{y}} - \bar{y}\dot{\bar{x}}) \right] \mathrm{d}\tau + \eta(\bar{x}(t)\bar{y}(t) - \bar{x}(0)\bar{y}(0)), \tag{3.41}$$

where the Morse and Feshbach Lagrangian spontaneously appears integrated over time. Thus, our expression (3.38) gives us a clue of how to interpret that Lagrangian correctly. The variables $\bar{x}$ and $\bar{y}$ (or x and y) cannot be thought as being representative of two different systems interacting with each other. Instead they represent coupled paths going forward and backward in time. These two paths are needed to describe the time evolution of $\tilde{\rho}(x, y, t)$. A diagrammatic expansion for the coupling of those paths is made in ref. 17 for a general interaction with a heat bath using the Kjeldysh formalism[26]).

Some years ago, Nemes and Piza[27]) created a phenomenological theory for dealing with damping in quantum mechanics based on the Morse and Feshbach Lagrangian. There, they regard $\bar{y}$ as an unphysical variable and trace it out. The procedure is very interesting; however, they end up with a result which contradicts the linear response theory, namely, the freezing of the width of the wave packet at long times.

In a context much closer to ours, Papadopoulos[28]) deduced an expression very similar to (3.38). Nevertheless, there are two main differences between our formulae. The first one concerns the real exponent in (3.38), which he writes as

$$(\text{real exponent}) = -\frac{1}{\hbar^2} M\gamma\hbar\omega \coth\frac{\hbar\omega}{2kT} \int_0^t [x(\tau) - y(\tau)]^2 \,\mathrm{d}\tau, \tag{3.42}$$

for the case of a harmonic oscillator with frequency ω. This can be shown to be a particular case of our expression. We shall exploit this point later on, in section 6. The second difference is that he does not have the γ dependent term in the imaginary exponent of (3.38). To account for the final effect of that sort of term he introduces an explicit time-dependent damping ad hoc. However, we think it is totally unnecessary since a γ-dependent term arises spontaneously from a microscopic calculation.

4. Coupling to velocities

Suppose we wish to study the motion of a particle coupled to a reservoir such that the total Lagrangian is given by

$$L(x, \dot{x}, \boldsymbol{q}, \dot{\boldsymbol{q}}) = \tfrac{1}{2} M\dot{x}^2 - v(x) + x \sum_i e_i \dot{q}_i + \sum_i \tfrac{1}{2} m\dot{q}_i^2 - \sum \tfrac{1}{2} m\omega_i^2 q_i^2 . \tag{4.1}$$

This expression differs from the one with which we dealt above only through the coupling term (compare (3.4) and (4.1)).

Consequently, we cannot apply the results of the previous section to this new model, at least directly. What we are going to show is that we can transform (4.1) into a very similar Lagrangian with a coordinate coupling instead.

In order to overcome this problem, let us introduce a new set of coordinates given by

$$y_i = m\dot{q}_i + e_i x\,. \tag{4.2}$$

If we write $L(x, \dot{x}, \boldsymbol{y}, \dot{\boldsymbol{y}})$ and use the Euler–Lagrange equations we shall not reproduce the correct equations of motion we obtain from (4.1). This means that L is not invariant under the transformation (4.2). It is a very simple exercise to prove that the correct Langrangian in the new set of variables is

$$\tilde{L}(x, \dot{x}, \boldsymbol{y}, \dot{\boldsymbol{y}}) = \tfrac{1}{2} M\dot{x}^2 - v(x) - \sum_i \frac{e_i^2 x^2}{2m} + \sum_i \frac{e_i y_i x}{m} + \tfrac{1}{2}\sum_i \frac{\dot{y}_i^2}{m\omega_i^2} - \tfrac{1}{2}\sum_i \frac{y_i^2}{m}\,. \tag{4.3}$$

Defining an extra variable R_i such that

$$R_i \equiv \frac{y_i}{m\omega_i}\,, \tag{4.4}$$

we can rewrite (4.3) as

$$\tilde{L}(x, \dot{x}, \boldsymbol{R}, \dot{\boldsymbol{R}}) = \tfrac{1}{2} M\dot{x}^2 - v(x) - \sum_i \frac{C_i^2 x^2}{2m\omega_i^2} + \sum_i C_i x R_i + \sum_i \tfrac{1}{2} m\dot{R}_i^2 - \sum_i \tfrac{1}{2} m\omega_i^2 R_i^2\,, \tag{4.5}$$

where $C_i \equiv e_i\omega_i$, which is exactly of the form of the Lagrangian we used in the previous section. The difference here is that the transformation (4.2) introduced a new quadratic term into the bare potential $v(x)$. Thus, the new potential is

$$\bar{v}(x) = v(x) + \sum_i \frac{C_i^2}{2m\omega_i^2} x^2\,. \tag{4.6}$$

Now we can proceed as we have done before. Our problem was reduced to the one of section 3. The propagator for the reduced density operator is once again given by the expression (3.38). What is worth noting here is the form of the renormalized potential $\bar{v}_{\mathrm{R}}(x)$ which is written as

$$\bar{v}_{\mathrm{R}}(x) = \bar{v}(x) - \tfrac{1}{2} M(\Delta\omega)^2 x^2\,. \tag{4.7}$$

