Evolution of Wave Function in a Dissipative System

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Abstract

For a dissipative system with Ohmic friction, we obtain a simple and exact solution for the wave function of the system plus the bath. It is described by the direct product in two independent Hilbert space. One of them is described by an effective Hamiltonian, the other represents the effect of the bath, i.e., the Brownian motion, thus clarifying the structure of the wave function of the system whose energy is dissipated by its interaction with the bath. No path integral technology is needed in this treatment. The derivation of the Weisskopf-Wigner line width theory follows easily.

The simplest example of a dissipative system, an harmonic oscillator coupled to the environment, which is a bath of harmonic oscillators, has been the subject of extensive studies[1-15]. We shall show in the present paper that in a special case, the Ohmic case (to be defined later), the dissipative system can be exactly treated both classically and quantum mechanically, thereby clarifying the sense in which the wave function is describable by an effective Hamiltonian. In this treatment path integral technology is not needed, and our presentation is self-contained.

We consider the problem discussed by Caldeira and Leggett (CL)[1], an harmonic oscillator system (the dissipative system) with coordinate q, mass M, and frequency $(\omega_0^2 + \Delta\omega^2)^{1/2}$, interacting with a bath of N harmonic oscillators of coordinates x_j, mass m_j, and frequency ω_j., where $\Delta\omega^2$ is a shift induced by the coupling already discussed by CL. The Hamiltonian of the system and the bath is:

$$H = \frac{p^2}{2M} + \frac{1}{2}M(\omega_0^2 + \Delta\omega^2)q^2 + q\sum_j c_j x_j + \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 x_j^2\right) \tag{1}$$

The dynamic equation for operators in the Heisenberg representation leads to the following set of equations of motions:

$$M\ddot{q} = -M\omega_0^2 q - M\Delta\omega^2 q - \sum_j c_j x_j , \tag{2}$$

$$m_j\ddot{x} = -m_j\omega_j^2 x_j - c_j q \quad (j = 1, 2, ...N). \tag{3}$$

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Now, applying the Laplace transform[2] (the bars are our notations for the Laplace transform, s is the Laplace transform of time t), equations (2), (3) can be used to eliminate bath variables $\bar{x}_j$ to obtain the equation for $\bar{q}$

$$M(s^2\bar{q} - sq_0 - \dot{q}_0) = -M\omega_0^2\bar{q} - M\Delta\omega^2\bar{q} - \sum_j c_j \frac{sx_{j0} + \dot{x}_{j0}}{s^2 + \omega_j^2} - \sum_j \frac{c_j^2}{m_j(s^2 + \omega_j^2)}\bar{q} , \qquad (4)$$

where q_0, $\dot{q}_0$, x_{j0}, $\dot{x}_{j0}$ are the initial values of the respective operators in the Heisenberg representation. Assuming the number of bath oscillators is large enough so that we can replace the sum over j by an integration over ω_j, the coefficient of the last term can then be separated into two terms:

$$\int_0^\infty \frac{\rho(\omega_j)c_j^2 d\omega_j}{m_j \omega_j^2} - s^2 \int_0^\infty \frac{\rho(\omega_j)c_j^2 d\omega_j}{m_j\omega_j^2(s^2 + \omega_j^2)} , \qquad (5)$$

where $\rho(\omega_j)$ is the bath oscillator density. Following an argument similar to the one pointed out by CL[1], the requirement that the system becomes a damped oscillator with frequency ω_0 and damping rate η in the classical limit, known as the "Ohmic friction" condition, leads to the following constraint:

$$\rho(\omega_j) = \frac{2\eta M}{\pi} \frac{m_j\omega_j^2}{c_j^2} . \qquad (6)$$

