

Nonperturbative expansion method for a quantum system coupled to a harmonic-oscillator bath

Yoshitaka Tanimura

*Beckman Institute and School of Chemical Sciences, University of Illinois at Urbana-Champaign,
405 North Mathews, Urbana, Illinois 61801*

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A method to determine the resolvent of a quantum system coupled to a harmonic-oscillator bath is derived by extending the continued-fraction theory of a Gaussian-Markovian bath that has been presented by Tanimura and Kubo [J. Phys. Soc. Jpn. **58**, 101 (1989)]. The results are expressed in terms of continued fractions and apply to an oscillator bath with a general spectral density, corresponding to colored noise, at various temperatures. Exact values of the resolvent can be calculated for arbitrary strength of the system-bath interaction by making use of the convergence properties of the continued fractions. For the weak-interaction case these results agree with the quantum master equation. The physical meaning of the results is also discussed by a diagrammatic method. As an application, the result of the Gaussian-Markovian system is extended to the case of the low-temperature bath. Correlated (unfactorized) initial conditions are also discussed.

I. INTRODUCTION

There has been renewed interest in the problem of dissipative systems following the work by Caldeira and Leggett.¹ The dissipation arises from the interaction between the system, which we call the test system, and the bath. When the bath variables are eliminated from the equation of motion of the whole system, the test system is assumed to follow dissipative dynamics.

One of the oldest approaches of this problem is based on the quantum master equation, in which a weak system-bath interaction and a Gaussian-white-noise bath are assumed (see, for example, Ref. 2). The weak-interaction assumption keeps the bath in the equilibrium state and greatly simplifies the problem. A Gaussian nature is endorsed in the case when the bath is regarded as a set of harmonic oscillators or when the interaction is a cumulative effect of a large number of weak interactions where some sort of a central-limit theorem can be applied. Many realistic cases are well described by the Gaussian approximation. The white-noise assumption, producing a δ -time-correlated noise, works well when the relevant time scale is very short compared with the dynamical time scale (time coarse grained). In quantum optics³ and spin-relaxation theory,⁴ the white-noise assumption has been successfully used to describe damping phenomena. However, with the recent progress in the high-speed optoelectronics, the dynamical time scales are becoming very short, thus prohibiting time coarse graining and motivating our interest in colored noise.^{5,6}

To treat this kind of problem, time-convolution type of equations are used.⁷⁻⁹ The assumption of a weak system-bath interaction is necessary to write this equation in a closed form, but this assumption strongly restricts the number of possible applications. Another new approach is based on the path-integral formalism and applies to colored noise,¹⁰⁻¹³ however, its evaluation is not easy.

Recently, Tanimura and Kubo have derived the equa-

tion of motion for the test system coupled to the Gaussian-Markovian bath from the dynamical point of view.^{14,15} The result was expressed in the form of simultaneous differential equations for the density matrices and the corresponding resolvent was written in the continued fraction form. The Markovian property assumes exponential relaxation of the response of the bath when it acts on the test system and corresponds to the high-temperature Debye relaxation bath. Note that, as was shown by Doob, the Markovian property is produced not only by the short correlated noise (the white noise) but also by the exponentially correlated noise (see Ref. 2). The advantage of this treatment is that this can treat both the colored noise and the strong system-bath interaction by using the convergent nature of the continued fraction. In the white-noise limit, this equation agrees with the quantum master equation. In Ref. 16, we have extended our theory to the two-time correlation functions and observed that the strong system-bath interaction causes special features of the two-time correlation functions. As applications of this theory, we have investigated optical processes.^{17,18}

The assumption of the Markovian process is not universal but is a reasonably good model for the realistic systems. However, there are many systems that cannot be described by a Markovian process, for example, the case of a low bath temperature. The purpose of this paper is to provide a method to determine the resolvent of the system coupled to a bath for a general spectral distribution and arbitrary temperature. The resolvent cannot be expressed in a compact form, however, we can expand it in a form of continued fraction. From a study of the Gaussian-Markovian case, these expansion terms are expected to converge not only for the weak-interaction case but also for the strong-interaction case. Then by calculating the resolvent until its value converges, we may obtain the exact value of the resolvent for a nonperturbative interaction.

This paper is organized as follows. In Sec. II we briefly

summarize the work previously done on Gaussian-Markovian systems, for later convenience. The correlated (unfactorized) initial condition is also discussed. In Sec. III, we present an expansion method of the resolvent for a general noise bath. By applying the method of Sec. III, we extend the formulation of the Gaussian-Markovian system where the bath temperature is assumed to be high, to the case of the low temperature in Sec. IV. In Sec. V, we mention the problems of positivity.

II. GAUSSIAN-MARKOVIAN SYSTEM AND CORRELATED INITIAL CONDITIONS

A. Equation of motion for a Gaussian-Markovian bath

Let us consider a test system A coupled to a harmonic oscillator bath B . The total Hamiltonian is given by

$$H = H_A(a, a^\dagger) + V(a, a^\dagger) \sum_j c_j x_j + \sum_j \left[\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 x_j^2 \right], \quad (2.1)$$

where $H_A(a, a^\dagger)$ is the Hamiltonian of A itself and $V(a, a^\dagger)$ is a coupling operator of the system A described by a creation and an annihilation operator a and a^\dagger . For a many-particle system, a and a^\dagger can be regarded as a set of operators $\{a_j, a_j^\dagger\}$. The parameters of the bath B are defined in the usual way. The initial state of the total system is chosen to factorize in the form

$$\hat{\rho}_{A+B}(t_i) = |\phi_i\rangle \langle \phi_i| \hat{\rho}_B^e = \hat{\rho}(t_i) \hat{\rho}_B^e, \quad (2.2)$$

where $\hat{\rho}(t_i)$ is the initial density operator of A denoted by coherent states $|\phi_i\rangle$ and $\langle \phi_i|$, and $\hat{\rho}_B^e$ is the equilibrium density operator of B itself. Note that here we use the factorized initial condition, but we will discuss the correlated (unfactorized) case at the end of this section. Consider the total density operator at time t expressed in the path integral form. The system A is described by using a coherent state ϕ and its conjugate ϕ^* . By performing the integration of the bath, we obtain the density element of A in the form^{10,15}

$$\rho(\phi_f, \phi_f'; t) = \int D[Q(\tau)] \int D[Q'(\tau)] \exp \left[\frac{i}{\hbar} S_A(Q; t, t_i) \right] F(Q, Q'; t, t_i) \exp \left[-\frac{i}{\hbar} S_A(Q'; t, t_i) \right], \quad (2.3)$$

where ϕ_f and ϕ_f' are the final states of the system, and $Q(t)$ represents a set of coherent state variables ($\phi^*(t), \phi(t)$). The functional $S_A(Q; t, t_i)$ is an action of H_A and $D[Q(\tau)]$ represents the functional integral of $Q(\tau)$. The influence functional $F(Q, Q'; t, t_i)$ has the form:

