

Derivation of exact master equation with stochastic description: Dissipative harmonic oscillator

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A systematic procedure for deriving the master equation of a dissipative system is reported in the framework of stochastic description. For the Caldeira-Leggett model of the harmonic-oscillator bath, a detailed and elementary derivation of the bath-induced stochastic field is presented. The dynamics of the system is thereby fully described by a stochastic differential equation, and the desired master equation would be acquired with statistical averaging. It is shown that the existence of a closed-form master equation depends on the specificity of the system as well as the feature of the dissipation characterized by the spectral density function. For a dissipative harmonic oscillator it is observed that the correlation between the stochastic field due to the bath and the system can be decoupled, and the master equation naturally results. Such an equation possesses the Lindblad form in which time-dependent coefficients are determined by a set of integral equations. It is proved that the obtained master equation is equivalent to the well-known Hu-Paz-Zhang equation based on the path-integral technique. The procedure is also used to obtain the master equation of a dissipative harmonic oscillator in time-dependent fields.

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I. INTRODUCTION

In the real world, physical systems are not exempt from the disturbance of their surrounding environment. Because of dissipation caused by system-environment couplings [1–5], the dynamics of open systems will change dramatically from reversible to irreversible behavior. The most representative model of the dissipative dynamics is Brownian motion, a subject extensively investigated in many academic areas ranging from natural sciences, to engineering, to social sciences [6–10]. As one observes that the environment makes the dynamics of the system a stochastic process, it is natural to use random noises to imitate the influence of the environment, which results in the phenomenological Langevin equation and Fokker-Planck equation methods [11]. The Langevin equation describes the motion of a classical Hamiltonian system subjected additionally to a noise due to the environment, while the Fokker-Planck equation depicts the evolution of the phase-space probability for an ensemble of the system. The most successful microscopic model for the environment consists of an infinite number of effective harmonic oscillators [12], which has been shown to be a generic heat bath [13,14]. The harmonic-oscillator bath with linear couplings to the system under study is called the Caldeira-Leggett model in the literature.

Traditionally dissipative dynamics is an essential subject of nonequilibrium processes and plays an indispensable role in condensed-phase dynamics and transport as well as spectroscopy [15–17]. Nowadays the rapid development of quantum information and quantum measurement provides extraordinary paradigms for exploring dissipative effect, especially the interplay of quantum coherence, dephasing, and relaxation [18–21]. Because it is an inherent many-body problem, dissipative dynamics is usually very difficult to solve exactly. There are, however, still several general frameworks available for investigating the diversified features of open systems [2,3]. For instance, the projection operator technique

developed by Nakajima [22] and Zwanzig [23] has been widely used in fields of spectroscopy and quantum optics where dissipation in general is weak and thereby perturbation treatment can be employed. The influence functional method based on the path integral, on the other hand, which was first proposed by Feynman and Vernon [24] and popularized by Caldeira and Leggett [13], has been shown to be a powerful tool for theoretical analysis [1]. This method has also been implemented as a numerical technique to simulate dynamics of dissipative two- and three-state systems [25,26]. Following Feynman, Stockburger *et al.* interpreted the influence functional in the Caldeira and Leggett model as a random field and put forward a stochastic formulation for the dissipative dynamics [27]. Along this line one of the authors extended the stochastic idea to general heat baths and was able to establish that the influence of the heat bath on the system can be fully characterized by its induced stochastic fields [28]. Based on the stochastic description, a deterministic approach comprising hierarchical equations of motion was developed [29–32]. This scheme is only applicable to specific dissipation where the bath-induced stochastic field is the Ornstein-Uhlenbeck type or the like. Fortunately it is shown that the hierarchy method combined with *stochastic realization* can be used to accurately simulate zero-temperature dynamics of dissipative two-state systems at strong dissipation [29].

Analytically solvable models are always desired because they provide deep insights into the understanding of dissipation and benchmark results for comparison when developing approximations. It is unfortunate that in dissipative dynamics only a few systems are analytically solvable. Good examples include models of the harmonic oscillator [33–50], the free particle [51], and the parabolic barrier [52–55]. In this paper we will show that the stochastic decoupling approach can be invoked to obtain the master equation of the dissipative harmonic oscillator with or without driving fields in a straightforward and elementary way. Although some results were already reported and the method was briefly outlined in previous work [38,39], a full procedure by which one can follow step by step has yet been supplied. This paper will fill this gap. We will give a detailed report on the derivation of the

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master equation for dissipative linear systems from the establishment of the stochastic differential equation of the dissipative system to the statistical averaging that leads to the desired master equation.

The paper is organized as follows. In Sec. II we briefly review the stochastic description of quantum dissipation. In Sec. III we apply the stochastic formulation to a dissipative harmonic oscillator and derive its exact master equation. In Sec. IV we prove the equivalence between our results and the known results, the Hu-Paz-Zhang master equation. In Sec. V we extend the scheme to the case of the harmonic oscillator in time-dependent external fields and work out the master equation. We conclude the paper in Sec. VI.

II. THEORY

A. Stochastic description: Primer

To study the dissipative dynamics, we start with a system-plus-bath model defined by the Hamiltonian

$$\hat{H} = \hat{H}_s + \hat{H}_b + \hat{H}_{\text{int}}, \quad (1)$$

where \hat{H}_s is the Hamiltonian of the renormalized system of interest, \hat{H}_b the Hamiltonian of the bath, and \hat{H}_{int} the interaction energy between the system and the bath. Without loss of generality the couplings can be written as $\hat{H}_{\text{int}} = \sum_{\alpha} \hat{f}_{\alpha} \hat{g}_{\alpha}$, where \hat{f}_{α} are the operators of the system and \hat{g}_{α} the operators of the bath. According to quantum mechanics the evolution of the total system obeys the Liouville equation, namely,

$$i\hbar \frac{\partial \rho(t)}{\partial t} = [\hat{H}, \rho(t)], \quad (2)$$

where $\rho(t)$ is the density matrix. Keep in mind that we are interested only in the dynamics of the system. The reduced density matrix $\tilde{\rho}_s(t) = \text{Tr}_b \rho(t)$ provides sufficient information that we require. Because the complexity of dissipative dynamics lies in the coupling between the system and the bath, it would be desired to decouple the interaction in such a way that the evolution of the bath will no longer be explicitly involved in the evolution of the system. Actually, it was shown by one of the authors that the Hubbard-Stratonovich transformation can be used to convert the system-bath coupling during the evolution to the correlation of stochastic processes for the separated but random system and bath [28]. Doing this, the price one has to pay is to introduce auxiliary stochastic fields in subsystems. Later it was recognized that a simpler and natural language way to formulate the dissipative dynamics as a stochastic one is the Itô calculus [28].

The Itô calculus is concerned with a Wiener process $W(t) = \int_0^t dt' \mu(t')$, where $\mu(t)$ is a Gaussian white noise with zero mean and delta function correlation, i.e., $M\{\mu(t)\} = 0$ and $M\{\mu(t)\mu(t')\} = \delta(t - t')$. Roughly speaking, the white noise $\mu(t)$ can be regarded as a series of independent random numbers at time slices $t_0 = 0, t_1, \dots, t_N = t$, where one can simply assume the time steps $\Delta t_j = t_j - t_{j-1} = \Delta t$ are uniform and $\Delta t \rightarrow 0$. Thus the distribution function for any $\mu_j = \mu(t_j)$ is

$$P(\mu_j) = \lim_{\Delta t \rightarrow 0} \sqrt{\frac{\Delta t}{2\pi}} e^{-\frac{\Delta t}{2} \mu_j^2}.$$

For a random process $F[\mu]$ or $F(\mu_1, \dots, \mu_N)$ in discrete-time representation, the stochastic averaging M means the expectation value of $F(\mu_1, \dots, \mu_N)$, i.e.,

$$M\{F[\mu]\} = \int_{-\infty}^{\infty} \prod_{j=1}^N [d\mu_j P(\mu_j)] F(\mu_1, \dots, \mu_N).$$

