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Failure of the displaced-squeezed state for spin-boson models in the thermodynamic limit

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We present an analysis of a variational coherent-squeezed state that has been discussed in the literature as a potential ground state for the spin-boson model. We show that when the system-size scaling of the spin-bath coupling is included properly, all squeezing effects and nonuniversal physics vanish in the thermodynamic limit. We also present finite-size corrections to the renormalization of the spin's coherence, showing that squeezing effects are also absent to leading order in the inverse bath size.

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INTRODUCTION

The spin-boson model is one of the most important theoretical models for studying dissipation and decoherence in quantum systems, and has been applied to numerous systems in chemistry,[1] biology,[2] and the emerging fields of quantum computation and quantum devices.[3] The model is simple, comprising a coherent two level system (TLS) that is coupled to a bath of harmonic oscillators, yet it is known to contain a rich array of physical phenomena, and continues to provide new insights into open quantum systems.

One particularly important issue, especially for practical quantum devices, is the robustness of the coherence of the TLS in equilibrium with the bath. Numerous studies on this have revealed some extremely interesting physics, including quantum phase transitions between coherent and incoherent TLS states, and unusual temperature dependence of the coherence.[4–11]

Amongst these studies, the use of trial wave functions has provided some very intuitive insights into the problem. There are two common states in the literature, both based on the adiabatic approximation discussed by Leggett *et al.*[4] The first was that of Silbey and Harris, who modified the adiabatic approximation to allow for simple nonadiabatic responses from the low frequency modes in the problem.[6] This state was shown to correctly describe the coherent-incoherent transition for ohmic coupling,[6] and has recently been used to study the transition in the sub-ohmic system, giving results in excellent agreement with those obtained by other methods.[7–10]

The second state is known as the displaced-squeezed state (DSS) and was proposed by Chen, Zhang, and Wong.[12] This state is based on two effects: adiabatic displacement of the bath modes, and spatial deformation of the oscillator wave functions. At zero temperature it has been shown that the energy of the DSS can be significantly lower than the Silbey-Harris state for the case of strong coupling between one oscillator and the TLS,[13] and this has also been claimed for strong coupling to a super-ohmic continuum of bath modes.[14]

This DSS also predicts coherent-incoherent transitions in ohmic and sub-ohmic systems,[15,16] but with significantly different critical properties than those found in the rest of the literature. Moreover, these critical properties depend on the explicit form of the TLS-bath coupling, which is unusual as it has been shown using path integral techniques that the spin-boson physics should be controlled solely by the spectral function of the bath.[4,17] As the DSS is claimed to be the most stable ground state for strong coupling, there has been much discussion of this breakdown of "universality" as a function of coupling strength,[14,15] a breakdown which we shall show does not exist thermodynamically.

In this paper we use an effective Hamiltonian theory to show that when the system-size scaling of the TLS-bath coupling is included properly, all squeezing and nonuniversal features of the DSS vanish in the thermodynamic limit. Finite-size effects are then discussed, with no evidence for squeezing found to leading order in the inverse system size.

THE SPIN-BOSON MODEL

The Hamiltonian for the spin-boson model is given by[4]

$$H_{sb} = -K\sigma_x + \sigma_z \sum_l g_l(a_l + a_l^\dagger) + \sum_l \omega_l a_l^\dagger a_l, \qquad (1)$$

where $\sigma_{x,z}$ are Pauli matrices for the TLS, $a_l^\dagger$ and a_l are the bosonic creation and annihilation operators for the bath modes, and ω_l is the frequency of mode l. The bath couples to the TLS with coupling constants g_l, and the coherent tunneling matrix element between the eigenstates of σ_z is K. We assume that the bath is truly macroscopic, and that the modes can be treated as a continuum with a smooth density of states up to some cutoff frequency ω_c.[4] The physics of the spin-boson model is then normally determined solely by the spectral function of the bath $J(\omega)$,

$$J(\omega) = \sum_l g_l^2 \delta(\omega - \omega_l), \qquad (2)$$

$$= \frac{1}{2}\alpha\omega_s^{1-s}\omega^s, \quad \omega < \omega_c. \qquad (3)$$

The right-hand side of Eq. (3) is a phenomenological power law where α is a dimensionless coupling strength, ω_s is a typical frequency scale of the interaction, and s is the exponent of the frequency dependence. This form for $J(\omega)$ can be derived for specific microscopic interactions, and many physical examples can be found in the literature.[3,5] The dynamical and thermodynamical behavior of the TLS depends critically on α and s. As a result, three types of baths are distinguished according to their value of s: the super-ohmic bath ($s>1$), the ohmic bath ($s=1$), and the sub-ohmic bath ($s<1$).[4]