The frequency shift $\Delta\omega$ is defined in eq. (3.37), however, to get it we have already assumed a specific distribution of oscillators. We can proceed more generally if we follow the steps (3.28) to (3.31) with $\alpha_{\mathrm{I}}(\tau - s)$ given by the more general

expression (3.11). In this way $\Delta\omega$ is such that

$$M(\Delta\omega)^2 = 2\sum_i \frac{C_i^2}{2m\omega_i^2}\cos\omega_i(\tau - s)\Big|_{\tau=s} = 2\sum_i \frac{C_i^2}{2m\omega_i^2}, \tag{4.8}$$

which clearly reduces to (3.37) if we assume the distribution (3.23) to be valid. The advantage of working with (4.8) is that we can show that the correction potential which depends on $\Delta\omega$, exactly cancels the extra bit in (4.6). Moreover, this fact is completely independent of the distribution of oscillators we are using. Thus, for the model proposed in (4.1) we can say that the renormalized potential is the same as the bare one, that is

$$\tilde{v}_R(x) = v(x)\,. \tag{4.9}$$

The physical interest of the apparently rather academic point discussed in this section lies in the conclusion that not every system which is dissipatively coupled to its environment need undergo a frequency shift (or potential renormalization) due to the coupling. This point is of some significance in the context of the quantization of LCR- circuits and similar systems (where a failure to appreciate it has, indeed, caused some unnecessary confusion in the recent literature), and is discussed further in ref. 21.

5. The Fokker–Planck equation

In the last two sections we derived an expression for the propagator of the reduced density operator of a particle interacting with a reservoir with some specific characteristics. We also showed that in classical limit, the real exponential of (3.38) reduces to the characteristic functional of the stochastic force acting on a Brownian particle. At the same time we gave a definite form for the additional imaginary part of the integrand, i.e. the term involving $x\dot{x}$, etc, in (3.38). The question we want to answer now is whether this term makes sense. In other words: is that term compatible with the classical Brownian motion of a particle? In order to answer this question we shall initially investigate the equation of motion for the reduced density operator in the semiclassical region. If we wish to compare this equation to the one of a classical Brownian particle we must find a way to write it down in the phase-space representation. That is the only way we can compare it to the equation of motion of the phase-space distribution in classical physics. The way we can perform the transformation from the Hilbert to the phase space is by using the so-called Wigner distribution function[29]). For recent reviews on Wigner's formalism we refer the reader to[3,30]).

Let us start by writing (3.38) when $2kT \gtrsim \hbar\Omega \gg \hbar\omega_R$, Ω being the cutoff

frequency of the reservoir oscillators. This reads

$$J(x,y,t;x',y',0)=\int\int \mathrm{D}x\,\mathrm{D}y\,\exp\frac{\mathrm{i}}{\hbar}\left\{S_{\mathrm{R}}[x]-S_{\mathrm{R}}[y]-M\gamma\int_0^t[x\dot{x}-y\dot{y}\right.$$

$$\left.+x\dot{y}-y\dot{x}]\,\mathrm{d}\tau\right\}\exp-\frac{2M\gamma kT}{\hbar^2}\int_0^t[x(\tau)-y(\tau)]^2\,\mathrm{d}\tau\,. \quad (5.1)$$

At this point one should worry about the meaning of this high temperature quantum-mechanical propagator. Of course this expression becomes meaningless if we consider the classical limit $kT\gg\hbar\omega_{\mathrm{R}}$ and still keep its quantal form. However, one must bear in mind that this is our first step to obtain an equation of motion for the reduced density operator in the classical limit. Later, we shall take the appropriate measures in order to be consistent with this approximation. We shall use (5.1) rather than (3.38) only to simplify our future expressions.

What we shall do now is to follow Feynman's procedure in[22]) when he derives the Schroedinger equation from the functional integration formalism. Here our problem is analogous to that one. While in[22]) one has the propagator for the wave function from which one gets the equation of motion for ψ, here we have the propagator for the density operator from which we intend to get a master equation for $\tilde{\rho}$.

Suppose we have the reduced density operator at a time t and wish to find its value at $t+\epsilon$ where $\epsilon\to 0$. By (2.14) we have

$$\tilde{\rho}(x,y,t+\epsilon)=\iint \mathrm{d}x'\,\mathrm{d}y'\,J(x,y,t+\epsilon;x',y',t)\tilde{\rho}(x',y',t)\,. \quad (5.2)$$

The propagator J in (5.2) can be written in a very simple form when ϵ is small. To do so we only need to remember that for small time intervals any regular path can be approximated by a straight line. Thus, functional integrations over paths in short time intervals can be put equal to the value of the integrand times a normalization constant[22]). Then,

$$J(x,y,t+\epsilon;x',y',t)\approx\frac{1}{A^2}\exp\frac{\mathrm{i}}{\hbar}\left\{\int_t^{t+\epsilon}(\tfrac{1}{2}M\dot{x}^2-v_{\mathrm{R}}(x))\,\mathrm{d}\tau\right.$$

$$\left.-\int_t^{t+\epsilon}(\tfrac{1}{2}M\dot{y}^2-v_{\mathrm{R}}(y)\,\mathrm{d}\tau-\int_t^{t+\epsilon}M\gamma[x\dot{x}-y\dot{y}+y\dot{x}-x\dot{y}]\,\mathrm{d}\tau\right\}$$

$$\times\exp-\frac{1}{\hbar^2}\int_t^{t+\epsilon}2M\gamma kT[x-y]^2\,\mathrm{d}\tau\,. \quad (5.3)$$