By observing eq.(4) and eq.(5), it can be shown that the second term of eq.(5) leads to damping with the damping constant η, while the first term of eq.(5) represents a frequency shift. If the frequency renormalization constant $\Delta\omega^2$ is chosen to satisfy:

$$M\Delta\omega^2 = \int_0^\infty \frac{\rho(\omega_j)c_j^2 d\omega_j}{m_j\omega_j^2} , \qquad (7)$$

the frequency is shifted to ω_0. Then equation (4) is simplified, and its inverse Laplace transform gives the quantum Langevin equation, valid at time t $>=$ 0+:

$$\ddot{q} + \eta\dot{q} + \omega_0^2 q = f(t) , \qquad (8)$$

with the Brownian motion driving force:

$$f(t) = -\sum_j c_j(x_{j0} \cos\omega_j t + \dot{x}_{j0}\frac{\sin\omega_j t}{\omega_j}) . \qquad (9)$$

During the derivation, in order to carry out the integral in eq.(5), we used the requirement of the inverse Laplace transform that s must pass all the singular points from right of the complex plane, and hence real(s) >0.

Equation (8) and (9) are the equations of a *driven damped harmonic oscillator,* the solution of which is well known as a linear combination of the initial values at q_0, $\dot{q}_0$, x_{j0}, and $\dot{x}_{j0}$:

$$q(t) = a_1(t)q_0 + a_2(t)\dot{q}_0 + \sum_j (b_{j1}(t)x_{j0} + b_{j2}(t)\dot{x}_{j0}) , \qquad (10)$$

$$x_i(t) = \alpha_{i1}(t)q_0 + \alpha_{i2}(t)\dot{q}_0 + \sum_j (\beta_{ij1}(t)x_{j0} + \beta_{ij2}(t)\dot{x}_{j0}) , \; with \qquad (11)$$

$$a_1(t) = \frac{\nu e^{-\mu t} - \mu e^{-\nu t}}{\nu - \mu} \, , \; a_2(t) = \frac{e^{-\mu t} - e^{-\nu t}}{\nu - \mu} \, , \tag{12}$$

$$\mu = \frac{\eta}{2} + \omega i \, , \; and \; \nu = \frac{\eta}{2} - \omega i \, , \tag{13}$$

and here $\omega = (\omega_0^2 - \eta^2/4)^{1/2}$ is the frequency shifted by damping. (All formulae are correct whether ω is real or imaginary. To avoid a minor detail of the initial value problem, we have redefined the initial time as t=0+.) The explicit expression for b_{j1}, b_{j2}, α_{i1}, α_{i2}, β_{ij1}, and β_{ij2} are well known in freshmen physics.

We emphasize that the use of the Laplace transform instead of the Fourier transform allows us to express q(t) and $x_j(t)$ explicitly in terms of the initial values, as in eq.(10) and eq.(11).

The equations (10) and (11) serve as the starting point of subsequent discussions. We will proceed to find the Green's function of the full system, and hence the solution of the wave function in Schoedinger representation. The result tells us *in what sense the damped oscillator is described by an effective Hamiltonian without the bath variables* and gives its specific form, it also shows that under this condition, the wave function can be factorized, and the main factor relevant to the damped oscillator is a solution of the Schoedinger equation with an effective Hamiltonian.

Equations (10) and (11) are correct both in classical mechanics and in quantum mechanics in the Heisenberg representation. We notice that q(t) and $x_j(t)$ are both linear superpositions of q_0, $\dot{q}_0$, x_{j0}, $\dot{x}_{j0}$ with c-number coefficients. The commutation rules between $q(t)$, $\dot{q}(t)$, $x_j(t)$, $\dot{x}_j(t)$ are $[q(t), \dot{q}(t)] = \frac{i\hbar}{M}$, $[x_j(t), \dot{x}_j(t)] = \frac{i\hbar}{m_j}$, and operators q(t) and $\dot{q}(t)$ commute with $x_j(t)$ and $\dot{x}_j(t)$. One can prove these commutation rules by two ways: (a). By direct computation, using the fact that at t=0, they are correct. (b). By the general principle that $q(t)$, $\dot{q}(t)$, $x_j(t)$, $\dot{x}_j(t)$ are related by a unitary transformation to q_0, $\dot{q}_0$, x_{j0}, $and \, \dot{x}_{j0}$.

