Generalized Polaron Ansatz for the Ground State of the Sub-Ohmic Spin-Boson Model: An Analytic Theory of the Localization Transition

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The sub-Ohmic spin-boson model possesses a quantum phase transition at zero temperature between a localized and a delocalized phase, whose properties have so far only been extracted by numerical approaches. Here we present an extension of the Silbey-Harris variational polaron ansatz which allows us to develop an analytical theory which correctly describes a continuous transition with mean-field exponents for $0 < s < 0.5$. The critical properties, couplings, and observables we obtain show excellent agreement with existing numerical results, and we give an intuitive microscopic description of the changing correlations between the system and bath which suppress the spin coherence and drive the transition.

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The spin-boson model (SBM) is one of the key models for the study of decoherence, relaxation, and many other effects which arise when a quantum system is coupled to environmental degrees of freedom [1,2]. While nonequilibrium dynamics are often of most relevance for the many practical applications of the SBM [1–3], the model also possesses rich ground state properties, including a quantum phase transition that has recently become the subject of intense research. This transition separates a degenerate ''delocalized'' phase from a doubly degenerate ''localized'' phase in which the environment induces a spontaneous magnetization on the spin. This transition is predicted to appear when the spin's environment, modeled in the SBM as a bath of harmonic oscillators, is described by a spectral function $J(\omega) \propto \omega^s$ with $s \leq 1$. In the literature, such environments are referred to as Ohmic ($s = 1$) and sub-Ohmic ($s < 1$). The details of the Ohmic transition are well understood [1,2]; however, despite several sophisticated numerical studies, a microscopic description of the sub-Ohmic case has not yet appeared.

The quantum-classical mapping predicts that the sub-Ohmic SBM should be equivalent to a classical Ising spin chain with long-range interactions [4,5] and predicts a continuous magnetic transition with mean-field critical exponents for $0 < s < 0.5$. In Ref. [4], a continuous transition in the sub-Ohmic SBM was observed by using the numerical renormalization group (NRG) technique for all values of $0 < s < 1$, but the critical properties of the transition were found to be non-mean-field for $0 < s < 0.5$. It was suggested that this implied a breakdown of the classical to quantum mapping, and some subsequent work has supported this [6]. However, it is now believed that the non-mean-field results found by NRG in $0 < s < 0.5$ are incorrect and arise from the truncation of the number of states N_b used to describe each oscillator in the Wilson chain [7,8]. Recent numerical studies of the sub-Ohmic quantum phase transition using quantum Monte Carlo calculations [5], the sparse polynomial space approach [9], and an extended coherent state technique have indeed found mean-field critical exponents for $0 < s < 0.5$ [10].

In this Letter, we propose a variational ansatz for the ground state of the sub-Ohmic SBM for $0 < s < 0.5$ which allows an *analytical*, microscopic treatment of the transition. We show how distinctive types of system-bath correlations characterize each phase and how they suppress spin coherence. Understanding such system-bath correlations is a central issue in designing error correction schemes in quantum information processing and is also important in the emerging fields of measures of non-Markovianity and quantum metrology [11–13]. Our ansatz generalizes the widely used variational method of Silbey and Harris, which was successfully applied to the Ohmic transition [14] but was shown to fail approaching criticality for sub-Ohmic baths [15,16]. Our generalization fixes this problem and thus might allow similarly generalized Silbey-Harris and polaron master equations to accurately treat Ohmic and sub-Ohmic baths at strong coupling and finite bias and temperature [15,17,18], including the recently observed ultraslow dynamics found in Ref. [19]. Importantly, our method does not require any truncation of the environment, an essential feature, as we shall show that the number of environmental bosons *diverges* above the transition. Our results agree extremely well with existing numerical results, and give an intuitive microscopic description of the transition that pinpoints a numerical issue that arises in naive numerical density matrix renormalization group (DMRG) approaches to this problem, and possibly several other numerical methods.