All the integrals appearing above can also be approximated when $\epsilon \to 0$. Calling $x(t+\epsilon) = x$, $y(t+\epsilon) = y$, $x(t) = x'$ and $y(t) = y'$ and using the fact that

$$\dot{x} \approx \frac{x - x'}{\epsilon}, \quad \dot{y} \approx \frac{y - y'}{\epsilon} \quad \text{and} \quad \int_t^{t+\epsilon} f(x(\tau))\,\mathrm{d}\tau \approx \epsilon f\left(\frac{x + x'}{2}\right) \tag{5.4}$$

in the expression for J, eq. (5.2) becomes

$$\begin{aligned}\tilde{\rho}(x, y, t+\epsilon) = \int_{-\infty}^{\infty} \int \mathrm{d}\beta_1\,\mathrm{d}\beta_2 \exp\Big\{ & \frac{\mathrm{i}M\beta_1^2}{2\epsilon\hbar} - \frac{\mathrm{i}\epsilon}{\hbar} v_{\mathrm{R}}\left(x - \frac{\beta_1}{2}\right) - \frac{\mathrm{i}M\beta_2^2}{2\epsilon\hbar} \\ & + \frac{\mathrm{i}\epsilon v_{\mathrm{R}}}{\hbar}\left(y - \frac{\beta_2}{2}\right) - \frac{\mathrm{i}M\gamma}{\hbar}\left(x - \frac{\beta_1}{2}\right)\beta_2 + \frac{\mathrm{i}M\gamma}{\hbar}\left(y - \frac{\beta_2}{2}\right)\beta_1 \\ & - \frac{\mathrm{i}M\gamma}{\hbar}\left(x - \frac{\beta_1}{2}\right)\beta_1 + \frac{\mathrm{i}M\gamma}{\hbar}\left(y - \frac{\beta_2}{2}\right)\beta_2 - \frac{2M\gamma kT\epsilon}{\hbar^2}(x - y)^2 \\ & - \frac{2M\gamma kT\epsilon}{\hbar^2}(x - y)(\beta_1 - \beta_2) - \frac{M\gamma kT\epsilon}{\hbar^2}(\beta_1 - \beta_2)^2\Big\} \\ & \times \tilde{\rho}(x - \beta_1, y - \beta_2, t)\,,\end{aligned} \tag{5.5}$$

where $x - x' \equiv \beta_1$ and $y - y' \equiv \beta_2$. Now we can evaluate (5.5) in the limit $\epsilon \to 0$. First of all we must notice that the integral in (5.5) contains two very fast oscillating terms with exponents proportional to ϵ^{-1}. It is clear the main contribution comes from β_1 and β_2 very small, otherwise the factor $\exp(\mathrm{i}M/2\epsilon\hbar)(\beta_1^2 - \beta_2^2)$ would oscillate wildly giving no finite contribution to (5.5). To be more specific, we want

$$\beta_1 \approx \beta_2 \approx \left(\frac{\epsilon\hbar}{M}\right)^{1/2}, \tag{5.6}$$

because in this region the phase of both exponentials will change by an amount of order 1. One might wonder at this point about the contribution of the region $\beta_1 \approx \beta_2 \approx \beta$ with finite β. In this case the phase of the two exponentials combined would change by an amount of order 1 when

$$\Delta\beta \equiv \beta_1 - \beta_2 \approx \frac{\epsilon\hbar}{M\beta}. \tag{5.7}$$

Now, if we define new variables $\beta_1' \equiv \beta_1 - \gamma(x - y)\epsilon$ and $\beta_2' \equiv \beta_2 + \gamma(x - y)\epsilon$ and expand the exponentials of (5.5) in ϵ we can easily show that in the limit $\epsilon \to 0$ all terms depending on $\Delta\beta$ in the integrand will be $\mathcal{O}(\epsilon^2)$. This means that we can safely forget the region $\beta_1 \approx \beta_2 \approx \beta$.

The procedure now is simple. Let us expand $\rho(x - \beta_1, y - \beta_2, t)$ for $\beta_1 \approx \beta_2 \approx 0$

and keep all terms $\mathcal{O}(\epsilon)$ in the product. In terms of β_1' and β_2' it reads

$$\tilde{\rho}(x,y,t) = \iint \frac{d\beta_1' \, d\beta_2'}{A^2} \exp \frac{iM\beta_1'^2}{2\epsilon\hbar} \exp -\frac{iM\beta_2'^2}{2\epsilon\hbar} \left[\tilde{\rho}(x,y,t) - \frac{\partial\tilde{\rho}}{\partial x}\beta_1' - \frac{\partial\tilde{\rho}}{\partial y}\beta_2' \right.$$
$$- \frac{\partial\tilde{\rho}}{\partial x}\gamma(x-y)\epsilon + \frac{\partial\tilde{\rho}}{\partial y}\gamma(x-y)\epsilon + \tfrac{1}{2}\frac{\partial^2\tilde{\rho}}{\partial x^2}\beta_1'^2 + \frac{\partial^2\tilde{\rho}}{\partial x\partial y}\beta_1'\beta_2'$$
$$\left. + \tfrac{1}{2}\frac{\partial^2\tilde{\rho}}{\partial y^2}\beta_2'^2 - \frac{i\epsilon}{\hbar}v_R(x)\tilde{\rho} + \frac{i\epsilon}{\hbar}v_R(y)\tilde{\rho} - \frac{2M\gamma kT\epsilon}{\hbar}(x-y)^2\tilde{\rho} \right]. \quad (5.8)$$

