Quantum critical point of spin-boson model and infrared catastrophe in bosonic bath

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An analytic ground state is proposed for the unbiased spin-boson Hamiltonian, which is non-Gaussian and beyond the Silbey-Harris ground state with lower ground state energy. The infrared catastrophe in Ohmic and sub-Ohmic bosonic bath plays an important role in determining the degeneracy of the ground state. We show that the infrared divergence associated with the displacement of the nonadiabatic modes in bath may be removed from the proposed ground state for the coupling $\alpha < \alpha_c$. Then α_c is the quantum critical point of a transition from non-degenerate to degenerate ground state and our calculated α_c agrees with previous numerical results. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4803661]

I. INTRODUCTION

Quantum impurity systems with competing interactions constitute a field of wide interest in the quantum physics. In recent years, the quantum two-level system coupled to dissipative bosonic environment (spin-boson model, SBM) attracts much attention in this field because it may be one of the simplest but nontrivial quantum impurity system for studying the physics of competing interactions. The Hamiltonian of SBM reads (we set $\hbar = 1$)

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

where $b_k^\dagger$ (b_k) is the creation (annihilation) operator of environmental bosonic mode with frequency ω_k, σ_x, and σ_z are Pauli matrices to describe the two-level system. The competing interactions in SBM are between the quantum tunneling Δ and the dissipative coupling g_k to the environment. The effect of the environment is characterized by a spectral density $J(\omega) = \sum_k g_k^2\delta(\omega - \omega_k) = 2\alpha\omega^s\omega_c^{1-s}\theta(\omega_c - \omega)$ with the dimensionless coupling strength α and the hard upper cutoff at ω_c. The index s accounts for various physical situations:[1,2] the Ohmic $s = 1$, sub-Ohmic $s < 1$, and super-Ohmic $s > 1$ baths.

The quantum critical point (QCP) and the quantum phase transition (QPT) are related to the ground state transition, which is usually triggered by competing interactions. As for SBM, the interesting phase transition is related to the transition of degeneracy of the ground state, that is, it is a transition between the non-degenerate and degenerate ground state.[1–5] The main theoretical interest of the QCP in SBM is to understand how the competing interactions influences the degeneracy of the ground state. Since the Hamiltonian (1) is invariant under $\sigma_z \to -\sigma_z$ (together with $b_k, b_k^\dagger \to -b_k, -b_k^\dagger$) and one must have $\langle\sigma_z\rangle_G = 0$ ($\langle\ldots\rangle_G$ means the ground state average). However, for the Ohmic bath $s = 1$ it is well known[1,2] that a Kosterlitz-Thouless quantum transition separates a degenerate ground state at $\alpha > \alpha_c$ from a non-degenerate one at $\alpha < \alpha_c$ ($\alpha_c = 1$ in the scaling limit $\Delta \ll \omega_c$).

The ground state of SBM Hamiltonian (1) was studied by many authors using various analytic and numerical methods. Silbey and Harris (SH)[6] proposed a variational ground state and predicted the QCP $\alpha_c = 1$ for $s = 1$. The SH ground state was used by Kehrein and Mielke[7] for sub-Ohmic ($s < 1$) bath to calculate the QCP α_c. In last ten years, various numerical techniques were used for calculation of the QCP in the SBM, such as the numerical renormalization group (NRG),[3–5] the quantum Monte Carlo (QMC),[8] the method of sparse polynomial space representation,[9] the extended coherent state approach,[10] and the variational matrix product state approach.[11] Besides, recently an extension of the Silbey-Harris ground state was proposed by Zhao *et al.*[12] and Chin *et al.*[13] to study the QPT in the $s = 1/2$ sub-Ohmic SBM.

In this work, we propose an analytic ground state wavefunction for the SBM, which is non-Gaussian for the bath modes and is an extension of the work of Zhao *et al.*[12] and Chin *et al.*[13] The QPT is usually not a weak coupling problem and people believe that the numerical techniques may be more powerful than approximate analytic methods for strong coupling problem. Then, why do we still try to find an approximate analytical solution? Generally speaking, our purpose is to see and understand the physics more clearly and straightforwardly. In particular, here our purpose is to understand the role played by the infrared divergence in the SBM Hamiltonian (1).

