Coherent-incoherent transition in the sub-Ohmic spin-boson model

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We study the spin-boson model with a sub-Ohmic bath using a variational method. The transition from coherent dynamics to incoherent tunneling is found to be abrupt as a function of the coupling strength α and to exist for any power $0<s<1$, where the bath coupling is described by $J(\omega)\sim\alpha\omega^s$. We find nonmonotonic temperature dependence of the two-level gap $\tilde{K}$ and a reentrance regime close to the transition due to nonadiabatic low-frequency bath modes. Differences between thermodynamic and dynamic conditions for the transition as well as the limitations of the simplified bath description are discussed.

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I. INTRODUCTION

The spin-boson model[1] is a paradigm model for the study of dissipation and decoherence in quantum mechanics, and as such it is has been applied in a wide range of systems. Such applications include the search for macroscopic quantum coherence,[2] electron transfer in chemical and biological physics,[3,4] and most recently, the problem of dephasing and relaxation in solid state qubits.[5]

The particular case of the sub-Ohmic spin-boson model has had an interesting development in the last few years. Compared to the Ohmic bath, the sub-Ohmic bath is characterized by an increased density of states for the low-frequency bath modes. This makes analysis of the dynamics difficult as the low-frequency modes generally lead to non-Markovian dynamics and strong memory effects, even for relatively weak coupling. One of the physical situations corresponding to the sub-Ohmic bath is the $1/f$ noise in Josephson qubits.[5,6] Although there are certain limitations and assumptions in describing $1/f$ noise by an equilibrium sub-Ohmic bath,[7] the study of the sub-Ohmic spin-boson model may be useful in this and other contexts.

In the earliest treatments of the sub-Ohmic model,[1] it was argued that the sub-Ohmic bath always destroys the coherence of superposition states and localizes the system in one state for any nonzero coupling. This conclusion was based on the non-interacting-blip approximation,[1,8] which fails in the weak-coupling limit to the bath. More recently, several works addressed the problem of the sub-Ohmic spin-boson model and found that coherent phases can exist for sufficiently weak coupling.[5,9,10]

In the light of these developments, we contribute to this discussion of the coherent dynamics of the sub-Ohmic model by demonstrating the existence of the coherent regime for arbitrary $s<1$ using a simple and intuitive variational method. This variational method was originally developed by Silbey and Harris for the problem of Ohmic damping.[11] We will show that such a treatment allows us to define precise criteria for the thermodynamic existence of a coherent phase, and also provides a means to quantitatively map out the parameter space of the sub-Ohmic coherent regime. Within the coherent regime, we also give results for the renormalization of the parameters that describe the coherent dynamics. A reentrance regime close to the coherent-incoherent transition is found. In addition, strong coupling to nonadiabatic modes is considered, showing the limitations of Silbey-Harris variational ansatz.

In Sec. I A we briefly give an outline of the spin-boson model and in Sec. II we describe the variational method and explain the simple physical picture behind the variational ansatz. Throughout this paper we are primarily concerned with finding the conditions under which coherent oscillations of the two-level system are possible, and in Secs. III and IV we give some quantitative results for the critical couplings and the renormalized parameters of the dissipative tunneling at zero and finite temperature. In Secs. V and VI, we highlight some of the conditions under which the variational method can fail, and compare the variational results to those obtained from studying the dynamics of the sub-Ohmic model. In Sec. VII we discuss our results and compare the findings with results obtained by other authors. We end with a brief conclusion and summary.

A. The spin-boson model

The spin-boson model consists of a single two-level system (TLS) coupled linearly to an infinite bath of harmonic oscillators. The TLS can be thought of as spanning the two lowest levels of a double-well potential, or in other contexts, the TLS may appear in the situation where the transition matrix element between two given energy levels is much larger than the transition matrix elements to all other energy levels of the system. The two levels are coupled by a tunneling matrix element K, and taking these levels to be eigenstates of $\hat{\sigma}_z$, the spin-boson Hamiltonian is given by

$$\hat{H}=K\hat{\sigma}_x+\epsilon\hat{\sigma}_z+\sum_l \omega_l(\hat{a}_l^\dagger\hat{a}_l+1/2)+\hat{\sigma}_z\sum_l g_l(\hat{a}_l^\dagger+\hat{a}_l). \tag{1}$$

ϵ is the bias energy between the minima of the wells, and for the rest of this paper we set $\epsilon=0$. $\hat{a}_l$ and $\hat{a}_l^\dagger$ are the bosonic annihilation and creation operations for the bath modes. The last term in Eq. (1), the linear coupling of $\hat{\sigma}_z$ to the coordinate displacement of the bath oscillators, is assumed.

In the absence of coupling, the eigenstates of the TLS are coherent superpositions of the left and right states, and the particle can oscillate between the wells at a frequency of $2K$. The coupling between the TLS and the oscillators generally leads to damping of this motion, or may even suppress tunneling entirely. For an in-depth discussion of the rich dynamics of spin-boson models, the reader is referred to the original review of Leggett *et al.*,[1] or the more recent collection of papers on this subject.[12] The observed dynamical behavior is determined by the spectral function of the bath, $J(\omega)$,

$$J(\omega) = \pi \sum_l g_l^2 \delta(\omega - \omega_l). \tag{2}$$

For frequencies below a high-energy cutoff ω_c, the spectral function can be modeled by the power law form,

$$J(\omega) = \frac{1}{2}\pi\alpha\omega_s^{1-s}\omega^s, \tag{3}$$

where α is a dimensionless parameter that measures the effective strength of the system-bath coupling and ω_s is an energy scale included to keep α dimensionless. In this paper we assume that the cutoff frequency ω_c is much greater than all other scales in the problem, but the scale ω_s can be large or small compared to the other scales, e.g., K or the thermal energy scale $k_b T$.

The case of a bath with $s=1$ is known as the Ohmic bath, and the dynamics and thermodynamics of this model have been studied extensively in the literature.[1,8] Baths described by $s>1$ are termed super-Ohmic and we will not discuss them further. Here we shall focus on the sub-Ohmic spin-boson model where the bath is characterized by $0<s<1$.

II. THE VARIATIONAL METHOD

In this section, we motivate the variational approach to this problem and outline the method.[11] Discussion of the regimes in which the method fails is deferred until Sec. VI.

In the absence of the tunneling term, the spin-boson Hamiltonian Eq. (1) reduces to an independent-boson model,[13] and the solutions of Eq. (1) correspond to the particle localized in one of the wells. The oscillator part of the Hamiltonian is then just a collection of displaced oscillators and can be diagonalized by a simple translation of the oscillators proportional $g_l\langle\hat{\sigma}_z\rangle$.

If the tunneling is switched back on, we propose that the approximate eigenstates of the system correspond to a dressed particle tunneling between the two levels carrying a dynamical cloud of such oscillator displacements. Our variational ansatz is therefore in the spirit of an adiabatic approximation,[1] but with a special treatment of the low frequency, nonadiabatic modes as we discuss in Sec. VII.

To describe this physical picture, we reproduce the method originally used by Silbey and Harris[11] for the Ohmic bath. We begin by performing a unitary transformation of the spin-boson Hamiltonian Eq. (1),

$$\tilde{\hat{H}} = \hat{U}\hat{H}\hat{U}^{-1}. \tag{4}$$

The unitary operator U is given by,

$$\hat{U} = \exp\left(-\hat{\sigma}_z \sum_l \omega_l^{-1} f_l (\hat{a}_l - \hat{a}_l^\dagger)\right). \tag{5}$$

The arbitrary coupling parameters $\{f_l\}$ introduced in Eq. (5) are proportional to the effective displacement or dressing of each bath mode due to the coupling to the TLS. If $f_l = g_l$ then the transformation diagonalizes the last three terms of Eq. (1), but as we demonstrate in Sec. VII, setting $f_l = g_l$ is often a suboptimal choice for $\{f_l\}$.