The spin-boson Hamiltonian can be written ($\hbar = 1$) as

$$H = -\frac{1}{2}\Delta\sigma_x + \frac{1}{2}\sigma_z\sum_l g_l(a_l + a_l^\dagger) + \sum_l \omega_l a_l^\dagger a_l, \quad (1)$$

where σ_i are the usual Pauli operators, which describe a tunneling two-level system (TLS), and the "environmental bath" is modeled as a collection of oscillators, where a_l and $a_l^\dagger$ are the bosonic annihilation and creation operators, respectively, of bath modes with frequency ω_l. The tunneling amplitude of the TLS is Δ, and g_l are the couplings between the TLS and the bath modes. It is well established that all effects of the bath on the reduced state of the TLS are completed determined by the spectral function $J(\omega) = \pi\sum_l g_l^2 \delta(\omega - \omega_l)$ [1,2]. Following Bulla *et al.* we consider the spectral function $J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s\Theta(\omega_c - \omega)$ [20], where ω_c is the maximum frequency in the bath. Super-Ohmic baths have $s > 1$, Ohmic baths $s = 1$, and sub-Ohmic baths $s < 1$.

By representing the $+1$ and -1 eigenstates of σ_z as $|+\rangle$ and $|-\rangle$, respectively, our variational ansatz $|\Psi\rangle$ is

$$|\Psi\rangle = C_+|+\rangle \otimes |\phi_+\rangle + C_-|-\rangle \otimes |\phi_-\rangle, \tag{2}$$

where $|\phi_\pm\rangle = \exp[-\sum_l f_{l\pm}(a_l - a_l^\dagger)]|0\rangle$ and $|0\rangle$ is the vacuum of the bath modes. This ansatz describes a superposition of the localized states $|\pm\rangle$ which are correlated (dressed) with bath modes displaced by $f_{l\pm}$. It is a generalization of the variational wave function of Silbey and Harris [14], in which the constants and displacements were fixed to obey $C_+ = C_-$ and $f_{l+} = -f_{l-}$. As we shall show, these constraints are broken in the localized phase, and we shall henceforth refer to the ansatz of Eq. (2) as the asymmetrically displaced-oscillator (ADO) state. The order parameter of the localization (magnetic) transition is the magnetization $M = \langle\Psi|\sigma_z|\Psi\rangle$, which can be expressed as $M = C_+^2 - C_-^2$. By using this relation and the standard properties of displaced oscillators, the ground state energy $E(M) = \langle\Psi|H|\Psi\rangle$ is given by

$$E(M) = -\frac{1}{2}\tilde{\Delta}\sqrt{1 - M^2} + \frac{(1 + M)}{2}\sum_l (f_{l+}g_l + f_{l+}^2\omega_l) - \frac{(1 - M)}{2}\sum_l (f_{l-}g_l - f_{l-}^2\omega_l). \tag{3}$$

In Eq. (3), we have introduced a renormalized tunneling amplitude $\tilde{\Delta} = \Delta\exp[-\frac{1}{2}\sum_l (f_{l+} - f_{l-})^2]$, which is a polaronic effect arising from the imperfect overlap of the displaced-oscillator wave functions $|\phi_\pm\rangle$ which dress the TLS states $|\pm\rangle$. We now minimize the energy at constant M with respect to the displacements $f_{i,l}$ to obtain

$$f_{l\pm} = -\frac{g_l(M\tilde{\Delta} \pm \sqrt{1 - M^2}\omega_l)}{2\omega_l(\tilde{\Delta} + \sqrt{1 - M^2}\omega_l)}. \tag{4}$$

These displacements are then substituted back into Eq. (3), and the spectral function can be used to compute $E(M)$ exactly. For simplicity, we shall now develop the analytical theory in the so-called scaling limit $\omega_c \to \infty$, although our numerical results do not use this approximation. In this limit, the ground state energy to leading order in $\frac{\Delta}{\omega_c}$ takes the form

$$E(M) = -\tilde{\Delta}\sqrt{1 - M^2} - \frac{\alpha\omega_c}{2s} \tag{5}$$

$$+ \frac{\alpha\pi\omega_c(1 - s)(1 - M^2)}{2\sin(\pi s)}\left(\frac{\tilde{\Delta}}{\omega_c\sqrt{1 - M^2}}\right)^s, \tag{6}$$

and the renormalized tunneling amplitude obeys the implicit equation

$$\tilde{\Delta} = \Delta\exp\left[-\alpha\omega_c^{1-s}\int_0^{\omega_c}\frac{(1 - M^2)\omega^s d\omega}{(\tilde{\Delta} + \sqrt{1 - M^2}\omega)^2}\right]. \tag{7}$$

