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Variational study of dissipative two-state systems

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Two variational states, the displaced state and the displaced-squeezed state, are compared for a two-state system with super-Ohmic dissipation, and their dependence on the form of the coupling strength $g_l \sim \omega_l^\lambda$ (ω_l is the phonon frequency) is analyzed. We find that, in the strong-coupling region, the displaced-squeezed state is more stable and the ground-state properties depend not only on the spectral density but also on the index λ. Moreover, we find that the stable area of the displaced-squeezed state increases as λ decreases.

The spin-boson Hamiltonian

$$H = -\Delta_0 \sigma_x + \sum_l \omega_l b_l^\dagger b_l + \sigma_z \sum_l g_l (b_l^\dagger + b_l) \tag{1}$$

has been used to study the dissipative effect of a bath in the quantum tunneling or two-state system.[1] In the Hamiltonian (1), σ_x and σ_z are Pauli matrices, and Δ_0 is the bare tunneling parameter, while the bath is described by a set of harmonic oscillators (phonons) with frequencies ω_l and coupling constants $g_l = g_0(\omega_l/\omega_0)^\lambda$ (where ω_0 is the upper cutoff).

It has been shown, on the basis of path-integral techniques,[1] that complete information about the dissipative effect of the bath is contained in the spectral density

$$J(\omega) \sim \sum_l g_l^2 \delta(\omega - \omega_l) \sim \omega^s , \tag{2}$$

with $s = 2\lambda + n - 1$, independent of the explicit form of the coupling constant g_l. Here n is the exponent of the phonon density of states $D(\omega) = \omega^{n-1}/\omega_0^n$. Recently this concept of universality was questioned by Chen and Yu.[2] Their work indicated that the static properties of an ohmic dissipative ($s = 1$) two-state system at zero temperature depends not only on the spectral density but also on the explicit form of the coupling constant. The main purpose of this paper is to extend this study to super-Ohmic dissipative cases $s = 2$ and 3 by a variational approach, and we want to find out at what conditions the universal description breaks down for super-Ohmic dissipation.

The basic assumption of the path-integral approach is that the bath degrees of freedom can be integrated out as Gaussian integrals with displaced centers.[3] It is implicitly assumed that the only effect of the two-state system on the bath is to displace the centers of the phonons. However, it is understood physically that the coupling of the bath to a two-state system may give rise to two different effects: displacement and deformation of the phonon states. The displaced-state approach only considers the former, and omits the latter. Recently, a displaced-squeezed state has been proposed for the variational ground state of phonons coupled with a two-state system.[4] Both the displacement and deformation effects are taken into account in the displaced-squeezed state. In the following, the stability of the displaced and the displaced-squeezed states, and their dependence on the indexes and λ will be studied for super-Ohmic dissipation.

The variational displaced state has the form[5]

$$|\phi_1\rangle = \exp\left[-\sigma_z \sum_l C_l (b_l^\dagger - b_l) \right] |\phi_{\rm vac}\rangle , \tag{3}$$

where the C_l's are variational parameters, $|\phi_{\rm vac}\rangle$ stands for both the vacuum state of phonons and the ground state of the two-state system ($\sigma_z |\phi_{\rm vac}\rangle = |\phi_{\rm vac}\rangle$). The energy of state $|\phi_1\rangle$ is

$$E_1 = -\Delta_1 + \sum_l (\omega_l C_l - 2g_l) C_l + \sum_l g_l^2/\omega_l , \tag{4}$$

where $\Delta_1 = \Delta_0 \kappa_1$ is the renormalized tunneling parameter with the phonon overlapping integral

$$\kappa_1 = \exp\left[-2\sum_l C_l^2 \right] . \tag{5}$$

The condition $\partial E_1/\partial C_l = 0$ gives

$$C_l = g_l/(\omega_l + 2\Delta_1) . \tag{6}$$

Inserting (6) into (4) and (5), we have

$$E_1 = -\Delta_0 \kappa_1 - \omega_0 \beta \left[\int_0^1 \frac{x + 4\alpha\kappa_1}{(x + 2\alpha\kappa_1)^2} x^s dx - \frac{1}{s} \right] , \tag{7}$$

$$\kappa_1 = \exp\left[-2\beta \int_0^1 x^s/(x + 2\alpha\kappa_1)^2 dx \right] , \tag{8}$$

with $\alpha = \Delta_0/\omega_0$, and $\beta = (g_0/\omega_0)^2$. From (7) and (8) one can see that, in the displaced-state approach, the ground-state properties of a dissipative two-state system depend only on the index s of the spectral density $J(\omega)$.

