

Quantum dynamics of the dissipative two-state system coupled with a sub-Ohmic bath

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The decoherence of a two-state system coupled with a sub-Ohmic bath is investigated theoretically by means of the perturbation approach based on a unitary transformation. It is shown that the decoherence depends strongly and sensitively on the structure of environment. Nonadiabatic effect is treated through the introduction of a function ξ_k which depends on the boson frequency and renormalized tunneling. The results are as follows: (i) the nonequilibrium correlation function $P(t)$, the dynamical susceptibility $\chi''(\omega)$, and the equilibrium correlation function $C(t)$ are analytically obtained for $s \leq 1$; (ii) the phase diagram of thermodynamic transition shows the delocalized-localized transition point α_l which agrees with exact results and numerical data from the numerical renormalization group; (iii) the dynamical transition point α_c between coherent and incoherent phase is explicitly given. A crossover from the coherent oscillation to incoherent relaxation appears with increasing coupling (for $\alpha > \alpha_c$, the coherent dynamics disappear); (iv) the Shiba's relation and sum rule are exactly satisfied when $\alpha \leq \alpha_c$; (v) an underdamping-overdamping transition point α_c^* exists in the function $S(\omega)$. Consequently, the dynamical phase diagrams in both ohmic and sub-Ohmic case are mapped out. For $\Delta \ll \omega_c$, the critical couplings (α_l , α_c , and α_c^*) are proportional to Δ^{1-s} .

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I. INTRODUCTION

A two-state system (TSS) coupled to a dissipative environment offers a unique testing ground for exploring fundamental physics of quantum mechanics behaviors such as tunneling and decoherence.^{1,2} It also provides a paradigmatic standard model for studying quantum computation.³ An interesting problem in this type of system is decoherence resulting from the influence of an environment, which is usually represented by an infinite set of harmonic oscillators. This system can be described by the spin-boson model (SBM), which reads

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

Here σ_x and σ_z are the usual Pauli spin matrices, Δ is the bare tunneling matrix element between the two states, ϵ describes the bias of the system. Throughout this paper we set $\hbar=1$ and $k_B=1$. The quantity g_k represents the coupling strength of TSS to the k th oscillator. Without dissipative environment, the TSS exhibits coherent tunneling between the two states, while the coupling to the environment will result in the lose of its phase coherence.

Impossible as an exact solution of SBM is, both the equilibrium and nonequilibrium dynamics in this model have been widely studied by using the Path-integral formalism, variational method, real time quantum Monte Carlo, numerical renormalization group (NRG), flow equations, etc.¹⁻²⁶ Much of the physics underlying the model has not been revealed by numerical methods, such as the coherent-incoherent transition.^{9,17} The main interest is to understand how the quantum environment influences the dynamics of TSS, in particular, how dissipation destroys quantum coherence. On the one hand, when the system can be prepared in one of the two states by applying a strong bias for times

$t < 0$ and then let it evolve for $t > 0$ in zero bias, the nonequilibrium correlation function $P(t)$ is of primary interest.^{1,24} Moreover, $P(t)$ can be directly measured by the technique of muon-spin rotation.²⁷ On the other hand, while the initial state preparation is not realizable, the interest lies in the equilibrium correlation function $C(t)$ related to the cross section of neutron scattering and the susceptibility $\chi(\omega)$.¹

The effect of a harmonic environment is characterized by a spectral density $J(\omega) = 2\alpha\omega_s^{1-s}\omega^s\theta(\omega_c - \omega)$ with the dimensionless coupling strength α , the upper cutoff ω_c , and the step function $\theta(x)$. An additional energy scale ω_s is introduced, but only the combination $\alpha\omega_s^{1-s}$ has fundamental significance. In this paper we assume that the high energy cutoff ω_c is much larger than all other scales. It is convenient to set $\omega_s = \omega_c/100$ in this paper except the special notation. The index s accounts for various physical situations around the TSS. For example, in solid materials where acoustic phonon provides the most efficient damping mechanism, according to the Debye model, $s=3$, which belongs to a super-Ohmic bath ($s > 1$). $s=1$ and $s < 1$ stand for Ohmic and sub-Ohmic bath, respectively. There are suggestions to model $1/f$ noise found in experiments by a limiting sub-Ohmic bath.²⁸⁻³⁰ In terms of the renormalization group, sub-Ohmic coupling represents a relevant perturbation.³¹ Moreover, there are various claims that the particle is always localized in the sub-Ohmic case for zero temperature based on noninteracting blip approximation (NIBA).^{1,2} As was pointed out in Ref. 6, the NIBA is unreliable for studying the long-time behavior of equilibrium correlation functions since it gives an exponential decay instead of an algebraic decay. Another tool for treating spin-boson problem, adiabatic renormalization, is invalid in the sub-Ohmic case.⁶ Due to technical difficulties, little result about long-time dynamics of $s < 1$ at zero temperature is known.

The study of SBM with a sub-Ohmic bath for zero bias case has attracted much attention recently.⁵⁻¹² The flow equation method has been applied by Kehrein, Mielke, and

Stauber to this model.⁶⁻⁸ Some important properties were predicted, such as a transition from delocalization for weak coupling to localization for strong coupling and the calculation on the equilibrium spectral function $C(\omega)$. However, as was pointed out by Stauber, this approach did not yield a correct normalization condition nor a satisfying result about the Shiba relation for a certain parameter regime.⁸ This approach seems difficult to calculate the quantum dynamics of SBM, especially the nonequilibrium correlation function $P(t)$. Besides, the NRG method, a powerful numerical tool, was employed by Bulla, Tong, Vojta, and co-workers to investigate the sub-Ohmic case and provide some reliable results for both static and dynamic quantities in the whole range of model parameters and temperatures.⁹⁻¹² They focused on the quantum critical behavior from a delocalized state to a localized one and found that the Shiba relation was fulfilled within an error of about 10% in the Ohmic case, but did not provide a check in the sub-Ohmic case.⁹ Very recently, the NRG study for sub-Ohmic case shows that the dynamical properties of the delocalized phase are not dominated only by a single energy scale Δ_r .¹² In their treatment, the energy scale ω_s was set equal to the high energy cutoff ω_c . Recently, Chin and Turlakov have used the variational method originally proposed by Silbey and Harris for the sub-Ohmic bath.⁵ They also paid more attention to the transition between delocalized phase (the effective tunneling $\Delta_r > 0$) and localized one ($\Delta_r = 0$) at both $T=0$ and $T>0$. They pointed out that dynamical and thermodynamics criteria for the transition should be expected to be different and sensitive to nonadiabatic mode. In their discussion, they have ignored the dynamical effect of the perturbation. Thus, it is difficult for the variational ansatz to make detailed statement about quantum dynamics beyond Born-Markov approximation. Moreover, they worked with $\omega_s \neq \omega_c$ and $\omega_c \rightarrow \infty$. In the present paper, we extend a unitary transformation proposed by one of our authors to investigate quantum dynamics of the sub-Ohmic SBM at $T=0$.¹⁴

The paper is organized as follows. In Sec. II, the Hamiltonian is separated into the unperturbed part and the perturbed one based on a unitary transformation and perturbation theory. In Sec. III A, the localization-delocalization transition point will be clarified, compared with the results of flow equations and NRG. The calculations of quantum dynamics $p(t)$ and $C(t)$ will be given explicitly in Sec. III B. Then, It is verified that real and imaginary parts of $\chi(\omega)$ satisfy the Shiba's relation analytically and numerically in Sec. III C. The coherent-incoherent transition is also discussed in detail in this part. Finally, Sec. IV gives discussion and further analysis of our results and approach. Usually, people believe that perturbation approach is not good for the dissipative SBM because of the infrared divergence in calculating the renormalized tunneling frequency and other physical quantities by perturbation expansion. Here we attempt to get rid of the divergence by using a unitary transformation. When one takes the scaling limit $\Delta \ll \omega_c$ from our obtained results, it will reproduce the known or exact one. This approach works well for the low-temperature region and weak coupling case with $0 < \Delta < \omega_c$ far away from the scaling limit.