All the integrals appearing in (5.8) are of the Fresnel type and can be evaluated from $-\infty$ to $+\infty$ since we know their main contribution will come from a tiny region about $\beta_1' = \beta_2' = 0$. Expanding the left-hand side of (5.8) up to terms $\mathcal{O}(\epsilon)$ and equating them to the corresponding ones on the right-hand side one concludes the following:

a) The zeroth order term in ϵ gives us the normalization constant

$$A^2 = \frac{2\pi\epsilon\hbar}{M}; \quad (5.9)$$

b) The first order term in ϵ gives us the desired equation of motion for $\tilde{\rho}$ in the semiclassical region,

$$\frac{\partial\tilde{\rho}}{\partial t} = -\frac{\hbar}{2Mi}\frac{\partial^2\tilde{\rho}}{\partial x^2} + \frac{\hbar}{2Mi}\frac{\partial^2\tilde{\rho}}{\partial y^2} - \gamma(x-y)\frac{\partial\tilde{\rho}}{\partial x} + \gamma(x-y)\frac{\partial\tilde{\rho}}{\partial y} + \frac{v_R(x)}{i\hbar}\tilde{\rho}$$
$$- \frac{v_R(y)}{i\hbar}\tilde{\rho} - \frac{2M\gamma kT}{\hbar^2}(x-y)^2\tilde{\rho}. \quad (5.10)$$

Once again, we wish to emphasize that (5.10) is not the most general equation for $\tilde{\rho}$. It is valid only when we have $2kT \gtrsim \hbar\Omega \gg \hbar\omega_R$. If we were interested in obtaining something more general we would not have been allowed to write (5.1) instead of (3.38) and the last term of (5.10) would involve a time integration (it would depend on the past history of the system).

The form (5.10) is not the most suitable one if we wish to compare it to previously developed master equations. We would rather write it as an operator equation independent of representation. This can be done with the help of some identities such as

$$\langle x \,|\, y \rangle = \delta(x-y), \quad \langle x|v(x')|y\rangle = v(y)\delta(x-y)$$
and (5.11)
$$\langle x|p|y\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-y).$$

Employing them one can check that (5.10) is the coordinate representation of the

operator equation

$$\frac{\partial\tilde{\rho}}{\partial t}=\frac{1}{\mathrm{i}\hbar}[H_{\mathrm{R}},\tilde{\rho}]+\frac{\gamma}{2\mathrm{i}\hbar}[\{p,x\},\tilde{\rho}]-\frac{1}{\hbar^2}D[x,[x,\tilde{\rho}]]+\frac{\Delta}{\hbar^2}([x,\tilde{\rho}p]-[p,\tilde{\rho}x]), \tag{5.12}$$

where H_{R} is the renormalized Hamiltonian of the system alone, $D=\eta kT$, $\Delta=-\mathrm{i}\hbar\gamma$ and $[,]$ stands for the commutators while $\{,\}$ for the anti-commutators.

Eq. (5.12) was deduced by Dekker[7]) by a completely different method. Actually his equation contains two additional diffusive terms (besides D) which he shows to vanish under certain conditions. Moreover those extra terms are due to the inclusion of noise sources in the equation of motion of the position as we mentioned in the introduction. Another difference is that Dekker's equation is valid for zero temperature with D given by some finite value while ours is valid only when T is high and $D=\eta kT$.

At the beginning of this section we have pointed out that once we had the master equation for $\tilde{\rho}$, another step would be necessary to compare it to the equation for the classical distribution in phase space. As we have said before what we need now is the Wigner distribution (or, the Wigner transform of $\tilde{\rho}$) defined by

$$w(x,p,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\left(\frac{\mathrm{i}py}{\hbar}\right)\left\langle x-\frac{y}{2}\right|\tilde{\rho}\left|x+\frac{y}{2}\right\rangle \mathrm{d}y\,. \tag{5.13}$$

In spite of presenting a purely quantal description of a system the Wigner distribution becomes very important when we are interested in the semiclassical region. This is because Wigner's theory is described directly in the classical phase space of the system. When $\hbar\to 0$, $w(x,p,t)$ tends to the classical distribution in phase space. For discussions on the validity of this assertion we refer the reader back to refs. 3 and 30.

If we take the Wigner transform of equation (5.12) and employ the identities (5.11) we shall find (see[7]) for details)

$$\frac{\partial w}{\partial t}=-\frac{\partial}{\partial x}pw+\frac{\partial}{\partial p}v_{\mathrm{R}}'w+2\gamma\frac{\partial}{\partial p}pw+D\frac{\partial^2 w}{\partial p^2}, \tag{5.14}$$

which is the well-known Fokker–Planck equation describing the time development of the Wigner transform of the reduced density operator of the system. This is a purely quantum mechanical equation. However, in order to be consistent with the fact that we are considering $D=\eta kT$ we need to take the limit $\hbar\to 0$ in the expression for w. As we said before, $w(p,x,t)$ tends to the classical phase space distribution in this limit. Then we conclude that (5.14) describes the time development of the phase space distribution of a classical Brownian particle when $\hbar\to 0$.

We also realize that the third term on the right-hand side of (5.14) is a direct consequence of the existence of the γ dependent term in the imaginary part of the exponent in (3.38). Therefore, the latter is responsible for the appearance of a force of the form $\eta\dot{x}$ in the classical equation of motion for the Brownian particle.

