Quantum Harmonic Oscillator In A Thermal Bath

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ABSTRACT

In this talk, we briefly review the influence functional path-integral treatment of quantum Brownian motion. We report on a newly derived exact master equation of a quantum harmonic oscillator coupled to a general environment at arbitrary temperature. We apply it to the problem of loss of quantum coherence.

INTRODUCTION

Recently there has been considerable interest in quantum Brownian motion. It was motivated by possible observation of macroscopic effects in quantum systems. Among them are quantum tunneling with dissipation [1], loss of quantum coherence due to system-environment interaction [2], just name a few. The newest application of quantum Brownian motion is in quantum cosmology, where the issue of quantum-to-classical transition of an open system is very important [3]. These issues also appear in semiclassical theory of early universe in which noise, fluctuation and dissipation play important roles in particle production, back reaction, phase transition, inflation and galaxies formation [4]. In these problems, the interaction between a system and its environment is quite complicated giving rise to nonlocal dissipation and colored noise.

The effect of nonlocal dissipation and colored noise in quantum Brownian motion is an outstanding problem, which has been studied only to a limited extent. In some limiting cases, the quantum master equation (the time evolution equation) for the reduced density matrix of the Brownian motion has been derived before by different authors with different methods. These cases are all in the class of ohmic environment, for which the dissipation is always local [5]. It corresponds to having a linear damping force proportional to the velocity of the Brownian particle classically. The noise associated with the dissipation is colored at low temperature.

Our contribution reported in this talk is the derivation of an exact master equation for the reduced density matrix of a Brownian harmonic oscillator linearly coupled to a general environment (with a general thermal bath spectral density) at arbitrary temperature [6]. In our model, the environment is a set of bath harmonic oscillators with different natural frequencies. The environment is at a thermal equilibrium state. The system (Brownian particle) is brought to contact with this thermal bath. The derivation is done from first principles of statistical and quantum physics with Feynman path-integral

method and Feynman-Vernon influence functional formalism [7]. This master equation can accommodate all possible forms of the nonlocal dissipation kernel and nonlocal noise kernel. It is a linear partial differential equation with time dependent coefficients. The non-Markovian character resides in these coefficients. In particular we examine the cases of ohmic, subohmic and superohmic environment and compute these time dependent coefficients numerically. We show that all the previous master equations obtained otherwise are just special examples of our master equation.

INFLUENCE FUNCTIONAL

Let us briefly review the Feynman-Vernon influence functional formalism of quantum open system. Consider a Brownian particle with mass $M = 1$ and natural (bare) frequency Ω. The environment is modeled by a set of harmonic oscillators with mass m_n and natural frequency ω_n. The Brownian particle is coupled linearly to each bath oscillator with strength C_n. The total action of the combined system plus environment is

$$
\begin{aligned}
S[x, q] &= S[x] + S_E[q] + S_{int}[x, q] \\
&= \int_0^t ds \left\{ \frac{1}{2}\dot{x}^2 - \frac{1}{2}\Omega^2 x^2 \right\} + \int_0^t ds \sum_n \left\{ \frac{1}{2}m_n\dot{q}_n^2 - \frac{1}{2}m_n\omega_n^2 q_n^2 \right\} \\
&\quad + \int_0^t ds \sum_n \left\{ C_n x q_n \right\}
\end{aligned}
\tag{1}
$$

where x and q_n are the coordinates of the particle and the n-th bath oscillators.