II. UNITARY TRANSFORMATION

In order to take into account the correlation between spin and bosons, we present a treatment based on the unitary transformation to H : $H' = e^S H e^{-S}$, where the generator of the transformation is

$$S = \sum_k \frac{g_k}{2\omega_k} \xi_k (b_k^\dagger - b_k) \sigma_z. \quad (2)$$

A k -dependent function ξ_k introduced in the transformation corresponds to the displacement of each boson mode due to the coupling to the TSS.^{14,32} Its form will be determined later by the perturbation theory.

The transformation can be done to the end and the result is $H' = H'_0 + H'_1 + H'_2$, where

$$H'_0 = -\frac{1}{2} \eta \Delta \sigma_x + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k} \xi_k (2 - \xi_k), \quad (3)$$

$$\eta = \exp \left[-\sum_k \frac{g_k^2 \epsilon_k^2}{2\omega_k^2 \xi_k} \right], \quad (4)$$

$$H'_1 = \frac{1}{2} \sum_k g_k (1 - \xi_k) (b_k^\dagger + b_k) \sigma_z - \frac{1}{2} \eta \Delta i \sigma_y \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k), \quad (5)$$

$$H'_2 = -\frac{1}{2} \Delta \sigma_x \left(\cosh \left\{ \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right\} - \eta \right) - \frac{1}{2} \Delta i \sigma_y \left(\sinh \left\{ \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right\} - \eta \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right). \quad (6)$$

H'_0 is the unperturbed part of H' . Obviously, since the spin and bosons are decoupled in this part, H'_0 can be solved exactly. The eigenstate of H'_0 is a direct product: $|s\rangle\{|n_k\rangle\}$, where $|s\rangle$ is the eigenstate of σ_x : $|s_1\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ or $|s_2\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, and $\{|n_k\rangle\}$ is the eigenstate of bosons with n_k bosons for mode k . In particular, $\{|0_k\rangle\}$ is the vacuum state in which $n_k=0$ for every k . The ground state of H'_0 is

$$|g_0\rangle = |s_1\rangle\{|0_k\rangle\}. \quad (7)$$

H'_1 (first-order terms) and H'_2 (including second order terms and higher ones) are treated as perturbation and they should be as small as possible. For this purpose ξ_k is determined as

$$\xi_k = \frac{\omega_k}{\omega_k + \eta \Delta}. \quad (8)$$

Substituting this form into Eq. (5), one has

$$H'_1 = \frac{1}{2} \eta \Delta \sum_k \frac{g_k}{\omega_k + \eta \Delta} [b_k^\dagger (\sigma_z - i \sigma_y) + b_k (\sigma_z + i \sigma_y)]. \quad (9)$$

It is easy to check that $H'_1|g_0\rangle=0$. Thus, by choosing the form of ξ_k , the matrix elements between the ground and the lowest

excited states are zero (we show them in the following). It will become possible to take a perturbation treatment based on the division of the transformed Hamiltonian. Besides, in the transformed Hamiltonian H' $\eta\Delta$ is the probability of diagonal transition of bosons which describes the coherent tunnelling motion of particle. η is determined in Eq. (4) to make $\text{Tr}(\rho_B H'_2) = 0$, where $\rho_B = \exp(-\beta H_B) / \text{Tr} \exp(-\beta H_B)$ is the equilibrium density operator of bosons ($H_B = \sum_k \omega_k b_k^\dagger b_k$). Thus one can see that the tunneling is renormalized by this factor η arising due to the dressing of bosons coupled with the TSS. In other words, the particle is surrounded by bosons cloud as it tunnels between the two states.

It is noticeable that $0 \leq \xi_k \leq 1$, which determines the intensity of the correlation between spin or particle presentive for subsystem and bosons in bath: $\xi_k \sim 1$ if the boson frequency (ω_k) is much larger than the renormalized tunneling of subsystem ($\eta\Delta$) while $\xi_k \ll 1$ for $\omega_k \ll \eta\Delta$. Since the transformation in Eq. (2) is essentially a displacement one, physically, one can see that high-frequency bosons ($\omega_k > \eta\Delta$) follow the tunneling particle adiabatically (instantaneously) because the displacement is $g_k \xi_k / \omega_k \sim g_k / \omega_k$, which leads to a dressed particle. On the other hand, low-frequency bosons $\omega_k < \eta\Delta$, in general, are not always in equilibrium with the tunneling particle, and hence the particle moves in a retarded potential arising from the low-frequency modes. When the nonadiabatic effect dominates, $\omega_k \ll \eta\Delta$, the displacement $g_k \xi_k / \omega_k \approx g_k / \eta\Delta \ll 1$, is substantially reduced. Therefore, the effects of each boson mode on subsystem are in nature treated separately by ξ_k .

The lowest excited states are $|s_2\rangle\{|0_k\rangle\}$ and $|s_1\rangle\{|1_k\rangle\}$, where $|1_k\rangle$ is the number state with $n_k = 1$ but $n_{k'} = 0$ for all $k' \neq k$. It is easy to check that $\langle g_0 | H'_2 | g_0 \rangle = 0$ [because of the form of η in Eq. (4)], $\langle \{0_k\} | \langle s_2 | H'_2 | g_0 \rangle = 0$, $\langle 1_k | \langle s_1 | H'_2 | g_0 \rangle = 0$, and $\langle \{0_k\} | \langle s_2 | H'_1 | s_1 \rangle | 1_k \rangle = 0$. Moreover, since $H'_1 | g_0 \rangle = 0$, we have $\langle \{0_k\} | \langle s_2 | H'_1 | g_0 \rangle = 0$ and $\langle 1_k | \langle s_1 | H'_1 | g_0 \rangle = 0$. Thus, we can diagonalize the lowest excited states of H' as

$$H' = -\frac{1}{2} \eta\Delta |g_0\rangle\langle g_0| + \sum_E E |E\rangle\langle E| + \text{terms with higher excited states.} \quad (10)$$

The diagonalization is achieved through the following transformation:²⁴

$$|s_2\rangle\{|0_k\rangle\} = \sum_E x(E) |E\rangle, \quad (11)$$

$$|s_1\rangle\{|1_k\rangle\} = \sum_E y_k(E) |E\rangle, \quad (12)$$

$$|E\rangle = x(E) |s_2\rangle\{|0_k\rangle\} + \sum_k y_k(E) |s_1\rangle\{|1_k\rangle\}, \quad (13)$$

where

$$x(E) = \left[1 + \sum_k \frac{V_k^2}{(E + \eta\Delta/2 - \omega_k)^2} \right]^{-1/2}, \quad (14)$$

$$y_k(E) = \frac{V_k}{E + \eta\Delta/2 - \omega_k} x(E), \quad (15)$$

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

$$E - \frac{\eta\Delta}{2} - \sum_k \frac{V_k^2}{E + \eta\Delta/2 - \omega_k} = 0. \quad (16)$$

III. QUANTUM DYNAMICS

A. Delocalization

The Ohmic spin-boson model has nontrivial dynamics only for $\alpha < 1$ when $\Delta \ll \omega_c$. Scaling arguments, flow equations and other methods give a renormalized tunneling, $\Delta_r = \Delta \left(\frac{\Delta}{\omega_c}\right)^{\alpha/1-\alpha}$.^{1,13} When α goes to 1, one gets $\Delta_r = 0$ which is a transition from delocalization for weak coupling to localization for strong coupling. However, for the sub-Ohmic bath $s < 1$, there is some confusion about the existence of such a transition within some various approximation approaches. On the one hand, the TSS is localized for nonzero sub-Ohmic coupling at $T=0$ which is predicted by the NIBA.^{1,2} On the other hand, from the mapping of SBM to Ising model, the corresponding results turn out a transition as a function of coupling.^{6,15} Moreover, the results of flow equations and numerical renormalization group also support it.^{6,9} However, the transition point is less clear for general Δ and s .

