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Sub-Ohmic spin-boson model with off-diagonal coupling: Ground state properties
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Sub-Ohmic spin-boson model with off-diagonal coupling: Ground state properties

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We have carried out analytical and numerical studies of the spin-boson model in the sub-ohmic regime with the influence of both the diagonal and the off-diagonal coupling accounted for, via the Davydov D1 variational ansatz. While a second-order phase transition is known to be exhibited by this model in the presence of diagonal coupling only, we demonstrate the emergence of a discontinuous first order phase transition upon incorporation of the off-diagonal coupling. A plot of the ground state energy versus magnetization highlights the discontinuous nature of the transition between the isotropic (zero magnetization) state and nematic (finite magnetization) phases. We have also calculated the entanglement entropy and a discontinuity found at a critical coupling strength further supports the discontinuous crossover in the spin-boson model in the presence of off-diagonal coupling. It is further revealed via a canonical transformation approach that for the special case of identical exponents for the spectral densities of the diagonal and the off-diagonal coupling, there exists a continuous crossover from a single localized phase to a doubly degenerate localized phase with differing magnetizations. © 2013 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4825205]

I. INTRODUCTION

As an archetype of open quantum systems popularized by Leggett,1 the spin-boson model (SBM) finds applications in condensed matter physics and chemistry in a wide variety of areas ranging from processes of electron transfer2 to dynamical aspects like damping which is accompanied by the transition from a delocalized state to a localized one.18 However, recent studies show that the nonequilibrium coherent dynamics can persist for ultrastrong coupling to a sub-Ohmic bath with s < 0.5.19,20

The SBM7 is similar to a one-exciton, two-site version of the Holstein molecular crystal model,21 which is among the most popular Hamiltonians for studying optical and transport properties of molecular and biological systems. In the Holstein Hamiltonian, the diagonal coupling is defined as a nontrivial dependence of the exciton site energies on the lattice coordinates, and the off-diagonal coupling, as a nontrivial dependence of the exciton transfer integral on the lattice coordinates.22 Off-diagonal interactions between
II. METHODOLOGY

The SBM Hamiltonian with simultaneous diagonal and off-diagonal coupling can be written as

\[ \hat{H} = \frac{\varepsilon}{2} \sigma_z - \frac{\Delta}{2} \sigma_x + \sum_l \omega_l b_l^\dagger b_l + \frac{\sigma_x}{2} \sum_i \lambda_i (b_i^\dagger + b_i) + \frac{\sigma_y}{2} \sum_i \phi_i (b_i^\dagger + b_i), \]  

where \( \hat{H} \) is set to unity, \( \sigma_i \) \((i = x, y, z)\) are the Pauli matrices of the TLS, \( b_l \) (\( b_l^\dagger \)) is the bosonic annihilation (creation) operator, \( \varepsilon \) is the bias to describe the influence of the external magnetic field, \( \Delta \) is the tunneling amplitude of the TLS, and \( \omega_l \) is the phonon frequency while \( \lambda_i \) and \( \phi_i \) are the corresponding diagonal and off-diagonal coupling strengths, respectively. The diagonal and off-diagonal coupling strengths can be determined by the corresponding bath spectral densities \( J_x(\omega) \) and \( J_y(\omega) \), respectively,

\[ J_x(\omega) = \sum_l \lambda_l^2 \delta(\omega - \omega_l) = 2\alpha \omega_l^{1-\delta} \omega^\delta \Theta(\omega_c - \omega), \]

\[ J_y(\omega) = \sum_l \phi_l^2 \delta(\omega - \omega_l) = 2\beta \omega_l^{1-\delta} \omega^\delta \Theta(\omega_c - \omega), \]

where \( \alpha \) and \( \beta \) are dimensionless coupling constants, \( \Theta(\omega_c - \omega) \) is the Heaviside step function, and \( \omega_c \) is the cut-off frequency which is set to be unity throughout this paper. The type of interactions between the TLS and the boson bath is characterized by the spectral exponents \( s \) and \( \bar{s} \) for diagonal and off-diagonal coupling, respectively. It should be noted that we use a common boson bath for both the diagonal and the off-diagonal coupling, but with different spectral densities. In the absence of off-diagonal coupling, the term \( s \omega^2 / 2 \) in the SBM describing the bias between the states \( |+\rangle \) and \(-\rangle \) forbids the continuous quantum phase transition. Introduction of the bias leads to the disruption of the symmetry of the SBM and accordingly, the ground state would tend to be spin-up or spin-down state. This implies the absence of a delocalized state, and that there may exist only a localized state which corresponds to nonzero magnetization. The off-diagonal coupling denotes the influence of the boson bath on the spin tunneling, and its introduction is believed to trigger competition with the bias. Therefore, it is anticipated that novel features may emerge in the ground state properties.

