Partial factorization of wave functions for a quantum dissipative system

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In this paper, a microscopic approach treating the quantum dissipation process presented by Yu and Sun [Phys. Rev. A **49**, 592 (1994); **51**, 1845 (1995)] is developed to analyze the wave function structure for the dynamic evolution of a typical dissipative system—a single-mode boson soaked in a bath of many bosons. The wave function of the total system is explicitly obtained as a product of two components of the system and bath in a coherent state representation. It not only describes the influence of the bath on the variable of the system through the Brownian motion, but also manifests the back-action of the system on the bath and the mutual interaction among the bosons of bath. Due to the back-action, the total wave function can only be partially factorizable even if the Brownian motion can be completely ignored in certain cases, e.g., weak coupling and large detuning. The semiclassical implication of the back-action, the mutual interaction, and the Brownian motion in the present model are also discussed by considering the wave packet evolution of the dissipative system in the coordinate representation. [S1063-651X(98)04604-2]

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I. INTRODUCTION

Historically, there are two different approaches to treat the quantum dissipative process, i.e., the system plus bath model in much of the literature [1–4], and the time dependent effective Hamiltonian model given by Kanai and Caldirola [5,6]. However, for quite a long time the problem of the relation between these two approaches, frequently appearing in the literature, has remained untouched. In two recent papers by Yu and one (C.P.S.) of the authors [7,8], based on the first approach, this problem was tackled by explicitly writing down the total wave function of the system plus the bath in a form of a product of the bath and system components. With this result the relation between the above mentioned approaches was clarified as that the product of the bath and system components becomes a direct product when the Brownian motion effects can be ignored in certain case. It was also shown that the system component is governed just by the Kanai and Caldirola effective Hamiltonian in this situation.

However, two questions about the discussions in Refs. [7,8] have to be answered. The first one concerns the fact that, as the mixed variables involving the physical coordinates of the system were chosen to describe the bath in the previous discussion, the wave function only manifested the influence of the bath on the system through the Brownian broadening of the width of the wave function for the system. Here we left the back-action of the system on the bath undiscussed. If there indeed exists a back-action of the system on the bath, it is reasonable to expect that, for individual particles comprising the bath, the mutual couplings among them should indirectly appear through coupling the system as an intermediate process. The second question involves the relation between quantum and classical systems. In many real situations, the classical or macroscopic states can be represented by coherent states in quantum optics and macroscopic quantum phenomena. Under the influence of the bath, it is significant to study how the system evolves with an initial coherent state, and to test if it can move in classical orbits

In this paper, we intend to consider the above two questions. In the rotating-wave approximation [9], a simple model of one boson interacting with a bath of many bosons is used to analyze the back-action of the system on the bath and the mutual couplings among the particles comprising the bath. In the presence of the back-action and indirect mutual coupling, the meaning of the wave function of the dissipative system is clarified by considering the dynamic evolution of the total system. A significantly different result from previous works [7,8] is the partial factorization structure, in which the total wave function is still a product of the system and bath components, but the coordinate of each individual particle in the bath component is entangled with the coordinates of the system and other bath particles. For instance, in the limit case with a very large width of the initial state and weak coupling or large detuning, the entanglement terms of the bath variables in the system component can be ignored up to the second order approximation, and the Brownian motion plays no role in the evolution of the system. However, in this case, the total wave function can only be partially factorized, because there still exist entanglement terms of the system variable in each bath component of the total wave function. It is also shown that, in this sense, the system component is only a function of the system variable governed by an effective Hamiltonian, which is equivalent to the Caldirola-Kanai Hamiltonian. With the Gaussian wave packet as an initial state of the system, the evolution of the wave packet can be explicitly calculated to mainifest the semiclassical features of the back-action and the mutual interaction.

The paper is organized into five sections. In Sec. II, the explicit expression for the total wave function is constructed in a coherent representation. In Sec. III, the physical meaning of the partial factorization of the wave function is discussed by deriving the Kanai and Caldirola effective Hamiltonian governing the system component. In Sec. IV, the semiclassical implications of the back-action and the mutual interaction, as well as the Brownian motion, are analyzed, with the wave packet evolution as an example.