It is well known that the time evolution of the total density matrix of the system plus environment $\hat{\rho}(t)$ is governed by the following quantum Liouville equation

$$
i\hbar \frac{d}{dt}\hat{\rho}(t) = \left[\hat{H}, \ \hat{\rho}(t) \right]
\tag{2}
$$

In the coordinate representation, the solution of the above quantum Liouville equation can

be written as

$$\rho(x_f, q_f; x'_f, q'_f; t) = \int\limits_{-\infty}^{+\infty} dx_i \int\limits_{-\infty}^{+\infty} dx'_i \int\limits_{-\infty}^{+\infty} dq_i \int\limits_{-\infty}^{+\infty} dq'_i$$

$$\times\, J(x_f, q_f, x'_f, q'_f, t \mid x_i, q_i, x'_i, q'_i, 0)\, \rho(x_i, q_i; x'_i, q'_i; 0) \tag{3}$$

where

$$J\left(x_f, q_f, x'_f, q'_f, t \mid x_i, q_i, x'_i, q'_i, 0\right)$$

$$= \int\limits_{x_i}^{x_f} Dx \int\limits_{x'_i}^{x'_f} Dx' \int\limits_{q_{ni}}^{q_{nf}} Dq \int\limits_{q'_{ni}}^{q'_{nf}} Dq\ \exp\frac{i}{\hbar}\Big\{ S[x,q] - S[x',q'] \Big\} \tag{4}$$

is the propagator of the total density matrix in path-integral form. Here q represents the full set of bath oscillator coordinates and the subscript i and f denote the initial and final variables.

We are only interested in how the dynamics of the system (the Brownian particle) under the influence of the environment (all bath oscillators). The quantity containing this information is the reduced density matrix of the system

$$\rho_r(x, x') = \int\limits_{-\infty}^{+\infty} dq \int\limits_{-\infty}^{+\infty} dq'\ \rho(x, q; x', q')\delta(q - q') \tag{5}$$

which is propagated in time by the the evolution operator

$$\rho_r(x_f, x'_f, t) = \int\limits_{-\infty}^{+\infty} dx_i \int\limits_{-\infty}^{+\infty} dx'_i\ J_r(x_f, x'_f, t \mid x_i, x'_i, 0)\, \rho_r(x_i, x'_i, 0) \tag{6}$$

If we assume that at $t = 0$ the system and the environment are uncorrelated

$$\hat{\rho}(t = 0) = \hat{\rho}_s(0) \times \hat{\rho}_e(0), \tag{7}$$

then

$$J_r(x_f, x'_f, t \mid x_i, x'_i, 0) = \int\limits_{x_i}^{x_f} Dx \int\limits_{x'_i}^{x'_f} Dx'\ \exp\frac{i}{\hbar}\Big\{ S[x] - S[x'] \Big\}\ F[x, x'] \tag{8}$$

Q-5

The functional factor $F[x, x']$ in (8), called influence functional, is defined as

$$F[x, x'] = \int\limits_{-\infty}^{+\infty} dq_f \int\limits_{-\infty}^{+\infty} dq_i \int\limits_{-\infty}^{+\infty} dq_i' \int\limits_{q_i}^{q_f} Dq \int\limits_{q_i'}^{q_f} Dq'$$

$$\times \exp \frac{i}{\hbar} \left\{ S_b[q] + S_{int}[x, q] - S_b[q'] - S_{int}[x', q'] \right\} \rho_b(q_i, q_i', 0) \tag{9}$$

It is first introduced by Feynman and Vernon [7].

For the problem described by (1), the influence functional can be computed exactly. The result is:

$$F[x, x'] = \exp \left\{ -\frac{i}{\hbar} \int\limits_0^t ds_1 \int\limits_0^{s_1} ds_2 \Big[x(s_1) - x'(s_1) \Big] \eta(s_1 - s_2) \Big[x(s_2) + x'(s_2) \Big] \right.$$

$$\left. -\frac{1}{\hbar} \int\limits_0^t ds_1 \int\limits_0^{s_1} ds_2 \Big[x(s_1) - x'(s_1) \Big] \nu(s_1 - s_2) \Big[x(s_2) - x'(s_2) \Big] \right\} \tag{10}$$

where

$$\nu(s) = \int\limits_0^{+\infty} d\omega \, I(\omega) \coth \frac{1}{2} \beta \hbar \omega \, \cos \omega s \tag{11}$$

is the noise kernel, also

$$\eta(s) = \frac{d}{ds} \gamma(s) \tag{12}$$

and

$$\gamma(s) = \int\limits_0^{+\infty} d\omega \, \frac{I(\omega)}{\omega} \cos \omega s \tag{13}$$

is dissipation kernel. Here $I(\omega)$ is the dissipation spectral density defined as

$$I(\omega) = \sum_n \delta(\omega - \omega_n) \frac{C_n^2}{2 m_n \omega_n} \tag{14}$$

