Analytical approach to dynamical behavior and phase diagrams in dissipative two-state systems

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An analytical approach is developed to investigate the phase transitions and the dynamical behaviors in dissipative two-state systems in a unified method for different bath indices with the view of understanding the effects of environments and tunneling on the systems. Analytic expressions of the current correlation function, the nonequilibrium correlation function, and the critical points of coherent-incoherent and delocalized-localized transitions for various bath indices are obtained by implementing perturbation treatment and employing the Green's function method. The phase boundaries can be precisely determined at both the scaling limit and the finite bare tunneling. The results of the dynamical behaviors of the correlation functions are consistent well with those of previous works and some well-established values are reproduced exactly. This theory is quite simple and may be applied as a potential method to study absorption spectra and photoluminescence in quantum dots and other confined quantum systems.

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I. INTRODUCTION

The influence of dissipation on quantum coherence is a crucial subject in the exploration of macroscopic quantum phenomena and the dissipation-induced decoherence remains the most important obstacle to the development of quantum information and quantum computer. Efforts to deal with the influence lead to the systematic study of the spin-boson model, which offers a unique testing ground for exploring the foundations of quantum mechanics and also serves as an elementary carrier of information in a quantum information processor in the form of a qubit.[1,2] Recently, the upsurge of interest in tunneling systems coupled to dissipative environment has renewedly stimulated extensive studies on the physical properties of dissipative two-state systems.[3–6] The dissipative two-state system is important for understanding numerous physical and chemical processes since it provides a universal model for these processes and has been used to describe a large class of problems ranging from Kondo impurities, superconductors, chemical reactions, to amorphous materials.[7,8] The main interest of these studies has been in understanding how the environment influences the dynamics of the system and, in particular, how the dissipation destroys quantum coherence.[9] The very recent exploitations of the properties of macroscopic quantum coherence in superconducting quantum interference devices, molecular magnets,[10] and entanglement of qubit with environment[11] and qubits in quantum computers[12] conduce to further interest of theoretical studies on intrinsic physics of this system. While considerable effort has been made to investigate the dynamic equilibrium and nonequilibrium correlations and the Shiba's relation, it is theoretically and experimentally significant to develop an accepted theory for the current correlation function, which contains useful information about excitation spectrum and therefore has been utilized to investigate the absorption spectra and photoluminescence in quantum dot[13] and the spin current in spin-cell device for spintronic circuits.[14] Since the two energy levels in this system cannot be completely decoupled from its environment, dissipation and decoherence effects are unavoidable.[15] The effect of environment on small quantum systems can induce mediate coupling of different electronic energy levels and results in many interesting phenomena. However, with the coupling to environment the dissipative two-state system is difficult to handle analytically, which has brought much uncertainty in the interpretation of experimental data and has limited our understanding of many interesting quantum phenomena of these systems. Although the dissipative two-state system has been dealt with by means of various analytical and numerical methods,[7,8,13–25] with respect to the current correlation function only numerical calculation has been performed.[23] An analytical study will make it possible to have an insight into the intrinsic properties of dissipative two-state systems.

In this work, we focus on the current correlation function and the phase diagrams of dissipative two-state systems with the view of understanding the effects of environment and tunneling on the dynamic behaviors of the correlation functions and the characteristics of the phase transitions. By developing an analytical approach, analytic expressions of the current correlation function and the phase-transition points are obtained. The validity of our theory is manifested by the very well agreement of our results with that of numerical calculations[23] of the current correlation function and the success in reproducing some well-established values well known as results of the nonperturbation in Ohmic case. More importantly, this mathematically simple and physically clear method may provide an analytic method to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems. The paper is organized as follows. In Sec. II, we introduce and diagonalize the Hamiltonian by using unitary transformation to obtain the ground- and the low-lying excited energy states. The equation determining the critical point of localized-delocalized phase transition is obtained. In Sec. III, by means of the Green's function and the residue theorem, analytic expressions of the current correlation function, the nonequilibrium correlation function, the critical value of the coherent-incoherent transition point, and the Q factor are obtained. The calculated results for different environments are presented and discussed In Sec. IV. In Sec. V, the properties of coherence-incoherence and localized-delocalized phase transitions are studied and the phase diagrams are illustrated. Finally, a brief summary will conclude our presentation in Sec. VI.

II. MODEL HAMILTONIAN

The dissipative two-state systems representing tunneling phenomena in condensed phase are often described by the spin-boson model,[7,8]

$$H = -\frac{1}{2}\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2}\sum_k g_k(b_k^\dagger + b_k)\sigma_z, \qquad (1)$$

where Δ is the bare tunneling matrix element, σ_i $(i=x,y,z)$ are the usual Pauli spin matrices, ω_k are the oscillator frequencies, and g_k is the strength of coupling of the system to the bath represented by an infinite set of harmonic oscillators, which are created by boson operators b_k and $b_k^\dagger$. The effects of the bath and the coupling are completely characterized by the spectral density

$$J(\omega) = \sum_k g_k^2 \delta(\omega - \omega_k) = 2\alpha\omega_c^{1-S}\omega^S\theta(\omega_c - \omega), \qquad (2)$$

where $\theta(x)$ is the usual step function and the index S denotes the different environment baths. The assumption of the environment bath reduces the characteristics of the bath and the coupling to two parameters: the dimensionless coupling (damping) constant α and the upper cutoff ω_c of the oscillator frequency. Though the Hamiltonian (1) seems quite simple, except for some special parameter values, it cannot be solved exactly.[26] Therefore, various approaches have been performed to this model and quite some progress in numerical methods has been done in recent years. The central techniques in these works include, for example, quantum Monte Carlo techniques,[27] quasiadiabatic path integral,[28] multilayer multiconfiguration time-dependent Hartree method,[29] noninteracting-blip approximation, Bloch-Redfield equation approach,[30] the self-consistent hybrid approach,[31] and numerical renormalization group.[32] However, up to now it is still a challenge to develop an analytical approach to produce correct physics in a unified way for various bath indices and the whole parameter ranges $0 \le \alpha$ and $0 \le \Delta < \omega_c$.

The isolated two-state system exhibits coherent tunneling and is trivial to diagonalize. The coupling of the system to the dissipative environment leads the tunneling between the two states to lose its phase coherence. This can happen even at zero temperature if the continuous spectrum of the macroscopic dissipative environment extends down to zero frequency. The transition from coherent to incoherent dynamics occurs at a critical damping $\alpha=\alpha_c$. To take into account the coupling of the system to the bath, a unitary transformation is applied to H,[33,34] $H' = \exp(A)H\exp(-A)$, with the generator

$$A = \sum_k \frac{g_k}{2\omega_k}\xi_k(b_k^\dagger - b_k)\sigma_z. \qquad (3)$$

The transformation can be done to the end and produces the transformed Hamiltonian as

$$H' = H_0' + H_1' + H_2', \qquad (4)$$

where

$$H_0' = -\frac{1}{2}\eta\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k}\xi_k(2-\xi_k), \qquad (5)$$

$$H_1' = \frac{1}{2}\sum_k g_k(1-\xi_k)(b_k^\dagger + b_k)\sigma_z - \frac{1}{2}\eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k), \qquad (6)$$

$$H_2' = -\frac{1}{2}\Delta\sigma_x\left(\cosh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right\} - \eta\right) - \frac{1}{2}\Delta i\sigma_y\left(\sinh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right\} - \eta\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right). \qquad (7)$$

For implementing perturbation treatment conveniently, the transformed Hamiltonian is separated into three parts according to their orders of the coupling strength. The first part H_0' contains the zeroth-order terms of the transformed Hamiltonian, H_1' the first-order terms, and H_2' the second as well as higher-order terms. H_0' is chosen as the unperturbed Hamiltonian and should include as more terms as possible to make the perturbation more efficacious on the premise of keeping it can be diagonalized exactly. H_1' and H_2' are treated as perturbation and they should be as small as possible. After collecting together the terms of the same order, the bare tunneling matrix element Δ in H_0' is multiplied by a factor

$$\eta = \exp\left(-\sum_k \frac{g_k^2}{2\omega_k^2}\xi_k^2\right) = \exp\left(-\alpha\omega_c^{1-S}\int_0^{\omega_c}\frac{\beta^S}{(\eta\Delta+\beta)^2}d\beta\right). \qquad (8)$$

Clearly, $0 \le \eta \le 1$. Compared with Hamiltonian (1), the tunneling matrix element in the transformed Hamiltonian is renormalized by the factor η due to the dissipative environment; therefore, the renormalized effective tunneling is given by[25]

$$\Delta_r = \eta\Delta. \qquad (9)$$

Because of the decoupled form of spin and boson operators, H_0' can be diagonalized exactly and its eigenstate is a direct product, $|s\rangle|\{n_k\}\rangle$, where $|s\rangle$ is $|s_1\rangle = \frac{1}{\sqrt{2}}\binom{1}{1}$ or $|s_2\rangle = \frac{1}{\sqrt{2}}\binom{1}{-1}$, i.e., the eigenstates of σ_x, and $|\{n_k\}\rangle$ means that there are n_k bosons for mode k. The ground state of H_0' is $|g_0\rangle = |s_1\rangle|\{0_k\}\rangle$, where $|\{0_k\}\rangle$ is the vacuum state of bosons in which $n_k=0$ for every k. Using the form of η given by Eq. (8), one can get $\langle g_0|H_2'|g_0\rangle = 0$, i.e., the contribution of H_2' to the perturbation calculation at second order of g_k is zero.

For a certain value of the index S, the localized-delocalized phase transition occurs at a critical value of the coupling constant α_l,[7,8] which separates a localized phase at $\alpha \ge \alpha_l$ from a delocalized phase at $\alpha < \alpha_l$. In the localized regime, the tunnel splitting between the two levels renormalizes to zero, whereas it is finite in the delocalized phase. For finite bare tunneling, when $\eta=0$ the renormalized tunneling frequency Δ_r becomes zero; thus, the transition point of the coupling constant between the delocalized and localized phases for different environment baths can be determined by increasing α in Eq. (8) until a critical value when η changes from finite to zero.

The form of the introduced parameter ξ_k in the generator of unitary transformation is determined by letting $H_1'|g_0\rangle=0$ as

$$\xi_k = \frac{\omega_k}{\omega_k + \eta\Delta}. \tag{10}$$

This choice of ξ_k leads to

$$H_1' = \frac{1}{2}\eta\Delta\sum_k \frac{g_k}{\omega_k}\xi_k[b_k^\dagger(\sigma_z - i\sigma_y) + b_k(\sigma_z + i\sigma_y)], \tag{11}$$

and the matrix element of H_1' between $|g_0\rangle$ and other eigenstates of H_0' to be vanished, $(H_1')_{m0}=0$, i.e., in the perturbation treatment H_1' has no perturbative contribution to both the ground state and the transition process between ground state and excited states. Thus, H_1' is related only to the higher-lying excited states of H_0' and under renormalization should be irrelevant to the ground state and the exciting process from the ground state. Therefore, the effect of the coupling term in the transformed Hamiltonian can be safely treated by the perturbation theory because the infrared divergence is eliminated by introducing the function ξ_k in unitary transformation.

