New Model for Dissipation in Quantum Mechanics

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We propose a new model for studying dissipation in quantum-mechanical systems. The mechanism of dissipation is solely due to the scattering of the environment excitations by the particle of interest. We treat the problem via the functional integral formalism. It is shown that the model gives a damping parameter which is temperature dependent.

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During the last few years there has been an increasing interest in the physics of dissipative systems [1–3]. The well-known standard model [1] for quantum Brownian motion deals with a particle coupled to a set of harmonic oscillators (the reservoir) via a coordinate-coordinate coupling. Moreover, the spectral function for these oscillators is assumed to have a specific form which must be compatible with the classical equation of motion of the particle. For example, it has a linear dependence on frequency in the Ohmic case.

This model exhibits two main characteristics: a nonlocal interaction, because all the oscillators are coupled to the particle, and nonconservation of the number of the reservoir excitations, that is, there is a transfer of energy from the particle to the set of oscillators by destruction and creation of quanta in the reservoir. One important consequence of this model is a damping parameter γ which is independent of temperature.

Nevertheless, in the majority of cases, the particle we are interested in is coupled only locally to the reservoir excitations and the main mechanism for dissipation is basically scattering. Consider, for instance, a heavy particle which is elastically scattered by light particles in a gas. The interaction is effective only very close to the heavy particle and the dissipation will take place by a sort of "effective recoil" of the particle.

In this Letter, we will show that an approximate form of a Hamiltonian which has currently been used in the theory of polaron dynamics [4,5] or, equivalently, quantization of nonlinear field theories by the collective coordinate method [6] can easily describe the above-mentioned mechanism for dissipation. Furthermore, we will also show that this model Hamiltonian is very suitable for the application of the path-integral methods in the well-known Feynman-Vernon [7] approach which has been extensively applied to the standard theory of the so-called quantum dissipation [1–3]. This method is known to be very convenient since it provides us with a systematic way of dealing with the quantum dynamics of nonisolated systems. It is also worth noticing that this method makes the use of kinetic theory unnecessary.

The model we are going to use is described by the following Hamiltonian:

$$H=\frac{[p-h(a_k^\dagger,a_k)]^2}{2m}+V(q)+H_R(a_k^\dagger,a_k)\,, \tag{1}$$

where

$$h(a_k^\dagger,a_k)=\frac{\hbar}{m}\sum_{kk'}G_{kk'}a_k^\dagger a_{k'}\,, \tag{2}$$

$$H_R(a_k^\dagger,a_k)=\sum_k \hbar\omega_k a_k^\dagger a_k\,, \tag{3}$$

and p and q are the momentum and position operators for the particle of interest. $V(q)$ is an external applied potential and the coupling parameters are such that

$$G_{kk'}^*=G_{k'k}$$

and

$$G_{k'k}=-G_{kk'}\,. \tag{4}$$

We will suppose that a_k and $a_k^\dagger$ are boson operators but the treatment can be easily generalized to fermion operators [8].

Observe that H commutes with the total number of excitations, $N=\sum_k a_k^\dagger a_k$, and due to (4) the interaction only couples excitations with different k. So, this Hamiltonian simulates the scattering of the excitations by the particle.

In order to apply the Feynman-Vernon approach we must define the reduced density operator for the particle by

$$\rho_s(t)=\mathrm{tr}_r[\rho(t)]\,, \tag{5}$$

where tr_r denotes the trace over the coordinates of the bosons and ρ denotes the density operator of the whole system.

Projecting (5) in the coordinate representation of the particle and using the coherent state representation for bosons, we get [9]

$$\rho_s(x,y,t)=\int dx'\int dy' J(x,y,t;x',y',0)\rho_s(x',y',0)\,,$$

where we have supposed, for simplicity, that before $t=0$ the particle and the bosons were decoupled and $\rho_s(0)$ is

the density operator of the particle at $t=0$.