Note that dW is of the order \sqrt{dt} and $(dW)^2 = dt$. To apply the Itô calculus we now consider the Liouville dynamics Eq. (2) with a disentangled initial state $\rho(0) = \rho_s(0)\rho_b(0)$. When calculating the time derivative of a composite stochastic process constructed from the Wiener process, one should take into account the second-order contribution of dW . Let us analyze the following stochastic differential equations:

$$\begin{aligned} i\hbar d\rho_s &= [\hat{H}_s, \rho_s]dt + \frac{\sqrt{\hbar}}{2} \sum_{\alpha} [\hat{f}_{\alpha}, \rho_s]dW_{1\alpha} \\ &+ i \frac{\sqrt{\hbar}}{2} \sum_{\alpha} \{\hat{f}_{\alpha}, \rho_s\}dW_{2\alpha}^* \end{aligned} \quad (3)$$

and

$$\begin{aligned} i\hbar d\rho_b &= [\hat{H}_b, \rho_b]dt + \frac{\sqrt{\hbar}}{2} \sum_{\alpha} [\hat{g}_{\alpha}, \rho_b]dW_{2\alpha} \\ &+ i \frac{\sqrt{\hbar}}{2} \sum_{\alpha} \{\hat{g}_{\alpha}, \rho_b\}dW_{1\alpha}^*, \end{aligned} \quad (4)$$

where $W_{1\alpha}(t) = \int_0^t dt' [\mu_{1\alpha}(t') + i\mu_{4\alpha}(t')]$ and $W_{2\alpha}(t) = \int_0^t dt' [\mu_{2\alpha}(t') + i\mu_{3\alpha}(t')]$ are complex Wiener processes with independent Gaussian white noises $\mu_{k\alpha}(t)$ ($k = 1 - 4$). Apparently there is no direct interaction between the two subsystems, and the equations of motion for the system and the bath Eqs. (3) and (4) are independent. Using the Itô calculus of the complex Wiener process, $dW_{\alpha}dW_k = dW_{\alpha}^*dW_k^* = 0$ and $dW_{\alpha}dW_k^* = 2\delta_{\alpha k}dt$, and the nonanticipating property, that is, that the combined stochastic process $\rho_s(t)\rho_b(t)$ is statistically independent of $dW_{1(2),t}$, $M\{\rho_s(t)\rho_b(t)dW_{1(2),t}\} = 0$, we can readily prove

$$\begin{aligned} i\hbar d(M\{\rho_s(t)\rho_b(t)\}) &= i\hbar M\{d\rho_s(t)\rho_b(t) + \rho_s(t)d\rho_b(t) + d\rho_s(t)d\rho_b(t)\} \\ &= \left[\hat{H}_s + \hat{H}_b + \sum_{\alpha} \hat{f}_{\alpha} \hat{g}_{\alpha}, M\{\rho_s(t)\rho_b(t)\} \right] dt. \end{aligned} \quad (5)$$

Therefore, $M\{\rho_s(t)\rho_b(t)\}$ satisfies the Liouville equation Eq. (2) and is, of course, identical with the density matrix $\rho(t)$ of the total system.

With the help of the Itô calculus, therefore, we are able to illustrate how the interaction between the system and bath is decoupled, as shown in Eqs. (3) and (4). As a consequence, the system as well as the bath is subjected to random fields. Again, it should be stressed that we want to calculate the reduced density matrix, $\tilde{\rho}_s(t) = \text{Tr}_b M\{\rho_s(t)\rho_b(t)\}$. To this end we change the operation order of the tracing over the degrees of freedom of the bath and the stochastic averaging to obtain

$$\tilde{\rho}_s(t) = M\{\rho_s(t)\text{Tr}_b \rho_b(t)\}. \quad (6)$$

The formal expression of $\text{Tr}_b \rho_b(t)$ can be feasibly acquired by solving its equation of motion [Eq. (4)],

$$\text{Tr}_b \rho_b(t) = \exp \left\{ \frac{1}{\sqrt{\hbar}} \sum_{\alpha} \int_0^t dt' [\mu_{1\alpha}(t') - i\mu_{4\alpha}(t')] \bar{g}_{\alpha}(t') \right\}, \quad (7)$$

where we introduce the bath-induced stochastic fields:

$$\bar{g}_{\alpha}(t) = \text{Tr}_b \{ \hat{g}_{\alpha} \bar{\rho}_b(t) \} \quad (8)$$

with $\bar{\rho}_b(t) = \rho_b(t)/\text{Tr}_b \rho_b(t)$ the normalized density matrix for the random bath. Now comes a crucial step. We can change the measure of stochastic processes to absorb the trace of the bath; that is, we modify the Wiener process $W_{1\alpha}(t)$ as $W_{1\alpha}(t) + 2 \int_0^t dt' \bar{g}_{\alpha}(t')/\sqrt{\hbar}$. Complying with this, $\rho_s(t)$ will also change accordingly. The mathematical manipulation is nothing but the Girsanov transformation [56,57]. To illustrate this transformation clearly, we again resort to the discrete-time representation. Now inserting Eq. (7) into Eq. (6), one has

$$\begin{aligned} \tilde{\rho}_s(t) &= \int_{-\infty}^{\infty} \prod_{\alpha} \prod_{k=1}^4 \prod_{j=1}^N d\mu_{j,k\alpha} P(\mu_{j,k\alpha}) \\ &\times \exp \left\{ \frac{\Delta t}{\sqrt{\hbar}} \sum_{\alpha} \sum_{j=1}^N [\mu_{j,1\alpha} - i\mu_{j,4\alpha}] \bar{g}_{\alpha}(t_j) \right\} \\ &\times \rho_s(t, \{\mu_{j,k\alpha}\}). \end{aligned} \quad (9)$$

Note that in this expression one can put the contribution due to the bath-induced field into the distribution function $P(\mu_{j,1(4)\alpha})$, namely,

$$\begin{aligned} &\prod_{\alpha} P(\mu_{j,1\alpha}) P(\mu_{j,4\alpha}) \exp \left\{ \frac{\Delta t}{\sqrt{\hbar}} \sum_{\alpha} [\mu_{j,1\alpha} - i\mu_{j,4\alpha}] \bar{g}_{\alpha}(t_j) \right\} \\ &= \prod_{\alpha} P \left[\mu_{j,1\alpha} - \frac{1}{\sqrt{\hbar}} \bar{g}_{\alpha}(t_j) \right] P \left[\mu_{j,4\alpha} + \frac{i}{\sqrt{\hbar}} \bar{g}_{\alpha}(t_j) \right]. \end{aligned}$$

Now we define new variables $\tilde{\mu}_{j,1\alpha} = \mu_{j,1\alpha} - \bar{g}_{\alpha}(t_j)/\sqrt{\hbar}$, $\tilde{\mu}_{j,2\alpha} = \mu_{j,2\alpha}$, $\tilde{\mu}_{j,3\alpha} = \mu_{j,3\alpha}$, and $\tilde{\mu}_{j,4\alpha} = \mu_{j,4\alpha} + i\bar{g}_{\alpha}(t_j)/\sqrt{\hbar}$. Because both $\mu_{j,1\alpha}$ and $\mu_{j,4\alpha}$ are independent of $\bar{g}_{\alpha}(t_j)$, the Jacobian of the variable change is equal to one. With these new variables, therefore, Eq. (9) becomes

$$\begin{aligned} \tilde{\rho}_s(t) &= \int_{-\infty}^{\infty} \prod_{\alpha} \prod_{k=1}^4 \prod_{j=1}^N d\tilde{\mu}_{j,k\alpha} P(\tilde{\mu}_{j,k\alpha}) \\ &\times \rho_s \left(t, \left\{ \tilde{\mu}_{j,1\alpha} + \frac{1}{\sqrt{\hbar}} \bar{g}_{\alpha}(t_j), \tilde{\mu}_{j,2\alpha}, \tilde{\mu}_{j,3\alpha}, \tilde{\mu}_{j,4\alpha} \right. \right. \\ &\quad \left. \left. - \frac{i}{\sqrt{\hbar}} \bar{g}_{\alpha}(t_j) \right\} \right) = M\{\rho_s[t, \{\tilde{\mu}_{k\alpha}\}]\}, \end{aligned}$$

where the second equality results from the continuous representation. Notice that $\rho_s(t) \equiv \rho_s[t, \{\mu_{k\alpha}\}]$ satisfies Eq. (3). Changing the underlying random processes in Eq. (3) from $\{\mu_{k\alpha}\}$ to $\{\tilde{\mu}_{k\alpha}\}$, one obtains the equation for the *new* density

matrix $\rho_s(t) \equiv \rho_s[t, \{\tilde{\mu}_{k\alpha}\}]$,

$$\begin{aligned} i\hbar d\rho_s &= \left[\hat{H}_s + \sum_{\alpha} \bar{g}_{\alpha}(t) \hat{f}_{\alpha}, \rho_s \right] dt + \frac{\sqrt{\hbar}}{2} \sum_{\alpha} [\hat{f}_{\alpha}, \rho_s] dW_{1\alpha} \\ &+ i \frac{\sqrt{\hbar}}{2} \sum_{\alpha} \{ \hat{f}_{\alpha}, \rho_s \} dW_{2\alpha}^*. \end{aligned} \quad (10)$$

For brevity, here and in the following, the functional dependence of the random density matrix $\rho_s(t)$ on $\{\tilde{\mu}_{k\alpha}\}$ will not indicated explicitly.