For sub-Ohmic baths, one of the self-consistent solutions of Eq. (7) is always $\tilde{\Delta} = 0$. This corresponds to the complete localization of the TLS ($M = \pm 1$) and is made self-consistent by the infrared divergence of the integrand in Eq. (7) for $s < 1$ and $\tilde{\Delta} = 0$ [1,2,14–16]. For sufficiently small α, there is also a finite solution for $\tilde{\Delta}$ [15,16], which can be expressed analytically in terms of the Lambert W function [21]. The ground state energy can now be expressed by using just the original system parameters and M. Taylor-expanding $E(M)$ about $M = 0$, we find that for small M the energy takes the Ginzburg-Landau form $E = c_0(\alpha) + c_1(\alpha)M^2 + c_2(\alpha)M^4 + O(M^6)$, where $c_i(\alpha)$ are constants for fixed α, ω_c, and Δ. This form for the ground state energy guarantees a second-order magnetic transition; above a critical coupling α_c, a magnetization grows continuously with $M \propto |\alpha - \alpha_c|^{1/2}$ and the magnetic susceptibility $\chi \propto |\alpha - \alpha_c|^{-1}$ [22]. The critical coupling α_c is the coupling for which $c_1(\alpha_c) = 0$. In the scaling limit, this equation can be solved analytically to find

$$\alpha_c = \frac{\sin(\pi s)e^{-s/2}}{2\pi(1 - s)}\left(\frac{\Delta}{\omega_c}\right)^{1-s}. \tag{8}$$

The values predicted from Eq. (8) agree well with those obtained by the recent quantum Monte Carlo, NRG, and sparse polynomial space approach studies and reproduces the scaling $\alpha_c \propto (\Delta/\omega_c)^{1-s}$ previously observed in other approaches [4,5,9,15,16,20].

Observables.—We show in Fig. 1 that the magnetization does indeed behave like $M \propto (\alpha - \alpha_c)^{1/2}$ close to the transition. The magnetization data are again in good agreement with the quantum Monte Carlo and sparse polynomial space approach results [5,9]. Figure 2 shows the behavior of the coherence $\langle\sigma_x\rangle$ as a function of α. We find that σ_x is always continuous at the transition, but $\frac{\partial\langle\sigma_x\rangle}{\partial\alpha}|_{\alpha_c}$ is discontinuous. In the scaling limit, the variational theory predicts $\langle\sigma_x\rangle = e^{-(s/2(1-s))}$ at the critical point and is thus independent of Δ/ω_c. Above the transition, $\langle\sigma_x\rangle$ decays faster but persists well into the localized

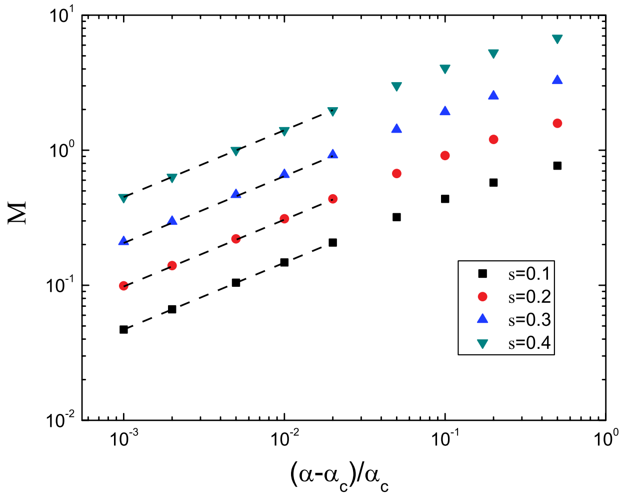

FIG. 1 (color online). Magnetization M as a function of $(\alpha - \alpha_c)/\alpha_c$ for $\alpha > \alpha_c$, $\Delta = 1$, and $\omega_c = 10$. For visibility, the curves have been multiplied by 1, 2, 4, and 8 for $s = 0.1, 0.2, 0.3$, and 0.4, respectively.