The kernels $\eta(s)$ and $\nu(s)$ are generally non-local. There exists an important relation between the noise and dissipation kernels, known as the fluctuation–dissipation relation. It can be written as

$$\nu(s) = \int\limits_{-\infty}^{+\infty} ds' \, K(s - s') \, \gamma(s') \tag{15}$$

where the kernel $K(s)$ is

$$K(s) = \int\limits_{0}^{+\infty} \frac{d\omega}{\pi} \; \omega \coth \frac{1}{2}\beta\hbar\omega \; \cos\omega s \tag{16}$$

which is independent of the dissipation spectral density $I(\omega)$

EXACT MASTER EQUATION

The detailed derivation of the exact master equation of a quantum harmonic oscillator with influence functional (10) has been published in Ref. [6]. Here we just give that equation below

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t} \; \rho_r(x,x',t) = & \left\{ -\frac{\hbar^2}{2}\Big(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2}\Big) + \frac{1}{2}\Omega^2\big(x^2 - x'^2\big) \right\} \rho_r(x,x',t) \\
& + \frac{1}{2}\delta\Omega^2(t)\big(x^2 - x'^2\big) \; \rho_r(x,x',t) \\
& - i\hbar\Gamma(t)(x - x')\Big(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}\Big) \; \rho_r(x,x',t) \\
& - i\Gamma(t)h(t)(x - x')^2 \; \rho_r(x,x',t) \\
& + \hbar\Gamma(t)f(t)(x - x')\Big(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}\Big) \; \rho_r(x,x',t)
\end{aligned} \tag{17}
$$

where the time dependent coefficients are

$$\Gamma(t) = \frac{d_1(t)}{2\dot{u}_1(t)} \tag{18}$$

$$\delta\Omega^2(t) = d_2(t) - 2\Gamma(t)\dot{u}_2(t) \tag{19}$$

$$f(t) = 2\frac{a_{12}(t)}{\dot{u}_2(0)} + \frac{e_2(t) - c_1(t)}{2\Gamma(t)\dot{u}_2(0)} \tag{20}$$

$$h(t) = \dot{u}_2(t) \; f(t) + 8 \; a_{11}(t) + \frac{e_1(t) - c_2(t)}{\Gamma(t)} \tag{21}$$

The time dependent functions $c_i(t)$, $d_i(s)$ and $e_i(t)$ in (18) to (21) are

$$c_i(t) = \int\limits_{0}^{t} ds_1 \int\limits_{0}^{t} ds_2 \int\limits_{0}^{t} ds_3 \; \eta(t - s_1)\Big[G_{12}(s_1,s_2) + G_{21}(s_2,s_1)\Big]\nu(s_2 - s_3)u_i(s_3) \tag{22}$$

$$d_i(t) = 2 \int_0^t ds \; \eta(t-s)u_i(s) \tag{23}$$

$$e_i(t) = \int_0^t ds \; \nu(s)u_i(s) \tag{24}$$

The elementary functions $u_i(s)$ satisfy the following boundary value problem

$$\begin{cases} \dfrac{d^2 u_i(s)}{ds^2} + 2\int_0^s ds'\eta(s-s')u_i(s') + \omega_0^2 u_i(s) = 0 \\[2mm] u_1(0)=1, \quad u_1(t)=0 \qquad u_2(0)=0, \quad u_2(t)=1 \end{cases} \tag{25}$$

and

$$v_1(s) = u_2(t-s) \qquad v_2(s) = u_1(t-s) \tag{26}$$

The Green function $G_{12}(s_1,s_2)$ in (22) is

$$G_{12}(s_1,s_2) = \frac{u_1(s_1)u_2(s_2)\theta(s_1-s_2) - u_2(s_1)u_1(s_2)\theta(s_2-s_1)}{\dot{u}_1(s_2)u_2(s_2) - u_1(s_2)\dot{u}_2(s_2)} \tag{27}$$

