Brownian motion of a quantum particle

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Proposed here is an exactly soluble model for the field-free motion of a quantum particle interacting with a heat bath. The heat-bath interaction includes a fluctuating random force and a frictional force of Langevin type. The momentum and position distributions obtained in the model have a close relation to the corresponding solutions of the Fokker-Planck equation of a free classical particle.

The study of the motion of a quantum particle in interaction with a randomly fluctuating medium is of importance in several different contexts and has received much attention in the past.[1-5] For a particle moving in a lattice according to a single-band tight-binding Hamiltonian, whose parameters have the Gaussian, δ-correlated randomness in time, the problem has been analyzed exactly and the solution exhibits a diffusive behavior for the mean-square displacement $\langle x^2(t)\rangle$ in the long-time limit.[6,7] However, for the corresponding problem in continuum, $\langle x^2(t)\rangle$ instead of being diffusive grows like t^3, if the effect of the medium is taken into account by introducing a time-dependent, random, Gaussian δ-correlated potential in the Schrödinger equation.[8] As is well known, the classical diffusive behavior arises only on introduction of a Langevin-type frictional term in the equation of motion. The introduction of friction in quantum mechanics has been done in a number of ways. The principle approach has been to develop operator versions of the Langevin equation with analogs of fluctuation-dissipation relations (see Refs. 1 to 5 for further references to the extensive literature). The quantum Langevin equation (QLE) approach has been questioned by Benguria and Kac,[4] who point out that most of the derivations fall short of being rigorous. More bascially, there is a question regarding the approach towards quantum canonical distribution which has not been resolved satisfactorily. Taking QLE as the starting point, much work has been devoted to deriving and solving the corresponding Schrödinger representations.[2,9] Early on this led to the introduction of a time-dependent Hamiltonian, and its early treatments encountered serious difficulties which have only recently been resolved.[2,10] Kostin introduced a nonlinear wave equation representation[11] for QLE which is satisfactory in many ways, but suffers from the conceptual disadvantage that the superposition principle for the wave function is lost. Many other attempts, reviewed by Messer,[2] employ Heisenberg representation directly in various ways. In short, the results in different approaches differ more or less, and as such there is no unique treatment for QLE. A somewhat different approach is due to Agarwal,[12] who uses quantum-classical mapping to derive equations for the phase-space distribution functions, which are close parallels of Fokker-Planck equations.

Our purpose here is to introduce quantum friction in a direct way into a time evolution equation for the quantum-mechanical density matrix. Since our method avoids the use of QLE and utilizes a conceptually simple picture of the role of the heat bath, we believe it affords a fresh perspective on the problem. We also use some stochastic assumptions which amount to putting in the principle of detailed balance.[13] Since the method is applicable in any dimension, in the following we describe it for one dimension. The random interactions due to the heat bath are visualized as a series of momentum impulses of fixed magnitude, δp, and variable sign, occurring in time according to a Poisson sequence.[14] This implies that the probability of an impulse occuring between time t and $t+dt$ is $\lambda\, dt$, and the probability $p(t_1,t_2)$ that no impulse occurs between times t_1 and t_2 is $\exp[-\lambda(t_2-t_1)]$. The action of impulses on the wave function is described in terms of unitary impulse operators $I_\pm$ such that

$$I_\pm|p) = |p \pm \delta p) \quad , \tag{1}$$

where $|p)$ and $|p+\delta p)$ are normalized momentum eigenstates. Clearly, $(I_+)^\dagger = I_-$. A given impulse is positive or negative with probabilities w_+ and w_-, respectively, which we allow to depend upon the momentum state of the particle, in order to simulate a systematic force due to the heat bath. The parameters λ, δp, w_+, and w_- are arbitrary at the moment, but a limiting procedure carried out below enables us to replace these by conventional heat-bath parameters such as temperature and diffusion coefficient. The impulses of a given sequence are independent of each other, and we would like to average the density matrix operator over all possible impulse sequences in a given interval of time.[14]