The Davydov D1 ansatz is often employed to describe the motion of an exciton accompanied by a phonon cloud on a finite one-dimensional lattice. Known to be numerically efficient, the hierarchy of Davydov wave functions including the Davydov D1 trial state has been widely used to study exciton-phonon dynamics in molecular and biological systems. Recently, Chin et al. have demonstrated that the Davydov D1 ansatz is capable to describe the ground state of the SBM in the sub-Ohmic regime. While quite accurate results in the sub-Ohmic regime \((s \leq 0.5)\) of the SBM with only diagonal coupling were obtained, results based on the same ansatz failed to reproduce the well known phase transition point \( \alpha_c = 1 \) in the Ohmic case. We thus focus only on the sub-Ohmic regime when considering both the diagonal and the off-diagonal coupling with \( s \) and \( \bar{s} \leq 0.5 \). It should further be noted that the original Davydov D1 ansatz has been projected onto momentum eigenstates to form Bloch states for the ground-state descriptions of the Holstein polaron.
Aimed at extending the application of the D1 ansatz to off-diagonal coupling and studying the ground state properties of the SBM, the trial wave function can be given as

\[ |D_s⟩ = A|+⟩ \exp \left[ \sum_l (f_l b_l^† - \text{H.c.}) \right] |0⟩_\text{ph}, \]

\[ + B|−⟩ \exp \left[ \sum_l (g_l b_l^† - \text{H.c.}) \right] |0⟩_\text{ph}, \]

where H.c. stands for Hermitian conjugate, |+⟩ (|−⟩) is the spin up (down) state, and |0⟩_\text{ph} is the vacuum state of the boson bath. A and B are real variational parameters representing occupation amplitudes in states |+⟩ and |−⟩, respectively, and \( f_l \) and \( g_l \) (\( l = 1, 2, 3, \ldots \)) label the corresponding phonon displacements with momentum \( ω_l \). Without loss of generality, \( A^2 + B^2 \), which is the norm of \( |D_s⟩ \), can be set to unity, and the system energy \( E = ⟨D_s|H|D_s⟩ \) can then be written as

\[ E = \frac{ε}{2} M + \frac{\sqrt{1 - M^2}}{2} \bar{λ} + \frac{1 + M}{2} \sum_l (f_l λ_l + f_l^2 ω_l) - \frac{1 - M}{2} \sum_l (g_l λ_l - g_l^2 ω_l), \]

(5)

where \( \bar{λ} = [Δ - \sum l φ_l(f_l + g_l)]\exp[-\sum_l(f_l - g_l)^2/2] \) is the renormalized tunneling amplitude that involves the modulations of the phonon bath, and \( M = ⟨D_s|σ_z|D_s⟩ = A^2 - B^2 \) is the magnetization parameter that will be used in this work to study the critical behavior of the SBM.

The ground state of the SBM can be obtained by minimizing the system energy of Eq. (5) with respect to the variational parameters \( M, f_l, \) and \( g_l \). Employing the minimization procedure with respect to phonon displacement \( f_l \) and \( g_l \), one obtains

\[ (1 + M) \left( ω_l f_l + \frac{λ_l}{2} \right) = \frac{\sqrt{1 - M^2}}{2} (\tilde{ϕ}_l - Δ(f_l - g_l)), \]

(6)

\[ (1 - M) \left( ω_l g_l - \frac{λ_l}{2} \right) = \frac{\sqrt{1 - M^2}}{2} (\tilde{ϕ}_l - Δ(g_l - f_l)), \]

(7)

where we have introduced an auxiliary function \( \tilde{ϕ}_l = ϕ_l \exp[-\sum_l(f_l - g_l)^2/2] \). Combining Eqs. (6) and (7), one arrives at

\[ f_l = -\frac{λ_l(M Δ + \sqrt{1 - M^2} ω_l)}{2ω_l(Δ + \sqrt{1 - M^2} ω_l)} - \frac{\tilde{ϕ}_l(\sqrt{1 - M^2} Δ + (1 - M)ω_l)}{2ω_l(Δ + \sqrt{1 - M^2} ω_l)}, \]

(8)

\[ g_l = -\frac{λ_l(M Δ - \sqrt{1 - M^2} ω_l)}{2ω_l(Δ + \sqrt{1 - M^2} ω_l)} - \frac{\tilde{ϕ}_l(\sqrt{1 - M^2} Δ + (1 + M)ω_l)}{2ω_l(Δ + \sqrt{1 - M^2} ω_l)}, \]

(9)

Similarly, energy minimization with respect to the magnetization \( M \) yields

\[ 0 = \frac{ε}{2} + \frac{Δ M^2}{2\sqrt{1 - M^2}} + \frac{1}{2} \sum_l (f_l^2 + f_l^4 ω_l) + \frac{1}{2} \sum_l (g_l^2 - g_l^4 ω_l). \]

(10)

Substituting Eqs. (8) and (9) into the system energy of Eq. (5) accompanied by the spectral densities from Eqs. (2) and (3), the system energy as a function of the magnetization, \( E(M) \), is obtained. Using the Taylor series expansion for \( E(M) \) about \( M = 0 \), we can write

\[ E = c_0 + c_1 M + c_2 M^2 + c_3 M^3 + c_4 M^4 + O(M^5), \]

(11)

where \( c_i \) are constant coefficients for fixed \( α, β, Δ \), and \( ω_c \). Chin et al. found that in the scaling limit \( ω_c \to ∞ \) for small \( M \), the energy expression takes the Landau form without considering the influence of the bias and the off-diagonal coupling. This implies \( c_1 = 0 \) and \( c_3 = 0 \), and thus, a second-order phase transition exists in the SBM with only the diagonal coupling. Further, the scaling property of the critical coupling \( α_c ∝ (Δ/ω_c)^{1−σ} \) is also in good agreement with other numerical approaches for the SBM.