ADIABATIC APPROXIMATION AND THE DISPLACED-SQUEEZED STATE

In the absence of tunneling, the TLS will remain permanently in an eigenstate of σ_z, and the spin-boson Hamiltonian can be solved exactly. The two degenerate ground states $|+\rangle,|-\rangle$ are given by

$$|+\rangle = U_A|\uparrow\rangle|0\rangle, \quad |-\rangle = U_A|\downarrow\rangle|0\rangle, \tag{4}$$

$$U_A = \exp\left(-\sigma_z \sum_l g_l \omega_l^{-1}(a_l - a_l^\dagger)\right), \tag{5}$$

where $|\uparrow\rangle,|\downarrow\rangle$ are the usual eigenstates of σ_z. These ground states can be understood intuitively; the TLS creates a static force which displaces all the bath modes, and this displacement is described by the action of the shift operator U_A on the vacuum of all bath modes $|0\rangle$. When K is finite, the TLS can tunnel, and no exact solution for the problem is known. However, bath modes with frequencies much higher than the tunneling rate 2 K can respond almost instantaneously to the relatively slow tunneling, and will be dynamically displaced as the TLS tunnels between states. In such an approximation, the TLS-bath interaction can be eliminated by simple renormalization of the bare TLS tunneling matrix element.

In the zeroth-order adiabatic approximation, where all modes are assumed to follow the TLS instantaneously, the tunneling of the bath-dressed TLS leads to a coherent ground state $|gs\rangle=\frac{1}{\sqrt{2}}(|+\rangle+|-\rangle)$, which is characterized by a renormalized coherent level splitting $\tilde{K}=\langle+|K\sigma_x|-\rangle$. Physically, the tunneling probability is reduced by the TLS-bath correlation, as the overlap between the states $|+\rangle$ and $|-\rangle$ is suppressed by the relative displacement of the oscillator wave functions. Calculating $\tilde{K}$ explicitly, and using the definition of the spectral function to write the sum over bath modes as an integral, we find that

$$\tilde{K} = K \exp\left[-\alpha\omega_S^{1-s}\int_0^{\omega_c}\omega^{s-2}d\omega\right]. \tag{6}$$

The integral in Eq. (6) is finite for super-ohmic baths, but has an infrared divergence for all ohmic and sub-ohmic baths. Therefore this approximation predicts that the TLS always remains coherent for super-ohmic coupling, and is always incoherent, i.e., $\tilde{K}=0$, for ohmic or sub-ohmic couplings. For ohmic and sub-ohmic baths this result is known to be incorrect.[7–11] This failure can be traced to the mistreatment of the slow modes in the problem, for which the adiabatic approximation is clearly not valid.

The DSS of Chen, Zhang, and Wu[12] attempts to improve on the adiabatic approximation by also allowing for spatial distortion of the oscillator wave functions as they adiabatically follow the TLS. As is discussed in Ref. 12, the distortion of the oscillator wave functions can be described using the generators of bosonic squeezed states, minimum uncertainty states commonly used in quantum optics.[18] The effective displaced-squeezed ground state they propose is given by $|\psi_S\rangle=U_AU_S\frac{(|\uparrow\rangle+|\downarrow\rangle)|0\rangle}{\sqrt{2}}$ where U_S is given by

$$U_S = \exp\left(-\sum_l \gamma_l(a_l^2 - a_l^{\dagger 2})\right). \tag{7}$$

The parameters γ_l describe the amount of spatial distortion of the oscillator wave function, or alternatively, the squeezing of the bosonic quadrature operators.[18] Once determined, the squeezing parameters modify the renormalization of the tunneling matrix element by altering the overlap integral of the adiabatically displaced oscillator states. This modification can lead to qualitatively different physical results, including the possibility of finite $\tilde{K}$ for ohmic and sub-ohmic systems.

VARIATIONAL METHOD AND THE EFFECTIVE HAMILTONIAN

We now use an adapted version of the variational method of Silbey and Harris to calculate the effective tunneling matrix element of the TLS in the DSS at $T=0$ K.[6] First we make a canonical transformation to generate the Hamiltonian in the basis of the DSS, $\tilde{H}=U_AU_SH_{sb}U_S^{-1}U_A^{-1}$,

$$\begin{aligned}\tilde{H} = &-\hat{K}_+\sigma_+ - \hat{K}_-\sigma_- + \sum_l \omega_l\sinh(2\gamma_l)\\ &-\sum_l g_l^2\omega_l^{-1} + \sum_l \omega_l a_l^\dagger a_l[\cosh^2(2\gamma_l)+\sinh^2(2\gamma_l)]\\ &+\sum_l \omega_l(a_l^2 + a_l^{\dagger 2})\cosh(2\gamma_l)\sinh(2\gamma_l),\end{aligned} \tag{8}$$

where the operators K_+,K_- obey

$$\hat{K}_+ = \hat{K}_-^* = K\exp[-2g_l\omega_l^{-1}e^{-2\gamma_l}(a_l - a_l^\dagger)]. \tag{9}$$