As we mentioned in the Introduction, we are primarily interested in establishing whether or not coherent oscillations can exist in the sub-Ohmic model and to answer this question, we introduce the quantity $\tilde{K}$ which is given by

$$\tilde{K} = K\left\langle \exp\left(-2\sum_l f_l \omega_l^{-1}(\hat{a}_l - \hat{a}_l^\dagger)\right)\right\rangle_{bath}, \tag{6}$$

where the angular brackets denote the thermal expectation value taken over the bath modes.

We interpret $\tilde{K}$ as the effective coherent tunneling matrix element of the dressed particle. The exponential factor in Eq. (6) suppresses the bare tunneling, and arises due to the partial overlap of the oscillators that dress the TLS as it tunnels between the wells. Adding and subtracting $\tilde{K}$ to Eq. (4), we rewrite the Hamiltonian as

$$\tilde{\hat{H}} = \hat{H}_0 + \hat{V}, \tag{7}$$

where the separation is into a main coherent part H_0,

$$\hat{H}_0 = \tilde{K}\hat{\sigma}_x + \sum_l \omega_l(\hat{a}_l^\dagger \hat{a}_l + 1/2) + \sum_l (f_l^2 - 2 f_l g_l), \tag{8}$$

and a series of perturbation terms $\hat{V}$, which contain the remaining weak coupling between the TLS and the bath,

$$\hat{V} = \hat{V}_+\hat{\sigma}_+ + \hat{V}_-\hat{\sigma}_- + \hat{V}_0\hat{\sigma}_z, \tag{9}$$

$$\hat{V}_0 = \sum_l (g_l - f_l)(\hat{a}_l + \hat{a}_l^\dagger) \tag{10}$$

$$\hat{V}_+ = \hat{V}_-^* = K\exp\left(-2\sum_l f_l\omega_l^{-1}(\hat{a}_l - \hat{a}_l^\dagger)\right) - \tilde{K}. \tag{11}$$

The introduction of $\tilde{K}$ and the separation of the Hamiltonian into a coherent part and perturbations is reminiscent of a mean-field-type theory, and our treatment is essentially in this spirit. Considering the main part of the Hamiltonian, Eq. (8), we see that if $\tilde{K}$ is finite, the eigenstates are coherent superpositions of the two levels and the TLS can undergo coherent oscillations between its levels. If $\tilde{K}$ vanishes, the degenerate levels become uncoupled and no coherent oscillations are possible. Therefore, at the mean-field level, we can use the existence of a finite effective tunneling matrix element as the signature for the existence of a thermodynamic coherent phase in the TLS. The point where $\tilde{K}$ vanishes as a function of the system parameters marks the transition to the incoherent phase.

However, this thermodynamic criterion for distinguishing between coherent and incoherent dynamics is only approximate, as we have not yet included the effects of the perturbation terms on the TLS dynamics. The effect of the perturbations and the general limitations of using $\tilde{K}$ as the criteria for the transition from coherence to incoherence will be discussed in Sec. V.

To calculate $\tilde{K}$, we must first determine the $\{f_l\}$. Following Silbey and Harris,[11] we compute the Bogoliubov-Feynman upper bound on the free energy of the system, A_B.[14] Bogoliubov's theorem states that the true free energy A of the Hamiltonian Eq. (7) is related to A_B by[15]

$$A \leqslant A_B,$$

$$A_B = -\beta^{-1}\ln \mathrm{Tr}\exp(-\beta\hat{H}_0) + \langle\hat{V}\rangle_{H_0} + O(\langle\hat{V}^2\rangle_{H_0}). \quad (12)$$

The angular brackets denote the thermal expectation value calculated with respect to H_0, and due to our choice of H_0, we have constructed the perturbations so that $\langle V_i\rangle_{H_0}=0$. In Sec. VI we explicitly calculate the second-order terms and find that they give a small contribution to A_B as $\omega_c\to\infty$. Therefore, dropping all higher-order terms, A_B is given by

$$A_B = -K_BT\ln[2\cosh(\tilde{K}\beta)] + \sum_l \omega_l^{-1}(f_l^2 - 2f_lg_l), \quad (13)$$

where we have left out the free energy of the bath which does not depend on $\{f_l\}$. A_B can then be minimized by varying the $\{f_l\}$ to find

$$f_l = g_l[1 + 2\tilde{K}\omega_l^{-1}\coth(\omega_l\beta/2)\tanh\beta\tilde{K}]^{-1}. \quad (14)$$

Notice already at this stage the limiting behavior of coefficients $\{f_l\}$:

$$f_l \approx \begin{cases} g_l & \text{if } \omega_l\beta \gg 1 \text{ and } \tilde{K}\beta \ll 1, \\ g_l\dfrac{\omega_l}{2\tilde{K}} & \text{if } \omega_l\beta \gg 1 \text{ and } \omega_l \ll \tilde{K}. \end{cases} \quad (15)$$

The coefficients of effective coupling $\{f_l\}$ vanish in the limit $\omega_l\to 0$ and finite $\tilde{K}$.

We now substitute this form for $\{f_l\}$ back into Eq. (6) and use the spectral function Eq. (3) to turn the sum over modes in Eq. (6) into an integral. We then obtain our key equation, the self-consistent equation for $\tilde{K}$,

$$\tilde{K} = K\exp(-2F[\tilde{K}]), \quad (16)$$

$$F[\tilde{K}] = \frac{1}{\pi}\int_0^{\omega_c}\frac{J(\omega)\coth(\omega\beta/2)d\omega}{[\omega + 2\tilde{K}\tanh(\beta\tilde{K})\coth(\omega\beta/2)]^2}. \quad (17)$$

III. RESULTS AT $T=0$

The appearance of $\tilde{K}$ on both sides of Eq. (16) means that we must solve self-consistently for $\tilde{K}$. At $T=0$, we can perform the integral in Eq. (16) exactly. The results below were calculated by extending the upper limit in Eq. (17) to infinity, an approximation that be easily dropped but which is valid for $s<1$. Calculating the integral and substituting into Eq. (16), we obtain

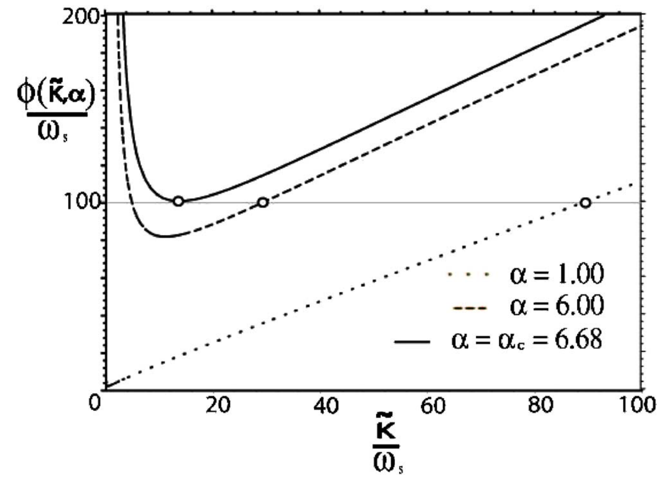

FIG. 1. (Color online) Solutions of the self-consistent equation for $s=1/2$ and $K/\omega_s=100$. Solutions exist where $\phi(\tilde{K})$ intersects the line $\tilde{K}=K$. As the coupling α is increased, the curve shifts until there is no intersection. The coupling where this occurs defines the critical coupling α_c.

$$\tilde{K}\exp\left(\frac{\alpha\omega_s^{1-s}\pi s}{(2\tilde{K})^{1-s}\sin(\pi s)}\right) = K. \quad (18)$$

The self-consistent values of $\tilde{K}$ can then be obtained by numerically solving Eq. (18) for general values of α. Note that $\tilde{K}=0$ is always a solution of Eq. (18).