The renormalization of tunneling can be calculated as

$$\begin{aligned} \eta &= \exp \left\{ -\alpha \omega_s^{1-s} \int_0^{\omega_c} \frac{\omega^s d\omega}{(\omega + \eta\Delta)^2} \right\} \\ &= \exp \left\{ -\alpha \omega_s'^{1-s} \frac{\pi s}{\sin(\pi s)} (\eta\Delta')^{s-1} \right. \\ &\quad \left. + \alpha \omega_s'^{1-s} \sum_{n=1}^{\infty} (-1)^n \frac{n}{s-n} (\eta\Delta')^{n-1} \right\}. \end{aligned} \quad (17)$$

Here $\omega_s' \equiv \omega_s / \omega_c$ and $\Delta' \equiv \Delta / \omega_c$. From this equation, it is self-consistent to determine η . It is clear to see that the eigenstates of the unperturbed part in H' are of superposition of the TSS if $\eta > 0$, while TSS becomes localized if $\eta = 0$, and no tunneling is possible. According to the analogical treatment of the transition condition in the work of Kohrein and Mielke,⁶ the critical transition condition from delocalization to localization can be derived

$$\begin{aligned} \eta &= \exp \left\{ -\alpha \omega_s'^{1-s} \left[(\eta\Delta')^{s-1} \frac{\pi s}{\sin \pi s} \right. \right. \\ &\quad \left. \left. + \sum_{n=0}^{\infty} \frac{n+1}{s-n-1} (-\eta\Delta')^n \right] \right\}. \end{aligned} \quad (18)$$

For the scaling limit $\Delta' \ll 1$, one gets

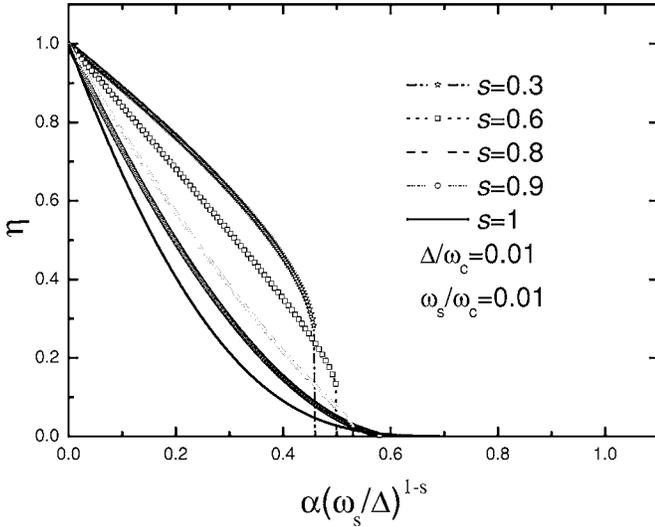


FIG. 1. η as a function of the dimensionless coupling strength $\alpha(\frac{\omega_s}{\Delta})^{1-s}$ for different bath types.

$$\eta = \exp \left\{ -\alpha \omega_s'^{1-s} \left[(\eta \Delta')^{s-1} \frac{\pi s}{\sin \pi s} + \frac{1}{s-1} \right] \right\}. \quad (19)$$

If the condition

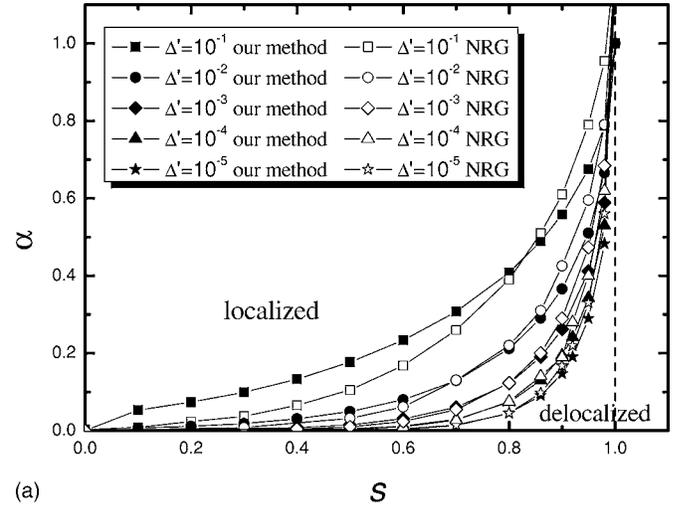
$$\alpha \omega_s'^{1-s} \frac{\pi s(1-s)}{\sin(\pi s) \Delta'^{1-s}} \leq e^{\alpha-1} \quad (20)$$

is satisfied, the solution for η is finite and satisfies

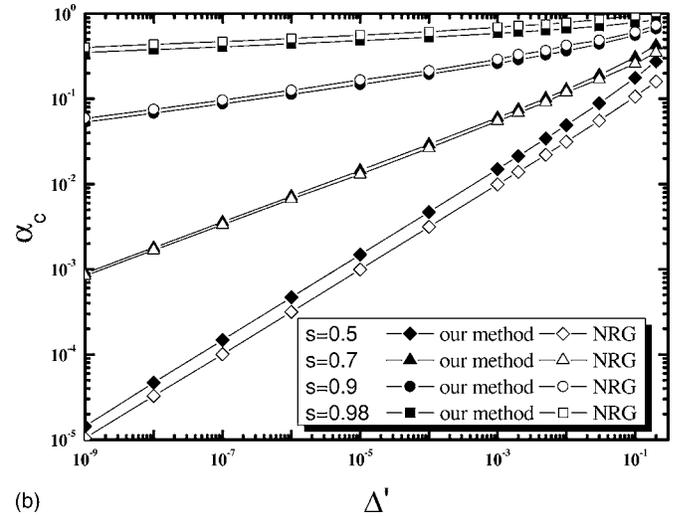
$$\eta^{1-s} \leq e^{\alpha-1} \quad (21)$$

otherwise $\eta=0$. It can be seen that, in the sub-Ohmic case, there exists a quantum transition boundary separating a delocalized phase for $\alpha < \alpha_l$ from a localized phase for $\alpha \geq \alpha_l$. In the delocalized region, the renormalized tunneling between the two states is finite, whereas it is renormalized to zero in the localized phase ($\eta=0$). When $s \rightarrow 1$, from the condition (20), it is easy to get $\alpha_l=1$ in the scaling limit, which agrees with the known results. Our results provide a direct evidence for a phase transition for all $0 < s \leq 1$. Furthermore, the transition point α_l is continuous as a function of s from the sub-Ohmic to Ohmic case, which is in good agreement with the NRG results.^{9,10} Compared with the transition condition Eq. (16) in Ref. 6 obtained by flow equations, it seems that there is a discontinuous behavior when s goes below to 1. Moreover, no transition happens for $s > 1$, in other words, the system is always delocalized in the super-Ohmic case. As is shown in the condition (20), the critical coupling α_l follows a power law as a function of the bare tunneling, $\alpha_l \propto \Delta^{1-s}$, which is in good agreement with the conjecture of NRG.¹⁰ From the above discussion, it indicates that the transition condition is sensitive to the index s in the sub-Ohmic case.

