Dynamics of the spin-boson model at zero temperature and strong dissipation

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Based on the stochastic decoupling framework and auxiliary function averaging technique, a functional integral equation for the zero-temperature population dynamics of the spin-boson model is established. This equation naturally displays the hierarchical structure of the dissipative dynamics and is amenable to nonperturbative approximations. It is shown that at strong dissipation the spin-boson model displays exponential decay with the rate decreasing from the maximum at the coherence-incoherence crossover to zero at the critical dissipation, a manifestation of quantum phase transition. Besides, the scaled time does not change in the whole regime of strong dissipation.

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I. INTRODUCTION

A two-state system (TSS) linearly coupled to a bath of infinite harmonic oscillators or a bosonic field is called the spin-boson model (SBM). It is a paradigmatic example exhibiting fruitful physics of quantum dissipation imposed by the bath on the TSS. We are usually interested in the behavior of the TSS, which may be a genuine physical entity of spin, or a quantum object projected from the low-energy approximation of a one-dimensional double-well system [1,2]. In particular, we want to understand how the heat bath affects quantum coherence, which may be specified by the population dynamics in the localized state of the TSS. It is well known that quantum coherence persists for weak dissipation and the TSS may act as a workable qubit in quantum computing. As dissipation increases, the dynamics of the TSS undergoes a coherence-incoherence crossover, which is reminiscent of a damped classical harmonic oscillator going through the critical damped point. Moreover, when dissipation reaches a critical strength, the zero-temperature dynamics is totally frozen. In other words, the TSS is always localized in the initial state. This is a demonstration of emergence of the local classicality from nonlocal quantumness, a *bona fide* quantum phase transition without a classical analog [3–5].

The SBM has been extensively investigated and applied in diversified fields such as quantum optics [6], electron or heat transfer [7–9], the Kondo problem [10], the interplay between driving and dissipation [11,12], and quantum computing [13] to name but a few. Notwithstanding the lasting efforts and progresses, the physics, especially the dynamical features of SBM, is still not fully understood. As Weiss stressed in his renowned monograph [2], "Despite its apparent simplicity, the spin-boson model cannot be solved exactly by any known method (apart from some limited regimes of the parameter space). Not only is the spin-boson model nontrivial mathematically, it is also nontrivial physically" (p. 261).

Studies on the dynamics of the SBM have been aroused by the pioneering work of Chakravarty and Leggett (CL) [14] and many theoretical and computational approaches have been used and developed since then [1,2]. For instance, the Feynman-Vernon influence functional [15,16], a powerful theoretical machinery for exploring quantum dissipation, was employed and popularized by CL and others, culminating in the celebrated noninteraction-blip approximation [14] (NIBA). This approximate result has been rederived over and over again and further developed, in particular by using those techniques based on the polaron transform plus the perturbation expansion method [17–20]. The NIBA is a good approximation only for weak dissipation or short times and predicts the correct form of time scaling and give the exact dissipation strength and exponential-decay dynamics at the coherence-incoherence crossover. Unfortunately, it cannot describe the strong-dissipation dynamics at low temperatures even qualitatively. That said, the zero-temperature dynamics in the regime of strong dissipation remains elusive and has been unsolved up to now [1]. Different numerical schemes have also been elaborated to study the dynamics of the SBM. The Monte Carlo simulation based on the path integral influence functional or the equivalence of SMB and the $1/r^2$ Ising model [21–24], the numerical renormalization group [25,26], the extended hierarchy approach [27], the stochastic equation of motion [28–33], and the multilayer multiconfiguration time-dependent Hartree methods [34,35] are among the frequently used methods. The last two techniques were employed to simulate zero-temperature, strong-dissipation dynamics of the SMB, producing results different not only from each other [31,35], but also from the analytic prediction in terms of the variational polaron transformation method and the conformal field theory [17,36].

The paper is organized as follows. In Sec. II we give a very short recapitulation of the stochastic decoupling method and show how to use it to unravel the global motion of the SBM, ending up with a stochastic differential equation (SDE) for the reduced density of the TSS. In Sec. III we formally solve the quantum expectation through the SDE and work out

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a stochastic integral-differential equation (SIDE) for the population dynamics. In Sec. IV we perform the random averaging by virtue of the auxiliary function technique and thus convert the SIDE to a deterministic equation in the functional form, an equation of motion displaying a hierarchical structure of multiple times. We further show that it gives an exponential decay at the coherence-incoherence crossover (exact Toulouse limit) and propose approximations to obtain the analytic result for strong dissipation. We summarize our findings and discuss their implications in Sec. V.