Using Eq. (18), it is possible to determine the critical coupling strength α_c for fixed K. α_c is the coupling strength above which the only possible solution of Eq. (18) is $\tilde{K}=0$.

To see the existence of this critical coupling, we define the left-hand side of Eq. (18) as $\phi(\alpha,\tilde{K})$. This function has the typical form shown in Fig. 1, and crucially, has only one minimum for any sub-Ohmic bath. Finite solutions for $\tilde{K}$ exist when the $\phi(\alpha,\tilde{K})$ intersects with the line $\tilde{K}=K$, and the point of intersection is controlled by the coupling strength α as shown in Fig. 1. The critical coupling strength can then be clearly identified as the coupling strength where the minimum of $\phi(\alpha,\tilde{K})$ just touches the line $\tilde{K}=K$ as shown in Fig. 1. When $\alpha>\alpha_c$ there is no longer any intersection with the line $\tilde{K}=K$ and the only self-consistent value of the renormalized tunneling matrix element is $\tilde{K}=0$.

The position and value of the minimum in $\phi(\tilde{K})$ can be determined by elementary calculus, and this gives the results

$$2\tilde{K}_{min} = \omega_s\left(\frac{\alpha_c\Delta(s)}{e}\right)^{1/(1-s)}, \quad (19)$$

$$\phi(\tilde{K}_{min}) = \tilde{K}_{min} e^{[1/(1-s)]} = K, \tag{20}$$

where $\Delta(s) = e\pi s(1-s)/\sin(\pi s)$. From these equations we then find that the critical coupling α_c is given by

$$\alpha_c = \frac{1}{\Delta(s)}\left(\frac{2K}{\omega_s}\right)^{1-s}. \tag{21}$$

Note that unlike the case of Ohmic damping, the sub-Ohmic critical coupling depends on the ratio of $2K/\omega_s$, and that the Silbey-Harris approach predicts a finite α_c as $s \to 0$. Note also that the above condition [Eq. (21)] can be rewritten so it is a condition on the coefficient $\alpha\omega_s^{1-s}$ appearing in the spectral function [Eq. (3)].

We also find that when $\alpha < \alpha_c$, $\tilde{K}$ satisfies

$$K \exp\left(\frac{1}{s-1}\right) \leq \tilde{K} \leq K \quad \text{if } \alpha < \alpha_c. \tag{22}$$

This inequality shows that at $T=0$, $\tilde{K}$ undergoes a discontinuous jump from a finite $\tilde{K}$ to $\tilde{K}=0$ as $\alpha \to \alpha_c$. Only at $s=1$ does this method predict that $\tilde{K} \to 0$ continuously.

In some other treatments of this problem,[10] the energy scale ω_s is set equal to the high-frequency cutoff ω_c. If this is done in this method, we find that we cannot send $\omega_c \to \infty$ in Eq. (17) as this leads to $\tilde{K}=0$ for all s and α. Keeping $\omega_c = \omega_s$ finite, we get the result

$$\alpha_c e^{-\alpha_c} = \frac{1}{\Delta(s)}\left(\frac{2K}{\omega_c}\right)^{1-s}. \tag{23}$$

The only modification to the previous result, Eq. (21), is the exponential factor and the replacement $\omega_s \to \omega_c$. The exponential factor is the correction for a finite cutoff. Note that as $s \to 1$, Eq. (23) correctly predicts the critical coupling for the Ohmic case, $\alpha_c = 1$.[1] We will not be too interested in the Ohmic case as this has already been thoroughly dealt with in the literature. Therefore for the rest of the this paper we work with $s < 1$, $\omega_s \neq \omega_c$ and $\omega_c \to \infty$ in the integral Eq. (17).

For $\alpha \ll 1$ we can make a perturbative expansion in α and determine $\tilde{K}(\alpha)$ to first order in α,

$$\tilde{K}(\alpha) = K\left[1 - \frac{\alpha s \pi}{\sin(\pi s)}\left(\frac{\omega_s}{2K}\right)^{1-s}\right]. \tag{24}$$

For general couplings to the bath, Eq. (16) needs to be solved numerically for $\tilde{K}$, and the typical behavior of $\tilde{K}(\alpha)$ across the whole range of coupling strengths is shown in Fig. 2.

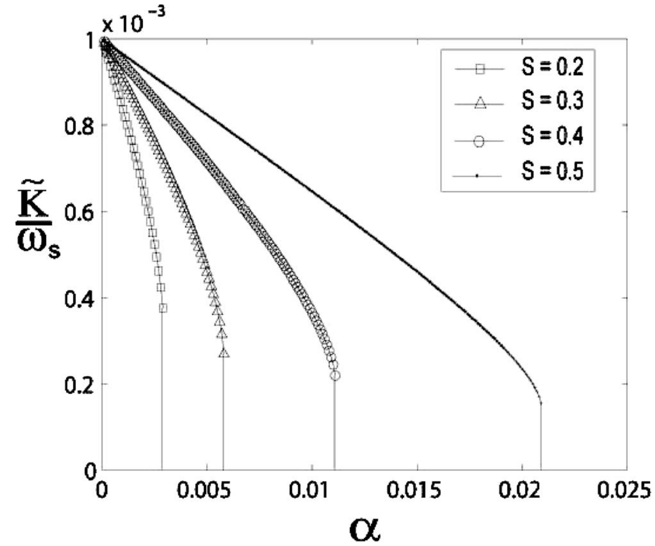

FIG. 2. Behavior of $\tilde{K}(\alpha)$ as a function of α at $T=0$. For this computation $K=10^{-3}\omega_s$ and $\omega_c \to \infty$.

IV. FINITE TEMPERATURES

A. High temperatures

Calculating the integral in Eq. (17) and solving Eq. (16) for the general case of finite temperatures can only be done numerically. However some analytical results can be extracted in certain limits. For the case of high temperatures and very weak coupling where $\tilde{K}\beta \ll 1$, we again find a coherent regime which crosses over to incoherent relaxation at a critical temperature T^*,

$$T^* = \frac{K}{\alpha f(s)}\left(\frac{2K}{\omega_s}\right)^{1-s}, \quad \alpha < \alpha_c, \tag{25}$$

where $f(s)$ is a slowly varying function of s which is always $\approx O(1)$. In this regime, we find that the transition from finite $\tilde{K}$ to $\tilde{K}=0$ occurs discontinuously at T^*.

For stronger coupling the relation given by Eq. (25) is violated, and a numerical study we have performed shows that $\tilde{K}$ vanishes at a significantly lower temperature than T^* as $\alpha \to \alpha_c$. For weak coupling, the numerical calculations of $\tilde{K}(T)$ give values of T^* in good agreement with Eq. (25).