Equation (10) and (11) show that the operators q(t) and $x_j(t)$ can each be written as a sum of two terms:

$$q(t) = Q(t) + \sum_j \xi_j(t) \, , \tag{14}$$

$$x_i(t) = \zeta_i(t) + \sum_j X_{ij}(t) \, , \tag{15}$$

where $Q(t)$ and $\zeta_i(t)$ are linear in q_0 and $\dot{q}_0$ and independent of x_{j0} and $\dot{x}_{j0}$, and ξ_j and $X_{ij}(t)$ are linear in x_{j0} and $\dot{x}_{j0}$, and independent of q_0 and $\dot{q}_0$. Thus $Q(t)$ and $\zeta_i(t)$ are operators in one Hilbert space S_Q, while $\xi_j(t)$ and $X_{ij}(t)$ are in an independent Hilbert space S_X, and the full Hilbert space is a direct product $S_Q \otimes S_X$.

We shall first analyze the structure of S_Q. We write that:

$$Q(t) = a_1 Q_0 + a_2 \dot{Q}_0 = a_1 Q_0 - a_2 \frac{i\hbar}{M} \frac{\partial}{\partial Q_0} \, . \tag{16}$$

To explicitly show that we are discussing the S_Q space, we define $Q_0 \equiv q_0$, $\dot{Q}_0 \equiv \dot{q}_0$. The eigenfunction of Q(t) with an eigenvalue denoted by Q_1, in the Q_0 representation, is easily calculated to be:

$$u_{Q_1}(Q_0, t) = \left(\frac{M \omega e^{\frac{1}{2} \eta t}}{2\pi \hbar \sin \omega t} \right)^{\frac{1}{2}} exp \left[-\frac{iM}{2\hbar a_2} \left(a_1 Q_0^2 - 2 Q_0 Q_1 + \phi(Q_1, t) \right) \right] \, , \tag{17}$$

with ϕ as an arbitrary phase, i.e., a real number. This eigenfunction is related to the Green's function $G(Q_1, Q_0; t, 0) \equiv < Q_1|U_Q(t)|Q_0 >$, by $u_{Q_1}(Q_0, t) = < Q_0|U_Q^{-1}(t)|Q_1 > = < Q_0|U_Q^\dagger(t)|Q_1 > = G^*(Q_1, Q_0; t, 0)$, where we denote the evolution operator by $U(t)$, which is unitary when we choose the eigenvectors of Q(t) to be orthonormal. Thus we have:

$$G(Q_1, Q_0; t, 0) = \left(\frac{M\omega e^{\frac{1}{2}\eta t}}{2\pi\hbar \sin\omega t} \right)^{\frac{1}{2}} exp\left[\frac{iM}{2\hbar a_2} \left(a_1 Q_0^2 - 2Q_0 Q_1 + \phi(Q_1, t) \right) \right] \ . \tag{18}$$

Next, we shall determine the arbitrary phase $\phi(Q_1, t)$, which is the phase of the eigenvectors of Q(t). Using eq.(16), we find the commutation rule for Q and $\dot{Q}$:

$$[Q, \dot{Q}] = (a_1 \dot{a}_2 - \dot{a}_1 a_2)[Q_0, \dot{Q}_0] = e^{-\eta t}[Q_0, \dot{Q}_0] = \frac{e^{-\eta t}}{M} i\hbar \ . \tag{19}$$