A similar expression for $G_{21}(s_1,s_2)$ can be written in terms of $v_i(s)$. In all the above equations, the index i runs from 1 to 2.

Let us take a closer look of this master equation. The first line corresponds to the usual unitary Liouvillian evolution, which is independent of the system-bath interaction. The second line corresponds to a time-dependent frequency shift (frequency renormalization). The third line contains a dissipative term with a time-dependent dissipative coefficient $\Gamma(t)$. The last two lines contain two diffusive terms with time-dependent coefficients. All of these terms depend on the system-bath coupling. Further, one can see that all these time-dependent coefficients vanish at $t=0$, when the initial uncorrelated condition is assumed valid. The frequency shift and the dissipation coefficient depend only on the dissipation kernel while the diffusion coefficients depend on the noise kernel. From (11), (12) and (13), we find all these time dependent coefficients are determined by the dissipation spectral density (14).

A simpler closed formula for the time-dependent coefficients in the master equation can be found in the weak coupling limit (up to the first order in the coupling constant between the system and the bath),

$$\delta\Omega^2(t) = 2 \int_0^t ds \, \eta(s) \, \cos\Omega s \tag{28}$$

$$\Gamma(t) = -\frac{1}{\Omega} \int_0^t ds \, \eta(s) \, \sin\Omega s \tag{29}$$

$$\Gamma(t)f(t) = \frac{1}{\Omega} \int_0^t ds \, \nu(s) \, \sin\Omega s \tag{30}$$

$$\Gamma(t)h(t) = \int_0^t ds \, \nu(s) \, \cos\Omega s \tag{31}$$

EXAMPLES

An important class of dissipation spectral density is

$$I(\omega) = \frac{2}{\pi}\gamma_0\omega\left(\frac{\omega}{\tilde{\omega}}\right)^{n-1} e^{-\frac{\omega^2}{\Lambda^2}} \tag{32}$$

where Λ is the physical cutoff frequency and $\tilde{\omega}$ is another frequency scale usually taken to be Λ. The environment is classified as ohmic if $n = 1$, as supra-ohmic if $n > 1$ or as sub-ohmic if $0 < n < 1$. It is important to introduce the physical cutoff frequency because, on physical grounds, one expects the spectral density to go to zero for very high frequencies. It is clear to see that after introducing the physical cutoff frequency, the dissipation kernel (13) is a non-local kernel even for the ohmic environment.

We have numerically computed the coefficients of the master equation given by (18) to (21) for three different environments, namely, ohmic ($n = 1$), subohmic ($n = 0.5$) and superohmic ($n = 3$). The damping constant is $\gamma_0 = 0.3$ and the cutoff frequency

is $\Lambda = 2000$. The bare frequency Ω is determined from the renormalized one, namely, $\Omega_p^2 = \Omega^2 + \delta\Omega^2 \rightarrow \Omega_r^2 = 1$ (see explanation in Ref. [6]). Both high temperature region $(T = 10^5)$ and low temperature region $(T = 10)$ have been studied. The numerical plots of these time dependent coefficients and detail analysis could be found in Ref. [6].

APPLICATION: QUANTUM DECOHERENCE

As a simple application, we discuss the damping of the interference between two Gaussian wave packets [8].