$$F(Q, Q'; t, t_i) = \exp \left[\left[-\frac{i}{\hbar} \right]^2 \lim_{M \rightarrow \infty} \sum_{k=2}^M \sum_{j=1}^{k-1} \epsilon^2 V^\times(Q, Q'; k\epsilon) \times [L_2(k\epsilon - j\epsilon) V^\times(Q, Q'; j\epsilon) - iL_1(k\epsilon - j\epsilon) V^\circ(Q, Q'; j\epsilon)] \right] \left[\epsilon = \frac{t_f - t_i}{M} \right] \\ = \exp \left[\left[-\frac{i}{\hbar} \right]^2 \int_{t_i}^t d\tau' \int_{t_i}^{\tau'} d\tau V^\times(Q, Q'; \tau') [L_2(\tau' - \tau) V^\times(Q, Q'; \tau) - iL_1(\tau' - \tau) V^\circ(Q, Q'; \tau)] \right], \quad (2.4)$$

where

$$iL_1(t) = i \int_{-\infty}^{\infty} d\omega J(\omega) \sin(\omega t), \quad (2.5)$$

and

$$L_2(t) = \int_{-\infty}^{\infty} d\omega J(\omega) \coth(\frac{1}{2}\beta\hbar\omega) \cos(\omega t) \quad (2.6)$$

with the spectral density for the bath oscillators

$$J(\omega) = \hbar\omega \sum_j \left[\frac{c_j^2}{4m_j\omega_j^2} \right] [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)], \quad (2.7)$$

and the inverse temperature of the bath $\beta = 1/k_B T$. The functional $V^\times(Q, Q'; \tau)$ and $V^\circ(Q, Q'; \tau)$ are the expressions of the commutator and the anticommutator operator of $V(Q(\tau))$ in the path-integral representation and are defined as

$$V^\times(Q, Q'; \tau) = V(Q(\tau)) - V(Q'(\tau)) \quad (2.8) \\ V^\circ(Q, Q'; \tau) = V(Q(\tau)) + V(Q'(\tau)).$$

Consider the following spectral function

$$J(\omega) = \frac{\hbar\eta}{2\pi} \frac{\omega\gamma^2}{\gamma^2 + \omega^2}. \quad (2.9)$$

This is essentially the Ohmic dissipation¹² with the Lorentzian cutoff (Drude dissipation¹). The constant η represents the coupling strength between A and B and, to compare the stochastic Gaussian-Markovian theory, we put $\eta = \hbar^2 \Delta^2 \beta / \gamma$ in Refs. 14–18. Then the functions Eqs. (2.5) and (2.6) can be calculated as

$$iL_1(t) = i \frac{\hbar\eta\gamma^2}{2} e^{-\gamma t} \quad (t > 0) \quad (2.10)$$

and

$$L_2(t) = \frac{\hbar\eta\gamma^2}{2} \left[\cot \left[\frac{\beta\hbar\gamma}{2} \right] e^{-\gamma t} - \sum_{k=1}^{\infty} \frac{4k\pi}{(\beta\hbar\gamma)^2 - (2\pi k)^2} e^{-(2\pi k t)/\beta\hbar} \right]. \quad (2.11)$$

If the initial temperature of the bath is high, the series terms of Eq. (2.11) can be neglected. From the numerical

consideration, this may be a good approximation for $\beta\hbar\gamma \lesssim 1$, which corresponds to $T \gtrsim 10$ K for a noise correlation time $t_c = 1/\gamma \sim 1$ ps. We will discuss the case of a low-temperature bath in Sec. IV. The function $L_1(t)$ has a singular point at $t=0$, however, from Eq. (2.4), it seems natural to compute it as

$$L_1(0) = \lim_{t \rightarrow 0^+} L_1(t) = \frac{\hbar\eta\gamma^2}{2}. \quad (2.12)$$

Then the influence functional is now written in the form

$$F(Q, Q'; t, t_i) = \exp \left\{ \frac{\hbar\eta\gamma^2}{2} \left[-\frac{i}{\hbar} \right]^2 \int_{t_i}^t d\tau' \int_{t_i}^{\tau'} d\tau e^{-\gamma(\tau'-\tau)} V^\times(Q, Q'; \tau') \times \left[\cot \left[\frac{\beta\hbar\gamma}{2} \right] V^\times(Q, Q'; \tau) - iV^\circ(Q, Q'; \tau) \right] \right\}. \quad (2.13)$$

Consider the following elements:

$$\begin{aligned} \rho_n(\phi_f, \phi'_f; t) &\equiv \int D[Q(\tau)] \int D[Q'(\tau)] \\ &\times \left\{ -i \frac{\eta\gamma^2}{2} \int_{t_i}^t d\tau e^{-\gamma(t-\tau)} \left[\cot \left[\frac{\beta\hbar\gamma}{2} \right] V^\times(Q, Q'; \tau) - iV^\circ(Q, Q'; \tau) \right] \right\}^n \\ &\times \left[\frac{i}{\hbar} S_A(Q; t, t_i) \right] F(Q, Q'; t, t_i) \exp \left[-\frac{i}{\hbar} S_A(Q'; t, t_i) \right], \end{aligned} \quad (2.14)$$

and the corresponding operator $\hat{\rho}_n(t)$ defined by

$$\hat{\rho}_n(t) = \int d\phi_f \int d\phi'_f |\phi_f\rangle \rho_n(\phi_f, \phi'_f; t) \langle \phi'_f|. \quad (2.15)$$

Then the first member $\hat{\rho}_0(t)$ agrees with $\hat{\rho}(t)$. The time differentiation of this operator becomes

$$\dot{\hat{\rho}}_0(t) = -\frac{i}{\hbar} \mathcal{L}_A \hat{\rho}_0(t) - \frac{i}{\hbar} V^\times \hat{\rho}_1(t), \quad (2.16)$$

$$\begin{aligned} \dot{\hat{\rho}}_n(t) &= -\left[\frac{i}{\hbar} \mathcal{L}_A + n\gamma \right] \hat{\rho}_n(t) - \frac{i}{\hbar} V^\times \hat{\rho}_{n+1}(t) \\ &\quad - \frac{ni}{\hbar} \Theta \hat{\rho}_{n-1}(t), \quad (n > 0) \end{aligned}$$

where

$$\Theta = \frac{\hbar\eta\gamma^2}{2} \left[\cot \left[\frac{\beta\hbar\gamma}{2} \right] V^\times - iV^\circ \right]. \quad (2.17)$$

Here, \times and \circ imply the commutator and the anticommutator operation, namely,

$$\begin{aligned} V^\times \hat{\rho} &= V\hat{\rho} - \hat{\rho}V, \\ V^\circ \hat{\rho} &= V\hat{\rho} + \hat{\rho}V, \end{aligned} \quad (2.18)$$

and we introduced the quantal Liouvillian defined by

$$\mathcal{L}_A \hat{\rho} = H_A^\times \hat{\rho}. \quad (2.19)$$

From the definition of $\hat{\rho}_n(t)$, the initial condition of Eq. (2.16) can be written as

$$\hat{\rho}_0(t_i) = \hat{\rho}(t_i), \quad \hat{\rho}_n(t_i) = 0 \quad \text{for } n > 0. \quad (2.20)$$

This corresponds to the factorized initial condition Eq. (2.2). We may evaluate Eq. (2.16) by neglecting the hierarchy operator $\hat{\rho}_{n+1}(t)$, which does not play a role for large number n .