The QPT in quantum impurity systems may be related to the infrared catastrophe in baths. Anderson[14] was the first to point out this relation for the Anderson model and Kondo model in fermionic bath. Our question is: What is the role played by the infrared catastrophe in the quantum phase transition in bosonic bath of SBM?

II. THE GROUND STATE

If $\Delta = 0$, Hamiltonian (1) is solvable and we have degenerate ground state

$$|\psi_{\uparrow(\downarrow)}\rangle = \exp\left[-\sum_k g_k\left(b_k^\dagger - b_k\right)\sigma_z/2\omega_k\right]|\uparrow(\downarrow)\rangle|\{0_k\}\rangle, \tag{2}$$

where $|\uparrow(\downarrow)\rangle$ is the eigenstate of σ_z: $\sigma_z|\uparrow(\downarrow)\rangle = +(-)|\uparrow(\downarrow)\rangle$ and $|\{0_k\}\rangle$ is the vacuum state of the bath. Then, for finite Δ it is naturally to use a superposed ground state to remove the degeneracy. But it is well known[1,2,6,7] that there exists an infrared divergence in the overlap between the degenerate states: $\langle\psi_\uparrow|\psi_\downarrow\rangle = \exp[-\sum_k g_k^2/2\omega_k^2] = 0$ for $s \le 1$. Silbey and Harris proposed a modified superposed ground state[6]

$$|G_{\rm SH}\rangle = \exp\left[-\sum_k g_k(b_k^\dagger - b_k)\sigma_z/2(\omega_k + \eta_0\Delta)\right]2^{-1/2} \times(|\uparrow\rangle + |\downarrow\rangle)|\{0_k\}\rangle, \tag{3}$$

with finite renormalized overlap $\eta_0 = \exp[-\sum_k g_k^2/2(\omega_k + \eta_0\Delta)^2]$ where the infrared divergence has been removed. The ground state energy is

$$E_g^{\rm SH} = -\eta_0\Delta/2 - \sum_k g_k^2(\omega_k + 2\eta_0\Delta)/4(\omega_k + \eta_0\Delta)^2. \tag{4}$$

For the SH ground state at the scaling limit $\Delta \ll \omega_c$, $\eta_0 = (e\Delta/\omega_c)^{\frac{\alpha}{1-\alpha}}$ for $s = 1$ and thus the QCP is at $\alpha_c^{\rm SH} = 1$ where $\eta_0 = 0$. For sub-ohmic bath $s < 1$ one can calculate the QCP by condition: $\eta_0 = 0$ at $\alpha \to \alpha_c^{\rm SH}$,[7,15] and some results are listed in the second column of Table I.

Zhao *et al.*[12] and Chin *et al.*[13] proposed an extension of the Silbey-Harris ground state to study the QPT in the $s = 1/2$ sub-Ohmic spin-boson model, with degenerate ground state when zero-biased and $\alpha > \alpha_c^D$ (superscript "D" means degenerate),

$$|\Psi_\pm\rangle = \exp(-S_\pm)(u_\pm|\uparrow\rangle + v_\pm|\downarrow\rangle)|\{0_k\}\rangle, \tag{5}$$

$$S_\pm = \sum_k \frac{g_k}{2\omega_k}\left(b_k^\dagger - b_k\right)[\xi_k\sigma_z \pm (1-\xi_k)\phi_k], \tag{6}$$

where $u_+ = v_- = 2^{-1/2}\sqrt{1+M}$, $u_- = v_+ = 2^{-1/2}\sqrt{1-M}$, $\xi_k = \omega_k/(\omega_k + W)$, $W = \eta\Delta/\sqrt{1-M^2}$, and

$$\eta = \exp\left[-\sum_k g_k^2\xi_k^2/2\omega_k^2\right], \tag{7}$$

TABLE I. QCP of different bath type s.