Given $\bar{g}_{\alpha}(t)$, one needs only to solve the stochastic differential equation Eq. (10) and calculate the random average to obtain the exact reduced density matrix $\tilde{\rho}_s(t)$. The bath-induced field in general evokes fast motion, and thus $\rho_s(t)$ as well as the white noises to which $\rho_s(t)$ is subjected displays a smaller time scale than its average $\tilde{\rho}_s(t)$. In the following section we will consider the Caldeira-Leggett (CL) model for which the bath-induced field can be worked out explicitly. We would like to emphasize that in the CL model there is only one interaction term, while within the stochastic description one can deal with many interaction terms.

B. Caldeira-Leggett model

The Hamiltonian of a CL model reads

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(\hat{x}) + \frac{1}{2} \sum_{j=1}^N \left[\frac{\hat{p}_j^2}{m_j} + m_j \omega_j^2 \left(\hat{x}_j + \frac{c_j}{m_j \omega_j^2} \hat{x} \right)^2 \right], \quad (11)$$

where the first two terms define the Hamiltonian of the system and the third one induces the Hamiltonian of the bath, the interaction, and a counterterm. The last can directly be read off as

$$V'(\hat{x}) \equiv \frac{1}{2} M \hat{x}^2 \tilde{\omega}^2,$$

where

$$\tilde{\omega}^2 = \sum_j \frac{c_j^2}{M m_j \omega_j^2} = \frac{2}{M\pi} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega}. \quad (12)$$

$J(\omega)$ is the spectral density function

$$J(\omega) = \frac{\pi}{2} \sum_j \left[\frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j) \right], \quad (13)$$

which exactly characterizes the effect of the environment. In general the system-bath linear coupling not only provides a dissipation mechanism for the system but also tends to renormalize the potential $V(\hat{x})$. To compensate for this renormalization effect the counterterm is introduced. It ensures that the system cannot lower its potential energy below the original uncoupled value [13].

Assume that the initial state of the bath is in a thermal equilibrium state for the noninteracting harmonic oscillators, that is, $\rho_b(0) = e^{-\beta \hat{H}_b} / \text{Tr}_b \{ e^{-\beta \hat{H}_b} \}$. Because of the linearity, the dynamics of the random bath described by Eq. (4) is analytically solvable. Moreover, since there are no interactions among the bath modes, the evolution of the bath is fully

determined by that of the individual mode. In other words, the solution of Eq. (4) can be written as

$$\rho_b(t) = \prod_j u_{j,1}(t,0)\rho_b(0) \prod_j u_{j,2}(0,t), \quad (14)$$

where $u_{j,1}(t,0)$ is the forward propagator of the mode j dictated by the Hamiltonian

$$\hat{h}_{1,j}(t) = \left(\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2}m_j\hat{x}_j^2\omega_j^2 \right) + \frac{\sqrt{\hbar}}{2}v_+(t)c_j\hat{x}_j,$$

and $u_{j,2}(0,t)$ is the backward propagator dictated by

$$\hat{h}_{2,j}(t) = \left(\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2}m_j\hat{x}_j^2\omega_j^2 \right) + \frac{\sqrt{\hbar}}{2}v_-(t)c_j\hat{x}_j$$

with the stochastic fields $v_{\pm}(t) = \mu_2(t) + i\mu_3(t) \pm i\mu_1(t) \pm \mu_4(t)$. For a driven harmonic oscillator

$$\hat{h}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 + v(t)\hat{x}, \quad (15)$$

its corresponding propagator $u(t,0)$ can be worked out in terms of the operator algebra method [58]. To do this, it would be better to work in the second quantization formalism. Now we introduce the creation and annihilation operators,

$$a^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2\hbar m\omega_0}}\hat{p} \quad (16)$$

and

$$a = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2\hbar m\omega_0}}\hat{p}. \quad (17)$$

From the commutation relation $[\hat{x}, \hat{p}] = i\hbar$, one readily finds $[a, a^\dagger] = 1$. The Hamiltonian Eq. (15) then becomes

$$\hat{h}(t) = \hat{h}_0 + \sqrt{\frac{\hbar}{2m\omega_0}}v(t)(a + a^\dagger),$$

where $\hat{h}_0 = \hbar\omega_0(a^\dagger a + 1/2)$ is the Hamiltonian of an isolated harmonic oscillator. The propagator $u_0(t,0)$ dictated by \hat{h}_0 has been well known, and the result can be found in several textbooks [24,59–61]. For the driven case one uses the interaction representation to have

$$i\hbar \frac{\partial u_I(t,0)}{\partial t} = \sqrt{\frac{\hbar}{2m\omega_0}}v(t)(ae^{-i\omega_0 t} + a^\dagger e^{i\omega_0 t})u_I(t,0)$$

with the initial condition $u_I(0,0) = 1$. Resorting to the Baker-Campbell-Hausdorff formula [62], we readily obtain

$$u_I(t,0) = \exp[d(t)a] \exp[b(t)a^\dagger] \exp[j(t)], \quad (18)$$

where

$$d(t) = -\frac{i}{\sqrt{2m\hbar\omega_0}} \int_0^t dt_1 \exp(-i\omega_0 t_1) v(t_1),$$

$$b(t) = -\frac{i}{\sqrt{2m\hbar\omega_0}} \int_0^t dt_1 \exp(i\omega_0 t_1) v(t_1),$$

and

$$j(t) = \frac{1}{2m\hbar\omega_0} \int_0^t dt_1 \int_0^{t_1} dt_2 v(t_1)v(t_2) \exp[i\omega_0(t_1 - t_2)].$$

Upon using Eqs. (16) and (17) and Baker-Campbell-Hausdorff formula again, the propagator $u_I(t,0)$ becomes

$$\begin{aligned} u_I(t,0) &= \exp \left\{ \sqrt{\frac{m\omega_0}{2\hbar}} [d(t) + b(t)] \hat{x} \right\} \\ &\times \exp \left\{ \frac{i}{\sqrt{2m\hbar\omega_0}} [d(t) - b(t)] \hat{p} \right\} \\ &\times \exp \left\{ \frac{1}{4} [d^2(t) - b^2(t)] \right\}. \end{aligned}$$

Finally with the given expressions of $u_0(t,0)$ and $u_I(t,0)$ the propagator $u(t,0) = u_0(t,0)u_I(t,0)$ is also available. Therefore, we propose a straightforward procedure to calculate $u_{j,1}(t,0)$ and $u_{j,2}(t,0)$. Inserting these results into Eq. (8) and calculating the trace we finally find

$$\begin{aligned} \bar{g}(t) &= \sqrt{\hbar} \int_0^t dt' \{ \alpha_R(t-t') [\mu_1(t') - i\mu_4(t')] \\ &+ \alpha_I(t-t') [\mu_2(t') + i\mu_3(t')] \}, \quad (19) \end{aligned}$$

where $\alpha_{R,I}(t)$ turn out to be the real and imaginary parts of the autocorrelation function of the “force” $\hat{g} = \sum_j c_j \hat{x}_j$, namely,

$$\begin{aligned} \alpha(t) &= \text{Tr}_b \{ \rho_b(0) \hat{g}(t) \hat{g}(0) \} = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \\ &\times \left[\coth \left(\frac{\hbar\beta\omega}{2} \right) \cos \omega t - i \sin \omega t \right] \quad (20) \end{aligned}$$

with $\hat{g}(t) = e^{i\hat{H}_b t/\hbar} \hat{g} e^{-i\hat{H}_b t/\hbar}$. One can see that $\alpha_R(t)$ is dependent on temperature, reflecting dissipation effects contributed from both quantum and “classical” motion, while $\alpha_I(t)$ is independent of temperature, embodying a pure quantum effect.

C. Formal solution

As one can understand, we start from Eq. (10), the working equation in the framework of stochastic description. The formal solution of this linear equation is [28]

$$\rho_s(t) = U_1(t,0)\rho_s(0)U_2(0,t), \quad (21)$$

where $U_1(t,0)$ is the forward propagator of the stochastic system associated with the Hamiltonian

$$\hat{H}_1(t) = \hat{H}_s + \sum_\alpha \left[\bar{g}_\alpha(t) + \frac{\sqrt{\hbar}}{2} \eta_{+\alpha}(t) \right] \hat{f}_\alpha, \quad (22)$$

while $U_2(0,t)$ is the backward propagator associated with the Hamiltonian

$$\hat{H}_2(t) = \hat{H}_s + \sum_\alpha \left[\bar{g}_\alpha(t) + \frac{\sqrt{\hbar}}{2} \eta_{-\alpha}(t) \right] \hat{f}_\alpha \quad (23)$$

with $\eta_{\pm\alpha}(t) = \mu_{1\alpha}(t) + i\mu_{4\alpha}(t) \pm i\mu_{2\alpha}(t) \pm \mu_{3\alpha}(t)$. When we can take stochastic average of random density matrix $\rho_s(t)$ in principle, we can obtain the exact reduced density matrix $\bar{\rho}_s(t)$. To derive the equation of motion for $\bar{\rho}_s(t)$ or the master equation, however, it would be better to start from Eq. (10). Whenever the statistical average of the right-hand side of Eq. (10) can be expressed explicitly in terms of $\bar{\rho}_s(t)$ and other known operators of the system, one obtains a master equation.