II. STOCHASTIC DIFFERENTIAL EQUATION OF EVOLUTION

The Hamiltonian of the SBM reads [1,2]

$$\hat{H}_{sb} = \hat{H}_s + \hat{H}_b + \hat{f}_s\hat{g}_b = -\frac{\hbar\Delta}{2}\sigma_x + \sum_j\left(\frac{\hat{p}_j^2}{2m_j} + \frac{m_j\omega_j^2}{2}\hat{x}_i^2\right) + \frac{1}{2}q_0\sigma_z\sum_j c_j\hat{x}_j, \tag{1}$$

where $\hat{H}_s$ denotes the the symmetric TSS, $\hat{H}_b$ indicates the bosonic bath, and $\hat{f}_s\hat{g}_b$ stands for the coupling between them. Here σ_x and σ_z are Pauli matrices and q_0 denotes the distance between the two local states and is set to unity for simplicity. The reorganization term is omitted because it is a constant, having no effect on time evolution. The dynamics of the SBM obeys the quantum Liouville equation, $i\hbar\partial\mathcal{D}/\partial t = [H, \mathcal{D}]$, where $\mathcal{D}(t)$ is the density matrix of the entire system. As usual, we assume an factorized initial condition $\mathcal{D}(0) = \rho_s(0)\rho_b(0)$, where ρ_s and ρ_b are the density matrices of the system and bath, respectively. Put differently, the system and the environment are initially disentangled. Because the bosonic degrees of freedom are infinite, directly solving the Liouville equation is difficult if not possible. Luckily, we do not need the detailed dynamics of the whole system, and it is sufficient to find out the equation of motion or master equation for the reduced density matrix $\tilde{\rho}(t) = \mathrm{Tr}_b\mathcal{D}(t)$ and to solve it, since we are interested only in the dynamics of the TSS. Notwithstanding, it is still unfortunate that the evolution of $\tilde{\rho}(t)$ in general does not satisfy a simple equation.

It has been shown that the effect of the bosonic bath on the TSS can fully be described by the spectral density function [1,2]

$$J(\omega) = \frac{\pi}{2}\sum_j\frac{c_j^2}{m_j\omega_j}\delta(\omega_j - \omega). \tag{2}$$

In the present work, we will adopt an Ohmic dissipation corresponding to the spectral density function, $J(\omega) = (2\pi\hbar K/q_0^2)\omega e^{-\omega/\omega_c}$, where the dimensionless K is the Kondo parameter measuring the strength of dissipation and ω_c is the high-frequency cutoff. Again, the whole system is supposed to evolve from a disentangled state $\rho_s(0)\rho_b(0)$, where the system of interest is initially in a localized state, $\rho_s(0) = \left(\begin{smallmatrix}1 & 0\\ 0 & 0\end{smallmatrix}\right)$, while the bath is in the ground state at zero temperature, prepared in the distant past. We want to reveal the universal feature of the population dynamics $\mathrm{Tr}\sigma_z(t)$ in the scaling limit, $\omega_c \to \infty$ at strong dissipation. Note that when the initial state of the bath is treated as the outcome of relaxation from a displaced ground state due to the coupling to the system, the mathematical treatment would be simpler, and we will discuss this point in a separate work.

Our strategy is to use the stochastic decoupling framework [30,37] to disentangle the real-time quantum evolution of the system and the bath. It is realized through introducing stochastic fields via either the Hubbard-Stratonovich transformation [28,30,37] or Itô calculus [38], and thereby the system and the bath separately evolve according to

$$i\hbar\frac{\partial\rho_s}{\partial t} = [\hat{H}_s, \rho_s] + \frac{\lambda_1\sqrt{\hbar}}{2}[\hat{f}_s, \rho_s][\mu_1(t) + i\mu_4(t)] + i\frac{\lambda_2\sqrt{\hbar}}{2}\{\hat{f}_s, \rho_s\}[\mu_2(t) - i\mu_3(t)], \tag{3}$$

$$i\hbar\frac{\partial\rho_b}{\partial t} = [\hat{H}_b, \rho_b] + \frac{\sqrt{\hbar}}{2\lambda_2}[\hat{g}_b, \rho_b][\mu_2(t) + i\mu_3(t)] + i\frac{\sqrt{\hbar}}{2\lambda_1}\{\hat{g}_b, \rho_b\}[\mu_1(t) - i\mu_4(t)], \tag{4}$$

where $\mu_j(t) (j = 1-4)$ are the Gaussian white noises and $\lambda_{1,2}$ are free scaling parameters. We notice that $\lambda_{1,2}$ may have units when Eqs. (3) and (4) are endowed with physical interpretation. But here we regard the decoupling scheme as a mathematical procedure and simply set $\lambda_{1,2} = 1$. Using Itô calculus, we readily prove that the equation for the average of the product of $\rho_s(t)$ and $\rho_b(t)$ over all the white noises is nothing but the original Liouville equation [38]. Therefore, there is $\langle\rho_s(t)\rho_b(t)\rangle = \mathcal{D}(t)$. Here and in the following brackets denote the average over the involving noises. The evolution of the whole system thus is unraveled into two separate motions of the system and of the bath respectively, subjected to common stochastic fields. Of course, the exact dynamics should be obtained by averaging all stochastic realizations. In other words, the effect of quantum interaction between the system and the bath on the dynamics is converted into correlations between their stochastic processes after unravelling. We go further to work out the equation for the stochastic reduced density matrix, $\rho(t) = \mathrm{Tr}_b\{\rho_s(t)\rho_b(t)\} = \rho_s(t)\mathrm{Tr}_b\rho_b(t)$ or its variants as long as their averages reproduce the exact reduced density matrix, $\langle\rho(t)\rangle = \tilde{\rho}(t)$. To this end, we calculate the formal expression of $\mathrm{Tr}_b\rho_b(t)$ via Eq. (4) and absorb it into the stochastic measure by using the Girsanov theorem [30,38,39]. As a consequence, Eq. (3) is changed accordingly, resulting in an equation for a more suitable form of the stochastic reduced density matrix [30,38],