By using the Laplace transform

$$\hat{\rho}_n[s] = \int_{t_i}^{\infty} dt \exp[-s(t-t_i)] \hat{\rho}_n(t), \quad (2.21)$$

we can also obtain the resolvent of the above equation in the continued fraction form as

$$\hat{\rho}_0[s] = Z_0[s] \hat{\rho}(t_i), \quad (2.22)$$

where we introduce

$$Z_k[s] = \frac{1}{s + k\gamma + \frac{i}{\hbar} \mathcal{L}_A + \frac{1}{\hbar^2} V^\times \frac{k+1}{s + (k+1)\gamma + \frac{i}{\hbar} \mathcal{L}_A + \frac{1}{\hbar^2} V^\times \frac{k+2}{s + (k+2)\gamma + \frac{i}{\hbar} \mathcal{L}_A + \dots} \Theta}, \quad (2.23)$$

for later convenience. The fractional expression of the above represents an inverse of an operator. We can evaluate these, for example, by using a matrix expression of \mathcal{L}_A , V^\times , and Θ (see Ref. 18). The calculation of the above continued fraction is expected to converge even though the system-bath interaction is very strong or the correlation time of the noise is very long. Then, we may nonperturbatively evaluate the resolvent by using this formulation.

B. Correlated initial conditions

We have used the factorized initial condition to obtain Eq. (2.16) but the result can apply in the case of correlated (unfactorized) initial conditions. To illustrate this point, consider an additional force F to the Hamiltonian Eq. (2.1), where operator F works only on the system A . Suppose that the total system is in the equilibrium state of the Hamiltonian $H'=H+F$ at time $t < t_i$ and the force F turnoff at time $t=t_i$. The time evolution of the system A after $t > t_i$ is written as

$$\hat{\rho}(t) = \text{Tr}_B \left[\exp \left[-\frac{i}{\hbar} H^\times(t-t_i) \right] \hat{\rho}'_{A+B} \right], \quad (2.24)$$

where

$$\hat{\rho}'_{A+B} = \lim_{t'_i \rightarrow -\infty} \exp \left[-\frac{i}{\hbar} (H+F)^\times(t_i-t'_i) \right] [\hat{\rho}(t'_i) \hat{\rho}_B^e], \quad (2.25)$$

and we have assumed that the system goes to the unique equilibrium state $\hat{\rho}'_{A+B}$ regardless of the choice of the initial condition when $t'_i \rightarrow -\infty$. In the above equations the density operator $\hat{\rho}'_{A+B}$ can be regarded as the initial condition $\hat{\rho}_{A+B}(t_i)$, but we cannot express this in the factorized form as Eq. (2.20), because the system-bath interaction mixes the A and B states. Here we are considering the correlated initial condition, however, the equation of motion for $t > t_i$ has the same form as Eq. (2.16). This can be shown by introducing the hierarchical elements at $t > t_i$ in the form

$$\begin{aligned} \rho_n(\phi_f, \phi'_f; t) &\equiv \int D[Q(t)] \int D[Q'(t)] \\ &\times \left\{ -i \frac{\eta\gamma^2}{2} \int_{t'_i}^t d\tau e^{-\gamma(t-\tau)} \left[\cot \left[\frac{\beta\hbar\gamma}{2} \right] V^\times(Q, Q'; \tau) - iV^\circ(Q, Q'; \tau) \right] \right\}^n \\ &\times \exp \left[\frac{i}{\hbar} [S_A(Q; t, t_i) + S'_A(Q; t_i, t'_i)] \right] F(Q, Q'; t, t_i) \\ &\times \exp \left[-\frac{i}{\hbar} [S'_A(Q'; t_i, t'_i) + S_A(Q'; t, t_i)] \right], \end{aligned} \quad (2.26)$$

where S'_A is the action of A including the force F . The initial condition is specified by the set of hierarchic operators $\hat{\rho}_n(t_i)$, which have nonzero elements as is easily seen from the above definition. By using the Laplace transform of $\hat{\rho}'_n(t)$ denoted by $\hat{\rho}'_n[s]$, the states $\hat{\rho}_n(t_i) = \hat{\rho}_n^e$ can be evaluated in the form¹⁶

$$\begin{aligned} \hat{\rho}_n^e &= \lim_{s \rightarrow 0} s \hat{\rho}_n[s] \\ &= \lim_{s \rightarrow 0} sn! \left[-\frac{i}{\hbar} \right]^n \left[\prod_{k=1}^n (Z_{n-k+1}[s] \Theta) \right] Z_0[s] \hat{\rho}(t'_i), \end{aligned} \quad (2.27)$$

where $Z_k[s]$ is given by Eq. (2.23). Above results suggest that correlated initial conditions can be taken into account by choosing nonzero elements of $\hat{\rho}_n(t_i)$. The correlated initial condition is a recent and not yet well ad-

ressed topic (see, for example, Ref. 19). The advantages of this simultaneous equation or the continued fractional approach is that we can treat not only the correlated noise but also the strong system-bath interaction. The example here we presented is a particular one, however the author believes that the appropriate set of $\hat{\rho}_n(t_i)$ allows us to study any correlated initial condition. The correlated initial condition also plays important role for the problem of the time correlation function.¹⁶ The importance of this condition has been investigated in the context of quantum optics and numerical results have been presented in Refs. 17 and 18.

III. NONPERTURBATIVE EXPANSION METHOD OF RESOLVENT FOR GENERAL SPECTRUM

For the general distribution $J(\omega)$, we cannot express the resolvent in the compact continued fraction form. In this case, as will be shown below, we can express the resolvent in the expansion form with terms in a continued fraction. The influence functional Eq. (2.4) is written in the Fourier form as

$$F(Q, Q'; t, t_i) = \exp \left[(-i)^2 \int_{t_i}^t d\tau' \int_{t_i}^{\tau'} d\tau \int_{-\infty}^{\infty} d\omega e^{-i\omega(\tau'-\tau)} V^\times(Q, Q'; \tau') \Theta(\omega; Q, Q'; \tau) \right], \tag{3.1}$$

where

$$\Theta(\omega; Q, Q'; \tau) = \frac{1}{\hbar^2} J(\omega) \left[\coth \left[\frac{\beta \hbar \omega}{2} \right] V^\times(Q, Q'; \tau) + V^\circ(Q, Q'; \tau) \right]. \tag{3.2}$$