B. Low temperatures

For temperatures close to zero where $\tilde{K}\beta \gg 1$, we can solve the self-consistent Eq. (16) for weak coupling by making a perturbation expansion in powers of α. The result to first order is

$$\tilde{K}(T,\alpha) = \tilde{K}(0,\alpha) + 2\alpha g(s)\frac{(K_B T)^2}{K}\left(\frac{\omega_s}{2K_B T}\right)^{1-s}, \tag{26}$$

where $\tilde{K}(0)$ is given by Eq. (24) and $g(s)$ is another function of s which is of order unity. Equation (26) shows the surprising result that $\tilde{K}$ becomes larger as the temperature is increased from zero. This result was also derived by Weiss for the Ohmic bath,[8] and was qualitatively described by Kehrein and Mielke for the sub-Ohmic bath.[9] However, we believe the quantitative result given in Eq. (26) has not been explicitly presented before for the sub-Ohmic bath. We shall discuss this effect in more detail in Sec. VII.

C. Intermediate temperatures

For intermediate values of α and T, we can determine $\tilde{K}$ numerically and the typical behavior is shown in Fig. 3. In

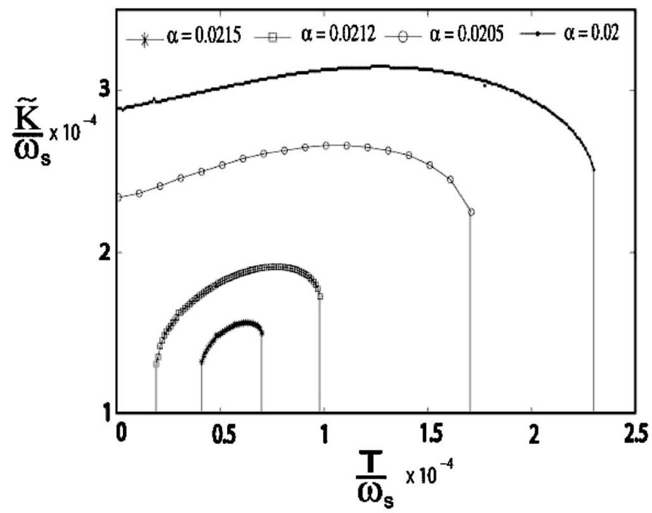

FIG. 3. $\tilde{K}$ as a function of temperature for a sub-Ohmic bath with $s=1/2$ and a range of different couplings. For this numerical computation $K=10^{-3}\omega_s$ and $\omega_c\to\infty$. Note that the two lowest curves have finite values of $\tilde{K}$ only between T^* and a lower reentrance temperature. For these curves, $\alpha>\alpha_c\approx 0.021$.

all cases we find that $\tilde{K}$ increases to a maximum and then drops discontinuously to $\tilde{K}=0$ at T^*. In Sec. VII we estimate that the peak in $\tilde{K}(T)$ should occur approximately at a temperature $K_BT_{max}\sim\tilde{K}(T_{max})$, which for sufficiently weak coupling can be approximated as $K_BT_{max}\sim K$. Comparing to the numerical results we find that this is a good order of magnitude estimate, but the peak typically occurs at a lower temperature $\sim T_{max}/2$ as illustrated in Fig. 3.

The numerical results also reveal an interesting feature if we look at the temperature dependence of $\tilde{K}$ for systems with $\alpha>\alpha_c$. We find that for couplings slightly above α_c, the TLS is incoherent at $T=0$, but then develops a finite $\tilde{K}$ between some reentrance temperature and T^*. In this reentrance regime, $\tilde{K}$ shows the same nonmonotonic temperature dependence described above, and some examples of the behavior of $\tilde{K}$ in this "supercritical regime" are shown in Fig. 3.

As the coupling between the TLS and bath is increased, the reentrance temperatures and T^* merge to one finite temperature and beyond this coupling, $\tilde{K}=0$ for all temperatures. This region is generally very small and together with the results for $\alpha<\alpha_c$, we obtain the schematic coherent and incoherent regions of the sub-Ohmic model as shown in Fig. 4. This reentrance phenomenon is a consequence of the same mechanism that causes the enhancement of $\tilde{K}$ at low temperatures, and we discuss this effect in Sec. VII.

V. TLS DYNAMICS AND LIMITATIONS OF THE VARIATIONAL METHOD

In Sec. II we defined the criteria for coherent dynamics as the existence of a finite renormalized tunneling matrix element $\tilde{K}$. However this criterion does not take into account the effect of the perturbation terms given in Eq. (11). These perturbation terms introduce dissipative dynamical effects which can alter the oscillatory behavior of the TLS in the coherent tunneling state. These effects can be calculated by a variety of methods, and for the Ohmic case are well understood.[1,5,8,11]

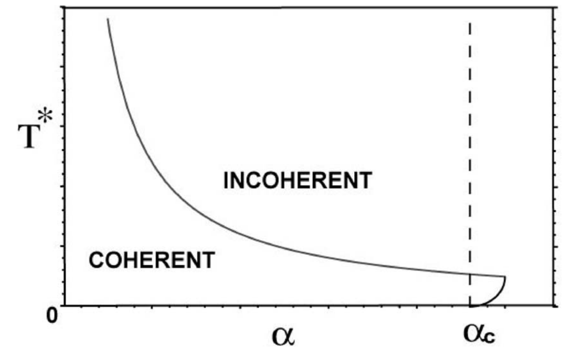

FIG. 4. Schematic plot of the boundary between coherent and incoherent regimes as found by the variational method. The curve is proportional to $1/\alpha$ for small α. The plot also shows the small reentrant region for coupling strengths greater than α_c.

For the sub-Ohmic problem, we are interested in the weak-coupling behavior, where approximations like the noninteracting-blip model are no longer valid.[1,5] However, the weak coupling should permit us to analyze the effects of perturbations using the perturbative reduced density matrix method.[14,16] To second order in the perturbations, the reduced density matrix of the TLS, $\rho_s(t)$, obeys the equation of motion

$$\dot{\rho}_s(t) = -\int_0^t dt'\,\mathrm{Tr}_b[\hat{V}(t),[\hat{V}(t'),\rho_s(t')\rho_b(0)]], \qquad (27)$$

where the operators are written in the interaction representation $\hat{V}(t)=\exp(i\hat{H}_0t)\hat{V}\exp(-i\hat{H}_0t)$, and $\hat{V}$ and $\hat{H}_0$ are defined in Eq. (11). $\rho_b(0)$ is the thermal density matrix for the unperturbed bath modes. Once $\rho_s(t)$ is known, all the observables of the TLS can be found using $\langle\hat{O}\rangle=\mathrm{Tr}[\rho_s(t)\hat{O}]$, where the trace is only over the states of the TLS.

As can be seen in Eq. (27), the time development of the reduced density matrix depends on the whole history of its motion, and such memory effects can lead to strong modification of the tunneling dynamics.[12] As a simple example of the dynamical effects that perturbation can cause, we consider very weak coupling and ignore the memory structure of the bath. This simplification is known as the Born-Markov approximtion,[16] and applying it to the spin-boson model, we find that $\hat{\sigma}_z$ obeys the simple equation of motion,[1,11]

$$\frac{d^2\langle\hat{\sigma}_z(t)\rangle}{dt^2} + 2\Gamma\frac{d\langle\hat{\sigma}_z(t)\rangle}{dt} + 4K^2\langle\hat{\sigma}_z(t)\rangle = 0. \qquad (28)$$

Therefore, in the Born-Markov approximation, the coherent oscillations of the TLS are exponentially damped with a decay rate given by

$$\Gamma = J(2\tilde{K})\coth(\tilde{K}\beta) \tag{29}$$

so that as $t \to \infty$ the TLS settles into an incoherent mixture of localized states. The coherence of the initial state is gradually destroyed by interactions with the environment on a time scale $1/\Gamma$. This is a generic phenomena for open quantum systems,[16] and for long enough times, the initial coherence of the superposition state is destroyed. Therefore when we talk about the coherent phase in the Silbey-Harris variational method, we mean that the initial ground state is coherent; the subsequent tunneling is then subject to decoherent and dissipative processes which eventually destroy the coherence.