II. STRUCTURE OF THE WAVE FUNCTION

In this section, we construct a partially factorized wave function for the system plus bath from the explicit solutions of the Heisenberg equations about the system operator and bath operators. Consider a simple model consisting of a single-mode boson and a bath of many bosons. The Hamiltonian is written as

$$H=\hbar\omega b^\dagger b+\sum_j \hbar\omega_j a_j^\dagger a_j+\hbar\sum_j [\xi_j b^\dagger a_j+\text{H.c.}], \quad (1)$$

where $\xi_j=|\xi_j|e^{i\sigma_j}$'s are the complex coupling constants and $b^\dagger$, $b;a_j^\dagger$, and a_j are the bosonic creation and annihilation operators for the system and bath, respectively. This model can be regarded as a rotating-wave approximation of the original oscillator model [7,8], with the linear coupling $\Sigma_j\xi_j q x_j \sim \Sigma_j[\xi_j b^\dagger a_j+\xi_j b^\dagger a_j^\dagger+\text{H.c}]$ of the system coordinate q to the bath variables x_j.

To obtain an explicit expression for the wave function of the total system formed by the system plus the bath, we invoke the well-known solutions given by Ref. [9],

$$b(t)=u(t)b(0)+\sum_j v_j(t)a_j(0), \quad (2)$$

$$a_j(t)=e^{-i\omega_j t}a_j(0)+u_j(t)b(0)+\sum_{s(\neq j)} v_{js}(t)a_s(0), \quad (3)$$

of the corresponding Heisenberg equation. Here, the time-dependent coefficients are

$$u(t)=\exp\left[-\frac{\gamma}{2}t-i(\omega+\Delta\omega)t\right], \quad (4)$$

$$v_j(t)=-\xi_j\exp(-i\omega_j t)\frac{1-\exp[i(\omega_j-\omega-\Delta\omega)t-\gamma t/2]}{\omega+\Delta\omega-\omega_j-i\gamma/2}, \quad (5)$$

$$u_j(t)=-\xi_j^* e^{-i\omega_j t}\frac{\exp[i(\omega_j-\omega-\Delta\omega)t-\gamma t/2]-1}{\omega_j-\omega-\Delta\omega+i\gamma/2}, \quad (6)$$

$$v_{js}(t)=\frac{-\xi_j^*\xi_s e^{-i\omega_j t}}{\omega+\Delta\omega-\omega_s-i\gamma/2}\times\left\{\frac{1-\exp[i(\omega_j-\omega-\Delta\omega)t-\gamma t/2]}{\omega+\Delta\omega-\omega_j-i\gamma/2}-\Lambda\right\}, \quad (7)$$

$$\Lambda=\begin{cases}\dfrac{\exp[i(\omega_j-\omega_s)t]}{\omega_j-\omega_s}, & j\neq s\\ t, & j=s.\end{cases} \quad (8)$$

Here the Lamb shift $\Delta\omega$ can be absorbed into ω to obtain the renormalized physical frequency $\tilde{\omega}=\omega+\Delta\omega$, and the damping constant γ is determined by the coupling $\xi_j$and the spectrum density $\rho(\omega_j)$ of the bath. If we chose an appropriate $\rho(\omega_j)$ similar to the Ohmic distribution of Caldeira and Leggett [1], the above solutions (2) and (3) are exact [7,8]; otherwise, the similar solution can be obtained by the Wigner-Weisskopf approach or the Markoff approximation [9].