$$i\hbar\frac{\partial\rho}{\partial t} = -\frac{\hbar}{2}\Delta[\sigma_x, \rho] + \omega_1(t)\sigma_z\rho - \omega_2(t)\rho\sigma_z, \tag{5}$$

where $\omega_{1,2}(t)$ are the effective stochastic fields defined by $\omega_{1,2}(t) = \bar{g}(t) + [\mu_1(t) \pm i\mu_2(t) \pm \mu_3(t) + i\mu_4(t)]/2$ with

$$\bar{g}(t) = \hbar\int_{t_0}^{t} dt'[\alpha_R(t-t')\nu_1^*(t') + i\alpha_I(t-t')\nu_2^*(t')]. \tag{6}$$

Here $\nu_1(t) = \mu_1(t) + i\mu_4(t)$ and $\nu_2(t) = i\mu_2(t) + \mu_3(t)$ are the (unnormalized) complex white noises, and $\alpha_{R,I}(t)$ are the real and imaginary parts of the correlation function of the bosonic bath, determined by the spectral density function given by Eq. (2). We take t_0 to be $-\infty$, which means the initial bath state $\rho_b(0)$ results from relaxation of a prepared state in the distant past. Note that the dissipative dynamics is very weakly dependent on t_0 [2].

At zero temperature the correlation function defining quantum dissipation reads

$$\alpha(t) = \alpha_R(t) + i\alpha_I(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)e^{-i\omega t} = \frac{\hbar}{2}K\omega_c^2(1+i\omega_c t)^{-2}. \tag{7}$$

Although a plain numerical implementation of Eq. (5) is feasible, it works only for very weak dissipation or short-time dynamics. As dissipation becomes strong, the lasting correlation between the stochastic density matrix $\rho(t)$ and the involving noises leads to the notorious difficulty: Numerical errors increase drastically with time. There have been continuous efforts to design more effective algorithms [29,31,33], but one that allows us to solve Eq. (5) for $K > 1/2$ and long times is yet to be available.

Instead of numerical treatments, the present work addresses analytical approximations to elucidate the dissipative dynamics dictated by Eq. (5). Again, we focus on the population dynamics described by the mean of $z(t) \equiv \mathrm{Tr}_s[\rho(t)\sigma_z(t)]$ with $z(0) = 1$. We will first derive the equation of motion for $z(t)$, starting from Eq. (5). To this end we define $I(t) \equiv \mathrm{Tr}_s[\rho(t)]$, $x(t) \equiv \mathrm{Tr}_s[\rho(t)\sigma_x(t)]$, and $y(t) \equiv \mathrm{Tr}_s[\rho(t)\sigma_y(t)]$ and obtain a set of stochastic differential equations,

$$\begin{aligned}\frac{dI}{dt} &= \frac{i}{\hbar}\nu_2(t)z(t)\\ \frac{dx}{dt} &= -\frac{1}{\hbar}\gamma(t)y(t)\\ \frac{dy}{dt} &= \Delta z(t) + \frac{1}{\hbar}\gamma(t)x(t)\\ \frac{dz}{dt} &= -\Delta y(t) + \frac{i}{\hbar}\nu_2(t)I(t),\end{aligned} \tag{8}$$

where the noises are regrouped for convenience as $\gamma(t) = 2\bar{g}(t) + \nu_1(t)$ and the initial condition is $I(0) = 1$, $x(0) = y(0) = 0$, and $z(0) = 1$. We readily find the correlations of the involved two stochastic fields $\nu_2(t)$ and $\gamma(t)$, namely, $\langle\gamma(t)\gamma(t')\rangle = 4\hbar\alpha_R(t-t')$, $\langle\nu_2(t)\nu_2(t')\rangle = 0$, and $\langle\gamma(t)\nu_2(t')\rangle = 4\hbar\theta(t-t')\alpha_I(t-t')$, where $\theta(t)$ is the Heaviside step function, which is unity for $t > 0$ and zero otherwise. We see that these two complex Gaussian noises fully specifying the effect of the heat bath on the dissipative system.

III. STOCHASTIC INTEGRAL EQUATION FOR $z(t)$

Using Green's function technique, we may feasibly manipulate Eq. (8) to obtain an integral equation for $z(t)$,

$$z(t) = e^{-i\phi_2(t,0)} - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2\cos[\phi_2(t,t_1)] \times \cos[\phi_1(t_1,t_2)]z(t_2), \tag{9}$$