s	$\alpha_c^{\rm SH}$	α_c^D	Our α_c	α_c[3]	α_c[8]	α_c[9]	α_c[10]
1/4	0.08554	0.02413	0.02744	0.0264	0.0254	0.0259	0.0256
1/2	0.1768	0.08555	0.1084	0.1065	0.0983	0.0977	0.0820
3/4	0.3537	0.2176	0.3076	0.3168	0.2951	0.2953	0.3205
1	1	0.5121	1	1	1	1	1

$$M = \sum_k g_k^2\phi_k(1-\xi_k)^2/(\omega_k W). \tag{8}$$

Zhao *et al.*[12] and Chin *et al.*[13] let $\phi_k = M$ to be a constant in Eqs. (6) and (8), where $M(>0) = \langle\Psi_+|\sigma_z|\Psi_+\rangle$ $(\langle\Psi_-|\sigma_z|\Psi_-\rangle = -M)$ is the bath-induced static displacement for the degenerate ground state $|\Psi_+\rangle$ and $|\Psi_-\rangle$ with degenerate ground state energy

$$E_g^D = -W/2 - \sum_k g_k^2\xi_k(2-\xi_k)/4\omega_k + \sum_k g_k^2M^2(1-\xi_k)^2/4\omega_k. \tag{9}$$

The first term in (9), $-W/2$ is the bath-renormalized energy of the two-level system from its bare form $-\Delta/2$. It was proposed[12,13] that the QCP is at $\alpha = \alpha_c^D$ where a nonzero M leads to lower ground state energy (note that when $\alpha \le \alpha_c^D$, $M = 0$, and $|\Psi_+\rangle = |\Psi_-\rangle = |G_{\rm SH}\rangle$). Some α_c^D values for different baths are listed in the third column of Table I. But, as mentioned above, since the Hamiltonian (1) is invariant under $\sigma_z \to -\sigma_z$ (together with $b_k, b_k^\dagger \to -b_k, -b_k^\dagger$) we should have $\langle\sigma_z\rangle_G = 0$.

III. INFRARED CATASTROPHE AND QPT

The wavefunction of every bath mode in $|G_{\rm SH}\rangle$ or $|\Psi_\pm\rangle$ is a Gaussian function, thus these ground states are in the Gaussian approximation. Following the proposal of Shore and Sander[16] we propose the following superposed ground state for the SBM, which is beyond the Gaussian approximation and takes into account the effect of quantum fluctuations,

$$|G\rangle = A(|\Psi_+\rangle + |\Psi_-\rangle), \tag{10}$$

where A is a normalization factor. Then, it is easy to check that $\langle G|\sigma_z|G\rangle = 0$. But if one choose $\phi_k = M$ in Eqs. (6) and (8), as was pointed out by Chin *et al.*,[13] there is an infrared divergence of the occupation number of the nonadiabatic (NA) modes. We show that this divergence leads to the orthogonality catastrophe between $|\Psi_+\rangle$ and $|\Psi_-\rangle$,

$$\begin{aligned}\rho &= \langle\Psi_-|\Psi_+\rangle \\ &= \langle\{0_k\}|\exp\left(-\sum_k \frac{g_k}{\omega_k}(1-\xi_k)\left(b_k^\dagger - b_k\right)M\right)|\{0_k\}\rangle \\ &= \exp\left(-\sum_k \frac{g_k^2}{2\omega_k^2}(1-\xi_k)^2M^2\right) \\ &= \exp\left(-\alpha M^2W^2\int_0 \frac{\omega^{s-2}d\omega}{(\omega+W)^2}\right) = 0\end{aligned} \tag{11}$$

for Ohmic ($s = 1$) and sub-Ohmic ($s < 1$) baths as the integration in the exponential is infrared divergent. This is similar to the infrared catastrophe in Fermi sea interacting with a quantum impurity.[14] Because of the orthogonality catastrophe the ground states, $|G_D\rangle = |\Psi_+\rangle$, $|G_D\rangle = |\Psi_-\rangle$, or $|G\rangle$ (Eq. (10)) are degenerate with ground state energy (9).

The way to avoid the infrared catastrophe is similar to the proposal of Anderson,[14] that is, quantum fluctuation of the NA modes leads to a k-dependent ϕ_k in Eqs. (6) and (8) removing the infrared divergence. Then the ground state energy E_g of the superposed ground state (10) is

$$E_g = (E_0 + \rho U)/(1 + \rho\sqrt{1 - M^2}), \tag{12}$$

where $E_0 = \langle\Psi_+|H|\Psi_+\rangle$, $\rho = \langle\Psi_+|\Psi_-\rangle$, and $\rho U = \langle\Psi_+|H|\Psi_-\rangle$. Here

$$E_0 = -W/2 - \sum_k g_k^2\xi_k(2-\xi_k)/4\omega_k + Y, \tag{13}$$

$$U = \sqrt{1-M^2}\left(-\eta^2\Delta^2/2W - \sum_k g_k^2\xi_k(2-\xi_k)/4\omega_k - Y\right)$$
$$-\eta\Delta\left[\cosh(M) - 1 - M(\sinh(M) - M)\right]/2, \tag{14}$$

and $Y = \sum_k g_k^2\phi_k^2(1-\xi_k)^2/4\omega_k$.