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The variational displaced-squeezed state is[4,6,7]

$$|\phi_2\rangle = \exp\left[-\sigma_z \sum_l (g_l/\omega_l(b_l^\dagger - b_l)\right] \times \exp\left[-\sum_l \gamma_l (b_l b_l - b_l^\dagger b_l^\dagger)\right] |\phi_{\text{vac}}\rangle , \qquad (9)$$

where the γ_l's are variational parameters. The energy of state $|\phi_2\rangle$ is calculated as

$$E_2 = -\Delta_2 + \sum_l \omega_l \sinh^2(2\gamma_l) , \qquad (10)$$

where $\Delta_2 = \Delta_0 \kappa_2$, and

$$\kappa_2 = \exp\left[-\sum_l (2g_l^2/\omega_l^2) e^{-4\gamma_l}\right] . \qquad (11)$$

Minimizing E_2 leads to

$$\gamma_l = \tfrac{1}{8}\ln(1 + 8\Delta_2 g_l^2/\omega_l^3) . \qquad (12)$$

Using (12), (10) and (11) become

$$E_2 = -\Delta_0\kappa_2 + \frac{\omega_0}{4}\int_0^1 x^{s-2\lambda+1}\{(1+8\alpha\beta\kappa_2 x^{2\lambda-3})^{1/2} + (1+8\alpha\beta\kappa_2 x^{2\lambda-3})^{-1/2} - 2\}dx , \qquad (13)$$

$$\kappa_2 = \exp\left[-2\beta\int_0^1 x^{s-2}(1+8\alpha\beta\kappa_2 x^{2\lambda-3})^{-1/2}dx\right] . \qquad (14)$$

Results (13) and (14) of the displaced-squeezed state indicate that, contrary to the displaced state, the ground-state properties of a dissipative two-state system depend not only on the index s of the spectral density $J(\omega)$ but also on the index λ of the coupling strength $g_l(\omega)$.

The stability of the displaced state and the displaced-squeezed state depend on the parameters s, λ, α, and β. For $S=3$, we have

$$E_1 = -\Delta_0\kappa_1\left[1 - \frac{2}{3}\left\{\ln\kappa_1 + \frac{\beta}{1+2\alpha\kappa_1}\right\}\right] , \qquad (15)$$

$$\kappa_1 = \left[\frac{2\alpha\kappa_1}{1+2\alpha\kappa_1}\right]^{24\alpha^2\beta\kappa_1^2} \times \exp\left\{-\frac{\beta}{1+2\alpha\kappa_1}[1-6\alpha\kappa_1 - 6(2\alpha\kappa_1)^2]\right\} , \qquad (16)$$

$$E_2(\lambda=\tfrac{1}{2}) = -\Delta_0\kappa_2(1 - \tfrac{1}{2}\ln\kappa_2) + \frac{\omega_0}{8}\left[\sqrt{1+8\alpha\beta\kappa_2} - 1\right] , \qquad (17)$$

$$E_2(\lambda=1) = -\Delta_0\kappa_2(1 - \tfrac{2}{3}\ln\kappa_2) + \frac{\omega_0}{6}\left[\sqrt{1+8\alpha\beta\kappa_2} - 1\right] , \qquad (18)$$

$$E_2(\lambda=\tfrac{3}{2}) = -\Delta_0\kappa_2 + \frac{\omega_0}{8}\left[\sqrt{1+8\alpha\beta\kappa_2} + \frac{1}{\sqrt{1+8\alpha\beta\kappa_2}} - 2\right] , \qquad (19)$$

$$\kappa_2(\lambda=\tfrac{1}{2}) = \left[\frac{1+\sqrt{1+8\alpha\beta\kappa_2}}{\sqrt{1+8\alpha\beta\kappa_2}}\right]^{8\alpha\beta^2\kappa_2} \times \exp(-\beta\sqrt{1+8\alpha\beta\kappa_2}) , \qquad (20)$$

$$\kappa_2(\lambda=1) = \left[\frac{\sqrt{8\alpha\beta\kappa_2}}{1+\sqrt{1+8\alpha\beta\kappa_2}}\right]^{96\alpha^2\beta^3\kappa_2^2} \times \exp\left[-\beta\sqrt{1+8\alpha\beta\kappa_2} - 12\alpha\beta\kappa_2\sqrt{1+8\alpha\beta\kappa_2}\right] , \qquad (21)$$

$$\kappa_2(\lambda=\tfrac{3}{2}) = \exp\left[-\frac{\beta}{\sqrt{1+8\alpha\beta\kappa_2}}\right] . \qquad (22)$$