η as a function of the dimensionless coupling strength $\alpha(\frac{\omega_s}{\Delta})^{1-s}$ is shown in Fig. 1. There is a discontinuous jump from a finite value to $\eta=0$ as $\alpha \rightarrow \alpha_l$ for $0 < s < 1$, namely, it is a first-order transition which is different from the NRG result.^{9,10} However, for $s=1$, η can continuously change



(a)



(b)

FIG. 2. (a) The delocalized-localized transition point α_l as functions of s . (b) Δ' dependence of the critical coupling α_l for various bath types s . The NRG data are also shown for comparison. NRG parameters here are $\Lambda=2$, $Nb=8$, and $Ns=100$.

from one to zero as α increases from zero to $\alpha_l \sim 1$. For $\alpha > 1$ in the scaling limit, the delocalized transition occurs which agrees with the known result in literature.

Our approach has given a clear evidence for the transition from a delocalized phase to a localized one in the sub-Ohmic case. The phase boundaries are shown in Fig. 2(a) which are determined by the vanishing of renormalized tunneling. NRG results are shown for comparison. It is seen that our data agree well with those of NRG for $s > 0.6$. At the same time, there is some deviation from our data for $s < 0.5$ due to the NRG discretization.^{9,10} As displayed in Fig. 2(b), the critical coupling α_l follows a power law as a function of the tunneling, $\alpha_l \propto \Delta'^{1-s}$ for $\Delta' \ll \omega_c$ [see Eq. (20)], also predicted by the NRG method.¹⁰ NRG data are provided for a fair comparison in Fig. 2(b), too. The calculated transition points are in agreement with those obtained by the NRG method. However, our result predicts a first-order transition, in contrast with the second-order transition predicted by the NRG.

B. Correlation function

The main interest of quantum dynamics is the nonequilibrium correlation $P(t)$ and the symmetrized equilibrium correlation $C(t)$. When the initial state can be prepared, the evolution of the state is of primary interest which can be described by $P(t)$. $P(t) = \langle b, +1 | \langle +1 | e^{iHt} \sigma_z e^{-iHt} | +1 \rangle | b, +1 \rangle$ is defined in Ref. 1, where $|+1\rangle$ is the state of bosons adjusted to the state of $\sigma_z = +1$.

Because of the unitary transformation ($e^S \sigma_z e^{-S} = \sigma_z$)

$$P(t) = \langle \{0_k\} | \langle +1 | e^{iH't} \sigma_z e^{-iH't} | +1 \rangle | \{0_k\} \rangle, \quad (22)$$

since $e^S | +1 \rangle | b, +1 \rangle = | +1 \rangle | \{0_k\} \rangle$. Using Eqs. (10)–(16) the result is

$$\begin{aligned} P(t) &= \frac{1}{2} \sum_E x^2(E) \exp[-i(E + \eta\Delta/2)t] \\ &\quad + \frac{1}{2} \sum_E x^2(E) \exp[i(E + \eta\Delta/2)t] \\ &= \frac{1}{4\pi i} \oint_C d\omega e^{-i\omega t} \left(\omega - \eta\Delta - \sum_k \frac{V_k^2}{\omega + i0^+ - \omega_k} \right)^{-1} \end{aligned}$$

$$+ \frac{1}{4\pi i} \oint_C d\omega e^{i\omega t} \left(\omega - \eta\Delta - \sum_k \frac{V_k^2}{\omega - i0^+ - \omega_k} \right)^{-1}, \quad (23)$$

where a change of the variable $\omega = E + \eta\Delta/2$ is made. The real and imaginary parts of $\sum_k V_k^2 / (\omega \pm i0^+ - \omega_k)$ are denoted as $R(\omega)$ and $\mp \gamma(\omega)$, respectively.

$$\begin{aligned} R(\omega) &= \sum_k \left(\frac{\eta\Delta}{\omega_k + \eta\Delta} \right)^2 \frac{g_k^2}{\omega - \omega_k} \\ &\quad - 2\alpha\omega_s^{1-s} \omega_c (\eta\Delta')^2 \int_0^1 \frac{x^s dx}{(x - \omega')(x + \eta\Delta')^2}, \end{aligned} \quad (24)$$

$$\gamma(\omega) = 2\alpha\pi\omega_s^{1-s} \omega_c \left(\frac{\eta\Delta'}{\omega' + \eta\Delta'} \right)^2 (\omega')^s \Theta(\omega_c - \omega), \quad (25)$$

where $\omega' \equiv \omega/\omega_c$ for simplicity. For general $s < 1$ the integration in Eq. (24) should be done by residue theorem,

$$\begin{aligned} R(\omega) &= -2\alpha\omega_s^{1-s} \omega_c \left(\frac{\eta\Delta'}{\omega' + \eta\Delta'} \right)^2 \left\{ \sum_{n=0}^{\infty} \frac{(1-s)(-\eta\Delta')^{n+2} + \omega' s (-\eta\Delta')^{n+1} - (\omega')^{n+2}}{n+2-s} - \frac{(\eta\Delta' + \omega')\eta\Delta'}{1 + \eta\Delta'} \right. \\ &\quad \left. - \frac{\pi}{\sin(\pi s)} [(s-1)(\eta\Delta')^s + s(\eta\Delta')^{s-1} \omega' + (\omega')^s \cos(\pi s)] \right\}. \end{aligned} \quad (26)$$

The integral in Eq. (23) can proceed by calculating the residue of integrand and the result is $P(t) = \cos(\omega_0 t) \exp(-\gamma t)$, where ω_0 is the solution of equation

$$\omega - \eta\Delta - R(\omega) = 0 \quad (27)$$

and $\gamma = \gamma(\eta\Delta) = \alpha\pi\omega_s^{1-s} (\eta\Delta)^s / 2$ (Wigner-Weisskopf approximation).³³ The behavior of $P(t)$ is of the form of damped oscillation. One can prove that the solution ω_0 of Eq. (27) is real for small coupling. As the coupling α increases, the solution ω_0 becomes imaginary, thus $P(t)$ demonstrates the incoherent dynamics. As a result, there exists a critical point corresponding to the coherent-incoherent transition. In other words, for the critical case, one can have $\omega_0 = 0$ and $P(t) = \exp(-\gamma t)$. For $\alpha > \alpha_c$, one has $P(t) > 0$ for all times. Meanwhile, oscillations disappears and that of pure incoherence displays. When $\Delta' \ll 1$, from Eq. (27), one gets

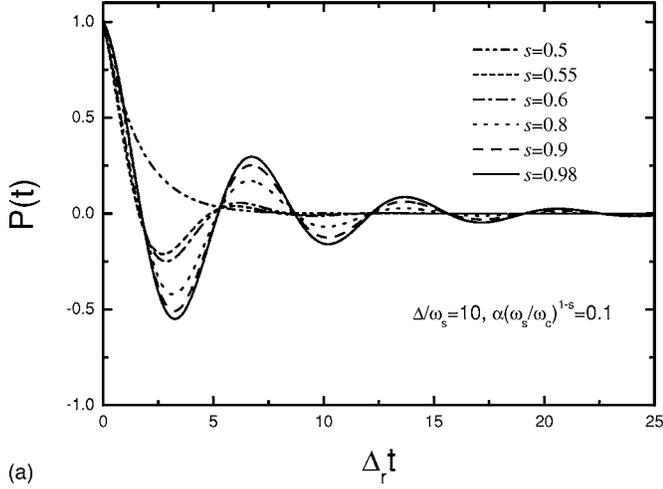
$$\alpha_c = \frac{\sin(\pi s)}{2\pi(1-s)} \left(\frac{\eta\Delta'}{\omega'_s} \right)^{1-s}. \quad (28)$$

For $s=1$, one gets $\alpha_c = \frac{1}{2}$ which is the same as known before. It is clear to see that α_c is also proportional to Δ^{1-s} for small Δ . It turns out the sensitivity of the critical coupling to bath structure.