In the absence of the medium, the density matrix operator $\rho(t) = |\psi(t))(\psi(t)|$ obeys the equation

$$\rho(t) = \exp\left(-\frac{i}{\hbar}H^\times t\right)\rho(0) \quad , \tag{2}$$

where $H^\times$ is the Liouville operator[14] associated with H, which is the free-particle Hamiltonian. When the effects of the heat bath are considered, we have to include the possibilities that the quantum evolution is interrupted by $0,1,2,\ldots,\infty$ force pulses with appropriate probabilistic weights. Thus

$$\begin{aligned}\rho(t) &= \Big(e^{-\lambda t}e^{-(i/\hbar)H^\times t} + \int_0^t dt_1 e^{-\lambda(t-t_1)}e^{-(i/\hbar)H^\times(t-t_1)}\lambda I \otimes e^{-i\lambda t_1}e^{-(i/\hbar)H^\times t_1} \\ &\quad + \int_0^t dt_2\int_0^{t_2} dt_1 e^{-(\lambda+iH^\times/\hbar)(t-t_2)}\lambda I \otimes e^{-(\lambda+iH^\times/\hbar)(t_2-t_1)}\lambda I \otimes e^{-(\lambda+iH^\times/\hbar)t_1} + \cdots\Big)\rho(0) \\ &= \sum_n Q_n(t,0)\rho(0) \quad ,\end{aligned} \tag{3}$$

where

$$Q_n(t,0)=\int_0^t dt_n\int_0^{t_n} dt_{n-1}\cdots\int_0^{t_2} dt_1 e^{-(\lambda+iH^\times/\hbar)(t-t_n)}\lambda I^\otimes e^{-(\lambda+iH^\times/\hbar)(t_n-t_{n-1})}\lambda I^\otimes\cdots\lambda I^\otimes e^{-(\lambda+iH^\times/\hbar)t_1} \quad . \tag{4}$$

Here $I^\otimes$ is the Liouville operator such that $I^\otimes\rho=I\rho I^\dagger$, and I is one of the operators defined in Eq. (1). Since the various impulses are independent, we can preform a further averaging and replace $I^\otimes$ by $\bar{I}^\otimes=w_+I_+^\otimes+w_-I_-^\otimes$ in Eqs. (3) and (4). Comparing these equations with standard perturbation expansion, one can equivalently write Eq. (3) as

$$\frac{\partial\bar{\rho}(t)}{\partial t}=\left(-\frac{iH^\times}{\hbar}+\lambda(\bar{I}^\otimes-1)\right)\bar{\rho}(t) \quad . \tag{5}$$

In momentum-space representaton, Eq. (5) can be written as

$$\frac{\partial}{\partial t}\bar{\rho}(p,q,t)=-\frac{i}{2m\hbar}(p^2-q^2)\bar{\rho}(p,q,t)+\lambda[\,w_-(p+\delta p,q+\delta p)\bar{\rho}(p+\delta p,q+\delta p,t)$$
$$+w_+(p-\delta p,q-\delta p)\bar{\rho}(p-\delta p,q-\delta p,t)-\bar{\rho}(p,q,t)] \quad , \tag{6}$$

where we have made use of Eq. (1) and let w's depend upon the momenta associated with the density matrix at the moment of impulse. We now take δp to be small and make a Taylor expansion to second order. Terms in the square bracket of Eq. (6) yield

$$-\lambda\,\delta p\left(\frac{\partial}{\partial p}+\frac{\partial}{\partial q}\right)\{[w_+(p,q)-w_-(p,q)]\bar{\rho}(p,q,t)\}$$
$$+\frac{\lambda}{2}(\delta p)^2x\left(\frac{\partial}{\partial p}+\frac{\partial}{\partial q}\right)^2\bar{\rho}(p,q,t) \quad . \tag{7}$$