The total number of phonons of the environment bath is usually temperature dependent. At low temperature, the multiphonon process is weak and the lowest-excited states are $|s_2\rangle|\{0_k\}\rangle$ and $|s_1\rangle|1_k\rangle$, where $|1_k\rangle$ is one phonon state with $n_k=1$ but $n_{k'}=0$ for all $k'\neq k$. It's easily to check that

$$\langle g_0|H_2'|g_0\rangle = 0,$$

$$\langle\{0_k\}|\langle s_2|H_2'|g_0\rangle = 0,$$

$$\langle 1_k|\langle s_1|H_2'|g_0\rangle = 0,$$

$$\langle\{0_k\}|\langle s_2|H_2'|s_1\rangle|1_k\rangle = 0, \tag{12}$$

and, since $H_1'|g_0\rangle=0$, we have also

$$\langle\{0_k\}|\langle s_2|H_1'|g_0\rangle = 0,$$

$$\langle 1_k|\langle s_1|H_1'|g_0\rangle = 0. \tag{13}$$

Thus, we can diagonalize the lowest-excited states of H' and rewrite it by means of projective description in Dirac notation as

$$H' = -\frac{1}{2}\eta\Delta|g_0\rangle\langle g_0| + \sum_E E|E\rangle\langle E| + \text{terms with higher excited states}. \tag{14}$$

The variational ground-state energy is supposed to be $E_g = \langle s_1|\langle\{0_k\}|H'|s_1\rangle|\{0_k\}\rangle$. ξ_k can also be obtained by the variational principle to minimize E_g and the result obtained in this way is the same as Eq. (10).

The polaron transformation is widely used in literature. The difference between the polaron transformation and our transformation is the form of the introduced parameter ξ_k in the generator of unitary transformation. In the polaron transformation $\xi_k=1$, which means that the phonons can follow completely the intrasite pseudospin tunneling, but this should not be the case when ω_k/Δ or ω_k/α is small. In spin-boson model, the bosons (bath modes) follow the tunneling motion only partly and there is a retardation effect. The low-frequency behavior of the spectrum density function in this model determines the long-time behavior of the two-state system. All quantum dynamic properties are very sensitive to the low-energy part in spectral structure, especially in the sub-Ohmic case. On the other hand, in the high-frequency limit, bath modes follow instantaneously to the tunneling motions, whereas near the low-frequency limit nonadiabatic modes couple weakly to the subsystem. In our transformation $0<\xi_k<1$, which means that the phonons follow the tunneling motion only partly and there is a retardation effect. In this sense, the theories using polaron transformation may overestimate the effect of quantum fluctuations of the environment, especially for the case when ω_k/Δ is small. Thus, while all boson modes are treated by the function ξ_k, their different contributions to the dressed two-state system have been distinguished with respect to the scale of boson energy. In this sense, the overestimate of quantum fluctuation effect of the environment, especially for the case when ω_k/Δ is small, can be overcome. In addition, the polaron transformation is divergent when the phonon energy is very small, whereas in our transformation this divergence is eliminated because of the chosen form of ξ_k.

The diagonalization of H' is as follows. Let $|E_0\rangle, |E\rangle, \cdots$ be the energy eigenstates of H' and denote the ground state, the low-excited states, and other higher-excited states, respectively,

$$H'|E_0\rangle = E_0|E_0\rangle,$$

$$H'|E\rangle = E|E\rangle,$$

$$\cdots. \tag{15}$$

They form a complete set of states and, consequently, H' can be expressed in the eigenstate representation,

$$H' = E_0|E_0\rangle\langle E_0| + \sum_E E|E\rangle\langle E| + \cdots. \tag{16}$$

The energy eigenstates $|g_n\rangle$ $(n=0,1,2,\cdots)$ of H_0' also form a complete set of states,

$$H_0' = \sum_n \langle g_n|H_0'|g_n\rangle|g_n\rangle\langle g_n|, \tag{17}$$

where $|g_0\rangle=|s_1\rangle|\{0_k\}\rangle$, $|g_1\rangle=|s_2\rangle|\{0_k\}\rangle$, $|g_{2k}\rangle=|s_1\rangle|\{1_k\}\rangle,\cdots$. Since $\langle g_m|H_1'+H_2'|g_0\rangle=0$, $(m=0,1,2,\cdots)$, H' and H_0' have the same ground state, i.e.,

$$|E_0\rangle = |g_0\rangle. \tag{18}$$

Thus, we have

$$E_0 = \langle E_0|H'|E_0\rangle = \langle g_0|H'|g_0\rangle = -\frac{1}{2}\eta\Delta \tag{19}$$

and obtain Eq. (14). $|g_n\rangle$ can be expanded by the energy eigenstates of H', and by neglecting the multiphonon process the lowest-excited states of H'_0 are expanded through the following transformation:[17]

$$|g_1\rangle = \sum_E x(E)|E\rangle, \tag{20}$$

$$|g_{2k}\rangle = \sum_E y_k(E)|E\rangle. \tag{21}$$

The inverse of the transformation formulas (20) and (21) is

$$|E\rangle = x(E)|s_2\rangle|\{0_k\}\rangle + \sum_k y_k(E)|s_1\rangle|1_k\rangle. \tag{22}$$

Here the coefficients $x(E)$ and $y_k(E)$ are given by

$$x(E) = \left[1 + \sum_k \frac{V_k^2}{(E + \eta\Delta/2 - \omega_k)^2}\right]^{-1/2},$$

$$y_k(E) = \frac{V_k}{E + \eta\Delta/2 - \omega_k} x(E), \tag{23}$$

with $V_k = \eta\Delta g_k \xi_k/\omega_k$. E's are the diagonalized excitation energies of H' and they are the solutions of the equation

$$E - \frac{\eta\Delta}{2} - \sum_k \frac{V_k^2}{E + \frac{1}{2}\eta\Delta - \omega_k} = 0 \tag{24}$$

obtained by the normalization condition $\langle E|E\rangle = 1$. The real and imaginary parts of the third term in left-hand side of this equation can be calculated by the residue theorem as

$$\sum_k \frac{V_k^2}{E + \frac{1}{2}\eta\Delta - \omega_k \pm i0^+} = R(\Omega) \mp i\gamma(\Omega), \tag{25}$$

where

$$R(\Omega) = P\sum_k \frac{V_k^2}{\Omega - \omega_k} = \int_0^\infty d\beta \frac{(\eta\Delta)^2}{(\eta\Delta + \beta)^2(\Omega - \beta)} \sum_k g_k^2 \delta(\beta - \omega_k) = 2\alpha \int_0^{\omega_c} \frac{(\eta\Delta)^2}{(\eta\Delta + \beta)^2(\Omega - \beta)} \omega_c^{1-S}\beta^S d\beta, \tag{26}$$

$$\gamma(\Omega) = \pi\sum_k V_k^2 \delta(\Omega - \omega_k) = \pi\int_0^\infty d\beta \frac{(\eta\Delta)^2}{(\eta\Delta + \beta)^2} \delta(\Omega - \beta)\sum_k g_k^2 \delta(\beta - \omega_k) = 2\alpha\pi \frac{\Omega^S \omega_c^{1-S}(\eta\Delta)^2}{(\Omega + \eta\Delta)^2}\theta(\omega_c - \Omega). \tag{27}$$

Here P denotes a Cauchy principal value and a change of the variable $\Omega = E + \eta\Delta/2$ is made in the calculations.

III. CORRELATION FUNCTIONS

In the studies of quantum dynamics in dissipative two-state systems, the time evolution of state and the tunneling property are two principal aspects. If the system is prepared in one of the two states at initial time and then let it evolve in zero bias, the nonequilibrium correlation function is of primary interest,[7,19] whereas if the initial-state preparation is not realizable, the interest then lies in the symmetrized equilibrium correlation function and the susceptibility.[16,20] Although both the equilibrium and the nonequilibrium dynamics are of interest for the different experimental realizations of two-state systems, it is the nonequilibrium correlation function from which the critical point of the coherent-incoherent transition can be directly derived. Therefore, the nonequilibrium correlation function and the current correlation function are chosen below as two typical quantum quantities to present our analysis to investigate the quantum dynamics in these systems.

The nonequilibrium correlation function is related to the macroscopic quantum coherence problem and is defined as the subsequent probability of system existing in an initially prepared eigenstate of σ_z (say $\sigma_z = +1$),[7]

$$P(t) = \langle b,+1|\langle +1|e^{iHt}\sigma_z e^{-iHt}|+1\rangle|b,+1\rangle, \tag{28}$$

where $|+1\rangle$ is the eigenstate of $\sigma_z = +1$ and $|b,+1\rangle$ is the state of bosons adjusted to the state of $\sigma_z = +1$. Since $\exp(A)|+1\rangle|b,+1\rangle = |+1\rangle|\{0_k\}\rangle$,

$$\begin{aligned} P(t) &= \langle\{0_k\}|\langle +1|e^{iH't}\sigma_z e^{-iH't}|+1\rangle|\{0_k\}\rangle \\ &= \frac{1}{2}\sum_E x^2(E)\exp[-i(E + \eta\Delta/2)t] + \frac{1}{2}\sum_E x^2(E)\exp[i(E + \eta\Delta/2)t] = \frac{1}{4\pi i}\oint_C d\Omega e^{-i\Omega t}\left(\Omega - \eta\Delta - \sum_k \frac{V_k^2}{\Omega + i0^+ - \omega_k}\right)^{-1} + \frac{1}{4\pi i}\oint_C d\Omega e^{i\Omega t}\left(\Omega - \eta\Delta - \sum_k \frac{V_k^2}{\Omega - i0^+ - \omega_k}\right)^{-1}. \end{aligned} \tag{29}$$

The integral can be proceed by calculating the residue of integrand and, finally, we obtain the simple result

$$P(t) = \cos(\omega_0 t)\exp(-\gamma t), \tag{30}$$

where ω_0 is the solution of equation

$$\Omega - \eta\Delta - R(\Omega) = 0. \tag{31}$$

When $\omega_0 = 0$, the decay of $P(t)$ is a pure exponential.[17] Substituting $\omega_0 = 0$ in Eq. (31), one can get a special value of damping constant. For α less than this value, the solution of ω_0 is real and $P(t)$ is the form of damped oscillation, but for α larger than this value, the solution of ω_0 is imaginary and one has an incoherent $P(t)$; that is to say, this value of damping constant is the critical point α_c, where there is a coherent-incoherent transition. Thus, the critical point of coherent-incoherent transition can be determined by letting variable of trigonometric function in $P(t)$ to be $\omega_0 = 0$,

$$\eta\Delta + R(\omega_0 = 0) = 0. \tag{32}$$

Thus, from Eq. (26), the coherent-incoherent transition point is given by

$$\alpha_c = \frac{1}{2\eta\Delta}\left[\int_0^{\omega_c} \frac{\omega_c^{1-S}\beta^{S-1}}{(\eta\Delta + \beta)^2} d\beta\right]^{-1}. \tag{33}$$

The expression of α_c only as function of the bare tunneling Δ/ω_c can be obtained by combining Eqs. (8) and (33) to eliminate η. In Sec. IV A, we will take the Ohmic bath as a concrete example to discuss in detail the influence of α on the behavior of $P(t)$.