To the best of our knowledge, the exploration of possible phase transitions in the SBM with the inclusion of off-diagonal coupling has not been systematically undertaken so far, and it thus forms the core of the current work. With the off-diagonal coupling incorporated in the SBM, the expressions of \( f_l \) and \( g_l \) acquire much more complex forms, presenting difficulties in obtaining analytical results at the phase transition point. The scaling limit in this case yields

\[ c_1 = \frac{ε}{2} - \frac{αβ}{2 \sin(π(s + δ)/2)} \left( \frac{Δ}{ω_c} \right)^{(s+δ)/2}, \]

(12)

which indicates the absence of a second-order phase transition in general, as \( c_1 \) and \( c_3 \) would be non-zero. However, by appropriately selecting \( ε, α, β, \) and \( Δ \), it is possible to set \( c_1 = 0 \), which may give rise to the possibility of a first-order phase transition as long as \( c_3 \neq 0 \). Even though obtaining an analytical expression for \( c_3 \) is indeed a difficult proposition, it is still possible to judge whether or not \( c_3 \) is equal to zero, by using results from numerical analysis, as will be elaborated in Sec. III.

The first requirement in our numerical calculation is to set \( c_1 = 0 \). Here we do not consider Eq. (12) in our numerical analysis as it is obtained in the scaling limit. An exact expression for \( c_1 \) can be written as

\[ c_1 = \left. \frac{dE}{dM} \right|_{M=0} = \left[ \frac{∂E}{∂M} + \sum_l \left( \frac{∂E}{∂f_l} \frac{∂f_l}{∂M} + \frac{∂E}{∂g_l} \frac{∂g_l}{∂M} \right) \right]_{M=0}. \]

(13)

Therefore, as long as Eqs. (6), (7), and (10) are satisfied in the condition that \( M = 0 \), \( c_1 \) would be zero and from it we can obtain a relation among the system parameters. Furthermore, the relaxation iteration technique was adopted to obtain numerical solutions to the set of the self-consistency equations.
[Eqs. (6), (7), and (10)] under the condition \( c_1 = 0 \). Once the variational parameters are obtained, we can get the ground state wave function, and other properties can be calculated subsequently.

III. RESULTS AND DISCUSSION

A. Diagonal coupling only

We first investigate the SBM with only the diagonal coupling considered. In this case, the existence of the second-order transition was demonstrated variationally by Chin et al., and an analytical expression for the phase transition point was also given.\(^{17}\) In this section, we present a detailed description of the magnetization and the ground state energy near the phase transition point for the purely diagonal coupling case by following the approach of Chin et al., for the sake of facilitating an easier distinction with the results upon inclusion of the off-diagonal coupling described in Sec. III B.

Figure 1(a) shows the magnetization corresponding to the extreme values of the system energy as a function of the strength of diagonal coupling \( \alpha \) with \( s = 0.2 \) and \( \Delta = 0.1 \) while ignoring the influence of the bias and off-diagonal coupling. There exists a critical coupling strength \( \alpha_c = 0.02998 \) which separates a non-degenerate delocalized phase \( (M = 0) \) from a doubly degenerate localized phase \( (M \neq 0) \) and leads to the bifurcation in the \( M(\alpha) \) plot. The solid line in Fig. 1(a) corresponds to the minima of the ground state energy, while the curve marked by solid triangles for \( \alpha > \alpha_c \) corresponds to its maxima. For \( \alpha < \alpha_c \), the system energy exhibits only one minimum at \( M = 0 \) and thus characterizes a delocalized state. This is evident in Fig. 1(b), which shows the detailed energy difference \( E(M) - E(M = 0) \) as a function of \( M \) for a representative value of \( \alpha = 0.0298 \). On the other hand, with \( \alpha > \alpha_c \), two minima begin to appear in the system energy plot, as can be observed for \( \alpha = 0.0302 \) in Fig. 1(b). The double-minimum indicates the transition of the system to a localized phase. In this case, \( M = 0 \) still corresponds to an extremum of the system energy, however not being a minimum, it does not correspond to the ground state.

Guided by the magnetization transition, it is straightforward to obtain the phase transition point. As shown in Fig. 2(a), the ground state magnetization will change from zero to nonzero at \( \alpha_c = 0.02998 \). Earlier studies have derived an expression for the dependence of the critical coupling strength on the bath spectral exponent as \( \alpha_c \propto (\Delta/\omega_c)^{1/\nu} \).\(^{9,12,13}\) To further characterize the quantum phase transition in terms of additional ground-state properties, we calculate the entanglement between the spin and the surrounding boson bath described by the von Neumann.