To acquire the deterministic equation from the corresponding stochastic differential equation for arbitrary noises is a challenging, if not impossible, task [63–66]. In the literature, one may find incorrect results about the derivation of the deterministic equation for Gaussian noises and similar statements in developing a master equation for open systems [67].

For the Caldeira-Leggett model, upon substituting the expression of the bath-induced fields Eq. (19) and carrying out the stochastic averaging, Eq. (10) becomes

$$i\hbar \frac{d\tilde{\rho}_s(t)}{dt} = [\hat{H}_s, \tilde{\rho}_s(t)] + \left[\hat{x}, \int_0^t dt' \alpha_R(t-t') M\{\rho_{s,1}(t, t')\} \right] + \left[\hat{x}, \int_0^t dt' \alpha_I(t-t') M\{\rho_{s,2}(t, t')\} \right], \quad (24)$$

where $\rho_{s,1}(t, t') = \sqrt{\hbar}[\mu_1(t') - i\mu_4(t')]\rho_s(t)$ and $\rho_{s,2}(t, t') = \sqrt{\hbar}[\mu_2(t') + i\mu_3(t')]\rho_s(t)$. In the above derivation the nonanticipating property of $\rho_s(t)$, namely, $M\{\rho_s(t) dW_{1(2)}(t)\} = 0$, is used. It is obvious that when there is no dissipation, only the first term remains on the right-hand side of Eq. (24). Of course, this is the Liouville equation of the system, as it should be. As the stochastic fields are added, the other two terms naturally come out. These terms lead to the irreversibility caused by the coupling to the bath *à la* its induced random fields. To obtain the expressions of $M\{\rho_{s,1(2)}(t, t')\}$ we resort to the Furutsu-Novikov theorem [68], that is,

$$M\{\mu(t')F[\mu]\} = M\left\{ \frac{\delta F[\mu]}{\delta \mu(t')} \right\} \quad (25)$$

for a white noise $\mu(t)$ and its arbitrary functional $F[\mu]$. Using this theorem allows us to write

$$M\{\rho_{s,1}(t, t')\} = \sqrt{\hbar} M\left\{ \frac{\delta \rho_s(t)}{\delta \mu_1(t')} - i \frac{\delta \rho_s(t)}{\delta \mu_4(t')} \right\} \equiv \hat{O}_{s,1}(t, t')$$

and

$$M\{\rho_{s,2}(t, t')\} = \sqrt{\hbar} M\left\{ \frac{\delta \rho_s(t)}{\delta \mu_2(t')} + i \frac{\delta \rho_s(t)}{\delta \mu_3(t')} \right\} \equiv \hat{O}_{s,2}(t, t').$$

Therefore, $M\{\rho_{s,1(2)}(t, t')\}$ in Eq. (24) can be replaced, respectively, by $\hat{O}_{s,1(2)}(t, t')$. For brevity, they are called the dissipation operators. With the formal solution of $\rho_s(t)$ [Eq. (21)], one can directly work out the expression of the functional derivatives

$$\hat{O}_{s,1}(t, t') = -iM\{\hat{x}_1(t, t')\rho_s(t) - \rho_s(t)\hat{x}_2(t, t')\} \quad (26)$$

and

$$\hat{O}_{s,2}(t, t') = M\{\hat{x}_1(t, t')\rho_s(t) + \rho_s(t)\hat{x}_2(t, t')\}, \quad (27)$$

where $\hat{x}_1(t, t') = U_1(t, t')\hat{x}U_1(t', t)$ and $\hat{x}_2(t, t') = U_2(t, t')\hat{x}U_2(t', t)$ are the Heisenberg operators. To build up a master equation, of course, we still need to find the expressions of $\hat{O}_{s,1(2)}(t, t')$ in terms of $\tilde{\rho}_s(t)$ and other known operators.

Some comments are in order. For arbitrary response functions $\alpha_{R(I)}(t)$, deriving the master equation relies on whether the explicit expressions of dissipative operators $\hat{O}_{s,1(2)}(t, t')$

can be worked out. However, when $\alpha_{R(I)}(t)$ are localized distribution functions, say, $\alpha_{R(I)}(t) = \tilde{\alpha}_{R(I)}\delta(t)$, Eq. (24) becomes

$$i\hbar \frac{d\tilde{\rho}_s(t)}{dt} = [\hat{H}_s, \tilde{\rho}_s(t)] + [\hat{x}, \tilde{\alpha}_R M\{\rho_{s,1}(t, t)\}] + [\hat{x}, \tilde{\alpha}_I M\{\rho_{s,2}(t, t)\}]. \quad (28)$$

From Eqs. (26) and (27), we know $M\{\rho_{s,1}(t, t)\} = -i[\hat{x}, \tilde{\rho}_s(t)]$ and $M\{\rho_{s,2}(t, t)\} = \{\hat{x}, \tilde{\rho}_s(t)\}$. Inserting into Eq. (28) yields the master equation

$$i\hbar \frac{d\tilde{\rho}_s(t)}{dt} = [\hat{H}_s, \tilde{\rho}_s(t)] - i\tilde{\alpha}_R[\hat{x}, [\hat{x}, \tilde{\rho}_s(t)]] + \tilde{\alpha}_I[\hat{x}, \{\hat{x}, \tilde{\rho}_s(t)\}]. \quad (29)$$

Therefore, both the specificities of the system and the bath-induced field determine the “existence” of the master equation.

III. DERIVATION OF MASTER EQUATION

Now we shall derive the master equation of a dissipative harmonic oscillator described by the Caldeira-Leggett model with $V(\hat{x}) = M\omega_0^2\hat{x}^2/2$. As discussed above, the system-bath coupling modifies the potential of the system by addition of a counterterm. In the present case the frequency of the harmonic oscillator becomes a renormalized one,

$$\omega^2 = \omega_0^2 + \tilde{\omega}^2.$$

To acquire the master equation we use the equation of motion in the Heisenberg representation to find the operators $\hat{x}_{1(2)}(t, t')$ in Eqs. (26) and (27). After some algebra we obtain

$$\hat{x}_{1(2)}(t, t') = \cos \omega(t-t')\hat{x} - \frac{\sin \omega(t-t')}{M\omega}\hat{p} - \frac{1}{M\omega} \int_{t'}^t dt_1 \times \sin \omega(t_1-t') \left[\tilde{g}(t_1) + \frac{\sqrt{\hbar}}{2}\eta_{\pm}(t_1) \right].$$

Inserting into Eqs. (26) and (27) and carrying out the involved stochastic averaging, we find

$$\begin{aligned} \hat{O}_{s,1}(t, t') &= -i \cos \omega(t-t')[\hat{x}, \tilde{\rho}_s(t)] + \frac{i}{M\omega} \sin \omega(t-t')[\hat{p}, \tilde{\rho}_s(t)] \\ &+ \frac{2}{M\omega} \int_{t'}^t dt_1 \int_{t_1}^t dt_2 \sin \omega(t_1-t')\alpha_I(t_1-t_2)\hat{O}_{s,1}(t, t_2) \end{aligned} \quad (30)$$

and

$$\begin{aligned} \hat{O}_{s,2}(t, t') &= \cos \omega(t-t')\{\hat{x}, \tilde{\rho}_s(t)\} - \frac{\sin \omega(t-t')}{M\omega}\{\hat{p}, \tilde{\rho}_s(t)\} \\ &- \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1-t')\alpha_R(t_1-t_2)\hat{O}_{s,1}(t, t_2) \\ &- \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1-t')\alpha_I(t_1-t_2)\hat{O}_{s,2}(t, t_2). \end{aligned} \quad (31)$$