The Q factor has been also used in literatures[35] to deduce the critical value of damping constant. From Eq. (30), the Q factor of the tunneling oscillations is given by[20,23]

$$Q = \frac{\omega_0}{\gamma} = \frac{\eta\Delta + R(\omega_0)}{\gamma}. \tag{34}$$

The transition from coherent to incoherent dynamics occurs at α_c at which the Q factor of the tunneling oscillations vanishes.

The current correlation function,

$$C(t) = \frac{1}{2}\langle j(t)j(0) + j(0)j(t)\rangle = \frac{\Delta^2}{8}\langle \sigma_y(t)\sigma_y(0) + \sigma_y(0)\sigma_y(t)\rangle, \tag{35}$$

is defined as correlation of the tunneling current $j=\frac{1}{2}\Delta\sigma_y$ and its correlation time implies the coherent oscillations in the position correlation function $\langle\{\sigma_z(t),\sigma_z(0)\}\rangle$, therefore, can predict correctly the coherent-incoherent transition.[23] Thus, the coherent-incoherent transition point can be investigated by both Eq. (33) and the current correlation function (35), and the results from these two calculations can prove each other to verify the effectiveness of our analytical method.

To calculate the current correlation function, we take g_k as the perturbation parameter and use the Green's function method to implement the perturbation treatment. The retarded Green's function is defined as

$$G(t) = -i\theta(t)\langle[\sigma_y'(t), \sigma_y']\rangle', \tag{36}$$

where

$$\sigma_i' = e^A \sigma_i e^{-A}, \tag{37}$$

$$\sigma_i'(t) = \exp(iH't)\sigma_i' \exp(-iH't), \tag{38}$$

and $\langle\ldots\rangle'$ means the average with thermodynamic probability $\exp(-\beta H')$. The Fourier transformation of $G(t)$ is denoted as $G(\omega)$, which satisfies a chain of equation of motion.[36] By means of the cutoff approximation for the equation chain,

$$\omega G(\omega) = \langle\langle[\sigma_y'(t), H'] \| \sigma_y'\rangle\rangle_\omega' \tag{39}$$

at the second order of g_k, a set of equations is obtained and from this set of equations the Green's function can be evaluated as

$$G(\omega) = \frac{\omega^2}{\Delta^2}\left(\frac{1}{\omega - \eta\Delta - \sum_k \frac{V_k^2}{\omega-\omega_k}} - \frac{1}{\omega + \eta\Delta - \sum_k \frac{V_k^2}{\omega+\omega_k}}\right). \tag{40}$$

Thus, the current correlation function

$$C(t) = -\frac{\Delta^2}{16\pi}\int_{-\infty}^{\infty} d\omega \exp(-i\omega t)\text{Im } G(\omega)$$
$$= \frac{1}{4\pi}\int_0^{\infty} \frac{\omega^2\gamma(\omega)\cos(\omega t)}{[\omega - \eta\Delta - R(\omega)]^2 + \gamma^2(\omega)} d\omega. \tag{41}$$

According to the property of Pauli matrices, $4C(t)/\Delta^2$ should be unity at initial time $t=0$ for any bath index S, which is well preserved by Eq. (41). For a general value of $\alpha \le \alpha_c$, $C(t)$ may contain both terms of the exponential decay and the algebraic decay, but the latter dominates at the long-time limit. The two relationships (30) and (41) allow us to identify coherence for damped cases, in which oscillations maybe masked by the incoherent background.

In our method, the approach treatment is perturbative in g_k, and at the end is equivalently perturbative in α because of their relation given by the spectral density (2). The nonequilibrium correlation function and the current correlation function are calculated to the second order of g_k. By applying unitary transformation and choosing the form of ξ_k to find a better way of dividing the transformed Hamiltonian into unperturbed and perturbative parts, the contributions of the perturbation to the ground-state correction and the exciting process from ground state (nondiagonal term) are zero and the expansion parameter $(g_k\xi_k/\omega_k)^2$ is smaller, which make the perturbation treatment more efficacious and valid for a wider range of coupling $\alpha < \alpha_c$.

IV. DYNAMICAL AND OSCILLATORY BEHAVIORS

The form of simple power-law behavior of the spectral density on frequency is defined by the index S in the expression of the spectral density (2). The index $S=1$ corresponding to the linear dissipation is well known in the literatures as the Ohmic case. The non-Ohmic bath consists of the sub-Ohmic case $0<S<1$ and the super-Ohmic case $S>1$. In this section, by making use of the formulas in previous sections to evaluate the current correlation function, the nonequilibrium correlation function, and the Q factor, we investigate the dynamical properties and the phase transitions in dissipative two-state systems for various values of S in a unified method.

A. Ohmic bath

The Ohmic form dissipation of two-state systems is experimentally the most relevant and theoretically the most interesting and has been widely studied because of its importance of not only being applied to numerous physical and chemical processes but also being a critical dimensionality, distinguishing totally different behaviors for the super-Ohmic and sub-Ohmic cases. A typical intriguing case described by Ohmic dissipation is that a particle couples to electron-hole excitations of a bosonic environment or equivalently a fermionic environment formed by conduction electrons.[16] For Ohmic bath, substituting $S=1$ into Eqs. (8), (26), and (27), we obtain

$$\eta = \exp\left(\frac{\alpha\omega_c}{\omega_c + \eta\Delta} - \alpha \ln\frac{\omega_c + \eta\Delta}{\eta\Delta}\right), \quad (42)$$

$$R(\omega) = -\frac{2\alpha(\eta\Delta)^2}{\omega + \eta\Delta}\left[\frac{\omega_c}{\omega_c + \eta\Delta} - \frac{\omega}{\omega + \eta\Delta}\ln\frac{\omega(\omega_c + \eta\Delta)}{\eta\Delta(\omega_c - \omega)}\right], \quad (43)$$

$$\gamma(\omega) = 2\alpha\pi\omega\frac{(\eta\Delta)^2}{(\omega + \eta\Delta)^2}. \quad (44)$$

The coherent-incoherent transition point α_c for Ohmic case, according to Eq. (33), is determined as

$$\alpha_c = \frac{1}{2}\left(1 + \frac{\eta\Delta}{\omega_c}\right). \quad (45)$$

Combining Eqs. (42) and (45) to eliminate η, we finally obtain α_c only as function of the bare tunneling Δ/ω_c

$$(2\alpha_c)^{\alpha_c}(2\alpha_c - 1)^{1-\alpha_c} = \sqrt{e}\frac{\Delta}{\omega_c}. \quad (46)$$

At the scaling limit $\Delta/\omega_c \ll 1$, $\alpha_c=1/2$. In fact, by substituting the expression (43) of $R(\omega)$ into Eq. (31), we have

$$\omega_0^2 = (\eta\Delta)^2\left[1 - \frac{2\alpha\omega_c}{\omega_c + \eta\Delta} + \frac{2\alpha\omega_0}{\omega_0 + \eta\Delta}\ln\frac{\omega_0(\omega_c + \eta\Delta)}{\eta\Delta(\omega_c - \omega_0)}\right], \quad (47)$$

and, therefore, $\omega_0 \to 0$ if $\alpha \to \alpha_c$. Obviously, the solution of ω_0 is real when $\alpha < \alpha_c$ but is imaginary when $\alpha > \alpha_c$. As α increases to cross α_c, the behavior of $P(t)$ changes from coherent oscillation to incoherent relaxation. Figure 1(a) shows the time evolution of the nonequilibrium correlation function $P(t)$ in the case of Ohmic dissipation for $\Delta/\omega_c=0.1$ and different values of the coupling constant α. By virtue of the analytic expression of the nonequilibrium correlation function, we can reveal the oscillatory behavior even for α very close to transition point α_c. The expanded view of $P(t)$ for $\Delta/\omega_c=0.1$ and $\alpha=0.5$ (near α_c) is shown in Fig. 1(b), and for comparison in the vicinity of the critical value α_c the results of $P(t)$ for $\alpha=0.5<\alpha_c$ and $0.51>\alpha_c$ are plotted in inset in this figure. One observes that the vibration period of $P(t)$ becomes larger as α increases to approach the critical point α_c since then $\omega_0 \to 0$ and performs the exponential decay for α larger than the critical point.

The Q factor in Ohmic case, according to its definition, can be calculated by substituting Eqs. (43) and (44) into Eq. (34). Figure 2(a) illustrates the oscillation frequency ω_0 and damping coefficient γ, respectively, as functions of the coupling constant α for $\Delta_r/\omega_c=0.0003$. For comparison with results of numerical simulations,[20] the calculated results for $\Delta_r/\omega_c=0.05$ and 0.2 are also plotted in this figure. Figure 2(b) shows the Q factor as function of the coupling constant α in the cases of the renormalized tunneling frequency $\Delta_r/\omega_c=0.0003$ and 0.2. The numerical data of Monte Carlo simulation[20] and the result of the path integral $Q = \cot[\pi\alpha/2(1-\alpha)]$ (Refs. 7 and 35) are also plotted in this