The condition $E_1 = E_2$ determines a critical curve $\alpha_c(\beta)$, which divides the α,β parameter space into two parts: $E_1 < E_2$ for $\alpha > \alpha_c(\beta)$, and $E_1 > E_2$ for $\alpha < \alpha_c(\beta)$. For the limit $\alpha \ll 1$, (15)–(22) become

$$E_1 = -\Delta_0\kappa_1(1 - 4\alpha\beta\kappa_1) , \qquad (23)$$

$$\kappa_1 = \exp[-\beta(1 - 8\alpha\kappa_1)] , \qquad (24)$$

$$E_2(\lambda=\tfrac{1}{2}) = -\Delta_0\kappa_2(1 + \alpha\beta^2\kappa_2) , \qquad (25)$$

$$E_2(\lambda=1) = -\Delta_0\kappa_2(1 - 4\alpha\beta^2\kappa_2) , \qquad (26)$$

$$E_2(\lambda=\tfrac{3}{2}) = -\Delta_0\kappa_2(1 - 2\alpha\beta^2\kappa_2) , \qquad (27)$$

$$\kappa_2(\lambda=\tfrac{1}{2}) = \exp\{-\beta[1 + 4\alpha\beta\kappa_2\ln(2\alpha\beta e^{1-\beta})]\} , \qquad (28)$$

$$\kappa_2(\lambda=1) = \exp[-\beta(1 - 8\alpha\beta\kappa_2)] , \qquad (29)$$

$$\kappa_2(\lambda=\tfrac{3}{2}) = \exp[-\beta(1 - 4\alpha\beta\kappa_2)] . \qquad (30)$$

The condition $E_1 = E_2$ gives

$$\beta_c = \begin{cases} 0 & (\lambda=\frac{1}{2}) \\ 1 & (\lambda=1) \\ 2 & (\lambda=\frac{3}{2}), \end{cases} \tag{31}$$

leading to $E_1 < E_2$ for $\beta < \beta_c$, and $E_1 > E_2$ for $\beta > \beta_c$. For ohmic dissipation ($S=1$), the previous study gave[2,7] $E_1 < E_2$ for $\lambda \geq 1$ and $0 < \beta < \frac{1}{2}$, and $E_1 > E_2$ for $\lambda < 1$ and $0 < \beta < \frac{1}{2}(3-2\lambda)$.

For $S=2$, we obtain

$$E_1 = -\Delta_0 \kappa_1 \left[1 - \tfrac{1}{2}\ln\kappa_1 - \frac{\beta}{1+2\alpha\kappa_1} \right] , \tag{32}$$

$$\kappa_1 = \exp\left\{ -2\beta \left[2 - \frac{1}{1+2\alpha\kappa_1} - 4\alpha\kappa_1 \ln\frac{1+2\alpha\kappa_1}{2\alpha\kappa_1} \right] \right\} , \tag{33}$$

$$E_2(\lambda=\tfrac{1}{2}) = -\Delta_0\kappa_2(1-\tfrac{1}{3}\ln\kappa_2) + \frac{\omega_0}{6}\left(\sqrt{1+8\alpha\beta\kappa_2} - 1 \right) , \tag{34}$$

$$E_2(\lambda=1) = -\Delta_0\kappa_2(1-\tfrac{1}{2}\ln\kappa_2) + \frac{\omega_0}{4}(\sqrt{1+8\alpha\beta\kappa_2} - 1) , \tag{35}$$

$$E_2(\lambda=\tfrac{3}{2}) = -\Delta_0\kappa_2 + \frac{\omega_0}{4}\left[\sqrt{1+8\alpha\beta\kappa_2} + \frac{1}{\sqrt{1+8\alpha\beta\kappa_2}} - 2 \right] , \tag{36}$$