In the derivation we have used the following functional derivatives:

$$M \left\{ \frac{\delta \rho_s(t)}{\delta \mu_1(t')} + i \frac{\delta \rho_s(t)}{\delta \mu_4(t')} \right\} = \frac{2}{\sqrt{\hbar}} \int_{t'}^t dt_1 \alpha_R(t_1 - t') \hat{O}_{s,1}(t, t_1)$$

and

$$M \left\{ \frac{\delta \rho_s(t)}{\delta \mu_2(t')} - i \frac{\delta \rho_s(t)}{\delta \mu_3(t')} \right\} = \frac{2}{\sqrt{\hbar}} \int_{t'}^t dt_1 \alpha_I(t_1 - t') \hat{O}_{s,1}(t, t_1),$$

which are also readily obtained with the formal solution of $\rho_s(t)$ and the Furutsu-Novikov theorem. For the integral equations (30) and (31) one can employ iteration to show that their solutions $\hat{O}_{s,1(2)}(t, t')$ possess the following forms:

$$\hat{O}_{s,1}(t, t') = x_{11}(t, t') [\hat{p}, \tilde{\rho}_s(t)] + x_{12}(t, t') [\hat{x}, \tilde{\rho}_s(t)] \quad (32)$$

and

$$\hat{O}_{s,2}(t, t') = x_{21}(t, t') \{\hat{x}, \tilde{\rho}_s(t)\} + x_{22}(t, t') \{\hat{p}, \tilde{\rho}_s(t)\} + x_{23}(t, t') [\hat{p}, \tilde{\rho}_s(t)] + x_{24}(t, t') [\hat{x}, \tilde{\rho}_s(t)]. \quad (33)$$

Because the operators $[\hat{x}, \tilde{\rho}_s(t)]$, $[\hat{p}, \tilde{\rho}_s(t)]$, $\{\hat{x}, \tilde{\rho}_s(t)\}$, and $\{\hat{p}, \tilde{\rho}_s(t)\}$ are arbitrary, their coefficients $x_{jk}(t, t')$ in Eqs. (32) and (33) are determined by Eqs. (30) and (31), which satisfy the following integral equations:

$$x_{11}(t, t') = \frac{i}{M\omega} \sin \omega(t - t') + \frac{2}{M\omega} \int_{t'}^t dt_1 \int_{t_1}^t dt_2 \sin \omega(t_1 - t') \times \alpha_I(t_1 - t_2) x_{11}(t, t_2), \quad (34)$$

$$x_{12}(t, t') = -i \cos \omega(t - t') + \frac{2}{M\omega} \int_{t'}^t dt_1 \int_{t_1}^t dt_2 \sin \omega(t_1 - t') \times \alpha_I(t_1 - t_2) x_{12}(t, t_2), \quad (35)$$

$$x_{21}(t, t') = \cos \omega(t - t') - \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1 - t') \times \alpha_I(t_1 - t_2) x_{21}(t, t_2), \quad (36)$$

$$x_{22}(t, t') = -\frac{\sin \omega(t - t')}{M\omega} - \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1 - t') \times \alpha_I(t_1 - t_2) x_{22}(t, t_2), \quad (37)$$

$$x_{23}(t, t') = -\frac{2}{M\omega} \int_{t'}^t dt_1 \sin \omega(t_1 - t') \left[\int_0^{t_1} dt_2 \alpha_R(t_1 - t_2) \times x_{11}(t, t_2) + \int_0^{t_1} dt_2 \alpha_I(t_1 - t_2) x_{23}(t, t_2) \right], \quad (38)$$

and

$$x_{24}(t, t') = -\frac{2}{M\omega} \int_{t'}^t dt_1 \sin \omega(t_1 - t') \times \left[\int_0^{t_1} dt_2 \alpha_R(t_1 - t_2) x_{12}(t, t_2) + \int_0^{t_1} dt_2 \alpha_I(t_1 - t_2) x_{24}(t, t_2) \right]. \quad (39)$$

With these expressions at hand, Eq. (24) immediately becomes the desired master equation, namely,

$$i\hbar \frac{d\tilde{\rho}_s(t)}{dt} = [\hat{H}_s, \tilde{\rho}_s(t)] + A_1(t) [\hat{x}, \{\hat{x}, \tilde{\rho}_s(t)\}] + A_2(t) [\hat{x}, \{\hat{p}, \tilde{\rho}_s(t)\}] + A_3(t) [\hat{x}, [\hat{p}, \tilde{\rho}_s(t)]] + A_4(t) [\hat{x}, [\hat{x}, \tilde{\rho}_s(t)]], \quad (40)$$

where $\hat{H}_s = \hat{p}^2/(2M) + M\omega^2 \hat{x}^2/2$ and the coefficients are

$$A_1(t) = \int_0^t dt' \alpha_I(t - t') x_{21}(t, t'), \quad (41)$$

$$A_2(t) = \int_0^t dt' \alpha_I(t - t') x_{22}(t, t'), \quad (42)$$

$$A_3(t) = \int_0^t dt' [\alpha_R(t - t') x_{11}(t, t') + \alpha_I(t - t') x_{23}(t, t')], \quad (43)$$

and

$$A_4(t) = \int_0^t dt' [\alpha_R(t - t') x_{12}(t, t') + \alpha_I(t - t') x_{24}(t, t')]. \quad (44)$$

As clearly clarified in the literature [38,39], $A_1(t)$ is the coefficient for the frequency shift because $[\hat{x}, \{\hat{x}, \tilde{\rho}_s(t)\}] = [\hat{x}^2, \tilde{\rho}_s(t)]$, $A_2(t)$ is a quantum dissipation term, $A_3(t)$ reflects the anomalous quantum diffusion, while $A_4(t)$ is the coefficient for the normal quantum diffusion.

IV. EQUIVALENCE TO THE HU-PAZ-ZHANG EQUATION

The master equation and the dynamics of the dissipative harmonic oscillator have been derived and studied by several researchers with diversified methods [35–50]. Dekker used the canonical quantization method [35], while Haake and Reibold employed the Wigner function method. The latter also studied the low-temperature and strong-damping anomalies [36]. Grabert, Schramm, and Ingold went beyond the factorized initial condition [37]. It would be stressed that the master equation in a general environment was derived by Hu, Paz, and Zhang (HPZ) by virtue of path-integral technique [38]. An elementary derivation of the HPZ equation was documented by Halliwell and Yu with the Wigner function approach [39]. Karrlein and Grabert pointed out that there is an exact dissipative Liouville operator for certain correlated initial conditions [40]. The master equation was also considered by Calzetta *et al.* through a stochastic method based on the quantum Langevin equation [41]. Ford and O'Connell [42] rederived the HPZ equation with the quantum Langevin equation method and also analyzed its solution. Strunz and Yu offered an alternative derivation, using the quantum trajectory method [43]. The HPZ master equation has recently been used by Chou, Yu, and Hu to derive the master equation of two and more coupled harmonic oscillators in a bosonic bath [44,45]. Furthermore, the HPZ master equation was extended by Xu *et al.* [46] to the case where time-dependent external fields are applied.

For convenience of comparison, we will always use the results in the paper by Halliwell and Yu [39]. The HPZ master

equation takes the same form as Eq. (40). The corresponding coefficients in our notation read

$$B_1(t) = \int_0^t dt' \alpha_I(t-t') \bar{x}_{21}(t, t'), \quad (45)$$

$$B_2(t) = \int_0^t dt' \alpha_I(t-t') \bar{x}_{22}(t, t'), \quad (46)$$

$$B_3(t) = \int_0^t dt' [\alpha_R(t-t') \bar{x}_{11}(t, t') + \alpha_I(t-t') \bar{x}_{23}(t, t')], \quad (47)$$

and

$$B_4(t) = \int_0^t dt' [\alpha_R(t-t') \bar{x}_{12}(t, t') + \alpha_I(t-t') \bar{x}_{24}(t, t')], \quad (48)$$

where

$$\bar{x}_{21}(t, t') = u_2(t') - \frac{\dot{u}_2(t)}{\dot{u}_1(t)} u_1(t'), \quad (49)$$

$$\bar{x}_{22}(t, t') = \frac{u_1(t')}{M \dot{u}_1(t)}, \quad (50)$$

$$\bar{x}_{11}(t, t') = \frac{i}{M} G_1(t, t'), \quad (51)$$

$$\bar{x}_{12}(t, t') = -i G'_1(t, t'), \quad (52)$$

$$\bar{x}_{23}(t, t') = \frac{2i}{M^2} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \alpha_R(t_1 - t_2) G_1(t, t_2) G_2(t', t_1), \quad (53)$$

and

$$\bar{x}_{24}(t, t') = -\frac{2i}{M} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \alpha_R(t_1 - t_2) G'_1(t, t_2) G_2(t', t_1). \quad (54)$$

Here the dot over $u_j(t)$ ($j = 1, 2$) stands for the derivative with respect to t , and the functions $u_j(t)$ are the solutions of the homogeneous integro-differential equation

$$\left(\frac{d^2}{dt^2} + \omega^2 \right) u(t) + \frac{2}{M} \int_0^t dt' \alpha_I(t-t') u(t') = 0 \quad (55)$$

with inhomogeneous boundary conditions $u_1(0) = 1$, $u_1(t) = 0$ and $u_2(0) = 0$, $u_2(t) = 1$ and $G_j(t_1, t_2)$ ($j = 1, 2$) are the Green's functions obeying

$$\left(\frac{d^2}{dt_1^2} + \omega^2 \right) G(t_1, t_2) + \frac{2}{M} \int_0^{t_1} dt_3 \alpha_I(t_1 - t_3) G(t_3, t_2) = \delta(t_1 - t_2) \quad (56)$$

with specified initial conditions at the fixed initial and final times $G_1(t_1 = 0, t_2) = 0$, $G'_1(t_1 = 0, t_2) = 0$ and $G_2(t_1 = t, t_2) = 0$, $G'_2(t_1 = t, t_2) = 0$. Here the prime in $G'_j(t_1, t_2)$ stands for the derivative with respect to the first variable, that is, $G'_j(t_1, t_2) = \partial G_j(t_1, t_2) / \partial t_1$. Because of causality $G_1(t_1, t_2) = 0$ for $t_1 < t_2$, while $G_2(t_1, t_2) = 0$ for $t_1 > t_2$.