where $\phi_1(t,t_1) = \frac{1}{\hbar}\int_{t_1}^t dt'\gamma(t')$ and $\phi_2(t,t_1) = \frac{1}{\hbar}\int_{t_1}^t dt'\nu_2(t')$. We want to study how the population difference $\tilde{z}(t) \equiv \langle z(t)\rangle$ changes in the two localized states, in particular when dissipation is strong, i.e., $K > 1/2$. Our task is to establish the equation of motion for $\tilde{z}(t)$ and find its solution. Because of the correlation of the involving noises there is not a straightforward way to transform the stochastic Eq. (9) into a closed-form, deterministic equation for $\tilde{z}(t)$. Notice that the first term on the r.h.s. of Eq. (9) represents a random phase that may be absorbed into the measure of the noises by employing the Girsanov transform [30,38,39]. Indeed, we recast $z(t)$ as $z(t) = e^{-i\phi_2(t,0)}z_1(t)$ and obtain the integral equation of $z_1(t)$,

$$z_1(t) = 1 - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2 e^{i\phi_2(t,t_2)}\cos[\phi_2(t,t_1)] \times \cos[\phi_1(t_1,t_2)]z_1(t_2). \tag{10}$$

We now apply the Girsanov transform, which is essentially equivalent to a change of variables for two white noises $\mu_2(t)$ and $\mu_3(t)$, namely, $\mu_2(t) \to \mu_2(t) - i/\hbar$ and $\mu_3(t) \to \mu_3(t) + 1/\hbar$. The factor $e^{i\phi_2(t,0)}$ then appears in the transformed statistical measure, which exactly cancels $e^{-i\phi_2(t,0)}$ in $z(t)$. We may further do direct calculations and check that terms containing only ϕ_2 are not affected, while terms containing ϕ_1 change according to $e^{\pm i\phi_1(t_1,t_2)} \to e^{\pm i[\phi_1(t_1,t_2)+A(t_1,t_2)]}$ where

$$A(t_1,t_2) = \frac{4}{\hbar}\int_{t_2}^{t_1} dt_3\int_{t_0}^{t_3} dt'\alpha_I(t_3-t') = -2K\omega_c(t_1-t_2), \tag{11}$$

which is readily evaluated by using Eq. (7) with $t_0 \to -\infty$. If t_0 is set to 0, $A(t_1,t_2)$ remains the same at the scaling limit $\omega_c \to \infty$. Note that $A(t_1,t_2)$ may be regarded as a contribution due to a delta function of the $\alpha_I(t)$, which does not affect the dynamics. As it will be canceled out by a counterterm in the following anyway, we will keep it as it is here. Upon finishing the Girsanov transform, $z(t)$ is changed to $\bar{z}(t)$, a direct result of $z_1(t)$ with the corresponding alternation of the noises,

$$\bar{z}(t) = 1 - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2 e^{i\phi_2(t,t_2)}\cos[\phi_2(t,t_1)] \times \cos[\phi_1(t_1,t_2) + A(t_1,t_2)]\bar{z}(t_2). \tag{12}$$

Obviously, when $A(t_1,t_2) = 0$, the equation of $\bar{z}(t)$ is identical to that of $z_1(t)$. In addition, since $z(t)$ and $\bar{z}(t)$ have the same average $\tilde{z}(t)$ yet to be determined, we will simply use the notation $z(t)$ for $\bar{z}(t)$ without any confusion and rewrite Eq. (12) in a compact form,

$$z(t) = 1 - \frac{\Delta^2}{4}\int_0^t dt_1\int_0^{t_1} dt_2 C(t,t_1,t_2)z(t_2), \tag{13}$$

where

$$C(t,t_1,t_2) = [1 + e^{2i\phi_2(t,t_1)}]\cos[\phi_1(t_1,t_2) + A(t_1,t_2)]e^{i\phi_2(t_1,t_2)}. \tag{14}$$

This stochastic integral equation is our working formula for obtaining the equation of $\tilde{z}(t)$. Because $z(t_2)$ and the stochastic kernel $C(t,t_1,t_2)$ are still correlated, there is no simple way to a closed-form equation for $\tilde{z}(t)$ from Eq. (13). To see the correlation more clearly and find an unraveling scheme, we first look at the noisy "angle" ϕ_1. With the definition of $\bar{g}$ given by Eq. (6) we may separate the acting time in ϕ_1 and divide it into two parts,

$$\phi_1(t_1,t_2) = \phi_{11}(t_1,t_2) + \phi_{12}(t_1,t_2), \tag{15}$$

where

$$\phi_{11}(t_1,t_2) = 2\int_{t_2}^{t_1} dt_3 \int_{t_2}^{t_3} dt_4[\alpha_R(t_3-t_4)\nu_1^*(t_4) + i\alpha_I(t_3-t_4)\nu_2^*(t_4)] + \frac{1}{\hbar}\int_{t_2}^{t_1} dt_3\nu_1(t_3), \tag{16}$$

$$\phi_{12}(t_1,t_2) = \frac{1}{2}\int_{t_0}^{t_2} dt_4\big[B'_{t_1,t_2}(t_4)\nu_1^*(t_4) + iB''_{t_1,t_2}(t_4)\nu_2^*(t_4)\big] \tag{17}$$