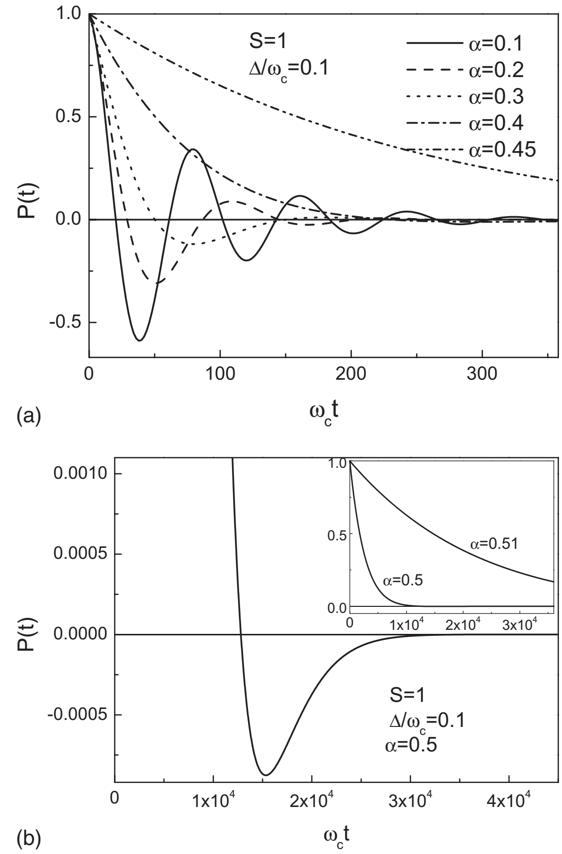


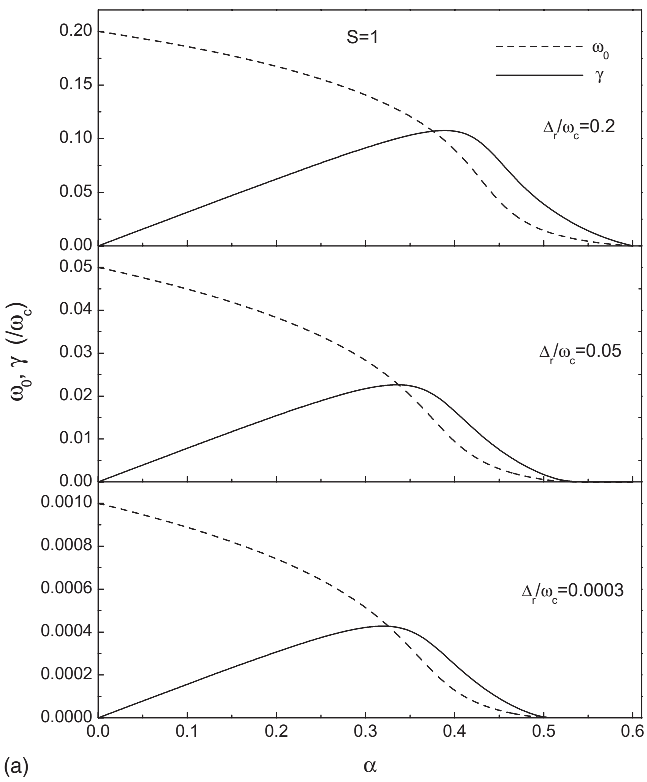
FIG. 1. (a) The time evolution of the nonequilibrium correlation function $P(t)$ in the case of Ohmic dissipation for bare tunneling frequency $\Delta/\omega_c=0.1$ and different values of the coupling constant α. (b) The expanded view of $P(t)$ in the Ohmic case for $\alpha=0.5$ (near α_c). Inset: the results of $P(t)$ in the vicinity of the critical value α_c for $\alpha=0.5<\alpha_c$ and $0.51>\alpha_c$.

figure for comparisons. As shown in the figure, the Q factor decreases as the coupling constant α increases and vanishes at the critical point α_c, where the coherent-incoherent transition occurs. The oscillation frequency ω_0 decreases to zero faster than that of damping coefficient γ as α increases to approach the critical point. The critical point α_c at the scaling limit, the line shape of ω_0, γ, and Q factor of our results are in agreement with those of path-integral and Monte Carlo simulations, but the dependence of the critical point on tunneling frequency is different. Figure 2(b) shows that the critical point α_c increases as the tunneling frequency Δ_r increases, which is contrary to that of numerical simulations.[20] In view of the fact that the tunneling frequency Δ enhances coherent oscillation of the system[24,37] and the coupling constant α acts against it, it is reasonable that the increase in the tunneling frequency conduces to the increase in the critical coupling constant α_c in Ohmic case.

At the scaling limit $\Delta/\omega_c \ll 1$, from Eq. (42) one obtains

$$\eta^{(1-\alpha)/\alpha} = \frac{e\Delta}{\omega_c}. \quad (48)$$

In this limit, the renormalized tunneling frequency approaches to zero (in other words, the system approaches to



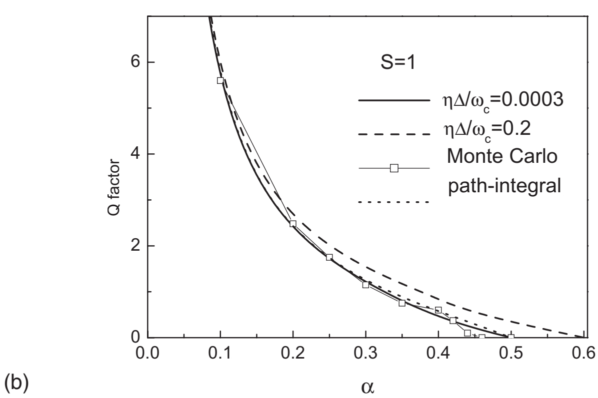


FIG. 2. (a) The oscillation frequency ω_0 and damping coefficient γ, respectively, as functions of the coupling constant α in the Ohmic case for the renormalized tunneling frequency $\Delta_r/\omega_c=0.0003$, 0.05, and 0.2. (b) The Q factor as function of the coupling constant α for the Ohmic bath in the cases of the renormalized tunneling frequency $\Delta_r/\omega_c=0.0003$ and 0.2. The dot line is the result of the path integral (Ref. 35) and the line with open square is the result of Monte Carlo simulations ($\Delta/\omega_c=0.05$) (Ref. 20).

the critical point of delocalized-localized transition) when $\eta=0$. At the scaling limit, the expression (48) holds at the critical point if and only if $\alpha=\alpha_l=1$. When $\alpha<\alpha_l$, the renormalized tunneling frequency (the effective tunneling)

$$\Delta_r=\eta\Delta=\Delta\left(\frac{e\Delta}{\omega_c}\right)^{\alpha/(1-\alpha)}. \tag{49}$$

This expression agrees with the result of the path-integral method.[23] The renormalized tunneling frequency is considered by scaling arguments[38] to be the only energy scale of the dynamics at zero temperature other than the upper cutoff ω_c.

Under the second-order approximation, from Eq. (44), one has $\gamma(\eta\Delta)=\alpha\pi\eta\Delta/2$. Substituting Eq. (48) and the critical value $\alpha=\alpha_c=1/2$ into this expression, the exponential decay rate at the scaling limit is obtained as

$$\gamma=\frac{e\pi\Delta^2}{4\omega_c}. \tag{50}$$

It agrees with result of noninteraction-blip approximation $\gamma=\pi\Delta^2/2\omega_c$ (Ref. 7) except for a constant $e/2$.

For finite bare tunneling Δ/ω_c, Eq. (42) can be rewritten as

$$\eta^{(1-\alpha)/\alpha}=\frac{\Delta}{\omega_c+\eta\Delta}\exp\left(\frac{\omega_c}{\omega_c+\eta\Delta}\right). \tag{51}$$

Obviously, when $\alpha<1$ the solution of η is finite, and at $\alpha=1$ one has the solution $\eta=0$, that is to say $\alpha_l=1$. In another way, we rewrite Eq. (42) as

$$\alpha=\frac{\ln\,\eta}{\ln\frac{\eta\Delta}{\omega_c+\eta\Delta}+\frac{\omega_c}{\omega_c+\eta\Delta}}, \tag{52}$$

and by letting $\eta\to 0$ the delocalized-localized transition point α_l also can be obtained as

$$\alpha_l=\lim_{\eta\to 0}\frac{\ln\,\eta}{\ln\,\eta+\ln\frac{\Delta}{\omega_c+\eta\Delta}+\frac{\omega_c}{\omega_c+\eta\Delta}}=1, \tag{53}$$

which is consistent with results of the renormalization group[7,37] and the continuous infinitesimal unitary transformations.[39] In one word, at both the scaling limit and the finite bare tunneling cases, we have $\alpha_l=1$ for Ohmic bath.

The current correlation function for Ohmic bath can be calculated by substituting the expressions (43) and (44) into the integral (41). In evaluation of the integral, the upper cutoff ω_c is used to determine the upper limit of the integration variable. Figure 3(a) shows the current correlation function as function of the evolution time Δt in the cases of $\Delta_r/\omega_c=0.01$ for different coupling constants $\alpha=0.2$, 0.3, 0.4, and 0.5. As shown in the figure, for finite renormalized tunneling, the oscillatory behavior of the current correlation function can be clearly observed up to $\alpha=0.5$, although its amplitude decreases rapidly with increasing α, which indicates that in Ohmic case the coherent-incoherent transition point $\alpha_c>1/2$ for $\Delta_r/\omega_c>0$. The comparisons of the coherent oscillation and the long-time decay of the current correlation function between numerical method[23] and our result in coherent phase are shown in Figs. 3(b) and 3(c). In these figures, the evolution time is scaled by the renormalized tunneling, the same as in the numerical simulations[23] for convenience of comparison, instead of the bare tunneling as in Fig. 3(a). One can see that for small alpha, our results agree very well with that of numerical simulations[23] (for example, for $\alpha=0.1$, the two lines are almost congruent), which is important for our theory as a potential method to be applied to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems

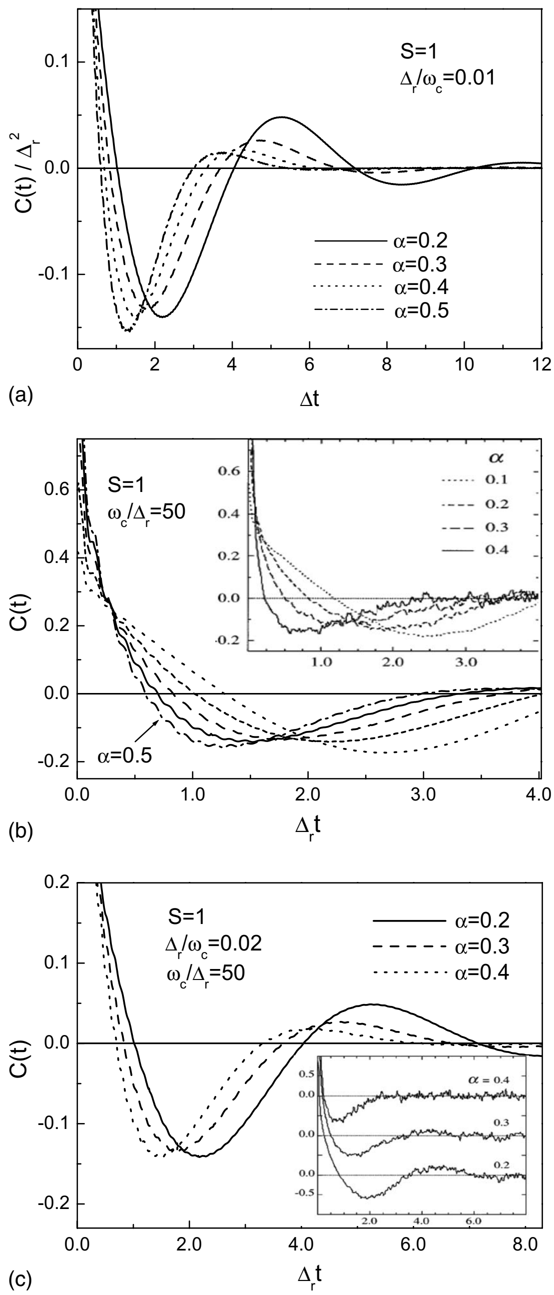


FIG. 3. (a) The current correlation function for the Ohmic bath as function of the evolution time Δt in the cases of $\Delta_r/\omega_c=0.01$ for different dampings $\alpha=0.2$, 0.3, 0.4, and 0.5. (b) The current correlation function for the Ohmic bath as function of the time $\Delta_r t$ for $\omega_c/\Delta_r=50$ and various dampings $\alpha=0.1$, 0.2, 0.3, 0.4, and 0.5. Inset: results of the numerical simulations (Ref. 23). (c) The coherent oscillation and the long-time decay of the current correlation function for the Ohmic bath for $\omega_c/\Delta_r=50$ and various dampings $\alpha=0.2$, 0.3, and 0.4. Inset: results of the numerical simulations (Ref. 23).