Now we show that the HPZ equation and that derived with the stochastic formulation are identical. To this end we need only to prove that $A_j(t) = B_j(t)$ ($j = 1 - 4$), respectively. As clearly shown in Eqs. (41)–(44) and (45)–(48), all functions $A_j(t)$ and the counterparts $B_j(t)$ are integrals over the time range $[0, t]$. Therefore, a sufficient condition for $A_j(t) = B_j(t)$ is that the corresponding integrands are the same. Besides,

because these integrands consist of factors $\alpha_{R(I)}(t)$ that are dependent on the specificity of the dissipation and can be arbitrary, one can further simplify the proof significantly.

A. Proof of $A_1(t) = B_1(t)$, $A_2(t) = B_2(t)$

To prove $A_1(t) = B_1(t)$, one should prove $x_{21}(t, t') = \bar{x}_{21}(t, t')$. Note that $u_j(t)$ satisfy linear differential Eq. (55). Because $\bar{x}_{21}(t, t')$ is a linear combination of $u_1(t')$ and $u_2(t')$, as a function of t' , it should also obey Eq. (55),

$$\left(\frac{\partial^2}{\partial t'^2} + \omega^2 \right) \bar{x}_{21}(t, t') = -\frac{2}{M} \int_0^{t'} dt_1 \alpha_I(t' - t_1) \bar{x}_{21}(t, t_1). \quad (57)$$

On the other hand, from the integral Eq. (36) we can show by a straightforward algebra that calculating the second-order derivative of $x_{21}(t, t')$ on both sides, one can obtain the equation that is the same as Eq. (57). Moreover, $x_{21}(t, t')|_{t'=t} = \bar{x}_{21}(t, t')|_{t'=t} = 1$ and $\partial x_{21}(t, t') / \partial t'|_{t'=t} = \partial \bar{x}_{21}(t, t') / \partial t'|_{t'=t} = 0$, and the initial conditions are the same. Therefore, $A_1(t)$ is identical with $B_1(t)$. Along the same line, one can prove $A_2(t) = B_2(t)$.

B. Proof of $A_3(t) = B_3(t)$, $A_4(t) = B_4(t)$

As pointed out above, the problem of proving $A_3(t) = B_3(t)$ can be changed to proving the equivalence of the two involved integrands. That is, one needs to show $x_{11}(t, t') = \bar{x}_{11}(t, t')$ and $x_{23}(t, t') = \bar{x}_{23}(t, t')$.

Let us look at Eq. (56) with the initial condition $G_1(0, t_2) = 0$ and $G'_1(0, t_2) = 0$. Suppose the second term on the left-hand side is given. Then Eq. (56) can be viewed as a function of t_1 and can be “solved” with the Green's function method. Now the required Green's function obeys

$$\left(\frac{d^2}{dt_1^2} + \omega^2 \right) \bar{G}(t_1, \tau) = \delta(t_1 - \tau)$$

with $\bar{G}(t_1, \tau)|_{t_1 < \tau} = 0$ and $\partial \bar{G}(t_1, \tau) / \partial t_1|_{t_1 < \tau} = 0$. Its solution is

$$\bar{G}(t_1, \tau) = \frac{\sin \omega(t_1 - \tau)}{\omega} \theta(t_1 - \tau).$$

Therefore, the “solution” of Eq. (56) can be written as

$$\begin{aligned} G_1(t_1, t_2) &= \int_0^{t_1} d\tau \bar{G}(t_1, \tau) \\ &\times \left[\delta(\tau - t_2) - \frac{2}{M} \int_{t_2}^{\tau} dt_4 \alpha_I(\tau - t_4) G_1(t_4, t_2) \right] \\ &= \frac{\sin \omega(t_1 - t_2)}{\omega} - \frac{2}{M\omega} \int_{t_2}^{t_1} dt_3 \\ &\times \int_{t_2}^{t_3} dt_4 \sin \omega(t_1 - t_3) \alpha_I(t_3 - t_4) G_1(t_4, t_2). \end{aligned}$$

Substituting into Eq. (51) yields

$$\begin{aligned} \bar{x}_{11}(t, t') &= \frac{i}{M\omega} \sin \omega(t - t') - \frac{2}{M\omega} \int_{t'}^t dt_1 \\ &\times \int_{t'}^{t_1} dt_2 \sin \omega(t - t_1) \alpha_I(t_1 - t_2) \bar{x}_{11}(t_2, t'). \quad (58) \end{aligned}$$

Note that from Eq. (20) one can see $\alpha_I(t_1 - t_2) = -\alpha_I(t_2 - t_1)$. Making a change of integration orders and variables in the double integral then leads to

$$\begin{aligned} \bar{x}_{11}(t, t') &= \frac{i}{M\omega} \sin \omega(t - t') + \frac{2}{M\omega} \int_{t'}^t dt_1 \\ &\times \int_{t_1}^t dt_2 \sin \omega(t - t_2) \alpha_I(t_1 - t_2) \bar{x}_{11}(t_1, t'), \end{aligned} \quad (59)$$

which is an integral equation of $\bar{x}_{11}(t, t')$ with respect to the first argument t . Now we show that $\bar{x}_{11}(t, t')$ determined by Eq. (59) is identical with $x_{11}(t, t')$ solved from Eq. (34), which is an integral equation with respect to the second argument t' . To this end, we discretize the variables t and t' so that $x_{11}(t, t')$ and $\bar{x}_{11}(t, t')$ can be represented as matrices. To be specific, the elements of matrices X_0 , X , X' , and α take the discretized values of $x_0(t, t')$, $x_{11}(t, t')$, $\bar{x}_{11}(t, t')$, and $\alpha(t - t')$, respectively. Here $x_0(t, t') = \sin \omega(t - t')$ is introduced. With these matrices, the integrals in Eqs. (34) and (59) become matrix products,

$$X = X_0 - X\alpha X_0 \quad (60)$$

and

$$X' = X_0 - X_0\alpha X'. \quad (61)$$

Solving these matrix equations with elementary algebraic manipulations, we find

$$X = X_0(\mathbf{1} + \alpha X_0)^{-1} \quad (62)$$

and

$$X' = (\mathbf{1} + X_0\alpha)^{-1} X_0. \quad (63)$$

Because $(\mathbf{1} + X_0\alpha)X_0 = X_0(\mathbf{1} + \alpha X_0)$, one immediately obtains $X = X'$. Therefore, we find $x_{11}(t, t') = \bar{x}_{11}(t, t')$. Thus, Eq. (51) can be recast as $G_1(t, t') = -iMx_{11}(t, t')$. Substituting into Eq. (53) leads to

$$\begin{aligned} \bar{x}_{23}(t, t') &= \frac{2}{M} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \alpha_R(t_1 - t_2) x_{11}(t, t_2) G_2(t', t_1). \end{aligned} \quad (64)$$

We now treat $G_2(t_1, t_2)$ in the same way as we did for $G_1(t_1, t_2)$ in the above. As a result, $G_2(t_1, t_2)$ satisfies the following integral equation:

$$\begin{aligned} G_2(t_1, t_2) &= \frac{\sin \omega(t_1 - t_2)}{\omega} - \frac{2}{M\omega} \int_{t_1}^t dt_3 \\ &\times \int_0^{t_3} dt_4 \sin \omega(t_3 - t_1) \alpha_I(t_3 - t_4) G_2(t_4, t_2). \end{aligned} \quad (65)$$

Inserting into Eq. (64) and rearranging, we find the integral equation of $\bar{x}_{23}(t, t')$ is identical with that of $x_{23}(t, t')$, Eq. (38). Therefore, $\bar{x}_{23}(t, t') = x_{23}(t, t')$. Similarly, we can demonstrate the equality $A_4(t) = B_4(t)$.