Corresponding to Eq. (2.14), we introduce the set of density elements by

$$\begin{aligned} \rho(\phi_f, \phi'_f; t; \omega_1, \omega_2, \dots, \omega_m) \equiv & \int D[Q(\tau)] \int D[Q'(\tau)] \prod_{k=1}^m \left[-i \int_{t_i}^t d\tau \exp[-i\omega_k(t-\tau)] \Theta(\omega_k; Q, Q'; \tau) \right] \\ & \times \exp \left[\frac{i}{\hbar} S_A(Q; t, t_i) \right] F(Q, Q'; t, t_i) \exp \left[-\frac{i}{\hbar} S_A(Q'; t, t_i) \right], \end{aligned} \tag{3.3}$$

and corresponding operators $\hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_m)$. Then the time derivation of $\hat{\rho}(t)$ can be expressed as

$$\dot{\hat{\rho}}(t) = -\frac{i}{\hbar} \mathcal{L}_A \hat{\rho}(t) - i \int_{-\infty}^{\infty} d\omega_1 V^\times \hat{\rho}(t; \omega_1). \tag{3.4}$$

The time derivation of $\hat{\rho}(t; \omega_1)$ yields the operator equation

$$\dot{\hat{\rho}}(t; \omega_1) = -\left[\frac{i}{\hbar} \mathcal{L}_A + i\omega_1 \right] \hat{\rho}(t; \omega_1) - i \int_{-\infty}^{\infty} d\omega_2 V^\times \hat{\rho}(t; \omega_1, \omega_2) - i\Theta(\omega_1) \hat{\rho}(t), \tag{3.5}$$

where we put

$$\Theta(\omega) = \frac{1}{\hbar^2} J(\omega) \left[\coth \left[\frac{\beta \hbar \omega}{2} \right] V^\times + V^\circ \right]. \tag{3.6}$$

We repeat the same process to get

$$\begin{aligned} \dot{\hat{\rho}}(t; \omega_1, \omega_2, \dots, \omega_m) = & -\left[\frac{i}{\hbar} \mathcal{L}_A + i \sum_{j=1}^m \omega_j \right] \hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_m) - i \int_{-\infty}^{\infty} d\omega_{m+1} V^\times \hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_{m+1}) \\ & - i\Theta(\omega_m) \hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_{m-1}) - i \sum_{k=1}^{m-1} \Theta(\omega_k) \hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_{k-1}, \omega_{k+1}, \dots, \omega_m). \end{aligned} \tag{3.7}$$

Here, we set $m > 1$ and $\omega_0 = 0$. Let us denote the Laplace transform of $\hat{\rho}(t; \omega_k, \omega_l, \dots)$ by $\hat{\rho}[s; \omega_k, \omega_l, \dots]$. The above equations are expressed in the matrix form as

$$\underline{P}[s] = \underline{R}[s] \underline{P}(t_i) + \underline{R}[s] \sum_k \Theta(\omega_k) \underline{P}_k[s], \tag{3.8}$$

where $\underline{P}[s]$ is a row vector with elements $\hat{\rho}(t; \omega_1, \omega_2, \dots, \omega_m)$,

$$\underline{R}[s] = \begin{pmatrix} s + \frac{i}{\hbar} \mathcal{L}_A & i \int d\omega_1 V^\times & 0 & 0 & 0 & \dots \\ i\Theta(\omega_1) & s + \frac{i}{\hbar} \mathcal{L}_A + i\omega_1 & i \int d\omega_2 V^\times & 0 & 0 & \dots \\ 0 & i\Theta(\omega_2) & s + \frac{i}{\hbar} \mathcal{L}_A + i(\omega_1 + \omega_2) & i \int d\omega_3 V^\times & 0 & \dots \\ 0 & 0 & i\Theta(\omega_3) & \ddots & & \\ \vdots & \vdots & 0 & & & \end{pmatrix}^{-1}, \tag{3.9}$$

$$\underline{P}(t_i) = \begin{pmatrix} \hat{\rho}(t_i) \\ 0 \\ \vdots \end{pmatrix}, \quad \underline{P}_k[s] = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hat{\rho}[s; \omega_1, \omega_2, \dots, \omega_{k-1}, \omega_{k+1}] \\ \hat{\rho}[s; \omega_1, \omega_2, \dots, \omega_{k-1}, \omega_{k+1}, \omega_{k+2}] \\ \vdots \end{pmatrix}, \tag{3.10}$$

where zeros are repeated $k + 1$ times in $\underline{P}_k[s]$. We denote the elements of $\underline{R}[s]$ by R_{jk} . Then $\hat{\rho}[s]$ can be expressed as

$$\begin{aligned} \hat{\rho}[s] = & R_{11}\hat{\rho}(t_i) + R_{13}\Theta(\omega_1)\hat{\rho}[s; \omega_2] + R_{14}\Theta(\omega_1)\hat{\rho}[s; \omega_2, \omega_3] + R_{15}\Theta(\omega_1)\hat{\rho}[s; \omega_2, \omega_3, \omega_4] + \dots \\ & + R_{14}\Theta(\omega_2)\hat{\rho}[s; \omega_1, \omega_3] + R_{15}\Theta(\omega_2)\hat{\rho}[s; \omega_1, \omega_3, \omega_4] + \dots \end{aligned} \quad (3.11)$$

The Laplace transform $\hat{\rho}[s; \omega_j, \omega_k, \omega_l, \dots]$ can be also expressed by using a set of differential equations. For example, $\hat{\rho}[s; \omega_2]$ is evaluated from

$$\begin{aligned} \dot{\hat{\rho}}(t; \omega_2) = & -i \left[\frac{1}{\hbar} \mathcal{L}_A + \omega_2 \right] \hat{\rho}(t; \omega_2) - i \int_{-\infty}^{\infty} d\omega_2' V^\times \hat{\rho}(t; \omega_2, \omega_2') - i\Theta(\omega_2)\hat{\rho}(t), \\ \dot{\hat{\rho}}(t; \omega_2, \omega_2') = & -i \left[\frac{1}{\hbar} \mathcal{L}_A + \omega_2 + \omega_2' \right] \hat{\rho}(t; \omega_2, \omega_2') - i \int_{-\infty}^{\infty} d\omega_2'' V^\times \hat{\rho}(t; \omega_2, \omega_2', \omega_2'') \\ & - i\Theta(\omega_2')\hat{\rho}(t; \omega_2) - i\Theta(\omega_2)\hat{\rho}(t; \omega_2'), \end{aligned} \quad (3.12)$$

etc. To simplify the notation, we denote $\hat{\rho}[s; \omega_j, \omega_k, \omega_l, \dots]$ by $\hat{\rho}[s; \nu_1, \nu_2, \dots, \nu_m]$, where m represents the argument number. By using similar form as in Eq. (3.8), these elements are expressed as

$$\underline{P}^m[s] = \underline{R}^m[s] \sum_k \Theta(\nu_k) \underline{P}_k^m[s]. \quad (3.13)$$