We now let $\lambda\to\infty$, $\delta p\to 0$ in such a way that $\lambda(\delta p)^2\to D$, where D has the usual interpretation of the momentum diffusion coefficient, and

$$\lambda(w_+-w_-)\delta p\to f(p,q)=-\gamma(p+q)/2 \quad , \tag{8}$$

where f is the systematic force for which we choose the form shown in Eq. (8). γ is the Langevin friction coefficient and in the case of thermal bath $\gamma=D/2mkT$. This particular form for force is chosen so that, for an initially pure momentum state, we obtain the Uhlenbeck-Orstein (UO) (Ref. 15) distribution for momentum. Equation (5) acquires the form

$$\frac{\partial}{\partial t}\bar{\rho}(p,q,t)=-\frac{i}{2m\hbar}(p^2-q^2)\bar{\rho}+\frac{\gamma}{2}\left(\frac{\partial}{\partial p}+\frac{\partial}{\partial q}\right)[(p+q)\bar{\rho}]$$
$$+\frac{D}{2}\left(\frac{\partial}{\partial p}+\frac{\partial}{\partial q}\right)^2\bar{\rho} \quad . \tag{9}$$

It can be easily verified that the procedures done between Eqs. (9) and (5) are such that the probability is conserved. Equation (9) can be solved exactly for arbitrary initial conditions. The convenient variables for solving the equation are $u=(p+q)/2$ and $v=(p-q)/2$, in terms of which Eq. (9) becomes

$$\frac{\partial}{\partial t}\bar{\rho}(u,v,t)=-\frac{2i}{m\hbar}uv\bar{\rho}+\gamma\frac{\partial}{\partial u}(u\bar{\rho})+\frac{D}{2}\frac{\partial^2}{\partial u^2}\bar{\rho} \quad . \tag{10}$$

Equation (10) can be reduced to an oscillatorlike equation with the help of the transformation

$$\rho(u,v,t)=\exp\left[-\frac{\gamma u^2}{2D}+\left(\frac{\gamma}{2}-\frac{2Dv^2}{(\gamma m\hbar)^2}\right)t\right]W(u,v,t) \quad . \tag{11}$$

With use of this fact it is simple to write the solution of Eq. (10). For the initial condition

$$\rho(u,v,0)=\delta(u-u_0)\delta(v-v_0) \quad , \tag{12}$$

the solution $G(u,v,t|u_0,v_0,0)$ of Eq. (10) is

$$G(u,v,t|u_0,v_0,0)=\left(\frac{\Gamma}{\pi}\right)^{1/2}\exp\left[-\frac{2Dv^2}{(\gamma m\hbar)^2}t+\frac{2iv(u-u_0)}{\gamma m\hbar}-\Gamma\left[u+\frac{2iDv}{\gamma^2m\hbar}(1-e^{-\gamma t})-u_0e^{-\gamma t}\right]^2\right]\delta(v-v_0) \quad , \tag{13}$$

where we have set $\Gamma=\gamma/D(1-e^{-2\gamma t})$. The physical significance of the solution comes forth nicely, if we study the evolution of a Gaussian wave packet given by

$$\psi(x,0)=(\pi^{1/4}\sigma^{1/2})^{-1}\exp[i\bar{p}x/\hbar-x^2/2\sigma^2] \quad . \tag{14}$$

With use of the equation

$$\bar{\rho}(u,v,t)=\int\int G(u,v,t|u_0,v_0,0)\rho(u_0,v_0,0)\,du_0dv_0 \tag{15}$$

it is seen that, for the wave packet of Eq. (14), one has

$$\bar{\rho}(u,v,t))=\left(\frac{\Gamma_1}{\pi}\right)^{1/2}\exp\left[-\left(\sigma^2+\frac{2Dt}{(\gamma m)^2}\right)\frac{v^2}{\hbar^2}+\frac{2iuv}{\gamma m\hbar}-\frac{\sigma^2\bar{p}^2}{\hbar^2}-\Gamma r^2+\eta\Gamma_1(1-e^{-2\gamma t})\left(\frac{iv}{\gamma mh}-\frac{\sigma^2\bar{p}}{\hbar^2}-\Gamma e^{-\gamma t}r\right)^2\right] \quad , \tag{16}$$