V. MASTER EQUATION OF DRIVEN HARMONIC OSCILLATOR

Consider a dissipative harmonic oscillator driven by general external time-dependent fields [46–49] with Hamiltonian

$$\hat{H}_s(t) = \frac{\hat{p}^2}{2M} + \frac{1}{2}M\omega^2 \hat{x}^2 + f_1(t)\hat{x} + f_2(t)\hat{p}.$$

We shall work out the master equation in the driving case along the same line of deriving the master equation of the dissipative harmonic oscillator in Sec. III. Note that for the external time-dependent fields that act only on the system, the bath-induced field is the same as that without driving fields. We can thus start from Eqs. (26) and (27). By solving the equations of motion for the Heisenberg operators and taking stochastic averaging, we find

$$\begin{aligned} \hat{O}_{s,1}(t, t') &= -i \cos \omega(t - t') [\hat{x}, \tilde{\rho}_s(t)] + \frac{i}{M\omega} \sin \omega(t - t') [\hat{p}, \tilde{\rho}_s(t)] \\ &+ \frac{2}{M\omega} \int_{t'}^t dt_1 \int_{t_1}^t dt_2 \sin \omega(t_1 - t') \alpha_I(t_1 - t_2) \hat{O}_{s,1}(t, t_2) \end{aligned}$$

and

$$\begin{aligned} \hat{O}_{s,2}(t, t') &= \cos \omega(t - t') \{\hat{x}, \tilde{\rho}_s(t)\} - \frac{\sin \omega(t - t')}{M\omega} \{\hat{p}, \tilde{\rho}_s(t)\} \\ &- \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1 - t') \alpha_R(t_1 - t_2) \hat{O}_{s,1}(t, t_2) \\ &- \frac{2}{M\omega} \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1 - t') \alpha_I(t_1 - t_2) \hat{O}_{s,2}(t, t_2) \\ &- \frac{2}{M\omega} \int_{t'}^t dt_1 \sin \omega(t_1 - t') f_1(t_1) \tilde{\rho}_s(t) - 2 \int_{t'}^t dt_1 \\ &\times \cos \omega(t_1 - t') f_2(t_1) \tilde{\rho}_s(t). \end{aligned}$$

Similar to the undriven case, these dissipation operators possess the following forms:

$$\hat{O}_{s,1}(t, t') = x_{11}(t, t') [\hat{p}, \tilde{\rho}_s(t)] + x_{12}(t, t') [\hat{x}, \tilde{\rho}_s(t)]$$

and

$$\begin{aligned} \hat{O}_{s,2}(t, t') &= x_{21}(t, t') \{\hat{x}, \tilde{\rho}_s(t)\} + x_{22}(t, t') \{\hat{p}, \tilde{\rho}_s(t)\} \\ &+ x_{23}(t, t') [\hat{p}, \tilde{\rho}_s(t)] + x_{24}(t, t') [\hat{x}, \tilde{\rho}_s(t)] \\ &+ x_{25}(t, t') \tilde{\rho}_s(t), \end{aligned}$$

where all coefficients $x_{jk}(t, t')$ except $x_{25}(t, t')$ are the same as that of undriven case [Eqs. (34)–(39)]. The new term is determined by

$$\begin{aligned} x_{25}(t, t') &= -\frac{2}{M\omega} \int_{t'}^t dt_1 \sin \omega(t_1 - t') f_1(t_1) - 2 \\ &\times \int_{t'}^t dt_1 \cos \omega(t_1 - t') f_2(t_1) - \frac{2}{M\omega} \\ &\times \int_{t'}^t dt_1 \int_0^{t_1} dt_2 \sin \omega(t_1 - t') \alpha_I(t_1 - t_2) x_{25}(t, t_2). \end{aligned}$$

Therefore, substituting $M\{\rho_{s,1(2)}(t,t')\}$ by $\hat{O}_{s,1(2)}(t,t')$ in Eq. (24) yields the required master equation:

$$\begin{aligned} i\hbar \frac{d\tilde{\rho}_s(t)}{dt} = & [\hat{H}_{\text{eff}}(t), \tilde{\rho}_s(t)] + A_1(t)[\hat{x}, \{\hat{x}, \tilde{\rho}_s(t)\}] \\ & + A_2(t)[\hat{x}, \{\hat{p}, \tilde{\rho}_s(t)\}] + A_3(t)[\hat{x}, [\hat{p}, \tilde{\rho}_s(t)]] \\ & + A_4(t)[\hat{x}, [\hat{x}, \tilde{\rho}_s(t)]], \end{aligned}$$

where the effective Hamiltonian $\hat{H}_{\text{eff}}(t)$ is

$$\hat{H}_{\text{eff}}(t) = \hat{H}_s(t) + \hat{x} \int_0^t dt' \alpha_I(t-t') x_{25}(t,t').$$

Here again, the coefficients $A_j(t)$ ($j = 1 - 4$) are the same as that of the undriven case, which are given through Eqs. (41)–(44). It is obvious that the second term in $\hat{H}_{\text{eff}}(t)$ reflects the very interplay between the system and the bath mediated by the driving fields.

VI. CONCLUSION

Classical dynamics of dissipative systems is traditionally described by the Langevin equation. It has been shown that the stochastic formulation provides a similar description of quantum dissipative systems [28]. In this framework the dissipative system obeys Liouville equations subjected to the stochastic fields due to the bath. Based on the stochastic formulation, flexible numerical methods have been proposed and used to solve dissipative dynamics [30]. As complementing previous work, the present paper provides conceptual and analytical results. We have illustrated how to obtain the bath-induced field of the Caldeira-Leggett model through an elementary solution of quantum linear systems. Furthermore, we have elaborated

a systematic approach to derive the master equation, if it exists.

The reduced density matrix can in principle be obtained by solving the stochastic Liouville equation and calculating stochastic average. Because it is difficult to have convergent stochastic averaging, a master equation describing the evolution of the reduced density matrix is highly desired. We have shown the existence of the master equation relies not only on the feature of the dissipation characterized by the spectral density function, but also on the dynamics of the stochastic system itself. For linear systems, we have found that the “dissipative operator” due to the interplay of the system and the stochastic field is exactly solvable and thereby derived the master equation. We have shown that the master equation is equivalent to the HPZ equation derived by Hu, Paz, and Zhang using the path-integral approach [38,39]. We would like to point out that the coefficients in our master equation are determined by a set of integral equations, which may not suffer from the mathematical problems concerned by Fleming, Roura, and Hu [50].

We have also shown that the master equation of driven harmonic oscillator can be derived similarly. In this case, the system is dressed by both the driving and the stochastic fields, although the dissipation operators appear the same as that of the undriven case.

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- [1] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987); **67**, 725(E) (1995).
- [2] U. Weiss, *Quantum Dissipative Systems*, 3rd ed. (World Scientific, Singapore, 2008).
- [3] H. P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University, Oxford, 2002).
- [4] T. Dittrich, P. Hänggi, G.-L. Ingold, B. Kramer, G. Schön, and W. Zwerger, *Quantum Transport and Dissipation* (Wiley-VCH, Weinheim, 1998).
- [5] P. Hänggi and G.-L. Ingold, *Chaos* **15**, 026105 (2005).
- [6] C. W. Gardiner, *Stochastic Methods: A Handbook for the Natural and Social Sciences*, 4th ed. (Springer-Verlag, Berlin, 2009).
- [7] M. F. M. Osborne, *Opns. Res.* **7**, 145 (1959).
- [8] J. A. Freund and T. Pöschel, *Stochastic Processes in Physics, Chemistry, and Biology* (Springer-Verlag, Berlin, 2000).
- [9] M. Kijima, *Stochastic Processes with Applications to Finance* (CRC, Boca Raton, 2002).
- [10] F. Beichelt, *Stochastic Processes in Science, Engineering, and Finance* (CRC, Boca Raton, 2006).
- [11] H. Risken, *The Fokker-Planck Equation Methods of Solution and Applications*, 2nd ed. (Springer-Verlag, Berlin, 1989).
- [12] V. B. Magalinskij, *Sov. Phys. JETP* **9**, 1381 (1959).
- [13] A. O. Caldeira and A. J. Leggett, *Physica A* **121**, 587 (1983); **130**, 374(E) (1985); *Ann. Phys.* **149**, 374 (1983).
- [14] P. Hänggi, *Quantum Dissipation: A Primer in: Dynamics of Open Quantum System* (CCP6, Daresbury, 2007).
- [15] A. Nitzan, *Chemical Dynamics in Condensed Phase: Relaxation, Transfer, and Reactions in Condensed Molecular Systems* (Oxford University Press, New York, 2006).
- [16] H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Mechanics* (Springer, Berlin, 1982).
- [17] C. H. Wang, *Spectroscopy of Condensed Media* (Academic Press, Orlando, 1985).
- [18] H. S. Goan, G. J. Milburn, H. M. Wiseman, and H. B. Sun, *Phys. Rev. B* **63**, 125326 (2001); J. Gambetta and H. M. Wiseman, *Phys. Rev. A* **66**, 012108 (2002).
- [19] M. P. Blencowe, *Phys. Rep.* **395**, 159 (2004).
- [20] M. D. Ventra, S. Evoy, and J. R. Heflin, *Introduction to Nanoscale Science and Technology* (Springer, Berlin, 2004).
- [21] H. G. Craighead, *Science* **290**, 1532 (2000).
- [22] S. Nakajima, *Prog. Theor. Phys.* **20**, 948 (1958).
- [23] R. Zwanzig, *J. Chem. Phys.* **33**, 1338 (1960).
- [24] R. P. Feynman and F. L. Vernon, *Ann. Phys.* **24**, 118 (1963); R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
- [25] C. H. Mak and R. Egger, *Adv. Chem. Phys.* **93**, 39 (1996).