Here $\underline{P}^m[s]$ is the row vector with the j th element defined by $\hat{\rho}[s; \nu_1, \nu_2, \dots, \nu_{m+j-1}]$ and

$$\underline{R}^m[s] = \begin{pmatrix} s + \frac{i}{\hbar} \mathcal{L}_A + i(\nu_1 + \dots + \nu_m) & i \int d\nu_{m+1} V^\times & 0 & \dots \\ i\Theta(\nu_{m+1}) & s + \frac{i}{\hbar} \mathcal{L}_A + i(\nu_1 + \dots + \nu_{m+1}) & i \int d\nu_{m+2} V^\times & \dots \\ 0 & i\Theta(\nu_{m+2}) & \ddots & \\ \vdots & 0 & \vdots & \end{pmatrix}^{-1}. \quad (3.14)$$

For $m \leq k$, the row vector $\underline{P}_k^m[s]$ is written as

$$\underline{P}_k^m[s] = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hat{\rho}[s; \nu_1, \dots, \nu_{k-1}] \\ \hat{\rho}[s; \nu_1, \dots, \nu_{k-1}, \nu_{k+1}] \\ \hat{\rho}[s; \nu_1, \dots, \nu_{k-1}, \nu_{k+1}, \nu_{k+2}] \end{pmatrix} \quad \text{for } m \leq k, \quad (3.15)$$

where in $\underline{P}_k^m[s]$, the zeros are repeated $k - m$ times. For $m > k$, $\underline{P}_k^m[s]$ is defined by its j th element $\hat{\rho}[s; \nu_1, \dots, \nu_{k-1}, \nu_{k+1}, \dots, \nu_{m+j-1}]$.

Then, for example, the terms $\hat{\rho}[s, \nu_1]$ and $\hat{\rho}[s, \nu_1, \nu_2]$ can be expressed as

$$\begin{aligned} \hat{\rho}[s, \nu_1] = & R_{11}^1 \Theta(\nu_1) \hat{\rho}[s] + R_{12}^1 \Theta(\nu_1) \hat{\rho}[s, \nu_2] + \dots, \\ \hat{\rho}[s, \nu_1, \nu_2] = & R_{11}^2 \Theta(\nu_1) \hat{\rho}[s, \nu_2] + R_{11}^2 \Theta(\nu_2) \hat{\rho}[s, \nu_1] + \dots \end{aligned} \quad (3.16)$$

The terms $\hat{\rho}[s, \nu_2]$, etc. can be evaluated in a similar way. By using the elements of $\underline{R}[s]$ and $\underline{R}^m[s]$ (see Appendix A), the resolvent can be expressed in the expansion form as

$$\hat{\rho}[s] = (G_1[s] + G_2[s] + G_3[s] + \dots) \hat{\rho}(t_i), \quad (3.17)$$

where

$$G_1[s] = Z[s], \quad (3.18)$$

$$G_2[s] = Z[s] \int d\omega_1 V^\times Z[s + i\omega_1] \int d\omega_2 V^\times Z[s + i(\omega_1 + \omega_2)] \Theta(\omega_1) Z[s + i\omega_2] \Theta(\omega_2) Z[s], \quad (3.19)$$

$$\begin{aligned} G_3[s] = & Z[s] \int d\omega_1 V^\times Z[s + i\omega_1] \int d\omega_2 V^\times Z[s + i(\omega_1 + \omega_2)] \Theta(\omega_1) Z[s + i\omega_2] \\ & \times \int d\omega_3 V^\times Z[s + i(\omega_2 + \omega_3)] \Theta(\omega_2) Z[s + i\omega_3] \Theta(\omega_3) Z[s] \\ & + Z[s] \int d\omega_1 V^\times Z[s + i\omega_1] \int d\omega_2 V^\times Z[s + i(\omega_1 + \omega_2)] \\ & \times \int d\omega_3 V^\times Z[s + i(\omega_1 + \omega_2 + \omega_3)] \Theta(\omega_1) Z[s + i(\omega_2 + \omega_3)] \\ & \times \{ \Theta(\omega_3) Z[s + i\omega_2] \Theta(\omega_2) Z[s] + \Theta(\omega_2) Z[s + i\omega_3] \Theta(\omega_3) Z[s] \} \\ & + Z[s] \int d\omega_1 V^\times Z[s + i\omega_1] \int d\omega_2 V^\times Z[s + i(\omega_1 + \omega_2)] \\ & \times \int d\omega_3 V^\times Z[s + i(\omega_1 + \omega_2 + \omega_3)] \Theta(\omega_2) Z[s + i(\omega_1 + \omega_3)] \\ & \times \{ \Theta(\omega_3) Z[s + i\omega_1] \Theta(\omega_1) Z[s] + \Theta(\omega_1) Z[s + i\omega_3] \Theta(\omega_3) Z[s] \}. \end{aligned} \quad (3.20)$$

Here $Z[s]$ is defined by

$$Z[s] = \frac{1}{s + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_1 V^\times \frac{1}{s + i\nu_1 + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_2 V^\times \frac{1}{s + i(\nu_1 + \nu_2) + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_3 V^\times \frac{1}{s + \dots} \Theta(\nu_3)} \Theta(\nu_2)} \Theta(\nu_1)}. \quad (3.21)$$

Note that we may also obtain similar results for the case of the deformation potential interaction. (See Appendix B.)

If we assume that the spectral width of $J(\omega)$ is very large, which corresponds to a short correlated noise, or the coupling strength of the system-bath interaction is very weak, the higher-order terms of Eq. (3.17) can be neglected. Then we have

$$\hat{\rho}[s] = \frac{1}{s + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_1 V^\times \frac{1}{s + i\nu_1 + \frac{i}{\hbar} \mathcal{L}_A} \Theta(\nu_1)} \hat{\rho}(t_i). \quad (3.22)$$

This equation is equivalent to the generalized master equation.

To discuss the meaning of Eq. (3.17), consider the expansion of the influence functional Eq. (3.1). To the first order in the expansion, the density elements of the system can be written as

$$\begin{aligned} \rho^1(\phi_f, \phi'_f; t) = & \int D[Q(\tau)] \int D[Q'(\tau)] \int_{t_i}^t d\tau' \int_{t_i}^{\tau'} d\tau \int_{-\infty}^{\infty} d\omega e^{-i\omega(\tau' - \tau)} V^\times(Q, Q'; \tau') \Theta(\omega; Q, Q'; \tau) \\ & \times \exp \left[\frac{i}{\hbar} S_A(Q; t, t_i) \right] \exp \left[-\frac{i}{\hbar} S_A(Q'; t, t_i) \right]. \end{aligned} \quad (3.23)$$

By performing a Laplace transform, we express the resolvent of this element in the form

$$\hat{\rho}^1[s] = Z_A[s] \int d\omega_1 V^\times Z_A[s + i\omega_1] \Theta(\omega_1) Z_A[s] \hat{\rho}(t_i), \quad (3.24)$$

where

$$Z_A[s] = \frac{1}{s + \frac{i}{\hbar} \mathcal{L}_A}. \quad (3.25)$$

This process corresponds to the one-phonon emission and the absorption processes. The corresponding diagrams are shown in Fig. 1.