since in these systems the coupling constant α is usually small. Deviations to some extent between our results and numerical data appear for relatively larger α. Our method may be less accurate in incoherent phase of $\alpha>\alpha_c$ due to the cutoff approximation for the Heisenberg equation of motion and the choice of the coupling strength as the perturbation parameter in perturbative treatment though our results of the Q factors are well even for relatively larger coupling constant, for example, in the cases of super-Ohmic baths. In comparison with results of numerical methods, in which the oscillatory behavior is visible up to $\alpha \simeq 0.4$ (Refs. 20 and 23) and the accuracy of numerical data does not allow one to resolve oscillatory behavior anymore after α passes that value,[20] our theory can reveal the oscillatory behavior even for α very close to transition point α_c by virtue of the analytic expression of the current correlation function (41). The coherent-incoherent transition point can be determined precisely at both the scaling limit and the finite renormalized tunneling. The use of finite upper cutoff introduced in calculations results in the emergence of the serrate dentation on the line of the current correlation function. This dentation is common in previous works using finite cutoff scale ω_c (Refs. 23 and 40) and is more apparent for relatively larger Δ_r/ω_c but disappears at the scaling limit.

Equations (42) and (46) are important expressions. By these two formulas, the coherent-incoherent and the delocalized-localized transition points in the Ohmic case can be determined precisely at both the scaling limit and the finite renormalized tunneling. Our theory, though simple, has been successful in obtaining exact results of the transition points at the scaling limit in Ohmic case $\alpha_c=1/2$ and $\alpha_l=1$, which are the well-established values and well known as results of nonperturbation. The dynamical behaviors of the calculated nonequilibrium correlation function and current correlation function consist well with that of previous works. In addition, the evaluated susceptibility[19,20] exactly satisfied the Shiba's relation,[26] and the calculated equilibrium correlation function decayed algebraically in the long-time limit the same as previous predictions.[8,19,34] Taking all of these as a check and verification of the effectiveness of our analytical method, we further apply the method to study the two-state systems with coupling to various environments.

B. Super-Ohmic bath

The cases $S=2$, 3, and 5 are the mainly concerned super-Ohmic baths in literatures. The latter two are called solid-state phonon heat bath and used to describe, for example, a defect tunneling in a solid with coupling to acoustic phonons. Because these cases have similar dynamic behaviors, for simplicity, we only chose $S=2$ as typical case to study the effect of the super-Ohmic bath. For super-Ohmic bath $S=2$, from Eqs. (8), (26), and (27), we obtain

$$\eta = \exp\left(-\frac{\alpha(\omega_c+2\eta\Delta)}{\omega_c+\eta\Delta} - \frac{2\alpha\eta\Delta}{\omega_c}\ln\frac{\eta\Delta}{\omega_c+\eta\Delta}\right), \qquad (54)$$

$$R(\omega) = -\frac{2\alpha(\eta\Delta)^2}{\omega_c(\omega+\eta\Delta)^2}\left[\omega^2\ln\frac{\omega_c-\omega}{\omega} + \eta\Delta(2\omega + \eta\Delta)\ln\frac{\omega_c+\eta\Delta}{\eta\Delta} - \frac{\eta\Delta\omega_c(\omega+\eta\Delta)}{(\omega_c+\eta\Delta)}\right]. \qquad (55)$$

From Eq. (33), the coherent-incoherent transition point is obtained as

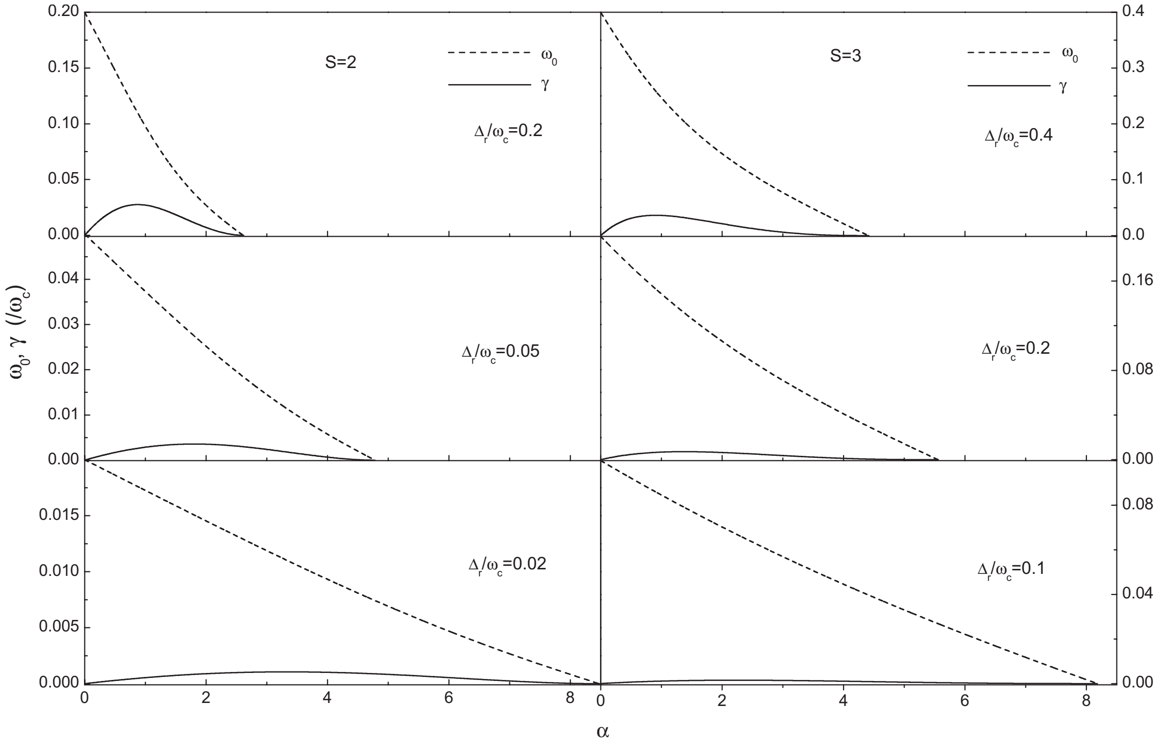


FIG. 4. The oscillation frequency ω_0 and damping coefficient γ, respectively, as functions of the coupling constant α in the cases of $S=2$ (left column) for $\Delta_r/\omega_c=0.2(\alpha_c=2.61)$, $0.05(\alpha_c=4.78)$, $0.02(\alpha_c=8.47)$, and $S=3$ (right column) for $\Delta_r/\omega_c=0.1$ $(\alpha_c=8.18)$, $0.2(\alpha_c=5.56)$, and $0.4(\alpha_c=4.41)$.

$$\alpha_c = -\frac{\omega_c}{2\eta\Delta}\left(\ln\frac{\eta\Delta}{\omega_c+\eta\Delta}+\frac{\omega_c}{\omega_c+\eta\Delta}\right)^{-1}. \tag{56}$$

Obviously, at the scaling limit $\alpha_c \propto -(\frac{\Delta}{\omega_c}\ln\frac{\Delta}{\omega_c})^{-1}$ is very large.

At the scaling limit $\Delta/\omega_c \ll 1$, from Eq. (54) one obtains

$$\eta = \exp\left[-\alpha\left(1+\frac{2\eta\Delta}{\omega_c}\ln\frac{\eta\Delta}{\omega_c}\right)\right], \tag{57}$$

thus, $\alpha_l \to \infty$ at this limit. This result agrees with the conclusion of previous works using various methods that there exists no delocalized-localized transition in a two-state system with super-Ohmic bath; in other words, α_l is at least very large in this case.

For finite bare tunneling Δ/ω_c, according to Eq. (54), the delocalized-localized transition point is obtained by letting $\eta \to 0$ as

$$\alpha_l = -\lim_{\eta\to 0}\frac{\ln\,\eta}{\frac{2\eta\Delta}{\omega_c}\ln\frac{\eta\Delta}{\omega_c+\eta\Delta}+\frac{2\eta\Delta+\omega_c}{\omega_c+\eta\Delta}} = \infty. \tag{58}$$

Therefore, in both the finite bare tunneling and the scaling limit cases, we have $\alpha_l=\infty$ (or at least very large) for super-Ohmic bath $S=2$. Since in real systems, the value of α is not so large, actually, the delocalized-localized transition will not happen in the two-state system with super-Ohmic bath. This supports the result obtained by mapping the two-state mode1 to the Ising model.[41]

Similarly, for $S=3$, one has

$$\eta = \exp\left(-\frac{\alpha(\omega_c^2-3\eta\Delta\omega_c-6(\eta\Delta)^2)}{2\omega_c(\omega_c+\eta\Delta)}-\frac{3\alpha(\eta\Delta)^2}{\omega_c^2}\ln\frac{\omega_c+\eta\Delta}{\eta\Delta}\right), \tag{59}$$

$$\alpha_c = \frac{\omega_c}{2\eta\Delta}\left(\frac{\omega_c+2\eta\Delta}{\omega_c+\eta\Delta}-\frac{2\eta\Delta}{\omega_c}\ln\frac{\omega_c+\eta\Delta}{\eta\Delta}\right)^{-1}. \tag{60}$$

Thus, $\alpha_c \propto (\frac{\Delta}{\omega_c})^{-1}$ is very large at the scaling limit and the system with solid-state phonon heat bath is never localized too for any bare tunneling.