- [26] N. Makri, *J. Math. Phys.* **36**, 2430 (1995).
- [27] J. T. Stockburger and C. H. Mak, *Phys. Rev. Lett.* **80**, 2657 (1998); *J. Chem. Phys.* **110**, 4983 (1999); J. T. Stockburger and H. Grabert, *Chem. Phys.* **268**, 249 (2001); *Phys. Rev. Lett.* **88**, 170407 (2002).
- [28] J. Shao, *J. Chem. Phys.* **120**, 5053 (2004); *Chem. Phys.* **322**, 187 (2006); **370**, 29 (2010).
- [29] Y. A. Yan, F. Yang, Y. Liu, and J. Shao, *Chem. Phys. Lett.* **395**, 216 (2004); Y. Zhou, Y. Yan, and J. Shao, *Europhys. Lett.* **72**, 334 (2005); Y. Zhou and J. Shao, *J. Chem. Phys.* **128**, 034106 (2008).
- [30] D. Lacroix, *Phys. Rev. E* **77**, 041126 (2008).
- [31] Y. Tanimura and R. Kubo, *J. Phys. Soc. Jpn.* **58**, 101 (1989); Y. Tanimura, *ibid.* **75**, 082001 (2006).
- [32] R. X. Xu, P. Cui, X. Q. Li, Y. Mo, and Y. J. Yan, *J. Chem. Phys.* **122**, 041103 (2005); Y. J. Yan and R. X. Xu, *Annu. Rev. Phys. Chem.* **56**, 187 (2005).
- [33] W. G. Unruh and W. H. Zurek, *Phys. Rev. D* **40**, 1071 (1989).
- [34] V. Ambegaokar, *J. Stat. Phys.* **125**, 1187 (2006).
- [35] H. Dekker, *Phys. Rev. A* **16**, 2126 (1977); *Phys. Rep.* **80**, 1 (1981).
- [36] F. Haake and R. Reibold, *Phys. Rev. A* **32**, 2462 (1985).
- [37] H. Grabert, P. Schramm, and G.-L. Ingold, *Phys. Rep.* **168**, 115 (1988).
- [38] B. L. Hu, J. P. Paz, and Y. Zhang, *Phys. Rev. D* **45**, 2843 (1992); **47**, 1576 (1993).
- [39] J. J. Halliwell and T. Yu, *Phys. Rev. D* **53**, 2012 (1996).
- [40] R. Karrlein and H. Grabert, *Phys. Rev. E* **55**, 153 (1997).
- [41] E. Calzetta, A. Roura, and E. Verdaguer, *Int. J. Theor. Phys.* **40**, 2317 (2001); *Physica A* **319**, 188 (2003).
- [42] G. W. Ford and R. F. O'Connell, *Phys. Rev. D* **64**, 105020 (2001).
- [43] W. T. Strunz and T. Yu, *Phys. Rev. A* **69**, 052115 (2004); T. Yu, *ibid.* **69**, 062107 (2004).
- [44] C. H. Chou, T. Yu, and B. L. Hu, *Phys. Rev. E* **77**, 011112 (2008).
- [45] C. H. Chou, B. L. Hu, and T. Yu, *Physica A* **387**, 432 (2008).
- [46] R. X. Xu, B. L. Tian, J. Xu, and Y. J. Yan, *J. Chem. Phys.* **130**, 074107 (2009).
- [47] P. S. Riseborough, P. Hänggi, and U. Weiss, *Phys. Rev. A* **31**, 471 (1985).
- [48] S. Kohler, T. Dittrich, and P. Hänggi, *Phys. Rev. E* **55**, 300 (1997).
- [49] C. Zerbe and P. Hänggi, *Phys. Rev. E* **52**, 1533 (1995).
- [50] C. H. Fleming, A. Roura, and B. L. Hu, *Ann. Phys.* **326**, 1207 (2011).
- [51] V. Hakim and V. Ambegaokar, *Phys. Rev. A* **32**, 423 (1985).
- [52] P. G. Wolynes, *Phys. Rev. Lett.* **47**, 968 (1981).
- [53] H. Dekker, *Phys. Rev. A* **38**, 6351 (1988).
- [54] J. Ankerhold, H. Grabert, and G.-L. Ingold, *Phys. Rev. E* **51**, 4267 (1995).
- [55] E. Pollak and J. L. Liao, *J. Chem. Phys.* **108**, 2733 (1998).
- [56] B. Øksendal, *Stochastic Differential Equations*, 6th ed. (Springer-Verlag, Berlin, 2003).
- [57] D. Gatarek and N. Gisin, *J. Math. Phys.* **32**, 2152 (1991); G. C. Ghirardi, P. Pearle, and A. Rimini, *Phys. Rev. A* **42**, 78 (1990).
- [58] W. H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973).
- [59] W. Dittrich and M. Reuter, *Classical and Quantum Dynamics*, 2nd ed. (Springer-Verlag, Berlin, 1992).
- [60] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th ed. (World Scientific, Singapore, 2009).
- [61] R. P. Feynman, *Statistical Mechanics* (Benjamin, New York, 1972).
- [62] G. Weiss and A. Maradudin, *J. Math. Phys.* **3**, 771 (1962); E. Wichmann, *ibid.* **2**, 876 (1961); W. Magnus, *Comm. Pure Appl. Math.* **7**, 649 (1954); D. Finkelstein, *ibid.* **8**, 245 (1955).
- [63] A. Brissand and U. Frisch, *J. Math. Phys.* **15**, 524 (1974).
- [64] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd ed. (Elsevier, Amsterdam, 2007).
- [65] V. I. Klyatskin, *Dynamics of Stochastic Systems* (Elsevier, Amsterdam, 2005).
- [66] M. Ban, S. Kitajima, and F. Shibata, *Phys. Lett. A* **374**, 2324 (2010).
- [67] We elucidate this point by using the following stochastic differential equation for an operator $\hat{O}(t)$, $i\partial\hat{O}/\partial t = \kappa(t)\hat{\mathcal{L}}(t)\hat{O}$, where $\kappa(t)$ is a scalar Gaussian noise determined by zero-mean and correlation $k(t,t') = M\{\kappa(t)\kappa(t')\}$, $\hat{\mathcal{L}}(t)$ is a deterministic operator, and the initial condition is nonrandom $\hat{O}(0) = \hat{O}_0$. Denote $\tilde{O}(t) = M\{\hat{O}(t)\}$. Using the Furutsu-Novikov theorem one obtains $i\partial\tilde{O}(t)/\partial t = \int_0^t dt' k(t,t')\hat{\mathcal{L}}(t)M\{\delta\hat{O}/\delta\kappa(t')\}$. The involved functional derivative can be formally solved in terms of the evolution operator $U(t,t_0) = \mathcal{T} \exp[-i \int_0^t dt' \kappa(t')\hat{\mathcal{L}}(t')]$, where \mathcal{T} is the chronological operator. Note that $\hat{O}(t) = U(t,t_0)\hat{O}(t_0)$. One readily obtains $\delta\hat{O}/\delta\kappa(t') = -iU(t,t')\hat{\mathcal{L}}(t')\hat{O}(t')$. For a general $\hat{\mathcal{L}}(t)$ this expression cannot be simplified further, and a closed-form equation of $\tilde{O}(t)$ is defied. The mistake one would make is $\delta\hat{O}/\delta\kappa(t') = -i\mathcal{L}(t')\hat{O}(t')$ [for instance, Eq. (11) in E. Torrente-Lujan, *Phys. Rev. D* **59**, 073001 (1999)], which leads to an approximate instead of exact evolution equation for $\tilde{O}(t)$.
- [68] E. A. Novikov, *Sov. Phys. JETP* **20**, 1290 (1965).