The variational function ϕ_k can be determined by

$$\frac{\partial E_g}{\partial \phi_k} = 0 = \frac{\partial E_g}{\partial M}\frac{\partial M}{\partial \phi_k} + \frac{\partial E_g}{\partial \rho}\frac{\partial \rho}{\partial \phi_k} + \frac{\partial E_g}{\partial Y}\frac{\partial Y}{\partial \phi_k} \tag{15}$$

for every mode k and the result is

$$\phi_k = \tau\omega_k/(\omega_k + \rho\delta), \tag{16}$$

where $\delta = 2(E_0\sqrt{1-M^2} - U)/[(1-\rho)(1+\rho\sqrt{1-M^2})]$ and τ is the variational parameter. In this way, the overlapping integral is

$$\rho = \exp\left(-\sum_k \frac{g_k^2}{2\omega_k^2}(1-\xi_k)^2\phi_k^2\right)$$
$$= \exp\left(-\alpha\tau^2W^2\int_0 \frac{\omega^s d\omega}{(\omega+W)^2(\omega+\rho\delta)^2}\right), \tag{17}$$

which is finite as long as $s > 0$.

For $s = 1$ the result of variational calculation is shown in Fig. 1. When α goes to 1, the variational parameter τ tends to 1 and the overlapping ρ decreases to zero as follows:

$$\rho = \left[\frac{\delta}{W}\right]^{\frac{\alpha\tau^2}{1-\alpha\tau^2}} \exp\left(\frac{\alpha\tau^2}{1-\alpha\tau^2}\left[\ln(1+W/\omega_c) + \frac{2+W/\omega_c}{1+W/\omega_c}\right]\right), \tag{18}$$

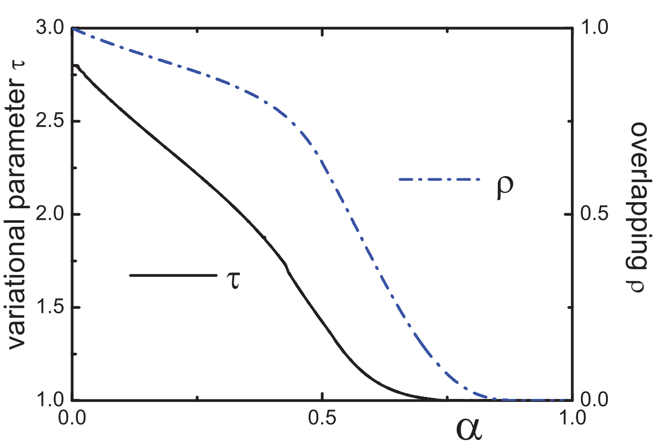

FIG. 1. The variation parameter τ and the overlapping ρ as functions of α for Ohmic bath $s = 1$.

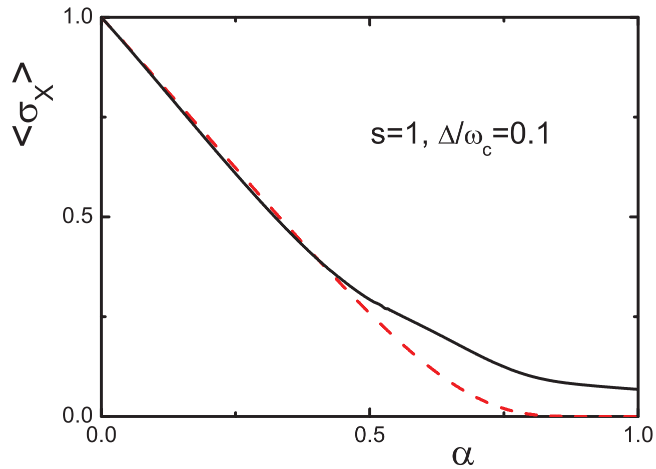

FIG. 2. The ground state average of σ_x as a function of α for Ohmic bath $s = 1$. The solid line is the result of our non-Gaussian ground state and the dashed line that of SH ground state.