phase. The persistence and the *increasing* value of $\langle\sigma_x\rangle$ around the transition as s decreases appears to be generally consistent with the dynamical NRG study of Anders, Bulla, and Vojta [23], where it was found that a coherent tunneling survives well into the localized phase for $0 < s < 0.5$ and becomes *more* robust as $s \to 0$. Note that the position of the cusps for $s = 0.4, 0.5$ appear shifted from the values predicted by Eq. (8) due to nonscaling limit corrections. These corrections scale like $(\Delta/\omega_c)^{1-s}$, and for the parameters used here they can perturb the analytical results for larger s.

Delocalized phase.—In the delocalized phase, the physics of the ADO state is determined only by the renormalization of $\tilde{\Delta}$ as we have $M = 0$ and $f_{l+} = -f_{l-}$. The variational solution separates the bath into adiabatic modes (A modes) and nonadiabatic modes (NA modes) which have different responses to the renormalized TLS tunneling. High frequency A modes ($\omega_l \gg \tilde{\Delta}$) can adiabatically adjust their displacements to maximize their interaction energy with the TLS ($f_{l\pm} \approx \pm g_l \omega_l^{-1}$) [1,2,15], while slow NA modes ($\omega_l \ll \tilde{\Delta}$) cannot respond fast enough to follow the tunneling, and their displacement is suppressed at low frequency ($f_{l\pm} \approx \pm g_l \tilde{\Delta}^{-1}$) [15,16]. From Eq. (7), one can see that this suppressed displacement of NA modes permits a finite solution for $\tilde{\Delta}$ by preventing the infrared divergence of the integrand in Eq. (7) [15,16]. Looking at Eq. (2), one sees that although the frequency dependence of the NA- and A-mode displacements are different, all modes are correlated with the TLS state, and the ground state is not separable into TLS and bath states. Inseparability of the ground state into TLS and bath states indicates the existence of quantum correlations, or entanglement $\mathcal{E}$, between the TLS and bath, which can be quantified by computing the von Neumann entropy of the reduced density matrix of the TLS [11]. This is given by $\mathcal{E} = -p_+ \log(p_+) - p_- \log(p_-)$, where $p_\pm = \frac{1}{2}(1 + \sqrt{\langle\sigma_x\rangle^2 + \langle\sigma_z\rangle^2})$. As shown in Fig. 3, entanglement between the TLS and bath increases monotonically with α due to the monotonic suppression of $\tilde{\Delta}$ in this phase by dressing correlations [24].

Localized phase.—Above the transition ($M \neq 0$), we find that a new energy scale appears in the problem. Modes with $\omega_l \gg M\tilde{\Delta}(1 - M^2)^{-1/2}$ continue to be adiabatic, while nonadiabatic modes with $\omega_l \ll M\tilde{\Delta}(1 - M^2)^{-1/2}$ now have displacements which have the *same* sign and *grow* at low

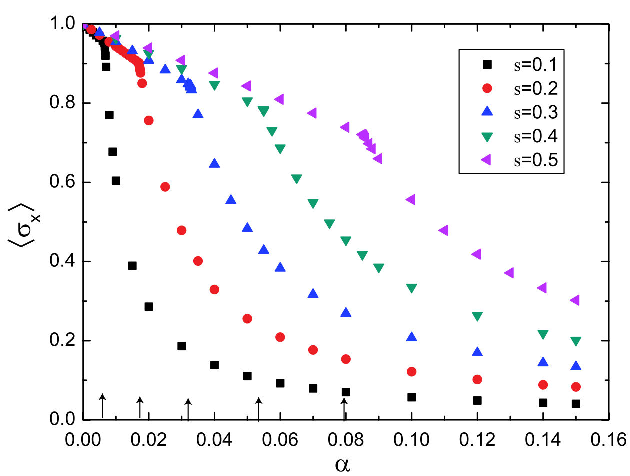

FIG. 2 (color online). Expectation value $\langle\sigma_x\rangle$ as a function of α for $\Delta = 1$ and $\omega_c = 10$. Cusps appear at the critical couplings α_c. The corresponding scaling limit critical couplings are indicated by arrows.