![Figure 1](image1.png)

**FIG. 1.** For \( s = 0.2, \Delta = 0.1, \) and \( \epsilon = 0 \) and without considering the off-diagonal coupling, (a) the magnetization \( M \) corresponding to the extreme values of the system energy as a function of the diagonal coupling strength \( \alpha \). The solid red curve corresponds to the minima (ground state) of the system energy, while the curve marked by solid triangles corresponds to energy maxima. (b) The system energy difference \( E(M) - E(M = 0) \) versus \( M \) for two values \( \alpha = 0.0298 \) (dashed, magenta) and 0.0302 (dotted, blue), which are also depicted by the two vertical arrows in (a) as a guide to eye.

![Figure 2](image2.png)

**FIG. 2.** (a) The positive component of the magnetization \( M \) (the negative part is symmetrically related) and (b) the entanglement entropy as a function of the diagonal coupling strength \( \alpha \) for \( s = 0.2, \Delta = 0.1, \) and \( \epsilon = 0 \) and without considering the off-diagonal coupling. The inset in each of the panels shows the corresponding plot over a larger range of \( \alpha \).
entropy (S), also known as the entanglement entropy, \( S = -\omega_+ \log_2 \omega_+ - \omega_- \log_2 \omega_- \), which is given for the spin-boson model as \( S = -\omega_+ \log_2 \omega_+ - \omega_- \log_2 \omega_- \), (14)

where

\[
\omega_\pm = (1 \pm \sqrt{(\sigma_x)^2 + (\sigma_y)^2 + (\sigma_z)^2})/2.
\] (15)

It should be noted that \( \langle \sigma_y \rangle = 0 \), as the spin-boson model is invariant under the transformation \( \sigma_y \rightarrow -\sigma_y \). The calculated entanglement entropy is plotted as a function of \( \alpha \) in Fig. 2(b). With an increase in \( \alpha \), \( S \) increases gradually until it reaches its maximum at the phase transition point and according to the formation of a cusp can be observed clearly in the inset of Fig. 2(b). We note that in the localized phase, the spin rapidly becomes frozen in one classical state while rapid disentanglement takes place.4, 17

B. Simultaneous diagonal and off-diagonal coupling

The inclusion of the off-diagonal coupling in the Holstein model is known to result in many interesting properties, which leads us to believe that similar implications will also be encountered upon its incorporation in the present work on the SBM. Furthermore, due to the similarity between the SBM and the Holstein model, we expect that our current approach of applying the Davydov D1 ansatz to the SBM can yield reliable results even upon the inclusion of the off-diagonal coupling.

As discussed earlier, in order to set \( c_1 = 0 \), a relation has to be established between the diagonal and the off-diagonal coupling strengths. Figure 3 depicts \( \alpha \) as a function of \( \beta \), which satisfies the required condition for different values of bias when \( s = \bar{s} = 0.2 \) and \( \Delta = 0.1 \). For a given \( \alpha \), the off-diagonal coupling strength \( \beta \) can be clearly observed to increase with an increase in the bias intensity. The role of applied bias in localization competes with that of the spin tunneling in delocalization. The modulation of the spin tunneling due to the off-diagonal coupling should thus increase with an increase in the bias. Furthermore, when \( \alpha \) tends to zero, \( \beta \) shows a tendency to diverge. This behavior emerges since the applied bias will be expected to destroy the possible transition if there is only off-diagonal coupling, as \( c_1 = 0 \) cannot be satisfied under such a condition [cf. Eq. (12)].

The coefficients \( c_i \) (1, 2, 3, and 4) in the Taylor series expansion of the system energy, plotted against the diagonal coupling strength \( \alpha \) for \( s = \bar{s} = 0.2, \epsilon = 0.01, \) and \( \Delta = 0.1 \), are shown in Fig. 4. The off-diagonal coupling strength \( \beta \) changes accordingly to guarantee that \( c_1 = 0 \) will always be satisfied. It is important to note here that \( c_1 \) is generally non-zero, which implies that the second-order phase transition does not exist under these conditions. A first-order phase transition may however still occur, when the condition of \( c_2 = 0 \) is satisfied at the critical coupling strength \( \alpha_c \).