J is the so-called superpropagator which can be expressed as a functional integral,

$$J=\int_{x'}^{x}Dx\int_{y'}^{y}Dy\exp\left\{\frac{i}{\hbar}(S_0[x]-S_0[y])\right\}F[x,y], \quad (6)$$

where the variable x (y) within brackets stands for a general path $x(t)$ ($y(t)$) connecting the intial point x' (y') to the final point x (y). The functional S_0 is the classical action of the particle,

$$S_0[x]=\int_0^t dt'\left(\frac{m\dot{x}^2(t')}{2}-V(x(t'))\right),$$

and F is the influence functional defined as

$$F[x,y]=\int\frac{d^2\alpha}{\pi^N}\int\frac{d^2\alpha'}{\pi^N}\int\frac{d^2\beta'}{\pi^N}\rho_R(\alpha'^*,\beta',0)\times\exp\left(-|\alpha|^2-\frac{|\alpha'|^2}{2}-\frac{|\beta'|^2}{2}\right)\int_{\alpha'}^{\alpha^*}D^2\gamma\int_{\beta'^*}^{\alpha}D^2\gamma'\exp\{-S_I[x,\gamma]-S_I^*[y,\gamma']\}. \quad (7)$$

In Eq. (7), $\boldsymbol{\alpha}$ is the vector $(\alpha_1,\alpha_2,\ldots,\alpha_N)$ and $\rho_R(0)$ is the density operator for bosons at $t=0$. Finally, S_I stands for the interaction action which reads

$$S_I[x,\boldsymbol{\alpha}]=-\int_0^t dt'\left\{\frac{1}{2}\left(\boldsymbol{\alpha}\cdot\frac{d\boldsymbol{\alpha}^*}{dt'}-\boldsymbol{\alpha}^*\cdot\frac{d\boldsymbol{\alpha}}{dt}\right)-\frac{i}{\hbar}(H_R-m\dot{x}h)\right\}. \quad (8)$$

The functional integrals in (7) can be exactly evaluated because the action in (8) is quadratic in the bosonic variables. So, we have transformed a nonlinear problem given by (1) into a linear one.

The Euler-Lagrange equations for (8) are given by

$$\begin{aligned}\dot{\alpha}_j+i\omega_j\alpha_j&=i\dot{x}\sum_k G_{jk}\alpha_k,\\ \dot{\alpha}_j^*-i\omega_j\alpha_j^*&=-i\dot{x}\sum_k G_{kj}\alpha_k^*.\end{aligned} \quad (9)$$

These equations represent a set of harmonic oscillators coupled by time-dependent terms. Observe that due to (4) the right-hand side of (9) does not contain the jth term of $\boldsymbol{\alpha}$. This fact allows us to solve these equations exactly.

The set of equations can be solved with the appropriate boundary conditions defined in (7) in terms of a new functional $W_{ij}[x]$ which obeys the following matrix equation:

$$W_{jk}[x]=W_{jk}^0[x]+\sum_{k'}W_{jk'}^0[x]W_{k'k}[x], \quad (10)$$

where

$$W_{jk}^0[x]=iG_{jk}\int_0^t dt'\dot{x}(t')e^{i(\omega_j-\omega_k)t'}. \quad (11)$$

Formally the equation above can be solved as

$$W=(1-W^0)^{-1}W^0, \quad (12)$$

where we have used matrix notation for W.

Of course (10) can be interpreted in terms of a scattering amplitude from mode k to mode j. The terms that appear in the sum (10) represent the virtual transitions between these two modes. Now, supposing that at $t=0$ the boson system is in thermal equilibrium at temperature T, that is,

$$\rho_R(0)=\exp\{-\beta H_R\}/Z,$$

with $\beta=1/k_BT$ and

$$Z=\mathrm{tr}_r(e^{-\beta H_R}),$$

we can evaluate (7) as

$$F[x,y]=\prod_k(1-n_k\Gamma_{kk}[x,y])^{-1}, \quad (13)$$

where

$$\Gamma_{kk}[x,y]=W_{kk}[x]+W_{kk}^*[y]+\sum_{k'}W_{k'k}[x]W_{k'k}^*[y] \quad (14)$$

and

$$n_k=(e^{\beta\hbar\omega_k}-1)^{-1}.$$

Although expression (13) is an exact result for the influence functional, its specific form makes the functional integral for J in (6) untractable. Therefore one must look for some reasonable approximation in order to evaluate the latter.