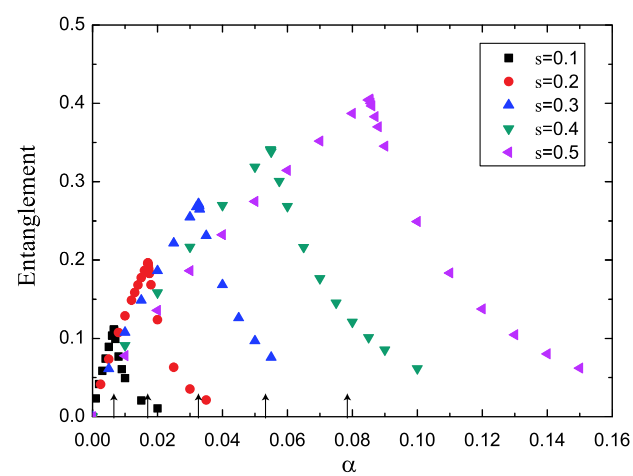

FIG. 3 (color online). Entanglement between the spin and bosonic environment as a function of α for $\Delta = 1$ and $\omega_c = 10$. The entanglement is defined here as the von Neumann entropy of the reduced density matrix of the TLS. Maxima occur at α_c, and the predicted scaling limit critical couplings are indicated by arrows.

frequency, $f_{l+} \simeq f_{l-} \simeq -Mg_l\omega_l^{-1}$. Because the nonadiabatic mode displacements have the same sign, they are not correlated with the state of the TLS, and the state of the system becomes a product state of NA modes and the correlated TLS–A-mode wave function. The NA-mode wave function has a finite displacement, and this appears to the TLS as an effective "mean-field-like" magnetic field in the z direction. While the total average displacement of NA modes is finite, there is an infrared divergence of the occupation number of these modes, as $\sum_l \langle a_l^\dagger a_l \rangle_{\rm NA} \propto M^2 \int_0^{\tilde{\Delta}} d\omega\omega^{s-2}$. However, the uncorrelated NA modes do not renormalize $\tilde{\Delta}$, and the coherence of the ground state remains *finite* at the transition, allowing M to grow continuously above the transition.

As the magnetization increases, the NA-mode character of the bath also increases, causing a monotonic decrease of entanglement above the transition. This allows us to intuitively understand the cusp in the entanglement shown in Fig. 3, which was numerically observed in Ref. [24]. The changing correlations also change the mechanism by which the TLS coherence is suppressed. In the localized phase, the growing NA-mode bias causes the effective magnetic field seen by the TLS to point away from the x axis, and, as the suppression of $\tilde{\Delta}$ due to dressing vanishes ($|M| \rightarrow 1$) in this phase, $\langle \sigma_x \rangle$ is determined solely by the rotation of the ground state to lie along the effective NA-mode magnetic field.

DMRG ground state.—The observation of an infrared divergence raises the question of whether simulations of the ground state using a truncated Fock space for the environment can converge above the transition. To explore this, we simulated the ground state by using imaginary-time TDMRG in conjunction with an exact mapping of the environment onto a 1D harmonic chain, as recently used by Prior *et al.* to look at real-time dynamics of open quantum systems with TDMRG [3,25,26]. Figure 4 shows results for the fidelity (overlap) between the ADO ansatz and the DMRG ground state. In the delocalized phase the TDMRG results converge very rapidly, and only the first few sites of the harmonic chain are appreciably excited. The fidelity with the ADO state is extremely high considering the many-body nature of the system.

Transforming the ADO ansatz into the chain representation, we find that the average occupation of site n in the chain $N_{\rm av}(n)$ decreases rapidly in the delocalized phase, and an accurate simulation of the ground state with a truncated Fock space, as confirmed by the DMRG results, is possible. However, as α approaches α_c, the decay of $N_{\rm av}(n)$ along the chain becomes much weaker, and contributions from many sites need to be included. Although $N_{\rm av}(n)$ is bounded along the chain, the convergence with respect to chain length in the DMRG simulations becomes much slower, and for a finite chain length we observe a reduced fidelity as $\alpha \rightarrow \alpha_c^-$. Above α_c, the fidelity suddenly becomes very small with increasing chain length.