The magnetization \( M \) corresponding to the extreme value of the system energy as a function of the diagonal coupling strength \( \alpha \) for \( s = \bar{s} = 0.2, \epsilon = 0.01, \) and \( \Delta = 0.1 \) is shown in Fig. 5(a). While both the solid curves correspond to the minima of the system energy, the red curve represents the ground state of SBM. The local maxima in the system energy are denoted by solid triangles. The differences in the magnetization behavior upon inclusion of the off-diagonal coupling as compared to that with only the diagonal coupling can be clearly observed. With the off-diagonal coupling considered, the symmetry about \( M = 0 \) is lost. For \( \epsilon = 0.01 \) and when \( \alpha \) is small, there exists a unique energy minimum at \( M = 0 \). However, when \( \alpha \) is large enough, two minima corresponding to different values of \( M \) appear. It should be noted that there are two branches, one of which corresponds to \( M > 0 \) showing a continuous change and the other corresponds to \( M < 0 \) showing a discontinuous change. Generally, the \( M < 0 \) branch corresponds to the lowest energy and thus to the ground state, which is likely due to the positive bias employed. The ground state of the SBM thus exhibits a discontinuous change in the magnetization from zero to nonzero values, at the critical point, which is found to be \( \alpha_c = 0.02967 \) for the set of parameters chosen here. In effect, we are witnessing the likely existence of a discontinuous first order transition between a zero-magnetization phase and a finite-magnetization

![Figure 3](image1)

FIG. 3. The inter-dependence of the diagonal coupling strength \( \alpha \) and the off-diagonal coupling strength \( \beta \) required in order to satisfy \( c_1 = 0 \). Behavior for different values of \( \epsilon = 0.01, 0.02, 0.03, 0.04, \) and 0.05 when \( s = \bar{s} = 0.2 \) and \( \Delta = 0.1 \) is shown. The arrow marks the direction of increasing \( \epsilon \).

![Figure 4](image2)

FIG. 4. The coefficients \( c_1 \) (squares, black), \( c_2 \) (circles, red), \( c_3 \) (up-triangles, green), and \( c_4 \) (down-triangles, blue) in the Taylor series expansion of the system energy, plotted against the diagonal coupling strength \( \alpha \) for \( s = \bar{s} = 0.2, \epsilon = 0.01, \) and \( \Delta = 0.1 \).
phase of the sub-Ohmic SBM in the presence of off-diagonal coupling. It should be noted, however, that for the special case of \( \bar{s} = \tilde{s} \), the SBM Hamiltonian can be subjected to a 90° rotation so that the transformed Hamiltonian assumes a form of the diagonal-coupling-only SBM with modified bias and tunneling amplitude. This leads to an ambiguity that compounds the difficulty of a purely variational approach in proving the existence of a first order phase transition in the SBM. This warrants a further careful analysis for adopting the notion of the Silbey-Harris ansatz, which itself is a special case of the Silbey-Harris method when applied to the biased SBM. Drawing attention to the limitations of the Silbey-Harris ansatz and the entanglement entropy may seem reminiscent of the tight-binding approach with a smaller value of diagonal coupling strength is needed to balance the off-diagonal coupling. Furthermore, the entanglement entropy can also be employed to characterize the discontinuous behavior. As shown in Fig. 6(b), the calculated entanglement entropy as a function of \( \alpha \) exhibits a discontinuity at the critical coupling point, \( \bar{s} \) which is to be presented in Sec. III C. The detailed energy difference \( E(M) - E(M = 0) \) as a function of \( \alpha \) including \( \alpha _c \). At a less than critical coupling strength, a new minimum appears at \( M = 0 \). With an increase in \( \alpha \), another minimum appears at \( M < 0 \) and gradually attains the lowest energy, signifying the ground state.

The ground state magnetization \( M \) as a function of the diagonal coupling strength for different \( \bar{s} \) is shown in Fig. 6(a) for \( s = 0.2, \Delta = 0.1, \) and \( \epsilon = 0.01 \). An abrupt jump in \( M \) at the critical coupling can be clearly noted. With an increase in \( \bar{s} \), the critical diagonal coupling strength decreases slightly. The dependence of the critical point on \( \bar{s} \) may be explained by considering the relaxation energy in the SBM given as \( \int _0 ^{\infty} \text{d} \omega , \mathcal{J}(\omega) / \omega = 2 \pi \alpha _w , \Gamma (s) \),43 where \( \Gamma (s) \) is the gamma function of \( s \) which decreases with an increase in \( s \) in the sub-Ohmic regime. If \( \bar{s} \) increases, the relaxation energy will decrease, implying that the influence of the off-diagonal coupling will also decrease. Accordingly, we may expect that a smaller value of diagonal coupling strength is needed to balance the off-diagonal coupling. Furthermore, the entanglement entropy can also be employed to characterize the discontinuous behavior. As shown in Fig. 6(b), the calculated entanglement entropy as a function of \( \alpha \) exhibits a discontinuity at the critical coupling. With an \( \alpha \) higher than the critical value, the SBM corresponds to the localized state for which rapid disentanglement, similar to that of the purely diagonal case, occurs. The discontinuous behavior of the magnetization and the entanglement entropy may seem reminiscent of similar discontinuous behavior in the results obtained with the Silbey-Harris method when applied to the biased SBM. Drawing attention to the limitations of the Silbey-Harris ansatz based variational approach, Nazir et al. proposed the discontinuous behavior to be regarded as artifacts arising from its excessive simplicity.37 The Davydov D1 ansatz employed in this work, on the other hand, is much more sophisticated and contains more flexible variational parameters as compared to the Silbey-Harris ansatz, which itself is a special case of the

![Graph](image-url)
Davydov D1 ansatz obtained by setting $A = B$ and $f_i = -g_i$ and is poorly equipped to deal with the asymmetry induced by the bias.