What we have achieved so far is that our quantum-mechanical expression (3.38) for the propagator J is in total accordance with the equations believed to describe the classical motion of a Brownian particle. It also means that the choice made for $\rho_D(\omega)\ C^2(\omega)$ in (3.23) is a very suitable one, allowing us to describe J solely in terms of the phenomenological damping constant η.

6. Some applications

In this section we shall study the behaviour of $\tilde{\rho}(x, y, t)$ for some specific examples, namely the damped simple harmonic oscillator and its special case, a damped free particle. We shall now drop the restriction of high temperatures because we are interested in the extreme quantum limit ($T \to 0$) as well. However, before starting it we would like to point out that the model presented in this paper is compatible with several kinds of motion. For example, suppose we start off from a harmonic potential $v(x) = \frac{1}{2}M\omega^2 x^2$. One can easily show that both underdamped and overdamped motions can be described by a proper choice of the microscopic parameters of the theory. This is valid for coordinate coupling as well as for velocity coupling. The difference between these two cases is that in the former one, it is the renormalized frequency ω_R given by $\omega_R^2 \equiv \omega^2 - (\Delta\omega)^2$ which is the frequency to be compared to γ, while in the latter this ω_R is such that $\omega_R = \omega$. For details we refer the reader to[31]).

Now, we shall proceed to evaluate (3.38) for the harmonic oscillator and the free patrticle ($\omega_R = 0$). To begin with let us rewrite (3.38) as

$$J(x_f, y_f, t; x_i, y_i, 0) = \int\int \mathrm{D}x\ \mathrm{D}y \exp\frac{\mathrm{i}}{\hbar}\tilde{S}[x, y] \exp -\frac{1}{\hbar}\phi[x, y], \tag{6.1}$$

where

$$\tilde{S}[x, y] = \int_0^t L(x, \dot{x}, y, \dot{y})\,\mathrm{d}\tau - \int_0^t M\gamma x\dot{x}\,\mathrm{d}\tau + \int_0^t M\gamma y\dot{y}\,\mathrm{d}\tau, \tag{6.2}$$

$$L = \tfrac{1}{2}M\dot{x}^2 - \tfrac{1}{2}M\dot{y}^2 - \tfrac{1}{2}M\omega_R^2 x^2 + \tfrac{1}{2}M\omega_R^2 y^2 - M\gamma x\dot{y} + M\gamma y\dot{x} \tag{6.3}$$

and

$$\phi[x, y] = \frac{2M\gamma}{\pi}\int_0^\Omega v \coth\frac{\hbar v}{2kT}\int_0^t\int_0^\tau [x(\tau) - y(\tau)] \times \cos v(\tau - s)[x(s) - y(s)]\,\mathrm{d}s\,\mathrm{d}\tau\,\mathrm{d}v. \tag{6.4}$$

The procedure to evaluate (6.1) is simple. We shall expand the whole integrand about the two-dimensional path which makes $\tilde{S}[x, y]$ an extremum. This path is found by

$$\frac{\delta \tilde{S}}{\delta x} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = M\ddot{x} + M\gamma\dot{y} + M\omega_{\mathrm{R}}^2 x = 0\,, \tag{6.5}$$

$$\frac{\delta \tilde{S}}{\delta y} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{y}} - \frac{\partial L}{\partial y} = M\ddot{y} + M\gamma\dot{x} + M\omega_{\mathrm{R}}^2 y = 0\,, \tag{6.6}$$

because the last two terms in (6.2) involve just end point variations. It is suitable to introduce new variables in order to solve (6.5) and (6.6). Then we define

$$X(\tau) = x(\tau) + y(\tau) \quad \text{and} \quad \xi(\tau) = x(\tau) - y(\tau) \tag{6.7}$$

and our equations become

$$\ddot{X} + 2\gamma\dot{X} + \omega_{\mathrm{R}}^2 X = 0\,, \tag{6.8}$$

$$\ddot{\xi} - 2\gamma\dot{\xi} + \omega_{\mathrm{R}}^2 \xi = 0\,. \tag{6.9}$$

When $X(t) = X_{\mathrm{f}}$, $\xi(t) = \xi_{\mathrm{f}}$, $X(0) = X_{\mathrm{i}}$ and $\xi(0) = \xi_{\mathrm{i}}$, their solutions are:

$$\tilde{X}(\tau) = (\sin \omega t)^{-1}\{X_{\mathrm{f}} \mathrm{e}^{\gamma t} \sin \omega\tau + X_{\mathrm{i}} \sin \omega(t-\tau)\}\, \mathrm{e}^{-\gamma\tau}\,, \tag{6.10}$$

$$\tilde{\xi}(\tau) = (\sin \omega t)^{-1}\{\xi_{\mathrm{f}} \mathrm{e}^{-\gamma t} \sin \omega\tau + \xi_{\mathrm{i}} \sin \omega(t-\tau)\}\, \mathrm{e}^{\gamma\tau}\,, \tag{6.11}$$

for the underdamped harmonic oscillator (UDHO from now on) with $\omega^2 \equiv \omega_{\mathrm{R}}^2 - \gamma^2$. For the overdamped case (ODHO) the solutions are obtained by substituting ω by $\mathrm{i}\tilde{\omega}$ in (6.10) and (6.11) where $\tilde{\omega}^2 \equiv \gamma^2 - \omega_{\mathrm{R}}^2$, while for the free particle (FP) the substitution is of ω by $\mathrm{i}\gamma$. Actually, these substitutions will be always valid for our subsequent expressions, however we warn the reader that in some of them (FP ones) the limit $\omega_{\mathrm{R}} \to 0$ must be taken carefully wherever it is necessary. Bearing this in mind we shall write the formulae in this section only for the UDHO.