Now we present a method in the coherent state representation to calculate the evolution of the wave function in the Schrödinger picture from explicit expressions of the canonical operators in the Heisenberg picture. It is different from that in our previous works [1,2], but quite direct and effective. If the initial state of the total system is a direct product $|\Psi(0)\rangle=|\phi\rangle\otimes\Pi_j|\phi_j\rangle$, and $U(t)$ is the evolution operator of the total system, the wave function $|\Psi(t)\rangle=U(t)|\Psi(0)\rangle$ at time t can be defined by its coherent state representation

$$\Psi(\lambda,\{\lambda_j\},t)=\langle\lambda,\{\lambda_j\}|\Psi(t)\rangle=\langle\Psi(0)|U(t)^\dagger|\lambda,\{\lambda_j\}\rangle^*. \quad (9)$$

Here, the overcomplete basis

$$|\lambda,\{\lambda_j\}\rangle=|\lambda\rangle\otimes\prod_j|\lambda_j\rangle =N(\lambda,\{\lambda_j\})\exp\left(\lambda b^\dagger(0)+\sum_j\lambda_j a_j^\dagger(0)\right)|0\rangle \quad (10)$$

has been constructed from the coherent states $|\lambda\rangle$ and $|\lambda_j\rangle$ for the annihilation operators $b(0)$ and $a_j(0)$, respectively. The normalization constant $N(\lambda,\{\lambda_j\})=\exp(-\frac{1}{2}|\lambda|^2-\Sigma_j\frac{1}{2}|\lambda_j|^2)$. To obtain explicit expressions of $U(t)|\lambda,\{\lambda_j\}\rangle$, we consider the role of the evolution matrix $U(t)$ in the Heisenberg picture. In fact, since $U(t)^\dagger O(0)U(t)=O(t)$ and $U(t)|0\rangle=|0\rangle$ for an operator O, it is easy to obtain

$$\begin{aligned}U(t)^\dagger|\lambda,\{\lambda_j\}\rangle &=N(\lambda,\{\lambda_j\})\exp\left(\lambda b^\dagger(t)+\sum_j\lambda_j a_j^\dagger(t)\right)|0\rangle\\ &=N(\lambda,\{\lambda_j\})\exp\left(\alpha(t)b^\dagger(0)+\sum_j\beta_j(t)a_j^\dagger(0)\right)|0\rangle\\ &=|\alpha(t)\rangle\otimes\prod_j|\beta_j(t)\rangle,\end{aligned} \quad (11)$$

where

$$\alpha(t)=u(t)^*\lambda+\sum_j \lambda_j u_j(t)^*, \tag{12}$$

$$\beta_j(t)=e^{i\omega_j t}\lambda_j+v_j(t)^*\lambda+\sum_{s(\neq j)} v_{s,j}(t)^*\lambda_s. \tag{13}$$

By substituting Eq. (11) into Eq. (9), a formal factorized wave function for the total system

$$\Psi(\lambda,\{\lambda_j\},t)=\phi\left(u(t)^*\lambda+\sum_j u_j(t)^*\lambda_j\right)\otimes\prod_j \phi_j\left(e^{i\omega_j t}\lambda_j+v_j(t)^*\lambda+\sum_{s(\neq j)} v_{s,j}(t)^*\lambda_s\right) \tag{14}$$

is obtained.

III. PARTIAL FACTORIZATION AND EFFECTIVE HAMILTONIAN

In this section we derive the effective Hamiltonian governing the evolution of the system component ϕ if the Brownian effect caused by the terms $\Sigma_j u_j(t)^*\lambda_j$ can be ignored, and then the total wave function Ψ is partially factorized. The above wave function (14) is not completely factorizable because of the entanglements of the variables λ and λ_j, which are implied by the term $\Sigma_j u_j(t)^*\lambda_j$ of the bath variables λ_j modifying the system variable λ, and the term $v_j(t)^*\lambda$ of the system modifying the bath variables λ_j. This former represents the bath fluctuation due to the Brownian motion, and the latter the back-action of the system on the bath. In fact the term $\Sigma_j u_j(t)^*\lambda_j$ is caused by the bath fluctuation operator $B(t)=\Sigma_j v_j(t)a_j(0)$ in the system operator $b(t)$. The bath fluctuation operator has a zero thermal average, but a nonzero correlation

$$\langle B(t)^\dagger B(t')\rangle=\sum_j 4|\xi_j|^2\frac{f_j(t,t')}{\gamma^2+4(\omega_j-\omega-\Delta\omega)^2}\times\left[\exp\left(\frac{\hbar\omega_j}{k_BT}\right)-1\right]^{-1}. \tag{15}$$

where $f_j(t,t')$ can be well defined by Eq. (5). The term $\Sigma_{j\neq s}v_{s,j}(t)^*\lambda_s$ shows the mutual interactions among the bosons of the bath through the system. Mathematically, if the coupling is weak with a small value of ξ_j, the mutual interactions are second order quantities, since $v_{s,j}(t)^*\propto\xi_j^*\xi_s$. Notice that the main difference between the present result and that in Refs. [7,8] is the back-action and the mutual interactions.