$$\kappa_2(\lambda=\tfrac{1}{2}) = \exp[-2\beta(\sqrt{1+8\alpha\beta\kappa_2} - \sqrt{8\alpha\beta\kappa_2})] , \tag{37}$$

$$\kappa_2(\lambda=1) = \exp\left[-2\beta \left[\sqrt{1+8\alpha\beta\kappa_2} - 8\alpha\beta\kappa_2 \ln\frac{1+\sqrt{1+8\alpha\beta\kappa_2}}{\sqrt{8\alpha\beta\kappa_2}} \right] \right] , \tag{38}$$

$$\kappa_2(\lambda=\tfrac{3}{2}) = \exp\left[-\frac{2\beta}{\sqrt{1+8\alpha\beta\kappa_2}} \right] . \tag{39}$$

The numerical results of the critical curve $\alpha_c(\beta)$ are shown in Fig. 1(a) for $S=3$, and in Fig. 1(b) for $S=2$. On the left side of the critical curve, we have $E_1 < E_2$ and the displaced state is more stable; while on the right side of it, we have $E_1 > E_2$ and the displaced-squeezed state is more stable. From Figs. 1(a) and 1(b), one can see that the stable area of the displaced-squeezed state increases as the index λ decreases. This result can be explained qualitatively in that the coupling strength $g_l(\omega) \sim (\omega_l/\omega_0)^\lambda$ increases as λ is reduced, and thus the deformation of the phonon state due to coupling with a two-state system becomes more important. From this picture, we may refer to the stable area of the displaced-squeezed sate as a strong-coupling region, and to that of

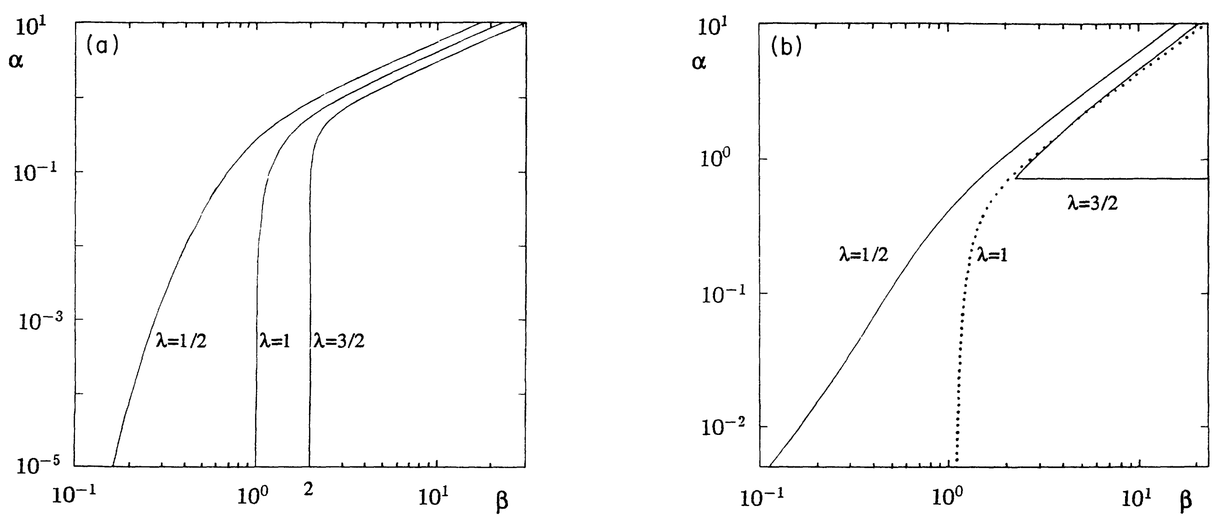

FIG. 1. The critical curve of $E_1 = E_2$ for $\lambda = \frac{1}{2}$, 1, and $\frac{3}{2}$. (a) $S=3$, (b) $S=2$. The displaced state is more stable on the left side of the curve, and the displaced-squeezed state is more stable on the right side.

the displaced state as a weak-coupling region.

In conclusion, the present variational study shows that, for a two-state system with super-Ohmic dissipation, in a weak-coupling region there is a universal behavior in the ground-state properties. The universality breaks down in the strong-coupling region, as the ground-state properties depend not only on the spectral density but also on the explicit form of the coupling strength.

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