The Q factor, the nonequilibrium correlation function, and the current correlation function for the case $S=2$ can be evaluated similarly as in the previous subsection. Figure 4 shows oscillation frequency ω_0 and damping coefficient γ, respectively, as functions of the coupling constant α in the cases of $S=2$ (left column) for $\Delta_r/\omega_c=0.2(\alpha_c=2.61)$, $0.05(\alpha_c=4.78)$, and $0.02(\alpha_c=8.47)$ and $S=3$ (right column) for $\Delta_r/\omega_c=0.1(\alpha_c=8.18)$, $0.2(\alpha_c=5.56)$, and $0.4(\alpha_c=4.41)$. The change tendency of ω_0 and γ indicates the same critical damping α_c as that calculated by Eq. (56). Figure 5 shows the time evolution of the nonequilibrium correlation function $P(t)$ in the case of $S=2$ for $\Delta/\omega_c=0.3$ with different values of the coupling constant α. The current correlation function as function of the time $\Delta_r t$ in the cases of $\alpha=0.1$ for different renormalized tunneling $\Delta_r/\omega_c=0.3$, 0.4, and 0.5 is shown in Fig. 6. In these figures, since α is less than the critical value α_c, the nonequilibrium correlation function and the current correlation function obviously display oscillatory behaviors. The time evolutions of the current correlation function and

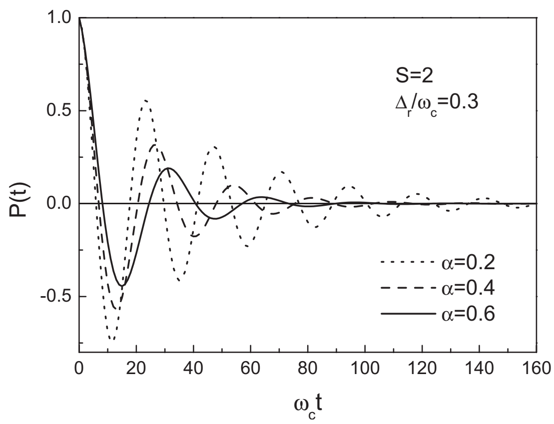


FIG. 5. The time evolution of the nonequilibrium correlation function $P(t)$ in the case of $S=2$ for $\Delta_r=0.3$ with different values of the coupling constant $\alpha=0.2$, 0.4, and 0.6.

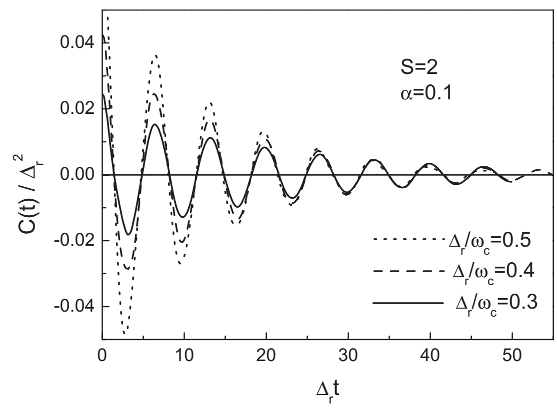


FIG. 6. The current correlation function as function of the time $\Delta_r t$ for the super-Ohmic bath $S=2$ in the cases of $\alpha=0.1$ for different renormalized tunneling $\Delta_r/\omega_c=0.3$, 0.4, and 0.5.

the nonequilibrium correlation function in the cases of $S=3$ and $S=5$ are similar as those of $S=2$ and therefore has not been illustrated. From Fig. 4, one observes that for super-Ohmic bath $S=2$ and 3 the change tendency in ω_0 and γ has been well described and, consequently, the coherent-incoherent transition point can be determined exactly by evaluating the Q factors, although in these cases the critical value of coupling constant is larger.

C. Sub-Ohmic bath

The case $0<S<1$ is called the sub-Ohmic bath. In this section, we take $S=1/2$ as a typical case to discuss the dynamic behaviors of two-state systems with coupling to sub-Ohmic bath. For $S=1/2$,

$$\eta = \exp\left(\frac{\alpha\omega_c}{\eta\Delta + \omega_c} - \alpha\sqrt{\frac{\omega_c}{\eta\Delta}}\arctan\sqrt{\frac{\omega_c}{\eta\Delta}}\right), \tag{61}$$

$$R(\omega) = -\frac{2\alpha\omega_c(\eta\Delta)^2}{(\omega+\eta\Delta)^2}\left[\frac{\omega+\eta\Delta}{\omega_c+\eta\Delta} - \frac{\omega-\eta\Delta}{\eta\Delta}\sqrt{\frac{\eta\Delta}{\omega_c}}\arctan\sqrt{\frac{\omega_c}{\eta\Delta}} - \sqrt{\frac{\omega}{\omega_c}}\ln\frac{\sqrt{\omega_c}-\sqrt{\omega}}{\sqrt{\omega_c}+\sqrt{\omega}}\right]. \tag{62}$$

The coherent-incoherent transition point is

$$\alpha_c = \frac{1}{2}\left(\frac{\omega_c}{\omega_c+\eta\Delta} + \sqrt{\frac{\omega_c}{\eta\Delta}}\arctan\sqrt{\frac{\omega_c}{\eta\Delta}}\right)^{-1}, \tag{63}$$

and, obviously, at the scaling limit

$$\alpha_c = \frac{\sqrt{\eta}}{\pi}\sqrt{\frac{\Delta}{\omega_c}}. \tag{64}$$

At the scaling limit $\Delta/\omega_c \ll 1$, from Eq. (61) one obtains

$$\eta = e^{2\alpha}\exp\left(-\frac{\alpha\pi}{2\sqrt{\frac{\Delta}{\omega_c}}\sqrt{\eta}}\right). \tag{65}$$

Thus,

$$\alpha_c = \frac{1}{\pi\sqrt[4]{e}}\sqrt{\frac{\Delta}{\omega_c}} \propto \left(\frac{\Delta}{\omega_c}\right)^{1-S}. \tag{66}$$

By letting $\sqrt{\eta}=e^{\alpha-x}$, it is easy to see that when

$$\frac{\alpha\pi}{4\sqrt{\frac{\Delta}{\omega_c}}} \le e^{\alpha-1}, \tag{67}$$

the solution of η in Eq. (65) is finite; otherwise, the solution is $\eta=0$.[42] Therefore, when taking the equal sign this relation gives the condition determining the critical point of delocalized-localized transition at the scaling limit. Substituting this condition into Eq. (65), we have

$$\frac{\pi\alpha_l}{4\sqrt{\frac{\Delta}{\omega_c}}} = e^{\alpha_l-1}, \tag{68}$$

and finally arrive at

$$\alpha_l = \frac{4}{\pi e}\sqrt{\frac{\Delta}{\omega_c}} \propto \left(\frac{\Delta}{\omega_c}\right)^{1-S}. \tag{69}$$

When $\alpha<\alpha_l$, the system is in the delocalized state, whereas when $\alpha \ge \alpha_l$ the system is in the localized state. This is in agreement with results of numerical renormalization-group[37] and infinitesimal unitary transformations.[42]

For finite bare tunneling, Eq. (8) cannot be used to directly calculate the delocalized-localized transition point because the integral in this equation is infrared divergent at $\eta=0$. The transition point for finite Δ/ω_c will be discussed in the next section by investigating the change tendency in η when characteristic parameter changes.

Figure 7 illustrates the Q factor as function of the coupling constant for the sub-Ohmic bath $S=1/2$ in the cases of renormalized tunneling frequency $\Delta_r/\omega_c=0.02$ and 0.05. As shown in the figure, the Q factor decreases as the coupling constant α increases and vanishes at the critical coupling constant α_c, which indicates that the coherent-incoherent transition occurs at a finite value of the coupling constant for finite Δ/ω_c.

For the sub-Ohmic bath, the critical coupling constant is relatively small even for moderately large tunneling fre-

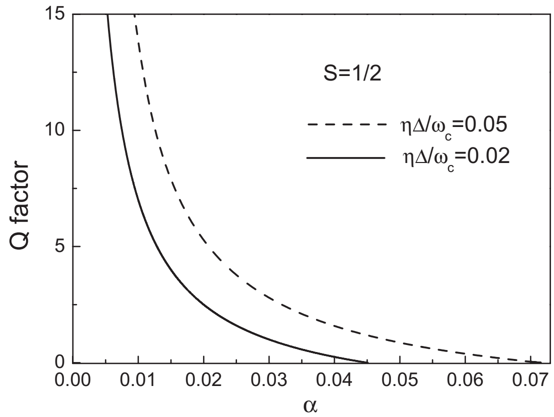


FIG. 7. The Q factor as function of the coupling constant α for the sub-Ohmic bath $S=1/2$ in the cases of renormalized tunneling frequency $\Delta_r/\omega_c=0.02$ and 0.05.

quency (for example, $\alpha_c=0.248$ for $\Delta_r/\omega_c=0.5$); therefore, our theory is suitable for studying the dynamical behaviors of the system even in the vicinity of the critical value α_c to reveal the change in $P(t)$ from coherent oscillation to incoherent exponential relaxation. This process is plotted in Fig. 8 by using the parameters $\Delta_r/\omega_c=0.4$ and different values of the coupling constant $\alpha=0.02$, 0.1, 0.2168, and 0.2169. From this figure, one observes a coherent-incoherent transition at the coupling constant $0.2168<\alpha<0.2169$. In fact, the calculated value of α_c by Eq. (63) for $\Delta_r/\omega_c=0.4$ is $\alpha_c=0.216801$.

The current correlation function as function of the time $\Delta_r t$ with the parameters $\Delta_r/\omega_c=0.1$ for different values of the coupling constant $\alpha=0.01$, 0.06, and 0.1 is shown in Fig. 9. As long as the coupling constant is relatively small, the system is maintained in the coherent state and, consequently, the current correlation function exhibits oscillatory dynamical behaviors.

The evaluation results in the foregoing subsections have shown that our theory describes well the dynamical behaviors and the phase transitions of the dissipative two-state sys-

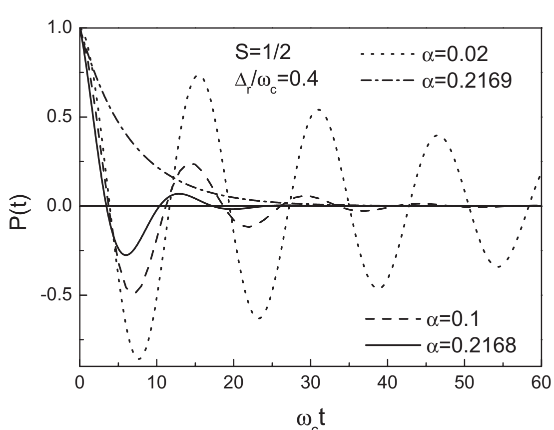


FIG. 8. Change in the dynamical behaviors of $P(t)$ from coherent oscillation to incoherent exponential relaxation in the vicinity of the critical value α_c with parameters $\Delta_r/\omega_c=0.4$ and $\alpha=0.02$, 0.1, 0.2168, and 0.2169 for the sub-Ohmic bath $S=1/2$. In this case, the calculated critical value $\alpha_c=0.216801$.