The purpose of these remarks on dynamics is to point out that in the thermodynamic coherent phase, these decoherent and dissipative processes can potentially drive the coherent tunneling of the TLS to become incoherent. Therefore it is possible that there is a transition to incoherent motion due to dynamical effects that may occur before or after the thermodynamic transition we have found at α_c or T^*. For example, the Silbey-Harris variational method predicts $\alpha_c=1$ for the Ohmic bath, whilst it is well known that for Ohmic baths at $T=0$, there is localization for $\alpha \geqslant 1$, incoherent tunneling for $0.5 < \alpha < 1$, and coherent oscillations are only observed for $\alpha < 0.5$.[1]

In order to find such a dynamical crossover in the variational method, we need to account for the perturbation terms and solve for the dynamics of the TLS. For Ohmic damping, Silbey and Harris calculated that the crossover to incoherent tunneling occurs when the equation of motion (28) becomes overdamped, which occurs at a coupling strength $\alpha_{inc}=2/\pi$ at $T=0$. If we apply the same procedure to the sub-Ohmic bath, we find that,

$$\frac{\alpha_{inc}}{\alpha_c} e^{s\alpha_c} = \frac{2es(1-s)}{\sin(\pi s)}, \quad T=0. \tag{30}$$

This result shows that $\alpha_{inc}/\alpha_c \sim O(1)$ for $0 < s \leqslant 1$.

However, this result only applies if the use of the Born-Markov approximation is valid, and this is not a good approximation for sub-Ohmic baths. The Born-Markov approximation fails for sub-Ohmic baths due to the presence of low frequency modes which cause large correlation times and strong memory effects. It is generally recognized that non-Markovian effects lead to stronger decoherence than that described by the simple Markov rate, and at present there is much discussion of non-Markovian dynamics in the context of qubit decoherence rates.[17–20]

As we mentioned in Sec. II, our method is based on a simple and intuitive variational ground state, and we have ignored the dynamical effects of the perturbations in our discussion of the transition between coherent and incoherent phases of this ground state. The existence of a finite $\tilde{K}$ as the signature for the coherent phase can be thought of as a thermodynamic criterion for an initial coherent phase, and in light of the discussion above, the critical couplings we have deduced from thermodynamical considerations can be different from those deduced from dynamics.

VI. CORRECTIONS AND FAILURES OF THE VARIATIONAL GROUND STATE

The determination of $\tilde{K}$ relies on the minimization of the free energy bound A_B given in Eq. (12). In this section we estimate the higher-order corrections to this free energy. We have already shown that the first-order term in powers of the perturbation vanishes and so the first corrections are given by second-order terms. The second-order term in the Bogoliubov-Feynman bound on the free energy is given by[14]

$$A_B^{(2)} = -\frac{1}{2}\left\langle \int_0^\beta e^{W\hat{H}_0}\hat{V}e^{-W\hat{H}_0}\hat{V}\,dW \right\rangle_0 . \tag{31}$$

The calculation of the second-order contribution to the free energy is outlined in Appendix A. For weak coupling at $T=0$, we find that the contribution to the free energy is small, $A_B^{(2)}/A_B \sim O((\tilde{K}/\omega_c)^s)$. Therefore we expect that our calculations based on the minimization of A_B to be accurate in the weak-coupling regime. For stronger coupling the corrections have to be calculated numerically, and again we find that corrections to A_B are small when ω_c is much larger than all other energy scales.

Another potential weakness of the method is that the variational ansatz may not be a particularly good guess at the true ground state in the first place. We can in fact demonstrate some cases where the variational solution is suboptimal. For simplicity, we shall show this by considering a spin-boson Hamiltonian with only one bath mode.

We call bosonic modes adiabatic if the frequency of such modes is much larger than TLS frequency $\omega_b \gg K$, because these modes can follow the TLS adiabatically. The Silbey-Harris approach is accurate in treating these adiabatic modes as well as being exact in the $K=0$ localized state. Now we turn to the opposite situation, the antiadiabatic case, where $K \gg \omega_b$.

We introduce a different variational wave function for the TLS in the basis of $\hat{\sigma}_z$. It is given by

$$|\Psi\rangle = \frac{1}{\sqrt{1+|\phi|^2}}\begin{pmatrix}1\\ \phi\end{pmatrix}, \tag{32}$$

where the number ϕ is a real variational parameter to be determined and $\phi=0$ corresponds to $|\uparrow\rangle$. Notice that in this ansatz we allow parity symmetry (up and down direction for the spin) to be broken unlike in the Silbey-Harris approach. We fix the TLS in the variational state, and this gives us an effective Hamiltonian for the bath mode given by[21]

$$H_{eff} = -\frac{2K\phi}{1+\phi^2} + g\left(\frac{1-\phi^2}{1+\phi^2}\right)(a+a^\dagger) + \omega a^\dagger a. \tag{33}$$

This is an example of an independent-boson Hamiltonian and can be diagonalized exactly.[13] The resultant ground-state energy is given by

$$E_{g.s.} = -\frac{2K\phi}{1+\phi^2} - \frac{g^2}{\omega}\left(\frac{1-\phi^2}{1+\phi^2}\right)^2 \quad (34)$$

and we minimize this energy with respect to ϕ to find the optimal ground-state wave function. The result is that the optimal value of ϕ is given by

$$\phi_{\pm} = \frac{2g^2}{\omega K} \pm \sqrt{\left(\frac{2g^2}{\omega K}\right) - 1}. \quad (35)$$

This result shows that the ground-state spin is a linear combination of the localized and delocalized states (cf. the variational method where the spin ground state is a purely delocalized or localized state). The part of the wave function corresponding to the localized state gains a displacement energy, whilst the tunneling energy is reduced as the tunneling part of the wave function has a reduced weight due to the normalization of the wave function.

We notice that the important parameter here is $g^2/(\omega K)$. When $g^2/(\omega K) \gg 1$, what we can call the strong-coupling case, the parity breaking (i.e., $\phi_+ \gg 1$) is large. Since we assumed $K \gg \omega$, the strong-coupling case implies that $g \gg \omega$. We will now show that when this strong-coupling condition is met, the Silbey-Harris method gives a suboptimal ground-state.

For $2g^2/\omega K \gg 1$, which corresponds to either strong coupling or a very low-frequency bath mode, the ground state energy of Eq. (34) is

$$E_{g.s} \approx -\frac{g^2}{\omega}\left[1 + \left(\frac{\omega K}{2g^2}\right)^2\right]. \quad (36)$$

The corresponding bound found using the Silbey-Harris method at $T=0$ is,

$$A_B \approx -K \exp\left[-\frac{g^2}{2\tilde{K}^2}\right] - \frac{g^2}{\tilde{K}}. \quad (37)$$

There is a large region of parameters that the ansatz of Eq. (32) has a lower ground-state energy than the Silbey-Harris ansatz. In particular, if we set $g^2/K^2 \ll 1$, then if ω is sufficiently small so that $\omega \ll g$, we find that

$$A_B \approx -K - \frac{g^2}{K} \gg E_{g.s}. \quad (38)$$

Therefore, when these conditions are satisfied, the Silbey-Harris variational method is suboptimal. For constant coupling g, we always enter this breakdown regime as $\omega \to 0$. However, since the coupling constant $g(\omega)$ can be frequency dependent, there can be (and are) many situations when weak coupling is valid as $\omega \to 0$, provided $g(\omega)$ vanishes quickly enough to maintain $g(\omega) \ll \omega$.