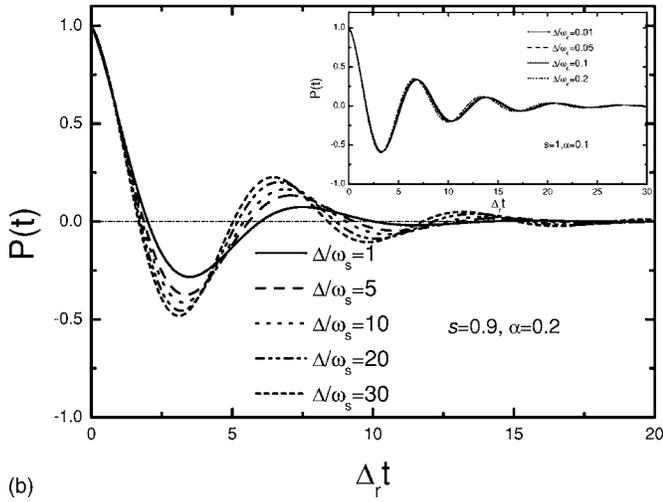
Figure 3(a) shows the time evolution of the nonequilibrium correlation $P(t)$ for the fixed coupling $\alpha\omega_s^{1-s} = 0.1$ and $\Delta/\omega_s = 10$ with different bath types. The damped oscillation exists when $\alpha < \alpha_c$, while it decays fast for $\alpha \sim \alpha_c$. That is to say, the tunneling regime $\alpha < \alpha_c$, namely $\eta > 0$, consists of two qualitatively different regions, distinguished by the presence (for $0 < \alpha < \alpha_c$) or absence (for $\alpha_c < \alpha < \alpha_c$) of tunneling oscillations in quantum dynamical quantities.²¹ It is predicted that there is a boundary between the phase coherent region and the pure incoherent one (the exponential decay), which is shown in Fig. 7(a).

The behavior of $P(t)$ is shown in Fig. 3(b) for $s=0.9$ and $\alpha=0.1$ with different tunneling $\Delta/\omega_s = 1, 5, 10, 20,$ and 30 , respectively. The less Δ is, the faster $P(t)$ decays. It indicates that there is a nonscaling behavior for dynamical quantities in the sub-Ohmic bath in contrast with a scaling one in the ohmic case.

Since $e^S \sigma_z e^{-S} = \sigma_z$, the retarded Green's function is



(a)



(b)

FIG. 3. (a) The time evolution ($\Delta_r t = \eta \Delta t$) of the nonequilibrium correlation $P(t)$ for $\alpha \omega_s^{1-s} = 0.1$ and $\Delta/\omega_s = 10$ with different bath types s . (b) $P(t)$ for $s = 0.9$ and $\alpha = 0.2$ with various values of Δ . The inset shows $P(t)$ for $\alpha = 0.1$ with different Δ in the Ohmic case.

$$G(t) = -i\theta(t) \langle [\exp(iH't)\sigma_z \exp(-iH't), \sigma_{z+}]' \rangle, \quad (29)$$

where $\langle \cdots \rangle'$ means the average with thermodynamic probability $\exp(-\beta H')$. The Fourier transformation of $G(t)$ is denoted as $G(\omega)$, which satisfies an infinite chain of equation of motion.³⁴ We have made the cutoff approximation for the equation chain at the second order of g_k and the solution at $T=0$ is

$$G(\omega) = \frac{1}{\omega - \eta\Delta - \sum_k V_k^2 / (\omega - \omega_k)} + \frac{1}{\omega + \eta\Delta - \sum_k V_k^2 / (\omega + \omega_k)}. \quad (30)$$

The equilibrium correlation function

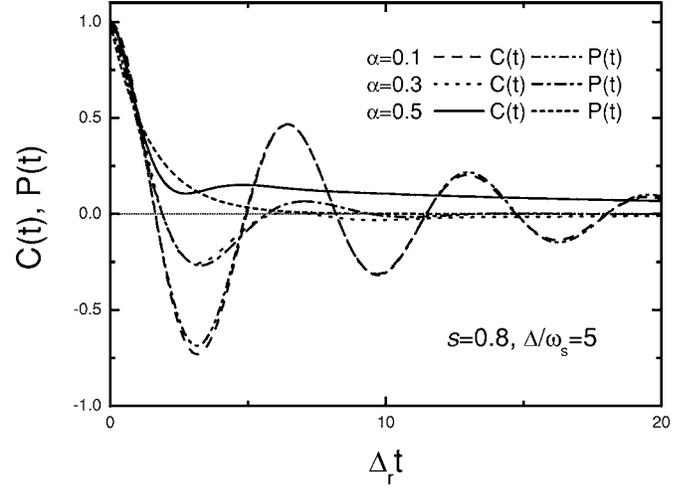


FIG. 4. The time evolution of $P(t)$ and $C(t)$ for $s = 0.8$ and $\Delta/\omega_s = 5$ with different couplings $\alpha = 0.1, 0.3,$ and 0.5 , respectively. Note that $\alpha_c = 0.53718$.

$$\begin{aligned} C(t) &= \frac{1}{2} \text{Tr} \{ \exp(-\beta H) [\sigma_z(t)\sigma_z + \sigma_z\sigma_z(t)] \} / \text{Tr} \{ \exp(-\beta H) \} \\ &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{\beta\omega}{2}\right) \text{Im} G(\omega) \exp(-i\omega t) \\ &= \frac{1}{\pi} \int_0^{\infty} d\omega \frac{\gamma(\omega)}{[\omega - \eta\Delta - R(\omega)]^2 + \gamma(\omega)^2} \cos(\omega t). \end{aligned} \quad (31)$$

For general value of $\alpha \leq \alpha_c$, $C(t)$ may contain both terms of the exponential decay ones and the algebraic decay ones. For the special value $\alpha = \alpha_c$, the exponential decay terms disappear. In the long-time limit the first nonzero algebraic decay term dominates, which is $\sim -1/t^{s+1}$. The time evolution of $C(t)$ is shown in Fig. 4 for $s = 0.8$, $\Delta/\omega_s = 0.1$ with different couplings $\alpha = 0.1, 0.3,$ and 0.5 , respectively. The time evolution of $P(t)$ is also provided to a fair comparison in this figure. It is remarkable that there are distinguishable characters between $C(t)$ and $P(t)$ for larger coupling, while the difference between them is not apparent for small coupling. This is an indication that $P(t)$ and $C(t)$ possess a similar structure for small coupling at intermediate times. However, they differ distinctively at long-time limit.

In Fig. 5 we show $C(\omega)$ for $s = 0.6$ [Fig. 5(a)] and $s = 0.3$ [Fig. 5(b)]. For weak coupling, there is a peak near the renormalized tunneling Δ_r . However, with increasing coupling, it is observed that part of the spectral weight has transferred to lower frequencies with a shoulder feature. It indicates that the dynamical properties in the sub-Ohmic case is not determined only by a single energy scale Δ_r , which agrees with the conclusion of the NRG.¹²

C. Shiba's relation and sum rule

The susceptibility $\chi(\omega) = -G(\omega)$, and its imaginary part is

$$\begin{aligned} \chi''(\omega) &= \frac{\gamma(\omega)\theta(\omega)}{[\omega - \eta\Delta - R(\omega)]^2 + \gamma^2(\omega)} \\ &+ \frac{\gamma(-\omega)\theta(-\omega)}{[\omega + \eta\Delta + R(-\omega)]^2 + \gamma^2(-\omega)}. \end{aligned} \quad (32)$$