with $B'_{t_1,t_2}(t_4) = 4\int_{t_2}^{t_1} dt_3\alpha_R(t_3-t_4)$ and $B''_{t_1,t_2}(t_4) = 4\int_{t_2}^{t_1} dt_3\alpha_I(t_3-t_4)$. As $\phi_{11}(t_1,t_2)$ comprises the white noises starting from t_2, it does not affect dynamic processes driven by those white noises at times earlier than t_2. By contrast, $\phi_{12}(t_1,t_2)$ does affect the stochastic processes up to time t_2, because it consists of the involving white noises from the distant past t_0 to t_2. We then define $\Phi_{1,2}(t_1,t_2) = \phi_{11}(t_1,t_2) \pm \phi_2(t_1,t_2) + A(t_1,t_2)$ and partition $C(t,t_1,t_2)$ accordingly to get

$$C(t,t_1,t_2) = \tfrac{1}{2}[1+e^{2i\phi_2(t,t_1)}][e^{i\Phi_1(t_1,t_2)}e^{i\phi_{12}(t_1,t_2)} + e^{-i\Phi_2(t_1,t_2)}e^{-i\phi_{12}(t_1,t_2)}]. \tag{18}$$

From this expression we may identify these two factors $e^{\pm i\phi_{12}(t_1,t_2)}$ that influence $z(t_2)$. Knowing this fact, we now return to Eq. (13) to work out a deterministic equation for $\tilde{z}(t)$, by virtue of the auxiliary function technique [41]. To this end we view $z(t)$ as a functional of the two stochastic processes γ and ν_2. Moreover, we add to them respectively the deterministic function B_1 and B_2 as auxiliary terms so that $\phi_{1,2}$ in Eq. (13) turn to be $\phi_1 \to \phi_{1B}(t_1,t_2) = \frac{1}{\hbar}\int_{t_2}^{t_1} dt'[\gamma(t') + B_1(t')]$ and $\phi_2 \to \phi_{2B}(t_1,t_2) = \frac{1}{\hbar}\int_{t_2}^{t_1} dt'[\nu_2(t') + B_2(t')]$. As a result, we obtain

$$z([\gamma+B_1,\nu_2+B_2],t) = 1 - \frac{\Delta^2}{2}\int_0^t dt_1\int_0^{t_1} dt_2 C_B(t,t_1,t_2)z([\gamma+B_1,\nu_2+B_2],t_2). \tag{19}$$

Because of the variation of partitioning factors in Eq (18), the integral kernel C in Eq. (13) is also modified as C_B, namely,

$$C_B(t,t_1,t_2) = \tfrac{1}{2}[1+e^{2i\phi_{2B}(t,t_1)}][e^{i\Phi_{1B}(t_1,t_2)}e^{i\phi_{12}(t_1,t_2)} + e^{-i\Phi_{2B}(t_1,t_2)}e^{-i\phi_{12}(t_1,t_2)}], \tag{20}$$

where

$$\Phi_{1B,2B}(t_1,t_2) = \phi_{11}(t_1,t_2) + \frac{1}{\hbar}\int_{t_2}^{t_1} dt' B_1(t') \pm \phi_{2B}(t_1,t_2) + A(t_1,t_2).$$

It is clear that in the kernel C defined by Eq. (18), the factors $e^{\pm i\phi_{12}(t_1,t_2)}$ impacting $z(t_2)$ in Eq. (13) remain unchanged. Taking into account these results in Eq. (19), we readily find

$$\begin{aligned}\langle C_B(t,t_1,t_2)z([\gamma+B_1,\nu_2+B_2],t_2)\rangle = \tfrac{1}{2}[1+\langle e^{2i\phi_{2B}(t,t_1)}\rangle][\langle e^{i\Phi_{1B}(t_1,t_2)}\rangle\langle e^{i\phi_{12}(t_1,t_2)}z([\gamma+B_1,\nu_2+B_2],t_2)\rangle \\ +\langle e^{-i\Phi_{2B}(t_1,t_2)}\rangle\langle e^{-i\phi_{12}(t_1,t_2)}z([\gamma+B_1,\nu_2+B_2],t_2)\rangle].\end{aligned} \tag{21}$$

Using the correlation relations for γ and ν_2 given above and the Novikov theorem [40], we perform the elementary algebra to finish the statistical average of the exponential processes determined by these two Gaussian noises, obtaining

$$\begin{aligned}\langle e^{2i\phi_{2B}(t,t_1)}\rangle &= e^{2\frac{i}{\hbar}\int_{t_1}^{t} dt' B_2(t')}, \\ \langle e^{i\Phi_{1B}(t_1,t_2)}\rangle &= Q(t_1-t_2)e^{\frac{i}{\hbar}\int_{t_1}^{t} dt'[B_1(t')+B_2(t')]} \\ \langle e^{-i\Phi_{2B}(t_1,t_2)}\rangle &= Q^*(t_1-t_2)e^{-\frac{i}{\hbar}\int_{t_1}^{t} dt'[B_1(t')-B_2(t')]},\end{aligned} \tag{22}$$

where $Q(t_1-t_2) = \exp[iA(t_1,t_2) - \frac{4}{\hbar}\int_{t_2}^{t_1} dt_3\int_{t_2}^{t_3} dt_4\alpha(t_3-t_4)] = [1+i\omega_c(t_1-t_2)]^{-2K}$.