Thus we define the canonical momentum P(t) as:

$$P(t) = Me^{\eta t}\dot{Q}(t) = M\, e^{\eta t}(\dot{a}_1 Q_0 + \dot{a}_2 \dot{Q}_0) = \dot{a}_1 Q_0 - \dot{a}_2 \frac{i\hbar}{M} \frac{\partial}{\partial Q_0} \ , \tag{20}$$

and get the commutation rule: $[Q(t), P(t)] = i\hbar$. The eigenfunction of P(t) can be calculated in two ways: (a). We can calculate the eigenvector of P(t) in the Q_0 representation using eq. (20) and then use the Green's function eq.(18) to transform it into the Q(t) representation; (b). The commutation rule $[Q(t), P(t)] = i\hbar$ requires that P(t)$=-i\hbar\frac{\partial}{\partial Q}$, so the eigenfunction of P(t) with eigenvalue P_1 is $exp[i\frac{P_1}{\hbar}Q]$. By comparing these two solutions, the arbitrary phase $\phi(Q_1, t)$ in the Green's function is determined to within a phase $\phi(t)$, which is independent of Q_1. $\phi(t)$ is an arbitrary real function of time, except that $\phi(0) = 0$ so that it satisfies the condition that at t=0, the Green's function becomes $\delta(Q_1 - Q_0)$. Thus we obtain the Green's function in the S_Q space:

$$G(Q_1, Q_0; t, 0) = \left(\frac{M\omega e^{\frac{1}{2}\eta t}}{2\pi i\hbar \sin\omega t} \right)^{\frac{1}{2}} exp\left[\frac{iM}{2\hbar a_2} \left(a_1 Q_0^2 + \dot{a}_2 e^{\eta t} Q_1^2 - 2Q_0 Q_1 \right) - \frac{i\phi(t)}{\hbar} \right] . \tag{21}$$

It is then straight forward to derive the Hamiltonian H_Q using the following relation:

$$H_Q = i\hbar \frac{\partial U_Q}{\partial t} U_Q^{-1} \ , \tag{22}$$

and remembering that the matrix elements of U_Q and U_Q^{-1} are the Green's function and its conjugate. The result is:

$$H_Q = e^{-\eta t} \frac{P^2}{2M} + \frac{1}{2} M\omega_0^2 e^{\eta t} Q^2 + \dot{\phi}(t) \ . \tag{23}$$

Since ϕ is arbitrary except that $\phi(0) = 0$, we can take $\phi(t) = 0$. Therefore we have derived the well known effective Hamiltonian for the dissipative system. *We emphasize that the expression for H_Q is here derived, while in usual literature it is introduced by more or less heuristic arguments.*

Next, we shall analyze the effect of the bath. Similar to eq. (17) we obtain the eigenfunctions $\theta_{\xi_{j1}}(x_{j0}, t)$ for ξ_j. Using Dirac's notation we have: $Q|u_{Q_1} >= Q_1|u_{Q_1} >$, $\xi_j|\theta_{\xi_{j1}} >= \xi_{j1}|\theta_{\xi_{j1}} >$.

Thus $|u_Q > \prod_j \bigotimes |\theta_{\xi_j} >$ is an eigenvector of q(t), with eigenvalue of $Q + \sum_j \xi_j$. In other words, the eigenvector of q(t) with eigenvalue q is $|q, \{\xi_j\} >= |u_{q - \sum_j \xi_j} > \prod_j \bigotimes |\theta_{\xi_j} >$.

If initially the wave function is $|\Psi_0 >= |\psi_0 > \prod_j \bigotimes |\chi_{j0} >$, to calculate the wave function at time t, we should expand Ψ_0 in terms of the eigenvectors $|q, \{\xi_j\} >$, i.e., we should calculate

$$\psi(Q, t) \equiv < u_Q | \psi_0 >= \int u_Q^*(q_0) \psi_0(q_0) dq_0 , \tag{24}$$

$$\chi_j(\xi_j, t) \equiv < \theta_{\xi_j} | \chi_{j0} >= \int \theta_{\xi_j}^*(x_{j0}) \chi_{j0}(x_{j0}) dx_{j0} . \tag{25}$$

Then the wave function in the Schoedinger representation at time t is

$$\Psi(q, \{\xi_j\}, t) =< q, \{\xi_j\} | \Psi_0 >= \psi(q - \sum_j \xi_j, t) \prod_j \chi_j(\xi_j, t) . \tag{26}$$