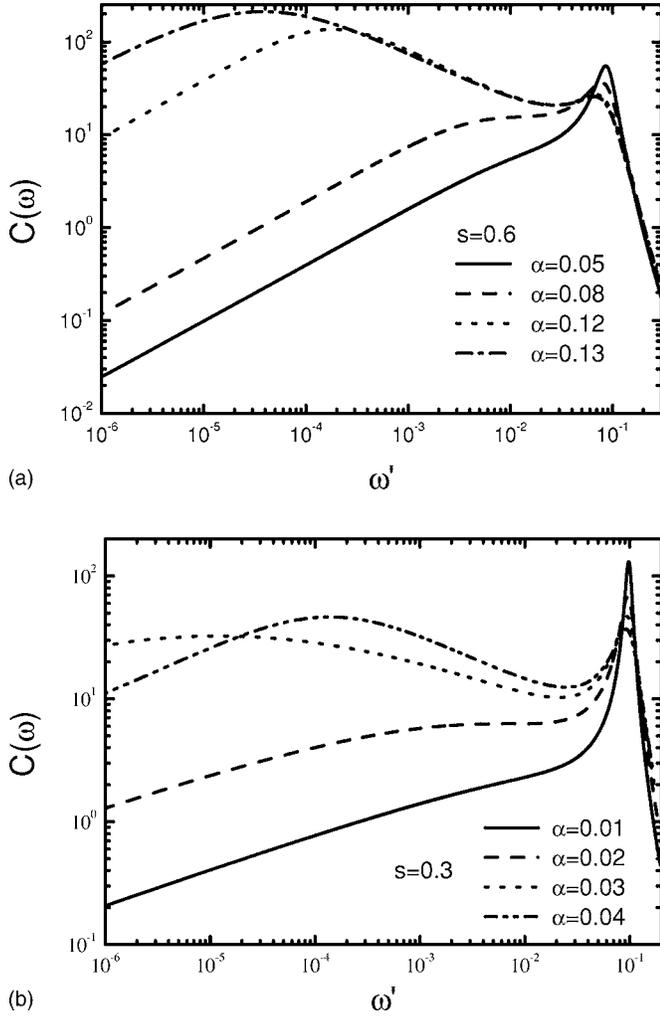


FIG. 5. The equilibrium correlation function $C(\omega)$ for (a) $s = 0.6$, $\Delta' = 0.1$ and $\alpha\omega_s^{1-s} = 0.05, 0.08, 0.12$, and 0.13 ; (b) $s = 0.3$ with various values of α , and $\Delta' = 0.1$ ($\omega_s = \omega_c = 1$). We find $\alpha_c = 0.1271$ for $s = 0.6$ and $\alpha_c = 0.0327$ for $s = 0.3$.

The $\omega \rightarrow 0$ limit of $S(\omega) = \chi''(\omega)/J(\omega)$ is

$$\lim_{\omega \rightarrow 0} \frac{\chi''(\omega)}{J(\omega)} = \frac{\pi}{(\eta\Delta + R(\omega=0))^2}. \quad (33)$$

With a Kramers-Kronig relation and a fluctuation-dissipation theorem, the static susceptibility χ_0 can be directly extracted

$$\chi'(\omega=0) = \frac{1}{2} \int_0^\infty d\omega \frac{C(\omega)}{\omega}. \quad (34)$$

Thus, there exist an important relation connecting the zero frequency behavior of the spectral function to static susceptibility, which is known as the Shiba's relation^{18–20,23,35}

$$\lim_{\omega \rightarrow 0} \frac{C(\omega)}{(2\chi_0)^2 J(\omega)} = 1. \quad (35)$$

It constitutes an important check of our approach.

Approximation schemes such as NIBA and numerical approaches based on Monte Carlo simulations cannot be used to verify the Shiba's relation since they failed to predict the long-time behavior.⁷ Results from both real time renormalization group and NRG in the Ohmic case have a maximal relative error of around 10%.^{9,19} Flow equation approach based on infinitesimal transformations gives its result for the sub-Ohmic case with error 10% or so.⁸ In Table I, the generalized Shiba relation is verified for various couplings, tunneling matrix and bath types. It shows that the Shiba's relation is exactly satisfied for $\alpha < \alpha_c$ in both the sub-Ohmic and Ohmic cases. Outside the range, the agreement is still good but no longer exact. In the present paper, we consider carefully the behavior of coherent dynamics for $\alpha < \alpha_c$. For $s = 1$, the Shiba's relation has been proved analytically by our approach in Ref. 14.

The sum rule $C(t=0) = 1$ is an important relation in the equilibrium correlation function which constitutes another significant check of our approach. The numerical solution of our approach can yield a satisfactory result, which is also shown obviously in Table I. As is told in the paper of Stauber,⁸ the sum rule is not fulfilled by the flow equation method. Independent of the bath type and the cutoff ω_c the sum rule is performed well in the present approach, while in the flow equations it only yields 80% or so.

Since different dynamical quantities may be associated with different initial preparations of the system, quantum coherence may be more or less sensitive to dissipation.²⁵ Therefore, there are disparate critical values of the damping strength for different coherence criterion. Considering the character of the spectral function $S(\omega)$, one gives its appropriate coherence criterion. For weak damping, $\alpha < \alpha_c^*$, the function $S(\omega)$ exhibits two inelastic peaks at finite frequency $\omega_p \approx \eta\Delta$. It can be seen that the width of peak $\gamma(\omega)$ is less than the value of ω_p . At the critical damping α_c^* , one has $\gamma(\omega) = \omega_p$, and the two peaks merge into a single quasielastic peak centered at $\omega = 0$. For instance, in the scaling limit, for $s = 1$, the critical damping value is determined by

$$\frac{\omega}{\eta\Delta} - 1 + \frac{1}{\pi} \left(1 + \frac{\omega}{\eta\Delta} - \frac{\omega}{\eta\Delta} \ln \frac{\omega}{\eta\Delta} \right) = 0, \quad (36)$$

and

$$2\alpha_c^* \left(\frac{1}{1 + \frac{\omega}{\eta\Delta}} \right)^2 = 1. \quad (37)$$

One gets $\alpha_c^* = 0.325$, which agrees well with $\alpha_c^* = \frac{1}{3}$ or $\alpha_c^* \approx 0.3$ obtained by the renormalization group numerical results⁹ and other conjectures.^{20,22} One can observe that the “quasiparticle peak” disappears at $\alpha = \alpha_c^*$ in Fig. 6(b). Physically, it indicates that the crossover between the underdamping oscillating behavior and overdamping decaying one occurs at $\alpha = 0.325$ at zero temperature.

In Fig. 6 the renormalized spectral function $S(\omega)\Delta^2$ is shown for $s = 0.8$ (a) and $s = 1$ (b) with $\Delta/\omega_s = 1$, $\omega_s/\omega_c = 0.1$ and various coupling strength α . $S(\omega)$ has a double-peak structure for $\alpha < \alpha_c^*$. Only the $\omega \geq 0$ part is shown in Figs.