The action $\tilde{S}[X, \xi]$ calculated along those paths (6.10–6.11) is found to be expressible as

$$\tilde{S}_{\mathrm{cl}} = K(t)[X_{\mathrm{f}}\xi_{\mathrm{f}} + X_{\mathrm{i}}\xi_{\mathrm{i}}] - L(t)X_{\mathrm{i}}\xi_{\mathrm{f}} - N(t)X_{\mathrm{f}}\xi_{\mathrm{i}} - \frac{M\gamma}{2}[X_{\mathrm{f}}\xi_{\mathrm{f}} - X_{\mathrm{i}}\xi_{\mathrm{i}}]\,, \tag{6.12}$$

where

$$K(t) = \frac{M\omega}{2}\cot \omega t, \quad L(t) = \frac{M\omega\, \mathrm{e}^{-\gamma t}}{2\sin \omega t} \quad \text{and} \quad N(t) = \frac{M\omega\, \mathrm{e}^{\gamma t}}{2\sin \omega t}\,. \tag{6.13}$$

Now, let us write our functional integral in terms of the translated paths

$$\xi'(\tau) = \xi(\tau) - \tilde{\xi}(\tau) \quad \text{and} \quad X'(\tau) = X(\tau) - \tilde{X}(\tau)\,, \tag{6.14}$$

with $\xi'(0) = \xi'(t) = 0$ and $X'(0) = X'(t) = 0$. Then one gets

$$J(X_\mathrm{i}, \xi_\mathrm{f}, t; X_\mathrm{i}, \xi_\mathrm{i}, 0) = \exp\frac{\mathrm{i}}{\hbar}\tilde{S}_\mathrm{cl}\exp-\frac{1}{\hbar}\{A(t)\,\xi_\mathrm{f}^2 + B(t)\xi_\mathrm{f}\xi_\mathrm{i} + C(t)\xi_i^2\}$$
$$\times\, G(X_\mathrm{f}, \xi_\mathrm{f}, t; X_\mathrm{i}, \xi_\mathrm{i}, 0)\,, \tag{6.15}$$

where

$$A(t) = \frac{M\gamma}{\pi}\int_0^\Omega \mathrm{d}\nu\nu\,\coth\frac{\hbar\nu}{2kT}A_\nu(t)\,, \tag{6.16}$$

$$A_\nu(t) = \frac{\mathrm{e}^{-2\gamma t}}{\sin^2\omega t}\int_0^t\int_0^t \sin\omega\tau\,\cos\nu(\tau - s)\sin\omega s\,\mathrm{e}^{\gamma(\tau+s)}\,\mathrm{d}\tau\,\mathrm{d}s\,, \tag{6.17}$$

$$B(t) = \frac{M\gamma}{\pi}\int_0^\Omega \mathrm{d}\nu\nu\,\coth\frac{\hbar\nu}{2kT}B_\nu(t)\,, \tag{6.18}$$

$$B_\nu(t) = \frac{2\mathrm{e}^{-\gamma t}}{\sin^2\omega t}\int_0^t\int_0^t \sin\omega\tau\,\cos\nu(\tau - s)\sin\omega(t-s)\,\mathrm{e}^{\gamma(\tau+s)}\,\mathrm{d}\tau\,\mathrm{d}s\,, \tag{6.19}$$

$$C(t) = \frac{M\gamma}{\pi}\int_0^\Omega \mathrm{d}\nu\nu\,\coth\frac{\hbar\nu}{2kT}C_\nu(t)\,, \tag{6.20}$$

$$C_\nu(t) = \frac{1}{\sin^2\omega t}\int_0^t\int_0^t \sin\omega(t-\tau)\,\cos\nu(\tau - s)\sin\omega(t-s)\,\mathrm{e}^{\gamma(\tau+s)}\,\mathrm{d}\tau\,\mathrm{d}s\,, \tag{6.21}$$

$$G(X_\mathrm{f}, \xi_\mathrm{f}, t; X_\mathrm{i}, \xi_\mathrm{i}, 0) = \int\!\!\int\frac{\mathrm{D}\xi'\,\mathrm{D}X'}{2}\exp\frac{\mathrm{i}}{\hbar}\tilde{S}[X', \xi']\exp-\frac{2}{\hbar}\phi_T[\xi', \xi']$$
$$\times\exp\frac{1}{\hbar}\phi_T[\tilde{\xi}, \xi'] \tag{6.22}$$

and

$$\phi_T[\tilde{\xi}, \xi'] = \frac{M\gamma}{\pi}\int_0^\Omega \mathrm{d}\nu\nu\,\coth\frac{\hbar\nu}{2kT}\int_0^t\int_0^t \tilde{\xi}(\tau)\cos\nu(\tau - s)\xi'(s)\,\mathrm{d}\tau\,\mathrm{d}s\,. \tag{6.23}$$