In the adiabatic approximations discussed previously, the TLS-bath interactions were eliminated to generate an effective noninteracting Hamiltonian characterized by a renormalized tunneling matrix element $\tilde{K}$. We derive this form of Hamiltonian, as a mean-field approximation to $\tilde{H}$, by introducing the expectation value of the tunneling operators $\tilde{K}=\langle 0|\hat{K}_+|0\rangle=\langle 0|\hat{K}_-|0\rangle$, which is given by

$$\tilde{K} = K\exp\left[-2\sum_l g_l^2\omega_l^{-2}e^{-4\gamma_l}\right]. \tag{10}$$

Adding and subtracting $\tilde{K}\sigma_x$ to $\tilde{H}$, we then write the Hamiltonian as $\tilde{H}=H_0+\tilde{V}$,

$$\begin{aligned}H_0 = &-\tilde{K}\sigma_x + \sum_l \omega_l\sinh(2\gamma_l) - \sum_l g_l^2\omega_l^{-1}\\ &+\sum_l \omega_l a_l^\dagger a_l[\cosh^2(2\gamma_l)+\sinh^2(2\gamma_l)],\end{aligned} \tag{11}$$

$$\tilde{V} = \tilde{H} - H_0. \tag{12}$$

Following Silbey and Harris,[6] we now compute the Bogoliubov-Feynman bound on the free energy of the system

A_B.[19] The true free energy A of the model is related to A_B by[19]

$$A \leqslant A_B, \tag{13}$$

$$A_B = -\beta^{-1}\ln \mathrm{Tr}\exp(-\beta H_0) + \langle \tilde{V}\rangle_{H_0}. \tag{14}$$

The angular brackets denote the thermal expectation value calculated with respect to H_0, and computing the trace using the simple eigenstates of H_0, we find that $\langle \tilde{V}\rangle_{H_0}=0$. The free energy bound at $T=0$ K is thus

$$A_B = -\tilde{K} + \sum_l \omega_l \sinh(2\gamma_l) - \sum_l g_l^2 \omega_l^{-1}. \tag{15}$$

We note here that, like all other variational studies in the literature, this variational method does not consider the possibility that the separation of the Hamiltonian into $H_0+\tilde{V}$ may lead to divergent fluctuations if higher order perturbations are calculated, i.e., that the variational state is an inappropriate starting point for analysis of this problem. This matter will be discussed in a forthcoming study of these variational methods.

The variational parameters γ_l are determined by minimizing A_B with respect to the set $\{\gamma_l\}$. We find that γ_l satisfies

$$e^{8\gamma_l} = 1 + \frac{8\tilde{K}g_l^2}{\omega_l^3}, \tag{16}$$

and substituting this into Eq. (10), we find that $\tilde{K}$ obeys the self-consistent equation

$$\tilde{K} = K\exp\left[-\sum_l \left(\frac{2g_l^2}{\omega_l^2}\right)\left(1+\frac{8\tilde{K}g_l^2}{\omega_l^3}\right)^{-1/2}\right]. \tag{17}$$

The presence of g_l^2 in two places in Eq. (17) means that the renormalization of K is determined by both $J(\omega)$ and g_l^2. In the literature,[12,14,15] g_l is taken to have a general power-law form $g_l = g_0\left(\frac{\omega_l}{\omega_c}\right)^n$, where g_0 is a constant. However, this form for the coupling constants cannot be valid, as it does not take into account the scaling of these constants with system size. From Eq. (2) we see that $J(\omega)$ is the product of g_l^2 at $\omega=\omega_l$ and the density of states per unit frequency. As the density of states per unit frequency is proportional to $\mathcal{N}$, where $\mathcal{N}$ is the total number of bath oscillators, the microscopic coupling constants have to scale as $\mathcal{N}^{-1/2}$ in order to ensure that the spectral function is well defined in the thermodynamic limit. This point is made very clear in the origin review of Leggett *et al.*[4]