Working again with the Girsanov transform, that is, $\mu_1 \to \mu_1 + iB'_{t_1,t_2}/2$, $\mu_2 \to \mu_2 - B'_{t_1,t_2}/2$, $\mu_3 \to \mu_3 - B''_{t_1,t_2}/2$, and $\mu_4 \to \mu_4 + iB''_{t_1,t_2}/2$, we are able to convert the correlation in two terms in Eq. (21) into spontaneous, deterministic fields, namely, $\langle e^{\pm i\phi_{12}(t_1,t_2)}z([\gamma+B_1,\nu_2+B_2],t_2)\rangle = \tilde{z}([B_1 \pm iB'_{t_1,t_2}, B_2 \mp B''_{t_1,t_2}],t_2)$. Taking the statistical average over γ and ν_2 on both sides of Eq. (19), we thus get

$$\begin{aligned}\tilde{z}([B_1,B_2],t) = 1 - \frac{\Delta^2}{4}\int_0^t dt_1\int_0^{t_1} dt_2[1+e^{2\frac{i}{\hbar}\int_{t_1}^{t} dt' B_2(t')}]\big\{Q(t_1-t_2)e^{\frac{i}{\hbar}\int_{t_2}^{t_1} dt'[B_1(t')+B_2(t')]}\tilde{z}\big(\big[B_1+iB'_{t_1,t_2}, B_2-B''_{t_1,t_2}\big],t_2\big) \\ + Q^*(t_1-t_2)e^{-\frac{i}{\hbar}\int_{t_2}^{t_1} dt'[B_1(t')-B_2(t')]}\tilde{z}\big(\big[B_1-iB'_{t_1,t_2}, B_2+B''_{t_1,t_2}\big],t_2\big)\big\}.\end{aligned} \tag{23}$$

This is the main result of the present work, and it shows that the fields B'_{t_1,t_2} and B'_{t_1,t_2} are spontaneously induced during the evolution, which, in turn, exert on the dynamics as a feedback. Therefore, the apparent dissipative dynamics may be regarded as an outcome of motion in self-generated fields.

Equation (23) may be solved as a infinite series of Δ^2 by iteration, which would reproduce the previously known result based on the path integral technique [1,2] and would be helpless in understanding strong dissipation. However, it may be dealt with nonperturbatively, thus presenting a global perspective on exploring the dynamics of the SBM. We would like to point out that the averaging procedure with auxiliary functions can directly be applied to Eq. (9). The result is the same as that of Eq. (23) transformed from $\tilde{z}([B_1, B_2], t) \to \exp\{\frac{i}{\hbar}\int_0^t dt' B_2(t')\}\tilde{z}([B_1, B_2], t)$.

In Eq. (23) the introduced deterministic functions $B_{1,2}$ can physically be viewed as auxiliary fields and will finally be set to zero for calculating the required quantity $\tilde{z}(t) = \tilde{z}([0, 0], t)$. As an integral functional equation, Eq. (23) says that new or self-induced fields arise as $\tilde{z}$ evolves, which conversely shapes the dynamics and defies a simple closed-form equation for $\tilde{z}(t)$. To be specific, the so-obtained formal equation of $\tilde{z}(t)$ includes two unknown functionals $\tilde{z}_1(t_1, t_2) \equiv \tilde{z}([iB'_{t_1,t_2}, -B''_{t_1,t_2}], t_2)$ and $\tilde{z}_1^*(t_1, t_2) = \tilde{z}([-iB'_{t_1,t_2}, B''_{t_1,t_2}], t_2)$ describing the dynamics of $\tilde{z}$ subjected to the pair of self-induced fields B'_{t_1,t_2} and B''_{t_1,t_2}. The equation of motion for $\tilde{z}_1(t_1, t_2)$ would also be determined through Eq. (23), which brings about further unknown functionals portraying the dynamics of $\tilde{z}$ with more accumulative self-induced fields exerting at different times. Repeating the procedure yields hierarchical equations for the ensuing yet-to-be-determined functionals, which may be terminated at a certain point to form a closed-form set. Instead of pursuing this way, we will analyze the speciality of functions B'_{t_1,t_2}, B''_{t_1,t_2}, and $Q(t_1, t_2)$ and thereby derive reasonably approximate equations for $\tilde{z}(t)$.

IV. EQUATION OF MOTION OF $\tilde{z}(t)$

Setting $B_{1,2} = 0$ in Eq. (23), we immediately acquire the expression for $\tilde{z}(t)$, which is identical to the integral-differential formulation

$$\frac{d\tilde{z}(t)}{dt} = -\frac{\Delta^2}{2}\int_0^t dt'[Q(t-t')\tilde{z}_1(t,t') + Q^*(t-t')\tilde{z}_1^*(t,t')] \tag{24}$$

with $\tilde{z}(0) = 1$. Here, as discussed above, the dissipative dynamics in the self-induced fields $\tilde{z}_1(t, t')$ are still unknown. We may resort to Eq. (23) to find the equations for them, but will end up with more unknown quantities representing dissipative dynamics ruled by a combination of self-induced fields. A simple and straightforward approximation is to assume that the self-induced fields B'_{t_1,t_2} and B''_{t_1,t_2} are negligible in Eq. (23). With vanishing auxiliary fields $B_{1,2} = 0$ Eq. (23) can then be recast as

$$\frac{d\tilde{z}(t)}{dt} = -\frac{\Delta^2}{2}\int_0^t dt'[Q(t-t') + Q^*(t-t')]\tilde{z}(t'). \tag{25}$$

This integral-differential equation is the result of the celebrated noninteracting blip approximation (NIBA) derived first with the path integral technique [14] and rederived afterwards by different methods [17–20]. Comparing it to Eq. (24), the exact one, we find the approximation adopted in NIBA may also be viewed as that of $\tilde{z}_1(t, t') \approx \tilde{z}(t')$. Although the validity of NIBA for describing short-time dynamics, weak dissipation, and other cases has been verified, its invalidity for describing long-time dynamics in the case of strong dissipation has been well known [1,2].