### C. Continuous crossover for $s = \bar{s}$

In this section, we carefully analyze the special case when the spectral densities for the diagonal and off-diagonal couplings are characterized by the same exponent. For this condition of $s = \bar{s}$, it is possible to transform the interaction to a purely diagonal form by employing a unitary matrix $\hat{P} \equiv \{(i, b) \}$, where $a = \sqrt{\frac{\gamma}{\varepsilon + \pi}}$ and $b = \sqrt{\frac{\gamma}{\varepsilon - \pi}}$. The transformed Hamiltonian can be rewritten as

$$
H_{\text{rot}} = \frac{\varepsilon}{2} \sigma_z + \frac{\bar{\Delta}}{2} \sigma_x + \sum_i \omega_i b_i^\dagger b_i + \frac{\sigma_z}{2} \sum_i g_i (b_i^\dagger + b_i).
$$

where

$$
\varepsilon = \sqrt{\gamma \varepsilon - \beta} \Delta, \\
\bar{\Delta} = \sqrt{\alpha \Delta + \sqrt{\beta} \varepsilon}.
$$

The interaction is characterized by the spectral density function $J(\omega)$,

$$
J(\omega) = \sum_i g_i^2 \delta(\omega - \omega_i) = 2(\alpha + \beta) \omega_i^{-1} \Theta(\omega_i - \omega).
$$

With this transformation, we have mapped the Hamiltonian (1) to that of the standard SBM with modified bias and tunneling amplitude via rotation. Therefore, the ground state of the Hamiltonian (1) is mapped to that of the regular SBM with modified control parameters, i.e., $|G(s, \alpha, \beta, \Delta, \varepsilon)\rangle = \hat{P}|G_{\text{SBM}}(s, \gamma, \Delta, \varepsilon)\rangle$, where $\gamma = \alpha + \beta$.

To obtain the ground state of this model, we adopt an analytical treatment previously developed, and subject $H_{\text{rot}}$ to a unitary transformation in order to take into account the correlation between the spin and bosons, yielding $H' = \exp(S)H_{\text{rot}}\exp(-S)$ with

$$
S = \sum_k \frac{g_k}{2\omega_k} (b_k^\dagger - b_k)[\xi_k \sigma_z + (1 - \xi_k)\sigma_0].
$$

Here, $\sigma_0$ is a constant, I is the identity matrix, and $\xi_k$ is a $k$-dependent function, the form of which can be found in Ref. 44. Following the transformation, one can write

$$
H' = H_0' + H_1' + H_2',
$$

$$
H_0' = \frac{\Delta_r}{2} \sigma_x + \frac{\varepsilon'}{2} \sigma_z + \sum_k \omega_k b_k^\dagger b_k
$$

$$
- \sum_k \frac{g_k^2}{4\omega_k}\xi_k(2 - \xi_k) + \sum_k \frac{g_k^2}{4\omega_k}\sigma_0^2(1 - \xi_k)^2,
$$

$$
H_1' = \frac{1}{2} \sum_k g_k (1 - \xi_k)(b_k^\dagger + b_k)(\sigma_z - \sigma_0) + i \frac{\Delta_r}{2} \sigma_y B,
$$

$$
H_2' = \frac{\Delta_x}{2} \sigma_y (\cosh(B) - \eta) + i \frac{\Delta}{2} \sigma_y (\sinh(B) - \eta) B,
$$

where $B = \sum_k \frac{\omega_k}{2} \xi_k(b_k^\dagger - b_k)$ and $\Delta_r = \eta \Delta$. The renormalized tunneling amplitude is determined as $\eta = \langle \cosh(B) \rangle$ (thermodynamically averaged with respect to the Bose-Einstein distribution), thereby yielding

$$
\eta = \exp \left[ - \sum_k \frac{g_k^2}{2\omega_k} \xi_k^2 \coth \left( \frac{\omega_k}{2T} \right) \right], \quad 0 \leq \eta \leq 1.
$$

Furthermore, the shifted bias is renormalized as

$$
\varepsilon' = \varepsilon - \tau \sigma_0, \quad \tau = \sum_k \frac{g_k^2}{\omega_k}(1 - \xi_k)^2.
$$

It becomes immediately clear that $H_0'$ can be solved exactly because the spin and the bosons in it are decoupled, and it is easy to obtain the ground state $|G\rangle$ with energy $E_g$. $H_0'$ is diagonalized by $U = u\sigma_z + v\sigma_x$, where $u = \sqrt{(1 - \varepsilon'/W)}$, $v = \sqrt{(1 + \varepsilon'/W)}$, and $W = \sqrt{\varepsilon'^2 + \Delta^2}$. After diagonalization, $H_0' \equiv U^\dagger H_0' U$ can be written as

$$
\tilde{H}_0 = \sum_k \omega_k b_k^\dagger b_k + \sum_k \frac{g_k^2}{4\omega_k} \left[ \sigma_0^2(1 - \xi_k)^2 - \xi_k(2 - \xi_k) \right] - \frac{W}{2} \sigma_z.
$$