What is left to evaluate now is the functional integral (6.22). As both $\xi'(\tau)$ and $X'(\tau)$ vanish at $\tau = 0$ and $\tau = t$, we can expand them in terms of an orthogonal

set obeying the same boundary conditions[22]),

$$X'(\tau) = \sum_n X_n \sin \omega_n \tau \quad \text{and} \quad \xi'(\tau) = \sum_m \xi_m \sin \omega_m \tau \,, \tag{6.24}$$

where $\omega_n = n\pi/t$. Now, inserting (6.24) in (6.22) one gets after some straightforward integrations (see[22]) for similar procedure)

$$G(X_f, \xi_f, t; X_i, \xi_i, 0) = F^2(t) = \lim_{N\to\infty} \frac{4\tilde{C}}{Mt} (2\pi\hbar)^N \prod_{i=1}^{N} \frac{1}{\omega_i^2 - \omega_R^2} \,, \tag{6.25}$$

where $\tilde{C}$ is the normalization constant. This result is exactly the square of the wave function amplitude for the undamped case. So, it means that the damping modifies just the exponent of $J(X_f, \xi_f, t; X_i, \xi_i, 0)$ and its final form is

$$J = F^2(t) \exp \frac{i}{\hbar} \left\{ \left[K(t) - \frac{M\gamma}{2} \right] X_f \xi_f + \left[K(t) + \frac{M\gamma}{2} \right] X_i \xi_i \right.$$
$$\left. - L(t) X_i \xi_f - N(t) X_f \xi_i \right\} \exp - \frac{1}{\hbar} \left\{ A(t) \xi_f^2 + B(t) \xi_f \xi_i + C(t) \xi_i^2 \right\} . \tag{6.26}$$

Now we have the tool we need to calculate the time development of the reduced density operator of the system in which we are interested. For example, suppose we initially have the system in a pure state described by a wave packet centered at the origin with initial momentum p and width σ. The reduced density operator is then

$$\tilde{\rho}(X_i, \xi_i, 0) = (2\pi\sigma^2)^{-1/2} \exp \frac{ip\xi_i}{\hbar} \exp - \frac{X_i^2 + \xi_i^2}{8\sigma^2} \tag{6.27}$$

and its time evolution reads

$$\tilde{\rho}(X_f, \xi_f, t) = \iint dX_i \, d\xi_i J(X_f, \xi_f, t; X_i, \xi_i, 0) \tilde{\rho}(X_i, \xi_i, 0) \,, \tag{6.28}$$

which can be evaluated with the insertion of (6.27) and (6.26). All the integrations in (6.28) are Gaussians and very simple. However, despite the simplicity the resulting expressions in the intermediate steps are quite lengthy, forcing us to quote only the final result

$$\tilde{\rho}(X_f, \xi_f, t) = F^2(t) \left[\frac{\pi^2\hbar^2}{2\sigma^2 K_1 + \hbar C_1} \right] \exp - \frac{N^2}{2\sigma^2 K_1^2 + 4\hbar C_1^2} \left(X_f - \frac{p}{2N} \right)^2$$
$$\times \exp - \left[\frac{A}{\hbar} + \frac{2\sigma^2 L^2}{\hbar^2} - \frac{(4\sigma^2 K_1 L - B\hbar)^2}{\hbar^2 (8\sigma^2 K_1^2 + 4\hbar C_1)} \right] \xi_f^2$$
$$\times \exp \frac{1}{\hbar} \left[K_2 X_f \xi_f - \frac{(4\sigma^2 K_1 L - B\hbar) N}{(4\sigma^2 K_1^2 + 2\hbar C_1)} \left(X_f - \frac{p}{N} \right) \xi_f \right] , \tag{6.29}$$

where we must remember that A, B, C_1, K_1, K_2, L and N are all functions of time and have defined

$$C_1(t) \equiv C(t) + \frac{\hbar}{8\sigma^2}, \quad K_1(t) \equiv K(t) + \frac{M\gamma}{2} \quad \text{and} \quad K_2(t) \equiv K(t) - \frac{M\gamma}{2}. \tag{6.30}$$

Of particular interest is the expression we can get from (6.29) by making $\xi_f = x_f - y_f = 0$ or $X_f = x_f + y_f = 2x_f$, that is

$$\tilde{\rho}(x_f, x_f, t) = F^2(t)\left[\frac{\pi^2\hbar^2}{2\sigma^2K_1^2 + \hbar C_1}\right]^{1/2} \exp - \frac{N^2}{2\sigma^2K_1^2 + \hbar C_1}\left(x_f - \frac{p}{2N}\right)^2. \tag{6.31}$$

This shows how the initial $|\psi(x)|^2$ develops in time. Its centre follows the path given by

$$x_0(t) = \frac{p}{2N(t)}, \tag{6.32}$$

which is the one of a classical damped particle, for example, for the UDHO it reads

$$x_0(t) = \frac{p}{M\omega} \sin \omega t \, e^{-\gamma t} \tag{6.33}$$

while its width obeys the equation

$$\sigma^2(t) = \tfrac{1}{2}\left(\frac{2\sigma^2K_1^2(t) + \hbar C_1(t)}{N^2(t)}\right). \tag{6.34}$$

This expression gives us the width of $\rho(x, x, t)$ at any time t. An interesting result is obtained when we study it at infinite times. The procedure is straightforward but extremely tedious. Inserting (6.13), (6.20), (6.21) and (6.30) into (6.34) one gets

$$\sigma^2(t \to \infty) = \langle (x - x_0(\infty))^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\nu \coth \frac{\hbar\nu}{2kT} \left(\frac{1}{M} \frac{2\gamma\nu}{(\omega_R^2 - \nu^2)^2 + 4\gamma^2\nu^2}\right), \tag{6.35}$$

where we took the limit $\Omega \to \infty$ at the upper limit of integration. Expression (6.35) is a very familiar one. The imaginary part of the response of a harmonic oscillator of frequency ω_R to an external force $F(t)$ is given by

$$\chi''(\nu) = \frac{1}{M} \frac{2\gamma\nu}{(\nu^2 - \omega_R^2)^2 + 4\gamma^2\nu^2} \tag{6.36}$$

Thus,

$$\sigma^2(\infty) = \frac{\hbar}{\pi} \int_0^\infty d\nu \coth \frac{\hbar\nu}{2kT} \chi''(\nu), \tag{6.37}$$

which is the well-known fluctuation–dissipation theorem[32].