To develop approximations beyond the NIBA, we need to know how the two-time function $\tilde{z}_1(t, t')$ relies on $\tilde{z}(t)$ in Eq. (24) and take advantage of the properties of the kernel $Q(t)$. Consider first $\tilde{z}_1(t, t')$. Upon substituting $B_1 = iB'_{t,t'}$ and $B_2 = -B''_{t,t'}$, Eq. (23) becomes

$$\tilde{z}_1(t,t') = 1 - \frac{\Delta^2}{4}\int_0^{t'} ds \int_0^s ds' P(t,t',s)\{Q(s-s')S(t,t',s,s')\tilde{z}([iB'_{t,t'} + iB'_{s,s'}, -B''_{t,t'} - B''_{s,s'}], s') + Q^*(s-s')[S^*(t,t',s,s')]^{-1}\tilde{z}([iB'_{t,t'} - iB'_{s,s'}, -B''_{t,t'} + B''_{s,s'}], s')\}, \tag{26}$$

where

$$P(t,t',s) = 1 + e^{-2\frac{i}{\hbar}\int_s^{t'} ds' B''_{t,t'}(s')} = 1 + e^{i4K\{\arctan[\omega_c(t-t')] - \arctan[\omega_c(t-s)] + \arctan[\omega_c(t'-s)]\}} \tag{27}$$

and

$$S(t,t',s,s') = \left[\frac{D(t-s)D(t'-s')}{D(t-s')D(t'-s)}\right]^K \tag{28}$$

with $D(t) = 1 + i\omega_c t$. If $t' = t$, then $P = S = 1$ and the above equation turns out to be the same as Eq. (24). In this case, therefore, $\tilde{z}_1(t, t) = \tilde{z}(t)$. For the special case $K = 1/2$ known as the Toulouse limit, there is $Q(t) = (i\omega_c)^{-1}[\mathcal{P}t^{-1} + i\pi\delta(t)]$, where $\mathcal{P}$ denotes the Cauchy principle value. As a result, Eq. (24) becomes

$$\frac{d\tilde{z}(t)}{dt} = -\frac{\pi\Delta^2}{2\omega_c}\tilde{z}(t) + i\frac{\Delta^2}{2\omega_c}\mathcal{P}\int_0^t dt'\frac{1}{t-t'}[\tilde{z}_1(t,t') - \tilde{z}_1^*(t,t')] = -\frac{\pi\Delta^2}{2\omega_c}\tilde{z}(t), \tag{29}$$

where we used the fact that for $t - t' > 1/\omega_c$ and in the scaling limit $\omega_c \to \infty$, the function $\tilde{z}_1(t, t')$ is real for almost all times. We readily obtain $\tilde{z}(t) = e^{-\frac{\pi\Delta^2}{2\omega_c}t}$, which is exact [1,2]. We thus showed the well-known results can be derived with ease by using the functional formulation Eq. (23).

Now we tackle the case of strong dissipation, $1/2 < K \leqslant 1$. We know $\tilde{z}_1(t, t) = \tilde{z}(t)$. For $t' < t$, in the evolution of $\tilde{z}_1(t, t')$ defined by Eq. (26) we neglect $B'_{t,t'}$ and $B''_{t,t'}$, the "driving" fields from the early time and keep the self-induced ones $B'_{s,s'}$ and $B''_{s,s'}$. This is loosely a Markovian approximation. Also, we approximately set $S(t, t', s, s') = 1$, which is exact for either $t = t'$ or $s = s'$. Further, let $t > t' \gg 1/\omega_c$. Note that $P(t, t', s)$ does not change much for $s < t'$. Resorting to Eq. (24), we approximate the integral in Eq. (26) by replacing the upper bound t' by $t' - \tau$, where $t' > \tau \gg 1/\omega_c$ to obtain

$$\tilde{z}_1(t,t') \approx 1 + \frac{1}{2}\int_0^{t'-\tau} ds \frac{\partial}{dt_1'}[P(t,t',s)z(s)]$$
$$= \frac{1}{2}\{1 - e^{i4K\arctan[\omega_c(t-t')]}\} + \frac{1}{2}e^{i2K\pi}z(t'). \quad (30)$$

The task now is to put these results into Eq. (24) to elicit the equation for $\tilde{z}(t)$. To simplify the manipulation, we treat $Q(t) \equiv Q_R(t) + iQ_I(t)$ as a pair of distribution functions, which is possible for both $Q_R(t)$ and $Q_I(t)$ being local in t. We first argue that there is no contribution from $Q_I(t)$ to $\tilde{z}(t)$. For $K > 1/2$, in fact, $Q_I(t)$ assumes its maximum at $t_I = \tan[\pi/2(1+2K)]/\omega_c < 1/\omega_c$, which becomes smaller for larger K and can be simply set to zero as a zeroth-order approximation for strong dissipation. As a consequence, since $\tilde{z}_1(t_1,t_1) = \tilde{z}(t_1)$ is real, the contributions in Eq. (24) result from the imaginary parts of $Q(t)$ and $Q^*(t)$ cancel out.