Furthermore, as $\tilde{H}_1 + \tilde{H}_2 \equiv U^\dagger (H_1' + H_2') U$ is treated as a perturbation, the transformation parameters $\sigma_0$ and $\xi_k$ are chosen in order to minimize $\tilde{H}_1 + \tilde{H}_2$. Note that in the unitary transformation approach, $\tilde{H}_1|G\rangle = 0$. Thus, one can write $\tilde{H}_0 + \tilde{H}_1|G_{\text{SBM}}\rangle = E_g|G_{\text{SBM}}\rangle$, where

$$
E_g = \sum_k \frac{g_k^2}{4\omega_k} \left[ (1 - \xi_k)^2 + (1 - \sigma_0^2) - 1 \right] - \frac{W}{2}.
$$

The above ground state energy, $E_g$, agrees well with that obtained by the numerical renormalization group (NRG) method for both the cases of zero and finite bias.44 The original Hamiltonian is exactly solvable in two limits, viz., the weak coupling limit of $\alpha \to 0$ and $\beta \to 0$ with $E_g(\alpha \to 0, \beta \to 0) = -\frac{1}{2} \sqrt{\Delta^2 + \epsilon^2}$, and the zero tunneling limit of $\Delta \to 0$ with $E_g(\Delta \to 0) = -|\epsilon|/2 - \sum_k g_k^2/4\omega_k$. It is easy to check that $E_g$ yields the correct values of the ground state energy in these two limits.

It is well known that there occurs a continuous phase transition for the unbiased SBM with only the diagonal coupling. With the introduction of a finite bias ($\epsilon \neq 0$), and simultaneous diagonal and off-diagonal couplings, the Hamiltonian (1) has no $Z_2$ symmetry, and thus $\langle \sigma_z \rangle_G$ is generally nonzero. However, there still exists an instability in the ground state if the modified bias $\tilde{\epsilon}$ is zero. The calculated energy difference [$E(M) - E(M_0)$] as a function of $M$ ($M_0$ corresponds to energy extremum) is shown in Fig. 7 for three values of $\alpha$ when $\bar{s} = \bar{s} = 0.3$ and $\Delta = 0.1$. At $\alpha = 0.028$, the system energy exhibits only a single minimum at $M = M_0 = -0.086$, and the system is in a localized state. For $\alpha = 0.029$ and 0.03, it is obvious to see that the system energy exhibits double minima, indicating the instability of the ground state. Moreover, with an increase in the diagonal coupling strength that is accompanied by a decrease in the off-diagonal coupling strength, there appears a continuous crossover of the SBM from a non-degenerate localized phase to double degenerate localized phase. We note that the
necessary condition of the continuous crossover of the ground state is $\tilde{\epsilon} = 0$.

In the framework of the transformed SBM with only diagonal coupling, the combined coupling strength $\gamma$, the modified bias $\tilde{\epsilon}$ and the tunneling amplitude $\Delta$ all depend on the diagonal and off-diagonal coupling strengths of Hamiltonian (1). As the coupling strengths $\alpha$ and $\beta$ change, $\tilde{\epsilon}$, $\Delta$, and $\gamma$ adopt new values. In the parameter space satisfying the condition $c_1 = 0$, the modified bias $\tilde{\epsilon}$ is always nonzero, while it is known that only for the requirement $\tilde{\epsilon} = 0$, there emerges a continuous crossover of the ground state from single localized phase to a doubly degenerate localized phase. It follows that the aforementioned continuous crossover does not contradict the discontinuous behavior revealed in Sec. III B using the Davydov $D_1$ ansatz, because the condition of $\tilde{\epsilon} = 0$ employed here is inherently different from the requirement of $c_1 = 0$ (in the expansion for $E(M)$ around $M = 0$) in the latter case. From a physical perspective, as the effect of the off-diagonal coupling may run counter to that of the bias, it is possible for the system to stay in a delocalized phase with $M = 0$ for a certain off-diagonal coupling strength under a finite bias. As the condition of $c_1 = 0$ implies that there exists a finite $\tilde{\epsilon}$, i.e., $\tilde{\epsilon} \neq 0$, the energy surface $E(M)$ is asymmetric about $M = 0$ as shown in Fig. 5. For weak off-diagonal coupling, there is only one minimum at $M = M_0 = 0$ on the energy surface, and the system is in a delocalized phase. On the other hand, with $\alpha$ and $\beta$ inter-related as shown in Fig. 3, for a certain special parameter regime, the energy exhibits two asymmetrically localized minima because $\tilde{\epsilon} \neq 0$, with either a finite $M$ or zero $M$ (cf. Fig. 5). The minimum with a lower energy corresponds to the stable ground state. At the same time, the maximum occurs at nonzero $M$. This implies the possibility of a phase transition showing an abrupt crossover from a delocalized state with $M = 0$ to a localized state with $M \neq 0$ provided that the diagonal and off-diagonal coupling strengths satisfy the condition $c_1 = 0$. It is thus likely that a discontinuous phase transition occurs as a result of the combined effect of the bias and the two competing forms of the spin-boson coupling, marking a behavior that is entirely different from the continuous phase transition in the unbiased SBM devoid of the off-diagonal coupling. Our work thus reveals the rich energy landscapes and transition properties emerging from the competition between the diagonal and the off-diagonal coupling in the extended sub-Ohmic SBM.