If the fluctuation can be ignored for certain cases, e.g., λ is very large in the initial state and the coupling is weak enough, the entanglement disappears, so that the wave function becomes a product

$$\Psi(\lambda,\{\lambda_j\},t)\approx\phi[u(t)^*\lambda]\prod_{j=1}^N \phi_j[e^{i\omega_j t}\lambda_j+v_j(t)^*\lambda]. \tag{16}$$

In this case, all influences of the bath on the system are represented by the damping constant γ, and then the wave function is partially factorizable due to the term $v_j(t)^*\lambda$. It is not difficult to prove that the system component $\phi[u(t)^*\lambda]$ is governed by an effective Hamiltonian which is also equivalent to the Caldirola-Kanai Hamiltonian.

To prove this, we need to return into the Heisenberg picture by dropping the bath operators $a_j(0)$ in $b(t)$, that is, $b(t)$ is replaced by $\tilde{b}(t)=u(t)b(0)$. However, $\tilde{b}(t)^\dagger$ and $\tilde{b}(t)$ are not canonical operators, since $[\tilde{b}(t),\tilde{b}(t)^\dagger]=e^{-\gamma t}$. Fortunately, the Bogoliubov transformation gives the general canonical operators

$$A(t)=\alpha\tilde{b}(t)+\beta\tilde{b}(t)^\dagger \tag{17}$$

satisfying $[A(t),A(t)^\dagger]=1$, where

$$|\alpha|^2-|\beta|^2=\exp(\gamma t). \tag{18}$$

To give the correct Heisenberg equations for operators $A(t)$ and $A(t)^\dagger$, the effective Hamiltonian is determined by definition (17) to be time dependent,

$$\begin{aligned}H_{\text{eff}}=i\hbar\exp(-\gamma t)(\bar{\alpha}\alpha^*-\bar{\beta}\beta^*)A(t)^\dagger A(t)\\+\tfrac{1}{2}(\bar{\beta}\alpha-\bar{\alpha}\beta)A(t)^\dagger A(t)^\dagger\\+\tfrac{1}{2}(\bar{\alpha}^*\beta^*-\bar{\beta}^*\alpha^*)A(t)A(t),\end{aligned} \tag{19}$$

where $\bar{\alpha}=\dot{\alpha}-(\gamma/2+i\tilde{\omega})\alpha$ and $\bar{\beta}=\dot{\beta}-(\gamma/2-i\tilde{\omega})\beta$. Notice that the number $\bar{\alpha}\alpha^*-\bar{\beta}\beta^*=\delta$ should be a pure imaginary number, i.e., $\delta^*=-\delta$. Here we should mention that the effective Hamiltonian is not unique because there is only one constraint [Eq. (18)] [10]. The different forms of the effective Hamiltonian correspond to the different realizations of the canonical variables. For instance, a specific solution

$$\alpha=\exp(\gamma/2+i\varphi)t,\quad \beta=0,\varphi=\tilde{\omega}-\sqrt{\gamma^2/4+\tilde{\omega}^2}$$

of Eq. (18) gives

$$H_{\text{eff}}=\hbar\exp(\gamma t)\Omega A(t)^\dagger A(t),$$

with $\Omega=\sqrt{\gamma^2/4+\tilde{\omega}^2}$. By formally introducing the canonical coordinate $Q=\sqrt{\hbar/2M\Omega}[A(t)+A(t)^\dagger]$ and momentum $P=-i\sqrt{M\Omega\hbar/2}[A(t)-A(t)^\dagger]$, with the varying mass $M=m\exp(\gamma t)$, this special effective Hamiltonian is just of the form given by Caldirola and Kanai. The same result can be also obtained in a purely quantized version in the Schrödinger picture by a direct calculation of matrix elements,

$$\langle\alpha|H_{\text{eff}}|\beta\rangle=\langle\alpha|i\hbar[\partial U(t)/\partial t]U(t)^\dagger|\beta\rangle.$$