7. Conclusions

Using a specific model for a particle interacting with a reservoir we have deduced the expression (3.38) for the propagator of the reduced density operator of that particle. Under certain circumstances we could get a closed expression for $\tilde{\rho}(x, y, t)$ at any instant t and for all temperatures as we have shown in the previous section. The centre of the packet $\tilde{\rho}(x, x, t)$ follows the motion of a classical Brownian particle (see (6.33)) and its width in the infinite time limit is shown to agree with the fluctuation–dissipation theorem (6.35). The latter result can be exploited a bit further.

To start with, (6.35) disagrees with ref. 27. There the authors claim that the width of the wave packet of a free particle "freezes" at infinite time. If we make $\omega_R \to 0$ in (6.35) we can show that when $T \to 0$, (6.35) diverges as $(-\ln v)$ as $v \to 0$. This is equivalent to say that $\sigma^2(t)$ behaves as $\ln t$ when $t \to \infty$. Consequently, $\sigma^2(t)$ spreads slower than it does in the undamped case ($\sigma^2(t) = \sqrt{A + Bt^2}$), however it does not freeze.

We attribute this difference between our approaches to the fact that, unlike us, the authors of[27]) do not take any sort of diffusive effects into account. By making $\phi[x, y] = 0$ in (6.1) we reproduce their results, despite the completely different physical interpretation of the two approaches.

Diffusion terms were also omitted from other attempts to quantize Brownian Motion starting from the Morse and Feshbach Lagrangian (see, for example, refs. 33 and 34 or sections 3 and 6 of ref. 35).

Our second comparison comes out when we study the extremely underdamped limit ($\gamma \to 0$). When this happens the final width at $t \to \infty$ can be worked out at any temperature as

$$\sigma^2(\infty) = \frac{\hbar}{2M\omega_R} \coth \frac{\hbar\omega_R}{2kT}, \tag{7.1}$$

which is the well-known result of equilibrium quantum statistical mechanics[22]). The same expression should be obtained if instead of working with the exact propagator J given by (3.38) we had worked with the one in (5.1) but with $2MkT\gamma$ replaced by $\hbar M\gamma\omega_R \coth(\hbar\omega_R/2kT)$. In other words, we should have a diffusion constant (in momentum space) given by

$$D = M\gamma\omega_R \hbar \coth \frac{\hbar\omega_R}{2kT}, \tag{7.2}$$

valid at all temperatures. When $T \to \infty$, (7.2) gives us the classical relation $D = 2M\gamma kT$, while when $T \to 0$ the diffusion constant becomes

$$D = M\gamma\hbar\omega_R = \tfrac{1}{2}\eta\hbar\omega_R, \tag{7.3}$$

which is the result found by Dekker[7]).

As we have pointed out in the introduction, Dekker applied canonical quantization to complex variables making use of explicit noise sources in the equations of motion of the position and momentum operators (however, see ref. 36 for an alternative derivation of expression (7.3)). It is true there are microscopic models which allow one to do so, nevertheless it can be shown[37]) that these equations have the same solutions as the usual ones (with noise sources only in the momentum equation) in the limit of very weak damping.

The trick proposed in (7.2) does not seem to be correct for finite γ. It means that the kernel $\alpha_R(t-t')$ appearing in the exponent of the influence functional in (3.9) can always be replaced by a function of the temperature times a delta function of $(t-t')$. However, this is not true for our specific model. Even if one can find a different model for the reservoir for which (7.2) is correct for any γ, our model serves as a counter-example to show that the procedure is not general.

A diffusion constant of the form (7.2) was proposed by Papadopoulos[28]) and Svin'in[38]). But, once again, their theories are valid only in the weak damping limit because this is a necessary condition for the validity of that expression.

Actually, it has been an old dream of many physicists to try to describe the relaxation to equilibrium by Markoffian equations (no time kernels involved) even in the quantum regime. However, we are a bit sceptical about the possibility of this, since as we have shown simple models can recover both equilibrium statistical mechanics and linear response theory asymptotically without being Markoffian at all. Ford et al.[16]) also achieved the same conclusion about the Markoffian assumption in the quantum limit. Notice that we are talking here only about the diffusion terms. Our drift term (the one involving γ) is always Markoffian. In order to find non-Markoffian corrections to the latter one needs to study the modifications of $\chi''(\nu)$ due to the sum rules which are important to describe the short time behaviour of the Brownian particle.

Finally, we should emphasize that although we have taken a model for the system-environment coupling that at first sight looks very arbitrary, the main features of our results should be fairly insensitive to its details. In particular, modification of the choice (3.23) for the quantity $\rho_D(\omega)C^2(\omega)$ should make little qualitative difference to the results provided only that the form (3.23) continues to hold for ω of the order of the characteristic frequencies of the system; all it will really affect is the frequency shift $(\Delta\omega)^2$, which is in any case not directly observable (cf. the discussion of the analogous point in the tunnelling problem in[21]).

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