Next we consider the second order in $F(Q, Q; t, t_i)$. The Laplace transform of a second term is written as

$$\begin{aligned}
\hat{\rho}^2[s] = & Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \Theta(\omega_1) Z_A[s] \int d\omega_2 V^\times Z_A[s+i\omega_2] \Theta(\omega_2) Z_A[s] \hat{\rho}(t_i) \\
& + Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \int d\omega_2 V^\times Z_A[s+i(\omega_1+\omega_2)] \Theta(\omega_2) Z_A[s+i\omega_1] \Theta(\omega_1) Z_A[s] \hat{\rho}(t_i) \\
& + Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \int d\omega_2 V^\times Z_A[s+i(\omega_1+\omega_2)] \Theta(\omega_1) Z_A[s+i\omega_2] \Theta(\omega_2) Z_A[s] \hat{\rho}(t_i) . \quad (3.26)
\end{aligned}$$

In the above equation we have rearranged the time ordering of the integration to perform the Laplace transform. Corresponding diagrams are shown in Fig. 2. In this figure the first, the second, and the third terms of Eq. (3.26) correspond to Figs. 2(a), 2(b), and 2(c), respectively. Note that for the Gaussian-Markovian case, each term of Eq. (3.26) gives the same contribution and merge into a single term, therefore the equation becomes very simple.

Now we consider the resolvent Eq. (3.17). The first term $Z[s]$ incorporates all the noncrossing diagrams. (See Fig. 3.) This is shown by expanding $Z[s]$ into the form

$$\begin{aligned}
Z[s] = & Z_A[s] + Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \Theta(\omega_1) Z_A[s] \\
& + Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \Theta(\omega_1) Z_A[s] \int d\omega_2 V^\times Z_A[s+i\omega_2] \Theta(\omega_2) Z_A[s] \\
& + Z_A[s] \int d\omega_1 V^\times Z_A[s+i\omega_1] \int d\omega_2 V^\times Z_A[s+i(\omega_1+\omega_2)] \Theta(\omega_2) Z_A[s+i\omega_1] \Theta(\omega_1) Z_A[s] + \cdots . \quad (3.27)
\end{aligned}$$

We denote these processes by the thick line as in Fig. 3.

As seen from the third term of Eq. (3.23) and corresponding diagram in Fig. 2(c), the term of Eq. (3.19) corresponds to the crossing diagram in Fig. 4. Similarly, the terms of Eq. (3.20) correspond to the diagrams in Fig. 5. Each term corresponds to a topologically different diagram. To derive the higher-order terms of Eq. (3.17), the diagram method is helpful.

As was shown in the Gaussian-Markovian case,¹⁸ the calculation of these continued fractions is expected to converge even though the system-bath interaction is very strong or the correlation time of noise is very long. Then, if we were to perform this calculation until the value of the terms converged, we then would obtain the correct value of the resolvent. For a simple system, numerical calculations of the resolvent can be performed by using the matrix expression for the operators. A simple example is illustrated in Appendix C.

The Laplace transform expression such as Eqs.

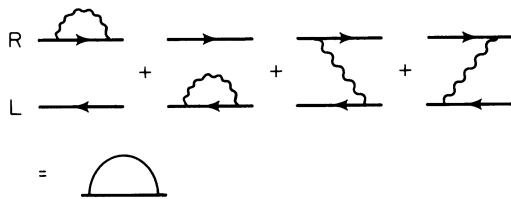


FIG. 1. The Feynman diagrams for the resolvent Eq. (3.24). In the upper part of the figure, the solid lines represent the wave functions of the system A , whereas the wavy lines the system B . The characters R and L , respectively, represent the time evolution of the right and the left parts of the density operator $\hat{\rho}(t)$. These diagrams are simply expressed by the half circle and the line as shown in the lower part of the figure.

(3.17)–(3.21) is useful to evaluate the power spectrum or the equilibrium value of the system. However, to evaluate the time evolution of system, solving the simultaneous differential equations such as Eqs. (3.4), (3.5), (3.7), (3.12), etc. can sometimes be performed more easily. In this case, since operators $\hat{\rho}(t; \nu_1, \nu_2, \dots, \nu_N)$ does not play a role for large number N even though the interaction is very strong, a set of differential equations are in closed form and we can solve these numerically.

We also notice that the correlated initial condition discussed in Sec. II can be applied to this general noise case. However, we do not address this issue here, since the extension is straightforward.

IV. LOW-TEMPERATURE CORRECTIONS FOR GAUSSIAN-MARKOVIAN SYSTEMS

In Sec. II, we neglected the series terms of Eq. (2.11) by assuming a high temperature bath $\beta\hbar\gamma \lesssim 1$ to produce the Markovian properties. However, by applying the method of Sec. III, we may discuss the case of a low-temperature bath. Let us take into account the series terms of Eq. (2.11) up to the m th terms. A similar consideration of Sec. III leads us to define the hierarchical elements as

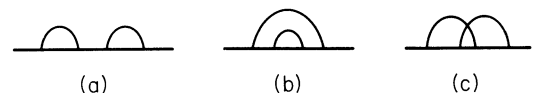


FIG. 2. The diagram representation of Eq. (3.26).

$$\rho(\phi_f, \phi'_f; t; n_0, n_1, \dots, n_m) \equiv \int D[Q(\tau)] \int D[Q'(\tau)] \times \prod_{j=0}^m \left[-\frac{i}{\hbar} \int_{t_i}^t d\tau \exp[-i\gamma_j(t-\tau)] \Theta_j(Q, Q'; \tau) \right]^{n_j} \times \exp \left[\frac{i}{\hbar} S_A(Q; t, t_i) \right] F(Q, Q'; t, t_i) \exp \left[-\frac{i}{\hbar} S_A(Q'; t, t_i) \right], \quad (4.1)$$

where $\gamma_0 = \gamma$, $\gamma_j = 2j\pi/\beta\hbar$ ($j > 0$), and

$$\Theta_0(Q, Q'; \tau) = C_0 V^\times(Q, Q'; \tau) + \frac{\hbar\eta\gamma^2}{2} V^\circ(Q, Q'; \tau), \quad \Theta_j(Q, Q'; \tau) = C_j V^\times(Q, Q'; \tau) \quad (j > 0) \quad (4.2)$$

with

$$C_0 = \frac{\hbar\eta\gamma^2}{2} \cot \left[\frac{\beta\hbar\gamma}{2} \right], \quad C_j = -\frac{\hbar\eta\gamma^2}{2} \frac{4j\pi}{(\beta\hbar\gamma)^2 - (2\pi j)^2} \quad (j > 0). \quad (4.3)$$

The hierarchal equation for the density operator $\hat{\rho}(t; n_0, n_1, \dots, n_m)$ is then

$$\dot{\hat{\rho}}(t; n_0, n_1, \dots, n_m) = - \left[\frac{i}{\hbar} \mathcal{L}_A + \sum_{j=0}^m n_j \gamma_j \right] \hat{\rho}(t; n_0, n_1, \dots, n_m) - \frac{i}{\hbar} \sum_{j=0}^m V^\times \hat{\rho}(t; n_0, \dots, n_j + 1, \dots, n_m) - \frac{i}{\hbar} \sum_{j=0}^m n_j \Theta_j \hat{\rho}(t; n_0, \dots, n_k - 1, \dots, n_m), \quad (4.4)$$

where Θ_j are the corresponding operators of the functional Eq. (4.2).