For the real part, $Q_R(t)$ (t is large) can be partitioned into two local functions, and the boundary is determined by $Q_R(t_b) = 0$, where $t_b = \tan(\pi/4K)/\omega_c$. The first one $Q_{1R}(t')$ defined as $Q_R(t')$ for $t' \in [0, t_b)$ is positive and assumes its maximum $t = 0$, while the second one $Q_{2R}(t')$ defined as $Q_R(t')$ for $t' \in [t_b, t)$ is negative, having the minimum at $t^* = \tan(\pi/1 + 2K)/\omega_c$.

As the physical time is a slow variable, i.e., $t \gg t^*$, the first distribution $Q_{1R}(t')$ dictates $\tilde{z}(t')$ and the second one $Q_{2R}(t')$ dictates the real part of $\tilde{z}_1(t,t')$ given by Eq. (30). Besides, the average of the first term on the r.h.s. of Eq. (30) is zero. Now we treat Q_{1R} and Q_{2R} as two delta functions with the plus and minus coefficient $\int_0^{t_b} dt' Q_R(t') = -C(K)/\omega_c$, where

$$C(K) = \frac{1}{1-2K}\left(1 + \tan^2\frac{\pi}{4K}\right)^{\frac{1}{2}-K} \sin\left[\frac{\pi}{4K}(1-2K)\right].$$

Substituting into Eq. (24), we obtain $d\tilde{z}(t)/dt = -R(K)\tilde{z}(t)$ with the solution $\tilde{z}(t) = e^{-R(K)t}$, where $R(K) = C(K)\sin^2(K\pi)\Delta^2/\omega_c$ is the decay rate. We may rewrite the result as $\tilde{z}(\bar{t}) = e^{-\bar{R}(K)\bar{t}}$ where $\bar{t} = (\Delta/\omega_c)t$ is the scaled time and $\bar{R}(K) = C(K)\sin^2(K\pi)\Delta$ is the corresponding decay rate. Therefore, the scaled time does not change in the strong-dissipation regime ($K > 1/2$), which is different from the weak-dissipation regime where the time is scaled as $\bar{t} = (\Delta/\omega_c)^{\frac{K}{1-K}}t$. Note that $\bar{R}(K)$ gives the exact value of Toulouse limit, $R(1/2) = \Delta\pi/2$. In addition, it also correctly predicts localization or a frozen state from a dynamical point of view at $K = 1$, i.e., $\bar{R}(1) = 0$. Localization of the dissipative system manifests a quantum-classical crossover, a genuine quantum phase transition in which the spin-boson model has a degenerate, parity-broken ground state. In between $\bar{R}(K)$ is a monotonically decreasing function of the Kondo parameter K. Our observation of the scaled time being invariant for strong dissipation is consistent with the former numerical finding [31] based on simulating the stochastic differential equation (5) with improved algorithms, but different from other reports [17,35,36]. Further studies will definitely be required.

V. SUMMARY AND DISCUSSION

The dynamical feature of the spin-boson system at zero temperature and strong dissipation has puzzled scientists for decades [1]. The difficulty is rooted in the involvement of different timescales in the quantum evolution, which defies a solution by available theoretical or numerical methods. Resorting to the stochastic decoupling framework, we show how to derive a stochastic Liouville equation for the two-state system of the SBM at zero temperature, for which the random average gives the exact reduced density matrix [28,30]. We then formally solve it using Green's function technique, obtaining a stochastic integral-differential equation for the population difference in two localized states. Its average directly reflects quantum coherence of the two-state system. We use the Girsanov theorem and auxiliary function techniques to convert this stochastic equation into a deterministic, functional form, which manifests the hierarchical structure with self-induced fields of the dissipative dynamics. Moreover, the functional equation allows for nonperturbative approximations. We demonstrate that it leads to the exact outcome in the Toulouse limit or the coherence-incoherence crossover with $K = 1/2$ and results in the NIBA when the self-induced fields is neglected. For strong dissipation $1/2 < K \leqslant 1$ we propose a Markovian-like approximations for the arising two-time function and observe that the dynamics follows an exponential decay, from the maximum in the Toulouse limit $K = 1/2$ to zero at the critical value $K = 1$ where the quantum phase transition takes places. In addition, the scaled time in the the whole range of decay dynamics is proportional to Δ/ω_c, which is in contrast to the weak-dissipation case where the scaled time is dependent on the Kondo parameter K. Our theoretical approach and findings would be helpful for understanding the quantum dissipation effects in particular the quantum-classical transition and quantum impurity dynamics.

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