that is, $\rho \to 0$ when $\alpha \to 1 - 0^+$ (0^+ is a positive infinitesimal) since $\tau \to 1$. This is to say that for $s = 1$ the ground state becomes doubly degenerate when $\alpha \to \alpha_c = 1$. We note that, although this is the same QCP for the Ohmic bath $s = 1$ as the prediction of Silbey and Harris,[6] the way to determine the QCP is different. Reference 6 determines the QCP by $\eta_0 \to 0$ when $\alpha \to \alpha_c$, while we determine the QCP by the vanishing overlapping $\rho \to 0$. Figure 2 shows the ground state average of σ_x as a function of α for Ohmic bath $s = 1$. One can see that our calculated average $\langle G|\sigma_x|G\rangle$,

$$\langle G|\sigma_x|G\rangle = \eta\left\{[\cosh(M) - M\sinh(M)]\rho + \eta\Delta/W\right\}/(1+\rho\eta\Delta/W), \tag{19}$$

is a finite quantity even if $\alpha = 1$, but that of Ref. 6, $\langle G_{SH}|\sigma_x|G_{SH}\rangle = \eta_0$, goes to zero when $\alpha < \sim 1$.

For sub-Ohmic bath $s < 1$ Eq. (17) has to be solved numerically and self-consistently, and the QCP α_c can be determined as the point where the ground state changes from non-degenerate ($\alpha < \alpha_c$) to doubly degenerate ($\alpha > \alpha_c$). Our results for some s values are shown in Table I. For

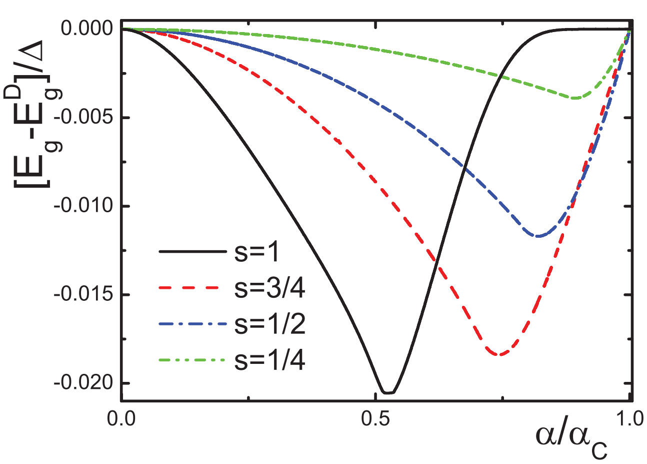

FIG. 3. $E_g - E_g^D$ is the difference between ground state energies calculated by Eqs. (12) and (9). $\Delta/\omega_c = 0.1$. See text for details.

comparison, the numerical results by NRG,[3] by QMC,[8] by the method of sparse polynomial space representation,[9] and by the extended coherent state approach[10] are also shown. One can see that our result compares well with these numerical results.

Figure 3 shows the difference between our calculation of the ground state energy and that of Zhao *et al.*[12] and Chin *et al.*,[13] $\delta E_g = E_g - E_g^D$. The lower ground state energy indicates that the ansatz of this work is a better one for the real ground state.

We note that when $s > 1$ (super-Ohmic bath) the overlapping ρ in Eq. (17) has always a finite solution. This is to say that the ground state of the SBM with super-Ohmic bath is always non-degenerate and there is no QPT.

IV. CONCLUSION

We propose an analytic ground state wavefunction for the unbiased spin-boson Hamiltonian, which is a superposition of the two degenerate state and is non-Gaussian for the bosonic bath modes. The infrared catastrophe in Ohmic and sub-Ohmic bosonic bath plays an important role in determining the degeneracy of the ground state and we show that the infrared divergence associated with the displacement of the nonadiabatic modes in bath may be removed from the proposed ground state for the coupling $\alpha < \alpha_c$. The QCP α_c is determined by the transition from non-degenerate to degenerate ground state. Our ground state energy is lower than previous authors' results. The calculation of α_c agrees well with previous numerical results.

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