These results show that the coherent state found by the Silbey-Harris method can be suboptimal for baths with finite couplings between the TLS and low-frequency modes. In appendix B we highlight this by comparing the variational ground state given by (32) and the Silbey-Harris state in the limit $s \to 0$.

VII. DISCUSSION

In Sec. II we stated that the physical picture behind the Silbey-Harris approach is that the tunneling particle drags along a cloud of displaced oscillators as it tunnels between the wells. For modes with frequencies much larger than the tunneling frequency we expect this adiabatic approximation to work well. The complications arise in this problem due to the presence of low-frequency modes in the bath, especially in the sub-Ohmic problem. These nonadiabatic modes cannot follow the tunneling motion and need to be treated separately from the adiabatic modes.

If we try and treat all modes with the same adiabatic approximation and set $f_l = g_l$, then it can be seen that the integral in Eq. (17) diverges in the infrared and always leads to $\tilde{K}=0$, i.e., no coherent oscillations. This complete suppression of tunneling for the sub-Ohmic bath was also obtained by Leggett *et al.*[1] using the technique of adiabatic renormalization.

However, the variational method goes beyond the adiabatic approximation and finds solutions with finite $\tilde{K}$. The appearance of a finite $\tilde{K}$ can be traced back to the free energy bound we calculated in Eq. (12) and it is shown explicitly in Eq. (A26). There are two competing processes; the choice $f_l = g_l$ maximizes the second term, the dressing or displacement energy. However, for sub-Ohmic baths this always renormalizes $\tilde{K}$ to zero and thus incurs an energy penalty. Equation (A26) is a nonlinear function of α, K, T and which process dominates depends sensitively on these parameters. When $\alpha < \alpha_c(T)$ it is energetically favorable to have a finite $\tilde{K}$.

For $\alpha < \alpha_c$ and $T=0$, we see from Eq. (14) that the variational method has loosely separated the bath modes into two distinct sets. Modes with $\omega > 2\tilde{K}$ respond adiabatically to the tunneling motion, i.e., have $f_l \approx g_l$. Nonadiabatic modes with $\omega < 2\tilde{K}$ couple more weakly to the TLS, with coupling strength $f_l \approx g_l \omega_l / 2\tilde{K}$ as $\omega_l \to 0$.

This vanishing of the coupling at low frequencies prevents the infrared divergence in Eq. (17) by fixing an effective cutoff at $2\tilde{K}\tanh(\tilde{K}\beta)$. In this method, the free energy minimization naturally determines the cutoff for the mode elimination, unlike in the adiabatic renormalization scheme.[1,9] We also note that while the nonadiabatic modes decouple from dressing the particle, they have not disappeared; they give the dominant contribution to the perturbation term $\hat{V}_0$, Eq. (10), and can cause significant dynamical effects.

The variational method also predicts interesting behavior for $\tilde{K}(T)$ at low temperatures. As we demonstrated in Sec. IV, $\tilde{K}(T)$ initially increases with temperature, and this behavior can be understood by looking at the temperature dependence of the coupling parameters $\{f_l\}$. We would normally expect that as the temperature is increased, the occupation of low-frequency oscillators would increase, and this should lead to increased renormalization through the hyperbolic cotangent factor in Eq. (17). However, from Eq. (14) we see that the dressing due to modes with $k_B T < \omega < 2\widetilde{K}$ decreases with temperature, and this decoupling leads to a net reduction in the renormalization of $\widetilde{K}$ from these nonadiabatic modes. The dressing parameters for the adiabatic modes are effectively independent of temperature, and so when they are thermally excited they always renormalize $\widetilde{K}$ towards zero.

At low temperatures only nonadiabatic modes are excited and the reduction in the renormalization due to nonadiabatic modes leads to the increase of $\widetilde{K}$ with temperature. This low-temperature reduction in the renormalization of $\widetilde{K}$ also gives a natural explanation for the reentrance of $\widetilde{K}$ at finite temperatures for systems with $\alpha > \alpha_c$. At higher temperatures, adiabatic modes become excited and the resulting increase in renormalization causes $\widetilde{K}$ to decrease until it goes discontinuously to zero at T^*.

The exact point at which the adiabatic modes halt the increase in $\widetilde{K}$ depends sensitively on the relative weight of adiabatic and nonadiabatic modes and thus depends on the spectrum of the bath. However, we can still estimate where the maximum occurs. From the discussion above, the turning point occurs around the temperature at which the adiabatic modes begin to be excited. This occurs approximately at a temperature $K_B T_{max} \sim \widetilde{K}(T_{max})$.

There have been several other recent treatments of the sub-Ohmic problem and we find that this simple variational method is consistent with several of the main results.[5,9,10] The flow equation analysis of Kehrein and Mielke also showed that a coherent phase exists for the sub-Ohmic model. They also point out, that on the basis of the well-known connection between the spin-boson model and Ising model in statistical mechanics,[9,22] the coherent phase corresponding to the high-temperature disordered phase of the Ising model, is expected to exist. Many results obtained from the flow equation method are in fact consistent with ours results, including the qualitative prediction of the rise in $\widetilde{K}(T)$ at low temperatures and the discontinuous transition at zero temperature.

It is important to remember that the transition in an infinite one-dimensional Ising model with long-range interactions as a function of temperature, is only related to the transition in the spin-boson model, as a function of α, at $T=0$. Therefore comparison of the nature of the transition (first order or second order) is limited to $T=0$. In this paper we are mostly concerned with the transition of spin-boson model at finite temperature, with several parameters describing the bath $(\alpha, \omega_s, \omega_c)$. Yet the comparison with the results known for the Ising model with $1/r^{1+s}$ interactions indicates that higher-order corrections to Silbey-Harris ansatz should be necessary to describe the close proximity of the transition, since for $s>0$ the transition in the Ising model is of second-order.[23,26–30]

The numerical renormalization group analysis by Bulla, Tong, and Vojta found that the system is localized at $s=0$,[10] and their perturbative RG results suggest that for $s>0$, the transition is continuous as a function of α. As our method is based on a variational ansatz, we cannot make any strong statement about the exact nature of the transition. As we noted in Sec. I there are several parameters which describe the bath, and the transition may depend on the constraints imposed between parameters and the assumptions used in the mappings to other models.

Shnirman, Makhlin, and Schon have also demonstrated that coherent oscillations are possible in the sub-Ohmic model,[5] but their work focuses on calculating the dephasing and relaxation times of the dynamics rather than renormalization effects. In contrast to Bulla, Tong, and Vojta, their diagrammatic approach predicts that the TLS can be coherent at $T=0$ and $s=0$. As we discussed, differences between thermodynamic and dynamic properties are expected for the spin-boson model with a sub-Ohmic bath, and further understanding of these questions is desirable.

VIII. CONCLUSIONS

We have studied the sub-Ohmic spin-boson model using the intuitive variational method of Silbey and Harris.[11] This method has allowed us to reproduce a number of previously known results about the coherent sub-Ohmic model, but without having to make lengthy or unduly complicated calculations. With this in mind, we note that this method may be useful for a first look at different types of environment for which there is some question about the existence of a coherent phase.