Notice that $\psi(Q, t)$ of eq.(24) is the wave function in the Schoedinger representation with the effective Hamiltonian eq.(23). Hence we have connected the effective Hamiltonian approach to the dissipative system problem with the other approaches that take both the system and the bath into account. We also notice that even though our $\Psi(q, \{\xi_j\}, t)$ is in a different representation from that of $\Psi(q, \{x_j\}, t)$, the usual probability interpretation is still valid: $\int \int ... \int |\Psi(q, \{\xi_j\}, t)|^2 \prod_j d\xi_j$ is the probability density of finding the particle at q. Since this solution is very simple, it provides a simple way to analyze other complicated problems, e.g., study the influence of Brownian motion on interference, which we shall not elaborate because of space.

Under certain conditions, eg., at low temperature and when the system q is in highly excited states so the range of q is large enough that for all the values of ξ_j which do not have vanishingly small probability, $q \gg |\sum_j \xi_j|$, we can approximately write: $\Psi(q, \{\xi_j\}, t) = \psi(q, t) \prod_j \chi_j(\xi_j, t)$. That is, the wave function is factorized, the dissipative system q can be described by the wave function $\psi(q, t)$ only, and the Brownian motion can be ignored. Therefore it is interesting to examine the width of the argument of the wave function ψ, due to the Brownian motion, i.e., the mean value of $(\sum_j \xi_j)^2$ at time t. It can be calculated using its expression in the Heisenberg representation as introduced by (10) and (18). At temperature T, this width is :

$$< (\sum_j \xi_j(t))^2 >= \sum_j \frac{\hbar}{2m_j \omega_j}(|b_{j1}(t)|^2 + \omega_j^2 |b_{j2}(t)|^2) \cot\left(\frac{\hbar \omega_j}{2kT}\right) . \tag{27}$$

This width is zero initially, then approaches its final equilibrium value in a time interval of the order of $1/\eta$. At low temperature limit, the equilibrium width is simplified to:

$$\sigma^2(t = \infty) = \frac{\hbar}{2\pi m \omega} \left[\frac{\pi}{2} + \arctan\left(\frac{\omega_0^2}{\eta \omega}\right)\right] . \tag{28}$$

If the damping rate η is much smaller than the frequency of the oscillator ω_0, this width happens to become the same as the width of the ground state of the system $\hbar/(2m\omega)$.

Finally, it is interesting to see the distribution of the dissipated energy of the harmonic oscillator in the bath, and check if it agrees with the Weisskopf-Wigner line width theory[16] For simplicity, we assume zero temperature. To calculate the energy dissipated by the system into the j'th bath oscillator, we use eq.(11) and its derivative to obtain the expression of $x_j(t)$ and $p_j = m_j\dot{x}_j(t)$, which are then substituted into the expression of the energy of the j'th oscillator: $h_j = \frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 x_j^2$. We then calculate the expectation value of h_j, assuming initially the system is in the n'th excited state, and the bath oscillators in the ground state. We calculate the contribution to the expectation value of h_j from the system, by keeping only terms which depend on q_0, and $\dot{q}_0$. The result is then the energy disspation by the system into the j'th oscillator. When multiplied by the density of states $\rho(\omega_j)$ eq.(6), it gives the dissipated energy spectrum. It is a function of ω_j, with a narrow peak near the resonance $\omega_j = \omega$, if the damping is small, i.e., if $\eta \ll \omega$. It is oscillatory with a frequency of $2\omega_j$. Its time average over a period is :

$$E_j = (n + \frac{1}{2})\hbar\omega \frac{\eta}{\pi} \frac{1}{\frac{\eta^2}{4} + (\omega - \omega_j)^2} A(\omega_j),\tag{29}$$

where $A(\omega_j)$ varies slowly near the resonance, i.e., over the width $\eta/2$ of the peak it changes very little. Therefore, we can replace ω_j by ω near the peak, and the result is simplified to: $A(\omega) \approx 1$. Thus eq.(29) shows that the dissipated energy has a Lorenzian distribution near the resonance, in agreement with the Weisskopf-Wigner line width theory.

Acknowledgements

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