TABLE I. Representative results from the numerical solution with parameters chosen by the spectral density $J(\omega)=2\alpha\omega_s^{1-s}\omega^s\Theta(\omega_c-\omega)$ and with the controlling precision 10^{-5} for iteration. $R \equiv [\lim_{\omega \rightarrow 0} C(\omega)/J(\omega)]/(2\chi_0)^2$. The numeric error for the Shiba relation and sum rule is at least less than 10^{-6} and can be improved by increasing the accuracy of numerical calculations.

s	ω'_s	$\frac{\Delta}{\omega_s}$	α	χ_0	$\frac{C(\omega)}{J(\omega)} \Big _{\omega \rightarrow 0}$	R	$C(t=0)$
1	1	0.01	0.1	93.275771	34801.4793	1	1
1	1	0.05	0.1	15.588677	972.0275	1	1
1	1	0.1	0.1	7.211567	208.0268	1	1
1	1	0.2	0.1	3.336971	44.54151	1	1
1	1	0.1	0.3	21.202413	1798.1694	1	1
1	1	0.1	0.4	54.393368	11834.5544	1	1
1	1	0.2	0.5	65.0612653	16931.8733	1	1
0.9	1	0.1	0.1	8.012265	256.7861	1	1
0.9	1	0.05	0.1	18.18289	1322.467	1	1
0.9	1	0.2	0.15	4.450706	79.23528	1	1
0.8	1	0.05	0.1	23.81572	2268.770	1	1
0.8	1	0.1	0.1	9.474312	359.0517	1	1
0.8	0.1	1	0.1	7.233729	209.3079	1	1
0.6	1	0.1	0.01	5.496693	120.8546	1	1
0.5	1	0.2	0.05	4.282478	73.35843	1	1
0.5	0.1	1	0.1	8.26555	273.2771	1	1

6(a) and 6(b). For $\alpha \geq \alpha_c^*$ there is only one peak at $\omega=0$. The critical coupling α_c^* corresponds to the crossover from underdamping to overdamping oscillations. We obtain $\alpha_c^*=0.34$ for a subohmic bath with $s=0.8$ which is in good agreement with $\alpha_c^* \approx 0.3$ obtained by the flow equations.⁷ Figure 6(c) shows the $S(\omega)$ versus ω relations for fixed $\alpha=0.3$ and $s=0.9$ with $\Delta/\omega_s=1, 5, 10$, and 30 , respectively.

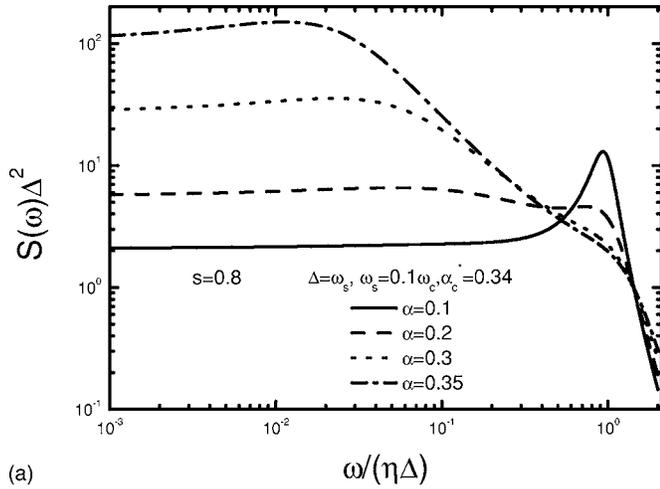
The dynamical phase diagrams are given in Fig. 7(a) ($s=1$) and Fig. 7(b) ($s=0.8$) for $\omega_s=\omega_c$. In both figures, the transition boundary between the incoherent relaxation and coherent oscillation is shown in a solid line, while that of underdamping-overdamping transition is shown in a dashed line. In the scaling limit ($\Delta' \ll 1$) for $s=1$, $\alpha_c=0.5$, and $\alpha_c^*=0.325$ are consistent with the known results.^{1,20,22} Further, in the Ohmic case, the coherent-incoherent transition coupling $\alpha_c = \frac{1}{2}[1 + \eta\Delta/\omega_c]$. With increasing tunneling, both α_c and α_c^* become larger, which presents a contrast with the tendency of the boundary obtained by Monte Carlo simulations.¹⁸ Moreover, note that the critical coupling is sensitive to the bath type, especially in the scaling limit. As displayed in Fig. 7(b), the critical couplings α_c^* and α_c nicely follow power laws as functions of the bare tunneling, $\alpha \propto \Delta^{1-s}$ for small Δ (in the case $s=0.8$). Our fit data for $\Delta' < 0.01$ are well consistent with the conclusion. It is pointed out by our approach that the critical couplings in addition to the delocalized-localized transition one are always proportional to Δ^{1-s} for small Δ , which hints that the critical value is sensitively dependent on the structure of bath.

IV. SUMMARY AND DISCUSSION

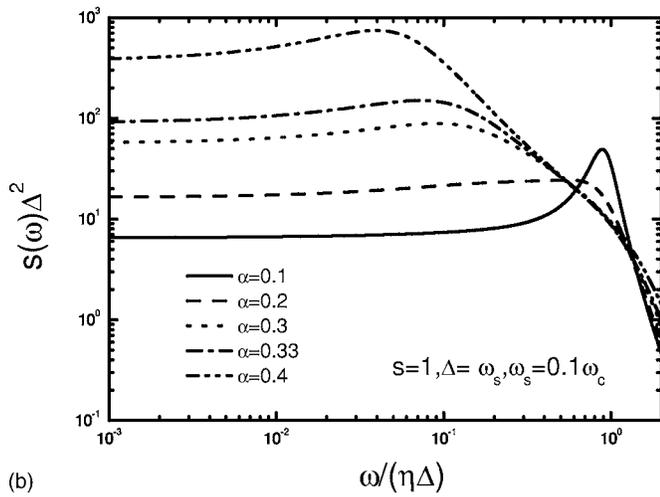
The dynamics of SBM with a sub-Ohmic bath is studied by means of the perturbation approach based on a unitary

transformation. Our approach is quite simple, whereas it correctly gives $P(t)$, $C(t)$, Shiba's relation, and reproduces nearly all results of previous authors that we note. By means of our approach, the dynamical transition point α_c is calculated. The main results include (i) the nonequilibrium correlation $P(t)$, the susceptibility $\chi''(\omega)$, and the equilibrium correlation $C(t)$ are analytically obtained for the general finite Δ/ω_c case; (ii) a critical transition point (α_l) from delocalization to localization exists in the sub-Ohmic case; (iii) for a fixed tunneling, as the coupling with environment increases, a crossover from coherent to incoherent tunneling appears. In other words, for $\alpha > \alpha_c$, the coherent dynamics disappear; (iv) there is a critical transition point α_c^* from underdamping oscillation to overdamping one in the susceptibility $\chi''(\omega)/\omega$. When $\alpha < \alpha_c^*$, the spectrum of susceptibility is of a double-peak structure, while there is only one peak at $\omega=0$ for $\alpha > \alpha_c^*$; (v) the Shiba's relation and sum rules are exactly satisfied for $\alpha \leq \alpha_c$; (6) the dynamical phase diagrams in both the sub-Ohmic and Ohmic cases are mapped out. For small tunneling, all of three critical coupling $\alpha_l, \alpha_c, \alpha_c^*$ are proportional to Δ^{1-s} .

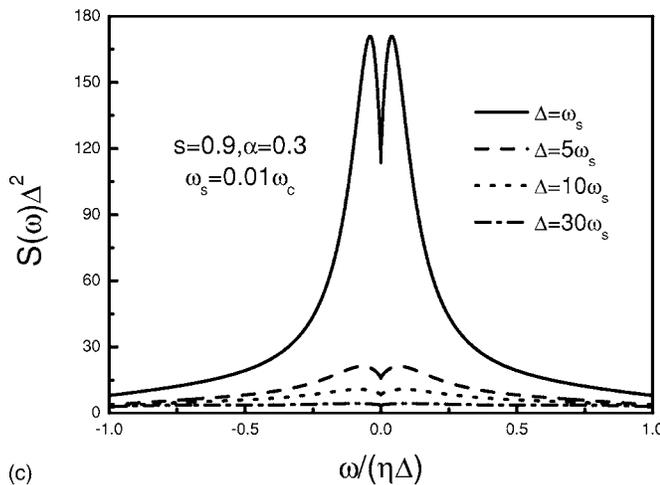
Our treatment is essentially a perturbation one. The transformed Hamiltonian is divided into the unperturbed part H'_0 and perturbation H'_1 and H'_2 . The unperturbed part gives the intrinsic coherent tunneling motion with diagonal transition of bosons. H'_1 is related to the single-boson nondiagonal transition and H'_2 to the multiboson transition. In our perturbation treatment we take into account only the single-boson nondiagonal transition (H'_1) which plays an important role for weak coupling and lower temperature. H'_2 with multiboson nondiagonal transition is neglected in our treatment. At strong coupling and high temperature, the multiboson nondi-