For the $T=0$ sub-Ohmic spin-boson model, we have shown that coherent oscillations exist if α is below a critical coupling α_c, which we have explicitly calculated in Eq. (21). When this condition is met, the renormalized tunneling matrix element satisfies, $Ke^{1/(s-1)} \leqslant \widetilde{K} \leqslant K$ and undergoes a discontinuous transition to $\widetilde{K}=0$ as $\alpha \to \alpha_c$.

We have also presented numerical results which show the dependence of $\widetilde{K}(T,\alpha)$ on temperature and coupling strength. We have shown that $\widetilde{K}(T)$ has a nontrivial dependence on temperature, initially rising to a maximum value and then decreasing to a discontinuous transition at a critical temperature T^*. We were able to show that this behavior arises from the temperature dependence of the effective dressing parameters $\{f_l\}$ [Eq. (14)], and we have highlighted the natural separation in this method of adiabatic modes $(\omega > 2\widetilde{K})$ and nonadiabatic modes $(\omega < 2\widetilde{K})$. Our numerical study of this theory also found a different phenomenon, a reentrant coherent phase that exists at finite temperatures for systems with $\alpha > \alpha_c$, when α is sufficiently close to the critical coupling.

Importantly, we showed that dynamical and thermodynamic criteria for the transition are different and sensitive to non-adiabatic modes. We also discussed several limitations of the description of the spin-boson model by an equilibrium bath characterized by the spectral function $J(\omega)$.

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APPENDIX A: CALCULATION OF SECOND-ORDER TERMS FOR THE FREE ENERGY BOUND

In Sec. VI we discussed the size of contributions to the free energy from higher-order terms in Eq. (12). In this appendix we outline the calculation of the lowest-order correction terms to the free energy bound. The fist corrections are second order in the perturbations (11) and are given by[14]

$$A_B^{(2)} = -\frac{1}{2}\left\langle \int_0^\beta e^{W\hat{H}_0}\hat{V}e^{-W\hat{H}_0}\hat{V}\,dW \right\rangle_0. \tag{A1}$$

The perturbation terms are shown in Eq. (11) and the Hamiltonian $\hat{H}_0$ is defined in Eq. (8). The average is explicitly given by

$$\langle A\rangle_0 = \frac{\mathrm{Tr}\exp(-\beta H_0)A}{\mathrm{Tr}\exp(-\beta H_0)}, \tag{A2}$$

where the trace is over all states of the TLS and bath. Each perturbation term is a product of a spin operator and a bath operator. As the thermal density matrix corresponding to H_0 is also separable into spin and bath parts, we can calculate each term in Eq. (A1) as the product,

$$\int_0^\beta dW \langle e^{W\hat{H}_0^s}\hat{V}_s e^{-W\hat{H}_0^s}\hat{V}_s\rangle_s \langle e^{W\hat{H}_0^b}\hat{V}_b e^{-W\hat{H}_0^b}\hat{V}_b\rangle_b. \tag{A3}$$

Here s refers to the spin part of H_0 and b is the bath part. Before discussing these factors, it is useful to re-write the perturbations in terms of the spin components x, y, z instead of the raising and lower operators. This gives the perturbations as

$$\hat{V}_0 = \sum_l (g_l - f_l)(\hat{a}_l + \hat{a}_l^\dagger)\hat{\sigma}_z, \tag{A4}$$

$$\hat{V}_1 = \tilde{K}\left[\cosh\left(2\sum_l f_l\omega_l^{-1}(\hat{a}_l - \hat{a}_l^\dagger)\right) - 1\right]\hat{\sigma}_x, \tag{A5}$$

$$\hat{V}_2 = -i\tilde{K}\sinh\left(2\sum_l f_l\omega_l^{-1}(\hat{a}_l - \hat{a}_l^\dagger)\right)\hat{\sigma}_y. \tag{A6}$$

1. Spin part

The spin factor is of the general form

$$I_s^{ijk} = \langle e^{W\tilde{K}\sigma_i}\sigma_j e^{-W\tilde{K}\sigma_i}\sigma_k\rangle_s, \tag{A7}$$

where $i=x,y,z$. The exponentiated spins can be written[24]

$$\exp(\theta\sigma_i) = \cosh(\theta) + \sinh(\theta)\sigma_i \tag{A8}$$

and using this and the Pauli spin algebra, one can derive the general relationship

$$e^{\theta\sigma_i}\sigma_j e^{-\theta\sigma_i} = \cosh(2\theta)\sigma_j + i\epsilon_{ijk}\sinh(2\theta)\sigma_k - 2\sinh^2(\theta)\delta_{ij}\sigma_j. \tag{A9}$$

Substituting this into Eq. (A7) we get,

$$I_s^{ijk} = \cosh(2\tilde{K}W)\langle\sigma_j\sigma_k\rangle_s + i\epsilon_{ijl}\sinh(2\tilde{K}W)\langle\sigma_l\sigma_k\rangle_s - 2\sinh^2(\tilde{K}W)\delta_{ij}\langle\sigma_j\sigma_k\rangle_s \tag{A10}$$

and finally, all the spin factors can be calculated using

$$\langle\sigma_x\rangle_s = -\tanh(\tilde{K}\beta), \tag{A11}$$

$$\langle\sigma_y\rangle_s = \langle\sigma_z\rangle_s = 0. \tag{A12}$$

2. Bath factors

If we define the operator $a_l(W) = \exp(WH_b)a_l\exp(-WH_b)$, then the bath terms contain only averages of the form

$$I_b = \langle V_i(W)V_j\rangle_b, \tag{A13}$$

where the V_i are the bath parts of the perturbation terms defined in Eq. (A6). To continue we need to calculate these expectation values. For the terms involving products of $V_{1,2}$ the following theorem is very useful. If the operators A and B are linear in the co-ordinates or momenta of an oscillator, then it can be shown,[25]

$$\langle e^A e^B\rangle_b = e^{(1/2)[\langle A^2\rangle_b + \langle B^2\rangle_b + 2\langle AB\rangle_b]}. \tag{A14}$$

For example, if we define $\Delta(W) = 2\sum_l f_l\omega_l^{-1}(\hat{a}_l(W) - \hat{a}_l^\dagger(W))$, then

$$\begin{aligned}\langle V_2V_2\rangle_b &= -\frac{K^2}{4}\langle(e^{\Delta(W)} - e^{-\Delta(W)})(e^{\Delta(0)} - e^{-\Delta(0)})\rangle \\ &= -\frac{K^2}{2}e^{\langle\Delta(0)^2\rangle}(e^{\langle\Delta(W)\Delta(0)\rangle} - e^{-\langle\Delta(W)\Delta(0)\rangle}) \\ &= -\tilde{K}^2\sinh[\gamma(W)],\end{aligned} \tag{A15}$$

where $\gamma(W)$ is given by

$$\begin{aligned}\gamma(W) &= \langle\Delta(W)\Delta(0)\rangle \\ &= -4\sum_l f_l^2\omega_l^{-2}[e^{\omega_l W}n_l + e^{-\omega_l W}(n_l+1)],\end{aligned} \tag{A16}$$

n_l are the Bose occupation factors for the bath modes, and we have used $\tilde{K} = K\exp(1/2\langle\Delta(0)^2\rangle)$.