As the dependence of $\tilde{K}$ on $\mathcal{N}$ is essential to our discussion, we assume a general power-law form for the couplings given by

$$g_l^2 = \frac{\alpha\omega_c^2}{\mathcal{N}}\left(\frac{\omega_l}{\omega_c}\right)^n, \tag{18}$$

where n is an exponent greater than zero.[5] We now use the definition of the spectral function given in Eq. (2) to write the sum in Eq. (17) as an integral over a continuous distribution of bath modes. In this limit, the self-consistent equation for $\tilde{K}$ takes the form

$$\tilde{K} = K\exp\left[-2\int_0^{\omega_c}\frac{J(\omega)\omega^{-2}d\omega}{(1+8\alpha\omega_c^{2-n}\tilde{K}\omega^{n-3}\mathcal{N}^{-1})^{1/2}}\right],$$

$$\tilde{K} = K\exp[-I(\tilde{K})]. \tag{19}$$

Using Eq. (3), we substitute the power-law form for $J(\omega)$ into $I(\tilde{K})$, and rewrite it in dimensionless form,

$$I(\tilde{K}) = \alpha\left(\frac{\omega_s}{\omega_c}\right)^{1-s}\int_0^1 \frac{x^{s-2}dx}{[1+\Delta(\tilde{K})x^{n-3}]^{1/2}}, \tag{20}$$

where we have defined the dimensionless numbers $x=\frac{\omega}{\omega_c}$ and $\Delta(\tilde{K})=\frac{8\alpha\tilde{K}}{\mathcal{N}\omega_c}$. Comparing Eq. (20) with Eq. (6), we can see that the inclusion of squeezing effects introduces a square root factor into the integrand which can have a profound effect on the renormalization of K. The squeezing provides an effective infrared cutoff to the integral, and thus prevents the infrared divergence if $n<2s+1$ and $\Delta(\tilde{K})$ is finite. Squeezing effects can therefore potentially lead to coherent ground states for ohmic and sub-ohmic baths, as well as sharp coherent-incoherent transitions, as is described for the ohmic case in Refs. 15 and 16.

However, as there can only be a true infrared divergence in the thermodynamic limit, we must consider what happens to the solutions of Eq. (19) as $\mathcal{N}\to\infty$. In this limit we see that $\Delta\to 0$, and thus the integral in Eq. (20) reverts to the form given by the adiabatic approximation.[4,5] Therefore for ohmic and sub-ohmic baths, the DSS always leads to an incoherent thermodynamic ground state, and there are no possible transitions from coherent to incoherent states. Interestingly, a recent variational study of squeezing effects in a weakly interacting Bose-Einstein condensate also found that the squeezing vanishes in the thermodynamic limit.[20]

We can also show that this conclusion is independent of when we choose to take the thermodynamic limit by solving the self-consistent equation at finite $\mathcal{N}$ and then sending $\mathcal{N}\to\infty$. At finite $\mathcal{N}$ there can be no phase transition as there will always be an infrared cutoff ω_{IR} arising from the finite size of the system. This frequency scales inversely with the linear dimensions of the system, and can be written $\omega_{IR}=\mathcal{N}^{-1/3}\omega_0$, where ω_0 is a nonuniversal frequency which depends on the density of oscillators in a given bath. The squeezing effects provide an effective infrared cutoff at a frequency of approximately $\omega_c\Delta^{1/(3-n)}\propto\mathcal{N}^{-1/(3-n)}$, which vanishes faster than ω_{IR} as $\mathcal{N}$ becomes very large. Thus in the limit of large $\mathcal{N}$, the squeezing factor can be ignored in the integrand of Eq. (20), and the renomalization is given by the adiabatic formula of Eq. (6), but with an infrared cutoff at ω_{IR}. The renormalized matrix element is then given by

$$\tilde{K} = K\exp\left[-\frac{\alpha}{1-s}\left(\frac{\omega_s\mathcal{N}^{1/3}}{\omega_0}\right)^{1-s}\right], \tag{21}$$

for the case of sub-ohmic coupling, and

$$\widetilde{K} = K\left(\frac{\omega_0}{\omega_c \mathcal{N}^{1/3}}\right)^{\alpha}, \tag{22}$$

for ohmic coupling.

As expected for finite $\mathcal{N}$, the TLS retains its coherence for arbitrary coupling strength, but this coherence always vanishes as $\mathcal{N}\to\infty$. Due to the fact that the infrared divergence is prevented by ω_{IR} rather than $\omega_c \Delta^{1/(3-n)}$, the coherence does not depend on the TLS-bath coupling, but the coherence is still nonuniversal through its dependence on ω_0.

Although we find no evidence for squeezing at finite $\mathcal{N}$, squeezing effects can be very important for coupling to a single mode,[13] or possibly a few discrete modes. For instance, such squeezing effects have recently been predicted for a TLS coupled to a single nanomechanical oscillator.[21]

In conclusion, when one uses the correct system-size scaling of the TLS-bath couplings, analysis of the DSS shows that all the squeezing and nonuniversal effects vanish in the thermodynamical limit. In thermodynamic equilibrium, this variational state thus reproduces the results of the basic adiabatic approximation, and fails to capture the interesting transition physics of ohmic and sub-ohmic systems. Squeezing effects are also found to be absent when one considers the leading order finite-size corrections around the zero-order adiabatic state.

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