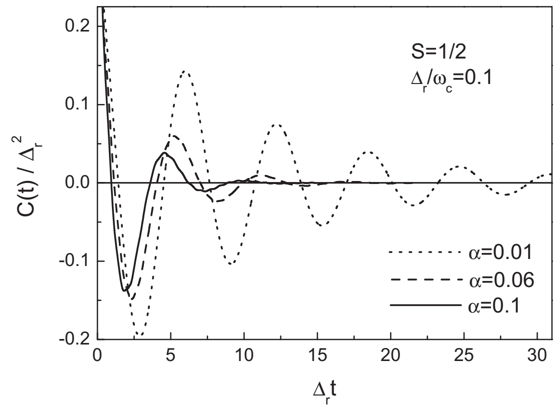


FIG. 9. The current correlation function as function of the time $\Delta_r t$ in the cases of $\Delta_r/\omega_c=0.1$ for different coupling constants $\alpha=0.01$, 0.06, and 0.1 for the sub-Ohmic bath $S=1/2$.

tems, especially in the Ohmic case. The change processes in $P(t)$ from coherent oscillation to incoherent exponential relaxation are very well represented in Ohmic and sub-Ohmic cases.

V. PHASE DIAGRAM

To the dissipative two-state systems, study interests in literatures concentrate mainly on the dynamical behaviors and the phase transitions, namely, the localized-delocalized and the coherent-incoherent transitions.

At the scaling limit $\Delta/\omega_c\ll 1$, for the coherent-incoherent and the localized-delocalized transitions, besides forenamed values $S=1/2$, 1, 2, and 3, Eqs. (8) and (33) can also be calculated exactly for, for instance, $S=0$, 1/3, 2/3, 4/3, 3/2, and 5, since in these cases their denominators can be integrated exactly and expressed by elementary functions. In sub-Ohmic cases, similarly as in Sec. IV C, we obtain the results as follows:

$$\alpha_c=\frac{3\sqrt{3}}{8\pi\sqrt[6]{e}}\left(\frac{\Delta}{\omega_c}\right)^{2/3}, \tag{70}$$

$$\alpha_l=\frac{9\sqrt{3}}{4\pi e}\left(\frac{\Delta}{\omega_c}\right)^{2/3}, \quad S=\frac{1}{3}; \tag{71}$$

$$\alpha_c=\frac{3\sqrt{3}}{4\pi\sqrt[3]{e}}\left(\frac{\Delta}{\omega_c}\right)^{1/3}, \tag{72}$$

$$\alpha_l=\frac{9\sqrt{3}}{4\pi e}\left(\frac{\Delta}{\omega_c}\right)^{1/3}, \quad S=\frac{2}{3}. \tag{73}$$

In all these cases, the critical values are in proportion to $(\Delta/\omega_c)^{1-S}$. In fact, for general values $0<S<1$, the integrals in Eqs. (8) and (33) can be integrated as

$$\eta=\exp\left[\frac{-\alpha\,{}_2F_1\left(S+1;2;S+2;-\frac{1}{\eta\Delta'}\right)}{(\eta\Delta')^2(S+1)}\right], \tag{74}$$

$$\alpha_c = \frac{(\eta\Delta')^2 S(S+1)}{2\eta\Delta'(S+1) - 2S\Big[{}_2\mathrm{F}_1\Big(S+1;1;S+2;-\frac{1}{\eta\Delta'}\Big) + {}_2\mathrm{F}_1\Big(S+1;2;S+2;-\frac{1}{\eta\Delta'}\Big)\Big]}, \tag{75}$$

where $\Delta' = \Delta/\omega_c$ and ${}_2\mathrm{F}_1$ is the hypergeometric function. After some straightforward calculations, it can be shown that the phase boundaries for general value of bath index in sub-Ohmic cases $0<S<1$ at the scaling limit yield for a universal exponential rule

$$\alpha_{c,l} \propto \left(\frac{\Delta}{\omega_c}\right)^{1-S}. \tag{76}$$

Taking all the results above together, we show that at the scaling limit the transition points and the system's states are as Table I.

These results indicate that the value $S=1$ is a "critical dimensionality" and for S larger or smaller than this value the behavior of the system is totally different.[7] At the critical dimensionality, the Ohmic case, the incoherent or coherent (the localized or delocalized) behavior of the system is determined by whether the coupling is larger or smaller than $\alpha_c = 1/2(\alpha_l = 1)$.

For $S \geq 1$, our results are consistent with that of the functional-integral approach,[7] whereas for $S<1$ the functional-integral approach predicts a localized state for any finite coupling constant at zero temperature. On the other hand, the spin-boson model can be mapped onto a one-dimensional Ising model with defects in the Ising system corresponding to spin flips of the original spin. Analysis of the Ising model by Kosterlitz using renormalization-group method suggested the existence of phase transition for $S<1$.[43] Carrying over this result to the spin-boson model, the existence of the localized-delocalized transitions for $S<1$ would be expected.[37,42] Therefore, efforts are inspired to investigate the transitions directly from the spin-boson model. Numerical simulation by the renormalization-group method has provided evidence of phase transition for all $S \leq 1$, and the simulated data of the critical coupling α_c closely follows the power-law relation $\alpha_l \propto \Delta^{1-S}$ for small bare tunneling,[37] which is in agreement with Eq. (76). Study by infinitesimal unitary transformations has obtained an analytic expression for α_c, but the method is valid only at the scaling limit.[42] In comparison with these method, our method can obtain analytic expressions for α_c and α_l for any values of the tunneling and the coupling constant.

In the case of finite bare tunneling, the critical value of coupling constant of coherent-incoherent transition varies with the tunneling frequency. In Fig. 10(a), as in previous works, we plot the dependence of the coherent-incoherent transition point α_c on the renormalized tunneling Δ_r for different bath indices according to Eqs. (45), (56), (60), and (63). Since the renormalization factor η and, consequently, the renormalized tunneling Δ_r vary with the coupling constant, the phase diagram in the $\alpha_c \sim \Delta/\omega_c$ plane is of advantage to directly exhibit phase boundary and critical value. The dependence of the coherent-incoherent transition point α_c on the bare tunneling Δ/ω_c for different bath indices is plotted in Fig. 10(b). The dependence of the coherent-incoherent transition point α_c on the bath index for different renormalized tunneling Δ_r, according to Eq. (33), is plotted in Fig. 10(c) and the inset in this figure depicts the move tendency of the phase boundary as the renormalized tunneling decreases to close the scaling limit. In these figures, for the convenience of having a full view of the phase diagrams for all bath indices, the ordinate is expanded into a wide range of coupling constant, though as mentioned before the results may be less accurate for larger α, and in the insets in Fig. 10(b) the abscissa is expanded into $\Delta/\omega_c \geq 1$, which in practice is already nonphysical. As shown in Fig. 10, the increase in the bath index leads the phase boundary of the coherent-incoherent transition to move to larger coupling constant. The phase diagrams of super-Ohmic cases [even for $1<S<2$, see the case $S=1.2$ shown in Fig. 10(a)] are different from that of $S \leq 1$ case. As the renormalized tunneling Δ_r increases, α_c increases monotonously for $S \leq 1$, but for $S>1$ α_c decreases first until it reaches its minimum at a definite value of Δ_r and thereafter increases. This definite value of Δ_r is the minimum point of α_c and can be obtained by applying the variational principle to Eq. (33) to minimize α_c. Let $\frac{\partial \alpha_c}{\partial(\eta\Delta)} = 0$, we get

$$\int_0^{\omega_c} \left(\frac{\beta}{\omega_c}\right)^{S-1} \frac{\beta - (\Delta_r)_{\min}}{[(\Delta_r)_{\min} + \beta]^3} d\beta = 0, \tag{77}$$

therefore, the minimum point $(\Delta_r)_{\min}$ is determined entirely by bath index S. Figure 11(a) shows the minimum point $(\Delta_r)_{\min}$ as function of the bath indices. When S changes from 1 to 2, the minimum point $(\Delta_r)_{\min}$ changes from zero to 0.46. In particular, for S little bit larger than 1, we call it the over-Ohmic case, the minimum point $(\Delta_r)_{\min}$ is small. In order to show this case clearly, the dependences of α_c on Δ_r

TABLE I. The transition points and the system's states at the scaling limit.

$0<S<1$	$\alpha_{c,l} \propto (\frac{\Delta}{\omega_c})^{1-S}$	$\alpha \geq \alpha_c$ incoherence, $\alpha<\alpha_c$ coherence $\alpha \geq \alpha_l$ localization, $\alpha<\alpha_l$ delocalization
$S=1$	$\alpha_c = \frac{1}{2}$, $\alpha_l = 1$	$\alpha \geq \frac{1}{2}$ incoherence, $\alpha < \frac{1}{2}$ coherence $\alpha \geq 1$ localization, $\alpha<1$ delocalization
$S>1$	$\alpha_{c,l} = \infty$ (or very large)	coherence and delocalization

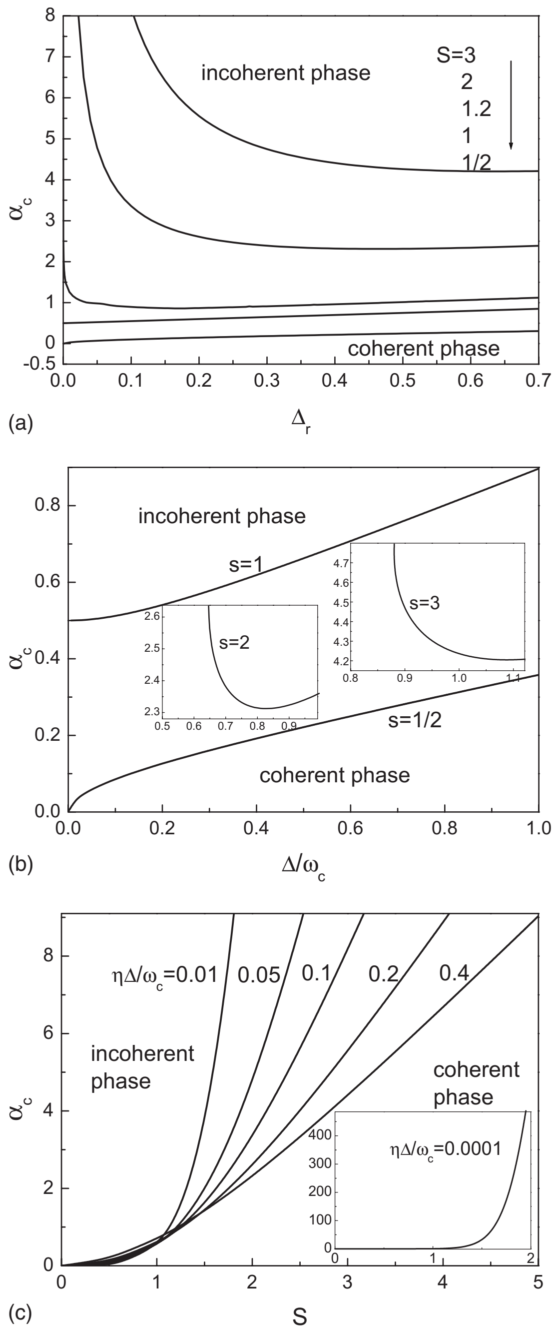


FIG. 10. (a) The dependence of the coherent-incoherent transition point α_c on the renormalized tunneling Δ_r for different bath indices. (b) The phase diagram of the coherent-incoherent transition in the $\alpha_c \sim \Delta/\omega_c$ plane for different bath indices. (c) The dependence of the coherent-incoherent transition point α_c on the bath index for different renormalized tunneling Δ_r. Inset: the move tendency of phase boundary as the renormalized tunneling decreases to approach the scaling limit.