Combining these results with the spin factors, we calculate that the second-order contribution to the free energy is

$$2A_B^{(2)} = -\tilde{K}^2\int_0^\beta dW[\cosh(\gamma(W)) - 1] \quad (A17)$$

$$+\tilde{K}^2\int_0^\beta dW\sinh(\gamma(W))$$

$$\times[\cosh(2\tilde{K}W) - \sinh(2\tilde{K}W)\tanh(\tilde{K}\beta)] \quad (A18)$$

$$-\int_0^\beta dW\langle V_2(W)V_0\rangle$$

$$\times[\sinh(2\tilde{K}W) - \cosh(2\tilde{K}W)\tanh(\tilde{K}\beta)] \quad (A19)$$

$$+\int_0^\beta dW\langle V_0(W)V_2\rangle$$

$$\times[\sinh(2\tilde{K}W) - \cosh(2\tilde{K}W)\tanh(\tilde{K}\beta)] \quad (A20)$$

$$-\sum_l (g_l - f_l)^2\int_0^\beta dW[e^{W\omega_l}\tilde{n}_l + (\tilde{n}_l + 1)e^{-W\omega_l}]$$

$$\times[\cosh(2\tilde{K}W) - \tanh\tilde{K}\beta\sinh(2\tilde{K}W)]. \quad (A21)$$

Note that the free energy correction $A_B^{(2)}$ is stated for the case of finite $\tilde{K}$.

3. Second-order terms at $T=0$

At $T=0$ we can calculate all expectation values explicitly and the free energy correction takes the form

$$A_B^{(2)} = -\frac{\tilde{K}^2}{2}\int_0^\infty dW\{\cosh[\gamma(W)] - 1\} \quad (A22)$$

$$+\frac{\tilde{K}^2}{2}\int_0^\infty dW\sinh[\gamma(W)]e^{-2\tilde{K}W} \quad (A23)$$

$$-6\tilde{K}^2\sum_l \frac{g_l^2}{(\omega_l + 2\tilde{K})^3}. \quad (A24)$$

We will show that the typical size of the correction term is small compared to the main free energy in the limit of large ω_c, which is the normal situation in this model. For the term (A24) we get a contribution of,

$$-6\tilde{K}^2\sum_l \frac{g_l^2}{(\omega_l + 2\tilde{K})^3} \approx -\frac{\alpha\omega_s}{2}\left(\frac{2\tilde{K}}{\omega_s}\right)^s\left(\frac{1}{1+s} + \frac{1}{s-2}\right), \quad (A25)$$

where we have introduced the spectral function and approximately calculated the integral. The other two terms (A22) and (A23) cannot be evaluated in a simple analytical form, but we note that as $\omega_c \to \infty$ these terms give finite contributions if $s<1$.

The main part of the free energy A_B is given by

$$A_B = -\tilde{K} + \sum_l (f_l^2 - 2f_lg_l) \quad (A26)$$

$$= -\tilde{K} - \frac{\alpha\omega_s^{1-s}}{2}\int_0^{\omega_c}\frac{(\omega + 4\tilde{K})\omega^s d\omega}{(\omega + 2\tilde{K})^2}, \quad (A27)$$

where again we have used the spectral function to convert the sum into an integral. Under assumption $\tilde{K} \ll \omega_c$, the leading term in ω_c of A_B is

$$A^B \approx -\frac{\alpha\omega_s}{2s}\left(\frac{\omega_c}{\omega_s}\right)^s. \quad (A28)$$

Comparing this to the second order correction $A_B^{(2)}$, we see that corrections due to the term given by (A24) are small, and are controlled by the small parameter $(\tilde{K}/\omega_c)^s$ for $s>0$. As we let $\omega_c \to \infty$, the corrections from terms (A23) and (A22) tend to a finite value, while A_B grows as ω_c^s. Therefore, the relative correction from (A23) and (A22) becomes small in this limit. However, these and higher-order perturbations may still be relevant in the proximity of the coherent-incoherent transition as $\tilde{K} \to 0$.

APPENDIX B: ALTERNATIVE VARIATIONAL TREATMENT OF SPIN-BOSON PROBLEM

In this section we give a treatment of the sub-Ohmic spin-boson model using the alternative variational solution given in Sec. VI. In the antiadiabatic or nonadiabatic situation of $K \gg \omega$, the TLS can be thought as creating effective potential for bosonic mode. As before we write a variational state for the spin,

$$|\Psi\rangle = \frac{1}{\sqrt{1 + |\phi|^2}}\begin{pmatrix}1\\ \phi\end{pmatrix}. \quad (B1)$$

We then calculate $\langle\Psi|H_{sb}|\Psi\rangle$ to get the effective Hamiltonian for the bath modes. This is given by

$$H_{eff} = -\frac{2K\phi}{1+\phi^2} + \left(\frac{1-\phi^2}{1+\phi^2}\right)\sum_l g_l(a + a^\dagger) + \sum_l \omega_l a^\dagger a. \quad (B2)$$

The first tunneling term is minimized for real ϕ, so that ϕ is chosen to be real although in general complex.

Again, this is a set of independent boson Hamiltonians and the energy of the variational ground state is given by

$$E_{g.s.} = -\frac{2K\phi}{1+\phi^2} - \left(\frac{1-\phi^2}{1+\phi^2}\right)^2\sum_l \frac{g_l^2}{\omega_l}. \quad (B3)$$

The sum over the bath couplings can be explicitly calculated by substituting the spectral function into the sum to get

$$\sum_l \frac{g_l^2}{\omega_l} = \frac{\alpha\omega_s^{1-s}}{2}\int_0^{\omega_c}\omega^{s-1}d\omega \quad (B4)$$

$$= \frac{\alpha\omega_s}{2s}\left(\frac{\omega_c}{\omega_s}\right)^s. \tag{B5}$$

Looking at the ground-state energy (B3) we see that as $s \to 0$, the static displacement energy of the oscillators [given by the second term of Eq. (B3)] diverges and becomes the dominant term for any nonzero coupling. Minimizing the free energy with respect to ϕ we always find that $\phi=0$ (or $\phi=\infty$) and therefore the particle is always localized for any nonzero coupling at $s=0$. This is due to the fact that these soft modes have no resistance to the static force due to the spin in the limit $\omega_l \to 0$.

For $s=0$, the Silbey-Harris variational method predicts a coherent phase with finite $\tilde{K}$ for sufficiently weak coupling. The free energy of this state is

$$A_B = -\tilde{K} - \frac{\alpha\omega_s}{2}\int_0^{\omega_c} \frac{(\omega + 4\tilde{K})d\omega}{(\omega + 2\tilde{K})^2} \tag{B6}$$

$$\approx -\tilde{K} - \alpha\omega_s \ln\left(\frac{\omega_c}{2\tilde{K}}\right). \tag{B7}$$

Comparing the energy of this coherent ground state to the energy of the localized ground state, we see that for $s=0$ and $\omega_c \to \infty$ the localized state is lower in energy for any nonzero coupling between the bath and the TLS. The coherent state is therefore never favorable when $s=0$ and the finite $\tilde{K}$ found by the variational method is an artifact of the method. This artifact occurs due to the divergence of the static displacement energy of the oscillators (singular limit for $\omega_c \to \infty$), which causes problems with the free energy minimization we use to determine f_l, $\tilde{K}$, etc. Notice though that $\tilde{K}=0$ is also a solution of the self-consistent Eq. (17), and so the Silbey-Harris method can correctly describe the $s=0$ state if we ignore the suboptimal solution with $\tilde{K}>0$.

To summarize, the divergence of the static displacement energy of the oscillators for $s \leqslant 0$ implies localization in the ground state and dramatic differences between thermodynamic and dynamic properties. Such differences due to nonadiabatic modes can also be seen for $s>0$.

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