(a)



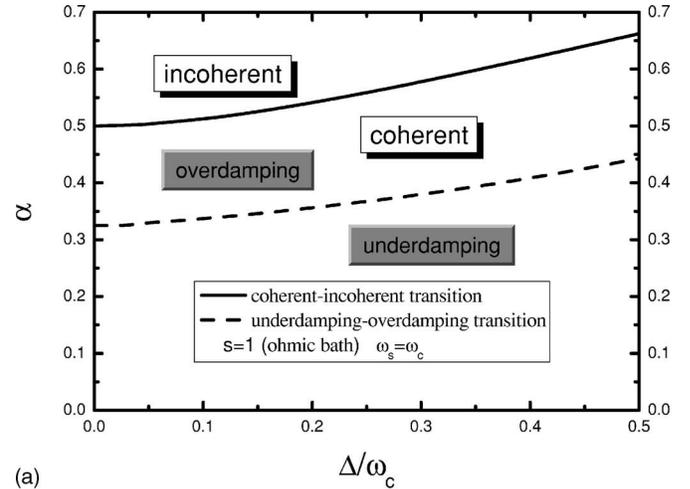
(b)



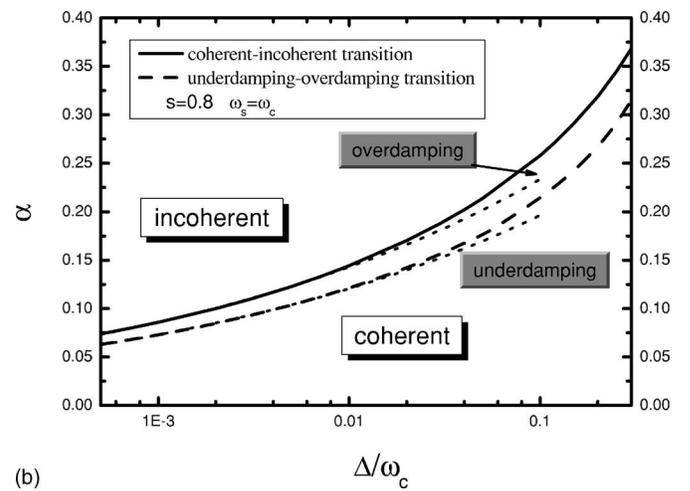
(c)

FIG. 6. The renormalized spectral function $S(\omega)\Delta^2$ as a function of ω for $s=0.8$ (a) and $s=1$ (b) with $\Delta/\omega_s=1$, $\omega_s/\omega_c=0.1$ and different α . (c) $S(\omega)\Delta^2$ as a function of ω for $s=0.9$, $\alpha=0.3$ with $\Delta/\omega_s=1, 5, 10$, and 30 , respectively.

agonal transition may play an important role. Since our perturbation treatment keeps the contribution of the single-boson nondiagonal transition and drops that of the



(a)



(b)

FIG. 7. The dynamical phase diagrams for $s=1$ (a) and $s=0.8$ (b) with $\omega_s=\omega_c$. The solid lines are the transition boundaries between the coherent oscillation and incoherent decay. The dashed lines stand for the boundaries between the underdamping oscillation and overdamping one in coherent region. The dotted lines in (b) are fits to the $\alpha \propto \Delta^{1-s}$ law using the $\Delta < 10^{-2}$ points only.

multiboson nondiagonal transition, we cannot make definite statement about the exact nature of the localization-delocalization transition. Our perturbation treatment could not be applied to study the localized phase beyond the critical point of the sub-Ohmic case ($\alpha > \alpha_l$). Thus, the approach cannot predict the oscillation behaviors on short times in the localized phase for strongly sub-Ohmic case. The recent NRG's results have captured the coherent oscillation even in the localized phase for small s and demonstrated it explicitly.¹² In principle, our approximation can be applied satisfactorily for $\alpha \leq \alpha_c$, whereas the approximation might fail when $\alpha \approx \alpha_l$.

At lower temperature and weak coupling, the diagonal transition of bosons dominates with coherent tunneling motion. As the coupling increases, single-boson and multiboson nondiagonal transitions come to prevail against the diagonal transition, which result in decoherence. Our perturbation treatment keeps the contribution of the single-boson nondiagonal transition and drops that of the multiboson nondiagonal

nal transition. Based on the perturbation treatment, our approach can reproduce the well-known results for the Ohmic case, such as $\alpha_I=1$ and $\alpha_c=1/2$. Besides, our result also points out that the dynamical property is not determined only by the single energy scale $\eta\Delta$. On the one hand, a nonscaling behavior of dynamical quantities is shown in Fig. 3(b). On the other hand, from the results of $C(\omega)$ for $s=0.6$ and $s=0.3$ [Figs. 5(a) and 5(b)], one can see that a pronounced shoulder in $C(\omega)$ comes to appear with increasing coupling which agrees with the NRG results. These complicated behaviors result from the nondiagonal transition, which is the contribution of H'_1 in our perturbation treatment. At the same time, Shiba's relation and sum rule are exactly satisfied for $\alpha \leq \alpha_c$ in both the Ohmic case and sub-Ohmic one (even for $s \ll 1$), which constitute important checks of the approach. In general, this method works well for weak coupling with $\alpha \leq \alpha_c$. Thus, this approach can be applied in the sub-Ohmic case to study the coherent-incoherent transition.

The function ξ_k plays an important role in our approach. It eliminates the infrared catastrophe completely. In conventional perturbation theory, from the original Hamiltonian H , the dimensionless expansion parameter is g_k^2/ω_k^2 . Thus, the renormalized tunneling becomes zero, and the system is always localized because

$$\sum_k \frac{g_k^2}{\omega_k^2} = \int_0^{\omega_c} \frac{2\alpha\omega_s^{1-s}}{\omega^{2-s}} d\omega. \quad (38)$$

For Ohmic bath $s=1$ the integrand becomes $2\alpha/\omega$ which is logarithmic divergent in the infrared limit. There also exists a low-energy divergence ($\frac{1}{\omega^{2-s}}$) for a sub-Ohmic bath $s < 1$. On the contrary, for the coupling in transformed Hamiltonian, H'_1 , the expansion parameter is $g_k^2\xi_k^2/\omega_k^2 \sim 2\alpha\omega^s\omega_s^{1-s}/(\omega + \eta\Delta)^2$, which is finite in the infrared limit for $s > 0$. There-

fore, from the viewpoint of mathematics, the introduction of ξ_k gets rid of the divergence. Physically, the disappearance of divergence arises due to the energy scale separation by ξ_k with a special treatment of the low frequency, nonadiabatic modes.

The low frequency behavior of the spectrum density function in SBM model determines the long-time behavior of TSS. All quantum dynamics 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 ($\omega_k \gg \Delta$), bath modes follow instantaneously to the tunneling motions, namely, the displacement of boson due to the coupling to subsystem is large, whereas near the low frequency limit ($\omega_k \ll \Delta$), nonadiabatic modes couple weakly to the subsystem with coupling strength $g_k \frac{\omega_k}{\eta\Delta}$, its displacement is small. Thus, while all boson modes are treated by the function ξ_k , their different contribution to the dressed TSS has been distinguished with respect to the scale of boson energy. Therefore, even if our approach is, in principle, a perturbation one, those reasons above give the intrinsic base of our present results, such as $P(t)$, $C(t)$, the dynamical transition points α_c and α_c^* and exact Shiba's relation. When $s \rightarrow 1$, our results agree well with exact or known ones. Besides, our approach can be straightforwardly extended to other more complicated coupling systems.

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