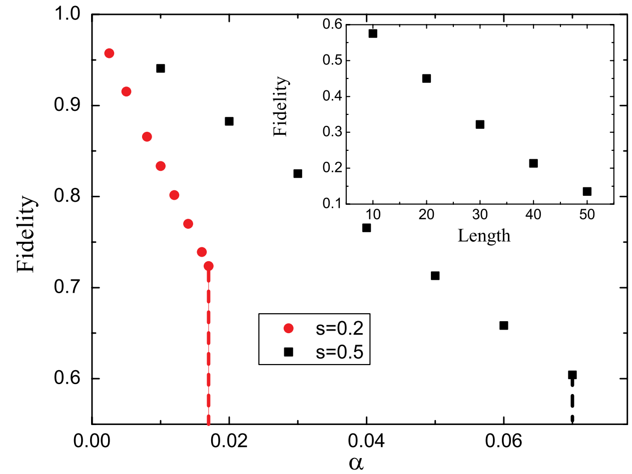

FIG. 4 (color online). Fidelity of the variational ansatz with the ground state determined by DMRG as a function of α for $\Delta = 1$ and $\omega_c = 10$. The DMRG simulation used 100 sites; $N_b = 15$ and 10 Schmidt coefficients were retained. At the critical coupling, the fidelity drops suddenly from finite values to zero. The inset shows the typically dramatic decrease in the fidelity with system size above the transition. Inset data correspond to $s = 0.3$ and $\alpha = 0.0328$ ($\alpha_c = 0.0316$).

This occurs because $N_{\rm av}(n)$ actually *diverges* along the chain in the magnetic phase, with our mapping predicting that $N_{\rm av}(n) \propto n^{1-2s}$ as $n \rightarrow \infty$ for finite M. The DMRG approach uses a finite N_b to represent each oscillator of the chain and cannot describe these diverging populations. Consequently, the norm of the projection of the ADO ansatz onto the truncated Fock space vanishes exponentially with increasing chain size, leading to the behavior shown in the inset in Fig. 4. The impossibility of finding a truncated representation of the ground state in the Fock basis also manifests itself through slow convergence of the DMRG algorithm for $\alpha > \alpha_c$.

DMRG in the Fock state basis of the harmonic chain appears to be unable to describe the localized phase for $s < 1/2$. However, the divergence of $N_{\rm av}(n)$ is a result of divergence of the NA-mode populations and could be cured by a unitary transformation $H \rightarrow UHU^{-1}$, where $U = \exp[-\sum_l (f_{l+}|+\rangle\langle+| + f_{l-}|-\rangle\langle-|)(a_l - a_l^\dagger)]$. This generalized polaron transformation effectively absorbs the mean-field displacement and dressing correlations in a new displaced-oscillator basis, thus removing the boson divergence and also greatly reducing the number of fluctuations of A modes that then need to be captured by the simulation method. This analysis confirms the idea originally proposed by Alvermann and Fehske that a unitary transform can greatly speed up convergence of simulations using truncated Hilbert spaces [9]; however, our microscopically derived transformation is quite different from that of Alvermann and Fehske, as it not only removes many of the quantum fluctuations, it also provides an accurate starting point for a more advanced method of determining the optimal basis of the simulation. Finally, we point out that the unitary transform U is the formal basis for defining an effective zeroth-order Hamiltonian which could be used in a polaron master equation approach to nonperturbative dynamics of multicomponent systems [17,18], extending these methods to the full parameter regimes of Ohmic and sub-Ohmic environments [15,16].

By generalizing the Silbey-Harris theory, we have given a detailed analytical description of the competing system-bath correlations which drive the quantum phase transition in the sub-Ohmic SBM and have extracted the correct mean-field critical exponents for $0 < s < 0.5$. All predicted observables were in good agreement with those found by sophisticated numerical approaches, the behavior of the coherences was given for the first time, and the effective Hamiltonian theory suggested by this ansatz should allow more efficient DMRG studies of this system and the extension of polaron theory to sub-Ohmic dynamics.

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