where $\eta=\hbar^2\gamma/\sigma^2 D$ is a dimensionless parameter,

$$r=u+(2iDv/\gamma^2 m\hbar)(1-e^{-\gamma t}) \ ,$$

and

$$\Gamma_1=(\gamma/D)[1+(\eta-1)e^{-2\gamma t}]^{-1} \ . \tag{17}$$

From Eq. (16), the probability densities for momentum and position can be derived. These are given as

$$|\psi(p,t)|^2=\bar{\rho}(u=p,v=0,t)$$
$$=\left(\frac{\Gamma_1}{\pi}\right)^{1/2}\exp[-\Gamma_1(p-\bar{p}e^{-\gamma t})^2] \tag{18}$$

and

$$|\psi(x,t)|^2=\int\int\bar{\rho}(u,v,t)e^{2ivx/\hbar}du\,dv/\hbar \tag{19}$$
$$=\left(\frac{\pi}{N(t)}\right)^{1/2}\exp\left[-\left[x-\frac{\bar{p}}{\gamma m}(1-e^{-\gamma t})\right]^2/N(t)\right] \ , \tag{20}$$

where

$$N(t)=\sigma^2+\frac{2kT}{m\gamma^2}[2\gamma t-3+4e^{-\gamma t}-e^{-2\gamma t}+\eta(1-e^{-\gamma t})^2] \ . \tag{21}$$

The following points about results contained in Eqs. (16) to (21) are worth indicating:

(i) As $t\rightarrow\infty$, Eq. (16) shows the off-diagonal elements of the density matrix in momentum space (i.e., $v\neq 0$) vanish.

(ii) The momentum distribution function (MDF) is like that obtained from the solution of the Fokker-Planck equation and, in fact, reduces to it exactly when parameter η is set to zero. For times of order $t>>\gamma^{-1}$, one obtains the Maxwell distribution.

(iii) The position distribution function (PDF) is Gaussian. At short times,

$$N(t)\approx\sigma^2+\frac{\hbar^2 t^2}{m^2\sigma^2} \ ,$$

which is what one gets from the Schrödinger equation. For large times,

$$N(t)\approx\sigma^2+\hbar^2/(m\gamma\sigma)^2+2kT(2\gamma t-3)/m\gamma^2 \ ,$$

the last term of which is the classical result (neglecting terms of order $e^{-\gamma t}$). Thus for $\gamma t>>1$, the solution reduces to the classical UO solution.[13] Considering the fact that the procedures employed for obtaining PDF in classical theory and our theory are very different,[16] this feature of the theory is indeed surprising.

(iv) Using the nonlinear Schrödinger equation, Messer[2] has derived results for MDF and PDF which can be compared with our results. For an initial Gaussian wave packet, Messer also finds that MDF and PDF are Gaussians with mean values the same as classical values. In the short-time limit, the widths of these Gaussians are the same as ours, but for $t>>\gamma^{-1}$, the widths of MDF and PDF go to values $(\hbar/\sigma)^2+2mkT$ and $\sigma^2+(4kT/m\gamma)+\hbar^2/m^2\gamma\sigma^2)t$, respectively. This is different from ours, as our widths exactly approach the UO limit.

To summarize, we have presented a model for the Brownian motion of a free quantum particle. The model yields explicit expressions for the momentum and position probability distributions. Though classical concepts are not used at any point, the incoherence of the stochastic process leads to classical distributions in the long-time limit. We feel that this approach may open the way to investigations where quantum and thermal effects compete. There is an obvious need to generalize this work to include an externally applied potential on the particle, and work is in progress in that direction.

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[16]In classical theory, the position distribution is obtained by integrating the momentum equation

$$p(t)=p(0)e^{-\gamma t}+\int_0^t e^{-\gamma(t-t')}f(t')dt \ ,$$

where $f(t)$ denotes the random force, whereas here the position distribution is obtained from the off-diagonal matrix elements of the quantum density matrix, for which there is no classical analog.