IV. MOTION OF THE CENTER OF THE WAVE PACKET WITH QUANTUM FLUCTUATION

In this section, we consider the classical counterpart of the factorization structure of a wave function, entangling a system variable with the bath variables. In the representation of the coordinate momentum determined by

$$q=\sqrt{\frac{\hbar}{2\omega}}(b+b^{\dagger}),\quad p=-i\sqrt{\frac{\hbar\omega}{2}}(b-b^{\dagger}),\tag{20}$$

$$x_j=\sqrt{\frac{\hbar}{2\omega_j}}(a_j+a_j^{\dagger}),\quad p_j=-i\sqrt{\frac{\hbar\omega_j}{2}}(a_j-a_j^{\dagger}),\tag{21}$$

the coherent states $|\lambda\rangle$ and $|\lambda_j\rangle$ are understood to be Gaussian wave packets of widths $\sqrt{\hbar/2\omega}$ centered in $q_0=\sqrt{\hbar/2\omega}(\lambda+\lambda^*)$ and $x_{j0}=\sqrt{\hbar/2\omega}(\lambda_j+\lambda_j^*)$, respectively. If the initial state of the total system is a direct product of such Gaussians,

$$|\Psi(0)\rangle=\left|\lambda=\sqrt{\frac{\omega}{2\hbar}}q_0\right\rangle\otimes\prod_j\left|\lambda_j=\sqrt{\frac{\omega_j}{2\hbar}}x_{j0}\right\rangle,\tag{22}$$

the wave function at time t,

$$\begin{aligned}|\Psi(t)\rangle&=|\lambda(t)\rangle\otimes\prod_j|\lambda_j(t)\rangle\\&=\left|u(t)\sqrt{\frac{\omega}{2\hbar}}q_0+\sum_j u_j(t)\sqrt{\frac{\omega_j}{2\hbar}}x_{j0}\right\rangle\\&\quad\otimes\prod_j\left|\sqrt{\frac{\omega_j}{2\hbar}}x_{j0}e^{i\omega_j t}\right.\\&\quad\left.+v_j(t)\sqrt{\frac{\omega}{2\hbar}}q_0+\sum_{j(\neq s)}v_{s,j}(t)\sqrt{\frac{\omega_s}{2\hbar}}x_{s0}\right\rangle,\end{aligned}\tag{23}$$

defines the position evolution of center of the Gaussian wave packet,

$$\begin{aligned}q_c(t)&=\sqrt{\frac{\hbar}{2\omega}}[\lambda(t)+\lambda^*(t)]=q_0\exp\left(-\frac{1}{2}\gamma t\right)\cos(\tilde{\omega})t\\&\quad+\sum_j|\xi_j|\sqrt{\frac{\omega_j}{\omega}}\frac{x_{j0}\Theta_j(t)}{\gamma^2/4+(\omega_j-\tilde{\omega})^2},\end{aligned}\tag{24}$$

where

$$\begin{aligned}\Theta_j(t)&=\exp\left(-\frac{1}{2}\gamma t\right)\left[\frac{\gamma}{2}\sin(\tilde{\omega}+\sigma_j)t+(\omega_j-\tilde{\omega})\right.\\&\quad\left.\times\cos(\tilde{\omega}+\sigma_j)t\right]-\left[\frac{\gamma}{2}\sin(\omega_j+\sigma_j)t+(\omega_j-\tilde{\omega})\right.\\&\quad\left.\times\cos(\omega_j+\sigma_j)t\right].\end{aligned}\tag{25}$$

It is known from Eq. (24) that the center of the wave packet moves along the classical trajectory of a damping harmonic oscillator. This motion is described by the first term in Eq. (24), and perturbed by the initial displacements x_{j0} of the bath oscillators shown in the second term in Eq. (24). This fluctuation effect is nothing but an explicit manifestation of the Brownian motion. If initial displacement q_0 is very large, this fluctuation effect can be ignored in the weak coupling case with small ξ_j, or in a sharp spectral distribution of the bath with a large detuning from the renormalized frequency $\tilde{\omega}$.