for S=1.01, 1.03, 1.05, and 1.1, according to Eq. (33), are plotted in Fig. 11(b). This figure indicates that for appropriate fixed values of α, there exist two critical values of renormalized tunneling $(\Delta_r)_{c1}$ and $(\Delta_r)_{c2}$. As Δ_r increases to cross the first critical value $(\Delta_r)_{c1}$, the state of the system changes from its original coherent state to incoherent state, and at the second critical value $(\Delta_r)_{c2}$ the system re-enters the coherent state. In this process, if S is larger than but very close to 1, the change in Δ_r is small and its value is in the physical meaningful range. For example, by using the input parameters α=0.564 and S=1.02, we obtain $(\Delta_r)_{c1}$=0.01 and $(\Delta_r)_{c2}$=0.03. Therefore, provided there exists a dissipative two-state system coupled to an over-Ohmic bath with S litter bit larger than 1, for an appropriate fixed value of α, by increasing Δ_r the system undergoes phase transition from coherent state to incoherent state or reversely and can even re-enter between the two states. Although α_c changes with Δ_r, its minimum value $(\alpha_c)_{\min}$ is determined only by the bath index. For a given index S, substituting $(\Delta_r)_{\min}$ in Eq. (33), one has

$$(\alpha_c)_{\min} = \alpha_c[(\Delta_r)_{\min}], \tag{78}$$

that is to say, for a fixed bath index the dissipative two-state system is certainly in the coherent state if the coupling constant α is smaller than $(\alpha_c)_{\min}$. The minimum value of coupling constant $(\alpha_c)_{\min}$ as function of the bath index is also shown in Fig. 11(a). As shown in the figure, in super-Ohmic case, $(\alpha_c)_{\min}$ is so large (for example, $(\alpha_c)_{\min}$=2.3 for S=2) that for real systems the coherent-incoherent transition will not occur in practice, which is similar to the delocalized-localized transition, where the critical coupling constant, as

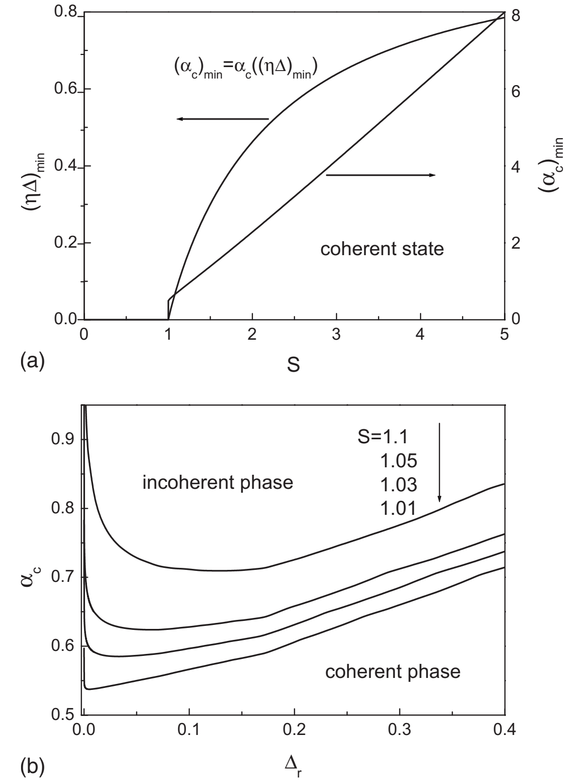


FIG. 11. (a) The minimum point $(\Delta_r)_{\min}$ (left) and the minimum value of the critical coupling constant $(\alpha_c)_{\min}$ (right) as function of the bath index. (b) The dependences of the coherent-incoherent transition point α_c on renormalized tunneling Δ_r in the over-Ohmic cases of S=1.01,1.03,1.05, and 1.1 according to Eq. (33). For appropriate fixed values of α, there exist two critical values of renormalized tunneling and the system can re-enter between coherent state and incoherent state.

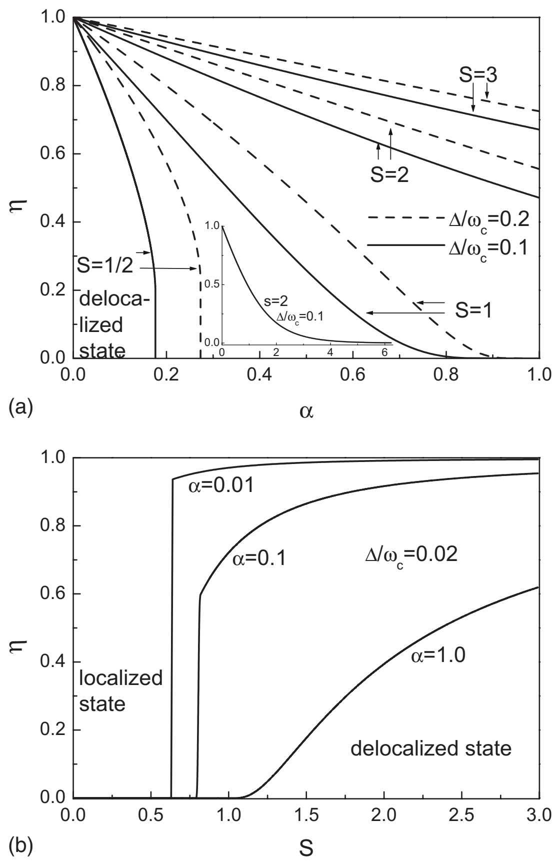


FIG. 12. (a) The change tendency in the renormalization factor η as function of the coupling constant α in the cases of $\Delta/\omega_c=0.1$ and 0.2 for different bath indices. Inset: a zoom out view of the change tendency of η for expanded range of α in the case $S=2$ and $\Delta/\omega_c=0.1$. (b) The change in the renormalization factor η as function of bath index S for different couplings. The delocalized-localized transition occurs only when $S\leq 1$.

has been discussed in previous subsections, is also too large. Therefore, it is generally accepted in literatures that for $S>1$, there exists no quantum phase transitions (though the coherent-incoherent transition may exists for the over-Ohmic case).

The delocalized-localized transition for finite bare tunneling, especially in the sub-Ohmic case, can be clearly identified by investigating the change tendency of η. In Fig. 12(a), the change tendency of η is plotted as function of the coupling constant α in the cases of $\Delta/\omega_c=0.1$ and 0.2 for different bath indices. In this figure, η is calculated by Eq. (42) for $S=1$, Eq. (54) for $S=2$, Eq. (59) for $S=3$, and Eq. (61) for $S=1/2$, respectively. For the $S=1/2$ case, because of the divergence of the terms in the right-hand side of Eq. (61) at $\eta=0$, the smallest value of η is only calculated to 10^{-4}, but the change tendency of η is already quite distinct. One can see that η decreases as α increases. In super-Ohmic case, η can be very small but never disappears for any finite value of coupling constant, which can be seen clearly in the inset in this figure by a zoom out view for an expanded range of α, whereas in Ohmic case η reduces to zero always at $\alpha=1$. In sub-Ohmic case, η decreases rapidly and becomes zero at a certain value of $\alpha_l<1$ for finite bare tunneling, which indicates a transition between the delocalized and localized states. When $\alpha<\alpha_l$, $\eta>0$ and the system is in the delocalized state, whereas when $\alpha\geq\alpha_l$, $\eta=0$ and the system is in the localized state. These features can also be identified from the change in η shown in Fig. 12(b), as function of bath index S for different couplings. This figure shows that only when $S\leq 1$, does the delocalized-localized transition in the system exist.

VI. CONCLUSION

By using the spin-boson model, an analytical approach is developed to investigate the properties of the correlation functions and the phase transitions in dissipative two-state systems in a unified method for different bath indices with the view of understanding the effects of environments and tunneling on the systems. We have theoretically studied the dynamical behaviors of the current correlation function and the nonequilibrium correlation function, and analytic expressions of these correlation functions are obtained by employing the Green's function method and residue theorem. Their behaviors of damped oscillation in coherent state and exponential relaxations in incoherent state are presented even for the coupling constant very close to the transition point. This analytical theory allows us to obtain the analytical expressions of the transition points for various bath indices and, therefore, the critical points and the phase boundaries of coherent-incoherent and delocalized-localized transitions can be determined precisely at both the scaling limit and the finite bare tunneling.

Our results of the dynamical behaviors of the current correlation function and the nonequilibrium correlation function are consistent with those of previous works. The calculation results show that for super-Ohmic baths, there exists no quantum phase transitions and the system is always in coherent and delocalized state; whereas for Ohmic and sub-Ohmic baths, the incoherent or coherent (the localized or delocalized) state of the system is determined by weather the coupling is larger or smaller than the critical value $\alpha_c(\alpha_l)$. In particular, in Ohmic case, some well-known results are obtained exactly, including the well-established values $\alpha_l=1$ and $\alpha_c=1/2$ at the scaling limit. In sub-Ohmic cases $0<S<1$ at the scaling limit, the universal exponential rule $\alpha_{c,l}\propto(\frac{\Delta}{\omega_c})^{1-S}$ is obtained. In the over-Ohmic case, for an appropriate fixed value of coupling constant, the system can even re-enter between coherent and incoherent states.

The validity of our theory has been discussed and manifested by the success in reproducing some well-established values, especially in the Ohmic case. Due to the choice of the coupling strength as the perturbation parameter in perturbative treatment, our results are more suitable in the relatively smaller coupling constant regime, which is significant for our theory as a potential method to be applied to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems since in these systems the coupling constant is usually small, although some of our results are well even for relatively larger coupling constant.

In this paper, we restrict our statements only at the zero temperature, but the effect of finite temperature on this model is an issue of much concern. The study for finite temperature is in progress and our preliminary investigation shows that, for example, α_c and α_l decrease as the temperature increases, and both the specific heat and the entropy are power function of temperature with powers for Ohmic and sub-Ohmic baths in the low-temperature region. Further investigation in this direction, for example, the analytical expression of temperature dependence of critical points, is needed.

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