Since (10) is basically a Dyson equation for W, it is suggestive that we solve it in the usual Born approximation. In terms of (12) this means that

$$W\simeq W^0+W^0W^0. \quad (15)$$

Now, if we use (15) in (14), we can approximate (13) by

$$F[x,y]=\prod_k\exp\{n_k\Gamma_{kk}\} \quad (16)$$

which coincides with the previous expression for F up to first order in $n_k\Gamma_{kk}$.

Substituting (16) into (6) we find

$$J=\int_{x'}^{x}Dx\int_{y'}^{y}Dy\exp\left\{\frac{i}{\hbar}S_{\mathrm{eff}}[x,y]+\frac{1}{\hbar}\phi[x,y]\right\}, \quad (17)$$

where

$$S_{\text{eff}}[x,y]=\int_0^t dt'\frac{m}{2}[\dot{x}^2(t')-\dot{y}^2(t')]-V(x(t'))+V(y(t'))+[\dot{x}(t')-\dot{y}(t')]\int_0^t dt''\Gamma_I(t'-t'')[\dot{x}(t'')+\dot{y}(t'')] \tag{18}$$

and

$$\phi[x,y]=\int_0^t dt'\int_0^t dt''\Gamma_R(t'-t'')[\dot{x}(t')-\dot{y}(t')][\dot{x}(t'')-\dot{y}(t'')]\,, \tag{19}$$

with

$$\Gamma_I(t)=\sum_{kk'}\hbar G_{kk'}^2 n_k\theta(t)\sin(\omega_k-\omega_{k'})t\,, \tag{20}$$

$$\Gamma_R(t)=\sum_{kk'}\hbar G_{kk'}^2 n_k\theta(t)\cos(\omega_k-\omega_{k'})t\,. \tag{21}$$

As usual, $\theta(t)$ is defined as

$$\theta(t)=\begin{cases}1 & \text{if } t>0\,,\\ 0 & \text{if } t<0\,.\end{cases}$$

As in the rest of this paper, we shall only be interested in the case of $V(q)=0$, we can define

$$R=\tfrac{1}{2}(x+y),\quad r=x-y\,,$$

in terms of which the Euler-Lagrange equations for (18) read

$$\ddot{R}+2\int_0^t dt'\,\gamma(\tau-t')\dot{R}(t')=0\,, \tag{22}$$

$$\ddot{r}-2\int_0^t dt'\,\gamma(t'-\tau)\dot{r}(t')=0\,, \tag{23}$$

where by (20),

$$\gamma(t)=\frac{1}{m}\frac{\partial\Gamma_I}{\partial t}$$

$$=\frac{\hbar\theta(t)}{m}\sum_{kk'}G_{kk'}^2 n_k(\omega_k-\omega_{k'})\cos(\omega_k-\omega_{k'})t \tag{24}$$

is the damping function.

In terms of these newly defined variables, we can easily see that (22) and (23) have the same form as the equations previously obtained in the case of quantum Brownian motion [1], except for the fact that they now present memory effects. It should be emphasized here that although (22) and (23) have only indirect physical meaning, through the study of the motion of the center of a wave packet and the spreading of its width, $\gamma(t)$ really plays the role of the damping parameter in the equation of motion of the former (see Ref. [1] for details).