It is interesting to consider the back-action of the system on the bath, and the mutual interaction among the bath bosons in the problem of the wave packet evolution. For each boson in the bath, the motion law of the center of Gaussian wave packet,

$$\begin{aligned}x_{jc}(t)&=\sqrt{\frac{\hbar}{2\omega_j}}[\lambda_j(t)+\lambda_j^*(t)]=x_{j0}\cos\omega_j t\\&\quad+q_0\sqrt{\frac{\omega}{\omega_j}}\mathrm{Re}[v_j(t)]+\sum_{s(\neq j)}\mathrm{Re}[v_{s,j}(t)]\sqrt{\frac{\omega_s}{\omega_j}}x_{s0},\end{aligned}\tag{26}$$

is given by the second component in Eq. (23). The back-action $q_0\sqrt{\omega/\omega_j}\mathrm{Re}[v_j(t)]$ is proportional to the initial displacement q_0 and a Lorentzian factor $\propto[\gamma^2/4+(\omega_j-\tilde{\omega})^2]^{-1}$ given by Eq. (5). It cannot be neglected for large q_0, or in the near-resonance case in which the bath spectral distribution $\rho(\omega_j)$ peaks in the renormalized frequency $\tilde{\omega}$ of the system. However, the last term $\Sigma_{s(\neq j)}\mathrm{Re}[v_{s,j}(t)]\sqrt{\omega_s/\omega_j}x_{s0}$ is of second order. It explicitly reflects the mutual coupling among the bosons of the bath, and can be neglected in the first order approximation.

V. DISCUSSIONS

In summary, we should mention that the Langevin approach serves as a standard treatment of the quantum dissipation process for the present model [2], but hardly concerns discussions about the structure of wave function, which is essentially important in zero temperature; the Markoff approximation is an effective method to treat the density operator related essentially to the wave function, but it only considers a few intuitional pictures based on the classical correspondence and the dissipation-fluctuation relation. This paper takes both aspects into account for the most simple model, and thus gives a direct and clean picture of the quantum dissipation process. This discussion not only concerns the necessary details in the dynamics of quantum dissipation, but also reveals the roles of the back-action of the bath and the mutual coupling among bosons in the bath. In fact, the Langevin approach is based on a stochastic equation,

$$\dot{b}(t)=\left[-\frac{\gamma}{2}-i(\omega_a+\Delta\omega)\right]b(t)+F(t),\tag{27}$$

with the stochastic force $F(t)=-i\Sigma_j\xi_j a_j(0)e^{-i\omega_j t}$. Its explicit solution is the starting point for finding the partially factorizable wave function of the total system in this paper. In this sense, the present study can be regarded as a generalization of quantum Langevin theory. From a view of the Markoff approximation theory, our explicit solutions (14) and (23) can be somewhat understood as the zero-temperature results of the density matrix approach, but they deal substantially with the dissipation-fluctuation relation in the framework of the wave function. Instead of understanding the effective wave function in terms of the complete factorization structure, as in previous works [7,8], another emphasis of this paper is the partially factorizable structure of the evolution wave function. This structure further clarifies the meaning of the wave function governed by the time-dependent effective Hamiltonian given by Caldirola and Kanai in the presence of the back-action and indirect mutual interactions.

To conclude this paper, it is worthwhile to point out that the methods used here and in previous works [7,8] are only limited to linear systems such as the harmonic oscillator, the inverse harmonic oscillator (the harmonic oscillator with an image frequency $\omega \rightarrow i\omega$), and a linear potential for a constant force. For these systems, the solutions of canonical Heisenberg operators are linear combinations of the system variable and the bath variables. Thus the wave functions of these systems are factorizable in the appropriate representations. The generalization of the idea and method of this paper to the nonlinear cases, except for linearizable systems, is still an open question.

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