The number m is chosen to approximate the function $iL_2(t)$, and will be small even for the case of the low temperature. If we set $m = 1$, this will be a good approximation for $\beta\hbar\gamma \lesssim 5$, which corresponds to $T \gtrsim 2$ K, for the noise correlation time $t_c = 1/\gamma \sim 1$ ps. In this case, the equation of motion (4.4) can be written as

$$\begin{aligned} \dot{\hat{\rho}}_{00}(t) &= -\frac{i}{\hbar} \mathcal{L}_A \hat{\rho}_{00}(t) - \frac{i}{\hbar} V^\times [\hat{\rho}_{10}(t) + \hat{\rho}_{01}(t)], \\ \dot{\hat{\rho}}_{10}(t) &= - \left[\frac{i}{\hbar} \mathcal{L}_A + \gamma_0 \right] \hat{\rho}_{10}(t) - \frac{i}{\hbar} V^\times [\hat{\rho}_{20}(t) + \hat{\rho}_{11}(t)] - \frac{i}{\hbar} \Theta_0 \hat{\rho}_{00}(t), \quad (4.5) \\ \dot{\hat{\rho}}_{01}(t) &= - \left[\frac{i}{\hbar} \mathcal{L}_A + \gamma_1 \right] \hat{\rho}_{01}(t) - \frac{i}{\hbar} V^\times [\hat{\rho}_{11}(t) + \hat{\rho}_{02}(t)] - \frac{i}{\hbar} \Theta_1 \hat{\rho}_{00}(t), \end{aligned}$$

etc., where we put $\hat{\rho}_{n_0 n_1}(t) = \hat{\rho}(t; n_0, n_1)$. The above equation may be numerically solved just as Eq. (2.16). We can also evaluate the resolvent by using a method similar to that of Sec. III, but we do not show it here.

V. SOME REMARKS

Finally, we should mention the requirement of dynamic positivity, conservation of the probability. Consider a time-evolution operator for a reduced density element ρ denoted by T_t . Then the time evolution of system can be written as $T_t: \rho \rightarrow \rho_t$. Because we are considering a physical process, there are some requirements on the operator T_t .²⁰ One such important restriction is positivity that if $\rho \geq 0$ then $T_t \rho_t \geq 0$ for all $t \geq 0$.^{21,22}

For a white-noise case, this requirement is well studied. It has been shown that for an off-diagonal interaction $(a + a^\dagger) \sum_j c_j (b_j + b_j^\dagger)$, (where we put $x_j = b_j + b_j^\dagger$), the quantum master equation, which can be obtained from Eq. (3.22) by taking the long-time limit for the dissipative part

$$\hat{\rho}[s] = \lim_{\epsilon \rightarrow 0^+} \frac{1}{s + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_1 V^\times \frac{1}{\epsilon + i\nu_1 + \frac{i}{\hbar} \mathcal{L}_A} \Theta(\nu_1)} \hat{\rho}(t_i) \quad (5.1)$$

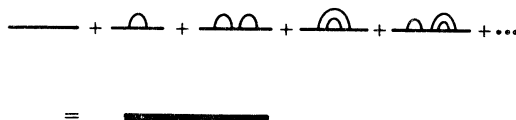


FIG. 3. The diagram representation of Eq. (3.27). We denote these diagrams by the thick line as in Fig. 4.

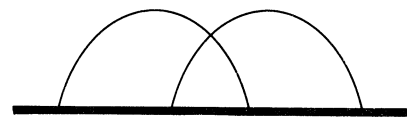


FIG. 4. The diagram representation of Eq. (3.19).

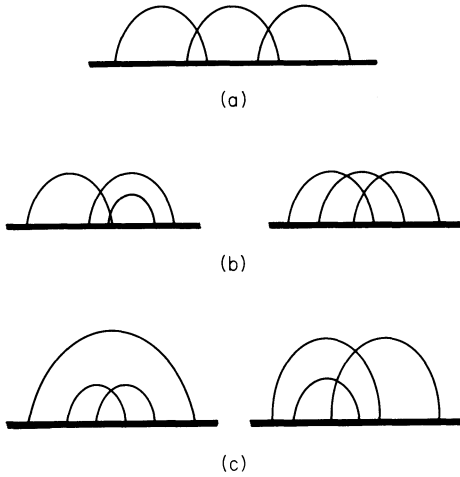


FIG. 5. The diagram representation of Eq. (3.20). (a), (b), and (c) represent the first, second, and third terms on the right-hand side of Eq. (3.20), respectively.

does not satisfy the property of positivity.^{23,24} Typically, one modifies an interaction in the resonant form as $ab_j^\dagger + a^\dagger b_j$ to keep positivity. The neglect of the off-resonant terms $ab_j + a^\dagger b_j^\dagger$ can be systematically performed by using the averaging method for the generalized master equation which corresponds to Eq. (3.22) before taking the long-time (white-noise) limit.^{25,26}

In our case, it is impossible to apply the discussion of the white-noise limit, since our system is described by a set of density elements $\{\rho_n\}$, and the interaction between the system and the bath is correlated and strong. For a

diagonal interaction $a^\dagger a \sum_j c_j (b_j + b_j^\dagger)$, which has been well used in the stochastic approach,²⁷ positivity may be satisfied. Our approach can treat the interaction in the resonant form as shown in Appendix B, but its validity is an open question since short correlated noise is essential in applying the averaging method, and there are no sufficient reasons to neglect off-resonant terms. The problem of positivity for the off diagonal, or more general interactions, is left for future study.

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APPENDIX A: EVALUATION OF INVERSE OPERATOR

Consider the following equations:

$$\begin{aligned}\hat{\rho}(t_i) &= \underline{A}\hat{\rho}[s] + \int d\nu \underline{B}\hat{\rho}[s, \nu], \\ \hat{\rho}(t_i, \nu) &= \underline{C}(\nu)\hat{\rho}[s] + \underline{D}(\nu)\hat{\rho}[s, \nu],\end{aligned}\quad (\text{A1})$$

where \underline{A} , $\underline{D}(\nu)$, $\hat{\rho}(t_i)$, etc., represent the operators or the matrices. The above equations can be expressed in the matrix form as

$$\begin{bmatrix} \hat{\rho}(t_i) \\ \hat{\rho}(t_i, \nu) \end{bmatrix} = \begin{bmatrix} \underline{A} & \int d\nu \underline{B} \\ \underline{C}(\nu) & \underline{D}(\nu) \end{bmatrix} \begin{bmatrix} \hat{\rho}[s, \nu] \\ \hat{\rho}[s, \nu] \end{bmatrix}.\quad (\text{A2})$$