Another important point about (17) is the real part of the exponent. This part is related to the diffusion function of the problem [1], which can be written here as

$$D(t)=\hbar\frac{\partial^2\Gamma_R}{\partial t^2}$$

$$=-\sum_{kk'}\hbar^2 G_{kk'}^2 n_k(\omega_k-\omega_{k'})^2\theta(t)\cos(\omega_k-\omega_{k'})t\,. \tag{25}$$

From (24) and (25) we clearly see that the memory effects will depend on the microscopic characteristics of our model, namely, the form of $G_{kk'}$. In what follows we shall define a function $S(\omega,\omega')$ which will, in analogy to the spectral function $J(\omega)$ of the standard model [1,2], allows us to replace all the summations over k by integrals over frequencies [cf. Eq. (29) below],

$$S(\omega,\omega')=2\pi\sum_{kk'}G_{kk'}^2\delta(\omega-\omega_k)\delta(\omega'-\omega_{k'})\,. \tag{26}$$

Notice, however, that unlike $J(\omega)$ in [1] or [2], this new function $S(\omega,\omega')$ is related to the scattering of the environmental excitations between states of frequencies ω and ω' (as seen from the laboratory frame). Moreover, due to (4) it is easy to see that

$$S(\omega,\omega')=S(\omega',\omega)\,. \tag{27}$$

From here on we shall call $S(\omega,\omega')$ the "scattering function."

Now, we will show that the specific ansatz

$$S(\omega,\omega')=\alpha\omega\omega'\theta(\omega_c-\omega)\theta(\omega_c-\omega') \tag{28}$$

is compatible with both the Markovian limit (time evolution without memory) and Ohmic dissipation (damping proportional to the velocity). In (28) ω_c is the cutoff frequency for the boson system (for example, if the bosons are phonons, ω_c must be the Debye frequency) and α is a constant.

In order to do so, we start by using the explicit form of $S(\omega,\omega')$ in (28) to rewrite (24) as

$$\gamma(t)=\frac{\hbar\theta(t)\alpha}{2\pi m}\int_0^{\omega_c}d\omega\int_0^{\omega_c}d\omega'\,\omega\omega' n(\omega)(\omega-\omega')\times\cos(\omega-\omega')t\,. \tag{29}$$

This expression can be further simplified in the low-temperature limit ($kT\ll\hbar\omega_0$) where we can approximate

$$n(\omega)\simeq e^{-\beta\hbar\omega}\,. \tag{30}$$

The form of (30) provides us with a natural cutoff frequency for the integrations in (29), namely, $kT/\hbar$. So, we can rewrite (29) as

$$\gamma(t)\simeq\frac{\hbar\theta(t)\alpha}{2\pi m}\int_0^{\infty}d\omega\int_0^{(\beta\hbar)^{-1}}d\omega'\,\omega\omega' e^{-\beta\hbar\omega}(\omega-\omega')\times\cos(\omega-\omega')t\,. \tag{31}$$

The integrals can be easily evaluated and in the limit of long times, $\tau \gg \beta\hbar$, we get

$$\gamma(t) = (a/2m\hbar^2)(kT)^4\delta(t).$$

So, for long times and low temperatures the particle behaves like a particle in a viscous environment with a damping parameter which increases as T^4. As a consequence, the mobility of the particle decreases as T^{-4}. For high temperatures we can approximate the occupation number by $n \simeq (\beta\hbar\omega)^{-1}$ and the damping parameter increases linearly with temperature. These results agree with those obtained some years ago for the mobility of the large acoustic polaron in one dimension [10]. Although the results in the latter have been achieved with the use of kinetic theory, we can make a connection between the two methods when applied to the specific example of polarons (optical or acoustical) [11].

In conclusion, we have established a new model for the study of dissipation in quantum mechanics where the mechanism of dissipation is given by the scattering of the quanta of the reservoir by the particle of interest. We used the functional integral formalism in the coherent state representation for the environmental bosons and obtained the reduced density matrix in the Born approximation. Through the definition of the scattering function $S(\omega,\omega')$, we have established the conditions under which the damping parameter is Ohmic in the long-time regime (Markovian approximation). It is also important to emphasize that in this new model the damping is naturally temperature dependent.

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