IV. CONCLUSIONS AND DISCUSSION

Off-diagonal exciton-phonon coupling is an important issue often neglected by the polaron community. Early treatments of the off-diagonal coupling in the Holstein Hamiltonian include the Munn-Silbey theory,46,47 the Toyozawa ansatz,32 and Sumi’s theory employing the dynamic coherent potential approximation (DCPA).48 Furthermore, the DCPA based theory was generalized by Kato et al.49 while an explicit expression was subsequently derived by Hannewald et al. for the temperature dependence of the polaron bandwidths by treating diagonal and off-diagonal coupling on an equal footing.50 More recently, the Global-Local Ansatz,51 formulated by Zhao et al. in the early 1990s, has been compared with DCPA with the Hartree approximation,52 and the delocalized form of the Davydov $D_1$ ansatz has been used to study the ground-state properties of the Holstein Hamiltonian with off-diagonal coupling.53 The absence of phase transitions in the Holstein model when only diagonal coupling is well known.27 Recent studies, however, indicate that novel nonanalyticities may emerge in the simultaneous presence of the diagonal and the off-diagonal coupling. For example, a sharp transition at the critical electron-phonon coupling strength of the Su-Schrieffer-Heeger model was revealed by Marchand et al.28 By employing linearized von Neumann entropy to quantify exciton-phonon correlations in the ground state, Zhang et al. uncovered the discontinuities in the presence of off-diagonal coupling of the antisymmetric form as opposed to the smooth crossover resulting from the symmetric off-diagonal coupling.59 Owing to the similarity between the SBM and the Holstein model, trial states from the hierarchy of Davydov ansätze may yield reliable results on the ground state properties upon inclusion of the off-diagonal coupling.

In this work, we have systematically explored the possibility of a phase transition in the SBM in the sub-Ohmic regime, under the simultaneous influence of the diagonal and off-diagonal spin-boson coupling. As the Davydov $D_1$ ansatz was employed successfully in studying the Holstein polaron, an analogous approach was taken in this work to investigate the SBM by drawing parallels to its relevance to the SBM. It is demonstrated that a Taylor series expansion of the system energy reveals the possible occurrence of the phase transition as well as its nature, if it does occur. The existence of a continuous phase transition in the SBM with purely diagonal coupling has been shown earlier;17 however, it is known to vanish in the presence of a bias. Primarily focussing on the influence of the off-diagonal coupling, the current work reveals the presence of a discontinuous transition between the states characterized by zero and finite magnetization for the sub-Ohmic SBM. It is to be noted, however, that the control parameters $\alpha$, $\beta$, $\Delta$, and $\tilde{\epsilon}$ must satisfy a certain interrelation to guarantee that the first order derivative of the system energy with respect to the magnetization $M$ is always zero. This
In the framework of the unitary transformation approach, a SBM model with modified bias and tunneling amplitude. The approach corresponding to the extreme values of the system energy is found to be asymmetrical about zero magnetization. At the critical coupling strength, there exists a discontinuous change in the ground state have been uncovered. In addition to the discontinuous crossover from zero magnetization to a finite one, a continuous phase transition also exists in some parameter regime which satisfies zero modified bias (\( \ell = 0 \)). With simultaneously considered diagonal and off-diagonal coupling, this work is thus hoped to shed new light on the emergence of interesting properties in the sub-ohmic regime of the SBM.

We note that in the absence of bias and off-diagonal coupling, the Hamiltonian of Eq. (1) is invariant under the transformation of \( \sigma_z \rightarrow -\sigma_z, b_i \rightarrow -b_i \), and \( b_i^\dagger \rightarrow -b_i^\dagger \). In this case, there exist two degenerate ground states with differing magnetization characteristics, and their wave functions can then be used to form symmetric and anti-symmetric wave functions which are similar to the Bloch states that are commonly employed in the study of the Holstein model. Very recently, Bera et al. have proposed a trial state to describe the adiabatic response of the high frequency bosonic modes to the spin tunneling as well as non-classical correlations due to the low frequency modes. With the new ansatz, comparable results to those from the NRG method were obtained, and new behavior in spin coherence and environmental entanglement was unveiled. Our current approach could well be extended to incorporate the influence of an “anti-polaron” state via the symmetric and anti-symmetric wave functions. The approach of utilizing such superposed wave functions may be expected to not only allow for improved descriptions of ground state properties in SBM but also lead to revelation of novel properties.

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