Equation (A1) is easily solved as the form

$$\begin{aligned}\hat{\rho}[s] &= \underline{Z}[s]\hat{\rho}(t_i) - \underline{Z}[s] \int d\nu \underline{B} \underline{D}(\nu)^{-1} \hat{\rho}[s, \nu], \\ \hat{\rho}[s, \nu] &= -\underline{D}(\nu)^{-1} \underline{C}(\nu) \underline{Z}[s] \hat{\rho}(t_i) + \{ \underline{D}(\nu)^{-1} + \underline{D}(\nu)^{-1} \underline{C}(\nu) \underline{Z}[s] \int d\nu \underline{B} \underline{D}(\nu)^{-1} \} \hat{\rho}[s, \nu],\end{aligned}\quad (\text{A3})$$

where

$$\underline{Z}[s] = \left[\underline{A} + \int d\nu \underline{B} \underline{D}(\nu)^{-1} \underline{C}(\nu) \right]^{-1}.\quad (\text{A4})$$

Then the inverse matrix of Eq. (A2) can be written as

$$\begin{bmatrix} \hat{\rho}[s] \\ \hat{\rho}[s, \nu] \end{bmatrix} = \begin{bmatrix} \underline{Z}[s] & -\underline{Z}[s] \int d\nu \underline{B} \underline{D}(\nu)^{-1} \\ -\underline{D}(\nu)^{-1} \underline{C}(\nu) \underline{Z}[s] & \underline{D}(\nu)^{-1} + \underline{D}(\nu)^{-1} \underline{C}(\nu) \underline{Z}[s] \int d\nu \underline{B} \underline{D}(\nu)^{-1} \end{bmatrix} \begin{bmatrix} \hat{\rho}[s] \\ \hat{\rho}[s, \nu] \end{bmatrix}.\quad (\text{A5})$$

Using above equation successively, we may evaluate the inverse operators of Eqs. (3.9) and (3.14) in the continued-fraction form.

APPENDIX B: DEFORMATION POTENTIAL INTERACTION

In this paper we focused on the problem described by the Hamiltonian Eq. (2.1). However, our results easily extend to the case of the deformation potential interaction described by

$$H = H_A + \sum_j (\alpha_j V_j^* b_j + \alpha_j^* V_j b_j^\dagger) + \sum_j \hbar \omega_j b_j^\dagger b_j,\quad (\text{B1})$$

where V_j and α_j are, respectively, the operator of the system A and the coupling constant with the phonon mode j . The other parameters and operators for the bath are defined in the usual way. The operators V_j and V_j^* are, for example, expressed by the creation and the annihilation operators with the electron frequency ν , namely, c_ν^\dagger and c_ν as the form

$$V(\omega_j) = \sum_\nu c_\nu^\dagger c_{\nu+\omega_j}, \quad V^*(\omega_j) = \sum_\nu c_\nu c_{\nu-\omega_j},\quad (\text{B2})$$

where we used the expression $V(\omega_j)$ and $V^*(\omega_j)$ instead of V_j and V_j^* , then $V^*(\omega) = V(-\omega)$.

The influence functional for this interaction is similarly expressed as Eq. (3.1).²⁸ However, in this case, the functional $V(Q(t))$ is not only the function of $Q(t)$ but also the function of the phonon mode j , that is, $V(\omega_j, Q(t))$. With the exception of this point, the method of obtaining the resolvent is similar to that of Sec. III. The final results are the same as Eqs. (3.17)–(3.21) except that the operator V becomes the function of ω_j , namely, $V(\omega_j)$. Then, for example, the corresponding equation of Eq. (3.21) is expressed as

$$Z[s] = \frac{1}{s + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_1 V^\times(\nu_1) \frac{1}{s + i\nu_1 + \frac{i}{\hbar} \mathcal{L}_A + \int d\nu_2 V^\times(\nu_2) \frac{1}{s + i(\nu_1 + \nu_2) + \dots} \Theta^*(\nu_2)} \Theta^*(\nu_1)}, \quad (\text{B3})$$

where

$$\Theta^*(\omega) = \frac{1}{\hbar^2} J(\omega) \left[\coth \left[\frac{\beta \hbar \omega}{2} \right] [V^*(\omega)]^\times + [V^*(\omega)]^\circ \right]. \quad (\text{B4})$$

APPENDIX C: SIMPLE EXAMPLE

Let us consider a two-level system described by an excited state $|1\rangle$ and a ground state $|0\rangle$. The density operator is expressed in the form

$$\hat{\rho}(t) = P_1(t)|11\rangle + P_2(t)|00\rangle + P_3(t)|10\rangle + P_4(t)|01\rangle, \quad (\text{C1})$$

where we have introduced the notation

$$|ij\rangle = |i\rangle \langle j|. \quad (\text{C2})$$

We assume the Hamiltonian of the system and the interaction operator of the system is in the form

$$H_A = \hbar \omega_A a^\dagger a, \quad (\text{C3})$$

and

$$V = a^\dagger a. \quad (\text{C4})$$

The operators \mathcal{L}_A , V^\times , and V° satisfy the following relations:

$$\begin{aligned} \mathcal{L}_A |11\rangle &= \mathcal{L}_A |00\rangle = V^\times |11\rangle = V^\times |00\rangle = 0, \\ \mathcal{L}_A |10\rangle &= \hbar \omega_A |10\rangle, \quad \mathcal{L}_A |01\rangle = -\hbar \omega_A |01\rangle, \\ V^\circ |10\rangle &= |10\rangle, \quad V^\circ |01\rangle = |01\rangle, \end{aligned} \quad (\text{C5})$$

etc. Then Eq. (3.17) can be written as

$$\underline{P}[s] = \underline{G}[s] \underline{P}(t_i), \quad (\text{C6})$$

where $\underline{P}[s]$ is the column vector with the elements $P_j[s]$ ($j=1, \dots, 4$) and the matrix $\underline{G}[s]$ is given by

$$\underline{G}[s] = \begin{pmatrix} 1/s & 0 & 0 & 0 \\ 0 & 1/s & 0 & 0 \\ 0 & 0 & F^+[s] & 0 \\ 0 & 0 & 0 & F^-[s] \end{pmatrix}, \quad (\text{C7})$$

where

$$F^\pm[s] = S^\pm[s] + S^\pm[s] \int d\omega_1 S^\pm[s + i\omega_1] \int d\omega_2 S^\pm[s + i(\omega_1 + \omega_2)] K^\pm(\omega_1) S^\pm[s + i\omega_2] K^\pm(\omega_2) S^\pm[s] + \dots \quad (\text{C8})$$

The elements $S^\pm[s]$ are defined by

$$S^\pm[s] = \frac{1}{s \pm i\omega_A + \int d\nu_1 \frac{1}{s + i\nu_1 \pm i\omega_A + \int d\nu_2 \frac{1}{s + i(\nu_1 + \nu_2) \pm i\omega_A + \int d\nu_3 \frac{1}{s + \dots} K^\pm(\nu_3)} K^\pm(\nu_2)} K^\pm(\nu_1)}. \quad (\text{C9})$$

Here

$$K^\pm(\nu) = \frac{1}{\hbar^2} J(\nu) \left[\coth \left[\frac{\beta \hbar \nu}{2} \right] \pm 1 \right]. \quad (\text{C10})$$

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