Let $\psi_{1,2}(x,t)$ be the wave functions of Gaussian wave packets located initially $(t = 0)$ at $x = \pm x_0$ respectively with the same initial spread σ

$$\psi_{1,2}(x,0) = Ne^{-\frac{(x \pm x_0)^2}{4\sigma^2}} \tag{33}$$

Let $\psi(x,t)$ be the wave function of a system consisting of the superposition of these two wave packets,

$$\psi(x,t) = \psi_1(x,t) + \psi_2(x,t) \tag{34}$$

The density matrix of the system can be written as the sum of three parts

$$\rho(x,x',t) = \psi(x,t)\psi^\dagger(x',t) = \rho_1(x,x',t) + \rho_2(x,x',t) + \rho_{int}(x,x',t) \tag{35}$$

The probability density function

$$P(x,t) = \mid \psi(x,t) \mid^2 = \rho(x,x,t) \tag{36}$$

can also be written as the sum of three parts

$$P_1(x,t) = P_1(x,t) + P_2(x,t) + P_{int}(x,t) \tag{37}$$

By using the influence functional (10) and the master equation (17), we get

$$P_{1,2}(x,t) = \tilde{N}(t)\exp\left[-\frac{(x \pm x_0(t))^2}{2\sigma^2(t)}\right] \tag{38}$$

and

$$P_{int}(x,t) = 2\sqrt{P_1(x,t)}\sqrt{P_2(x,t)}e^{-D(t)}\cos\phi(t) \tag{39}$$

where

$$x_0(t) = -\frac{\dot{u}_1(0)}{\dot{u}_2(0)}x_0 \tag{40}$$

and

$$\sigma(t) = \left[\frac{\dot{u}_1^2(0)}{\dot{u}_2^2(0)} + \frac{2a_{11}(t)}{\sigma^2\dot{u}_2^2(0)} + \frac{1}{4\sigma^4\dot{u}_2^2(0)}\right]^{1/2} \tag{41}$$

are respectively the position and spread of the wave packet at time t,

$$\phi(t) = \frac{2x_0[\dot{u}_2(0)x + \dot{u}_1(0)x_0]}{1 + 8a_{11}(t)\sigma^2 + 4\dot{u}_1^2(0)\sigma^4} \tag{42}$$

is the oscillatory angle (which is present even in the absence of the environment) and

$$D(t) = \frac{4a_{11}(t)x_0^2}{1 + 8a_{11}(t)\sigma^2 + 4\dot{u}_1^2(0)\sigma^4} \tag{43}$$

is the decay factor (which is present only because of the environment). It is this last term depicting the decay of interference between the two wave packets which is usually regarded as providing a measure of decoherence.

We have numerically computed the decay factor $e^{-D(t)}$ for all the cases described in the previous section. The results could be found in Ref. [6].

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REFERENCES

[1] A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) 149, 374 (1983); A. J. Leggett et al, Rev. Mod. Phys. 59, 1 (1987).

[2] W. H. Zurek, Phys. Rev. D24, 1516 (1981); D26, 1862 (1982).

[3] J. B. Hartle and S. W. Hawking, Phys. Rev. D28, 1960 (1983); A. Vilenkin, Phys. Lett. 117B, 25 (1985); Phys. Rev. D27, 2848 (1983) D30, 509 (1984).

[4] A. A. Starobinsky, in Field Theory, Quantum Gravity and Strings, ed. H. J. deVega and N. Sanchez (Springer, Berlin 1986).

[5] W. G. Unruh and W. H. Zurek, Phys. Rev. D40, 1071 (1989).

[6] B. L. Hu, J. P. Paz and Y. Zhang, Phys. Rev. D 45, 2843 (1992).

[7] R. P. Feynman and F. L. Vernon, Ann. Phys. 24, 118 (1963); A. O. Caldeira and A. J. Leggett, Physica 121A, 587 (1983); Grabert, P. Schramm, and G. -L. Ingold, Phys. Rep. 168, 115 (1988).

[8] A. O. Caldeira and A. J. Leggett, Phys. Rev. A 31, 1059 (1985)