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Variational ground state of the model of a two-state system coupled with phonons

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The ground state of the model of a two-state system coupled with phonons is studied by a variational method. Two trial states, the displaced state, and the displaced-squeezed state, for the phonon subsystem are compared, and their dependence on tunneling parameter Δ, phonon frequency ω, and coupling strength g is analyzed. We find that for $\Delta/\omega \ll 1$ the displaced state is more stable for $g/\omega < 1$, while the displaced-squeezed state is preferable for $g/\omega > 1$.

Recently, great interest has been raised in the dissipative effect of a bath on a quantum tunneling problem or on a two-state system,[1] e.g., dissipative macroscopic tunneling phenomena[2] and atomic tunneling states in solids.[3,4] Using a renormalization-group procedure, Chakravarty[5] and Bray and Moore[6] have shown that, for the Ohmic dissipation and at zero temperature, there exists a sharp localization-delocalization transition. It is believed that such a transition is the result of infrared divergence induced by the low-frequency phonons of the bath and that it depends strongly on the phonon behavior, especially the low-frequency phonons of the coupling system. Unfortunately, we know little about the ground states of phonons under coupling with a two-state system. Only a displaced state has been proposed[7,8] as the variational ground state, and it gave[9] precisely the same conditions for the localization-delocalization transition as that of the renormalization-group procedure. Such a method was also extended to a system of dissipative quantum tunneling diffusion.[10] It is understood physically that the coupling with a two-state system has two different influences on the wave function of phonons: displacement and deformation. The displaced state only considers the former and omits the latter. For high-frequency modes and weak coupling, the displaced-state approximation may be good, while for low-frequency modes and strong coupling, such an approximation is not sufficient, and one must take account of the effect of the deformation. Recently, we have proposed[11] a displaced-squeezed state as the variational ground state of phonons coupled with a two-state system. This new state includes both displacement and deformation effects. The main purpose of this Brief Report is to compare these two variational ground states, the displaced state, and the displaced-squeezed state, and to show which is more stable.

For simplicity, we only consider the model of a two-state system coupled with one phonon mode. It is not difficult to extend the method to a many-mode problem. The Hamiltonian is[1]

$$H=-\Delta\sigma_x+\omega b^\dagger b+g(b^\dagger+b)\sigma_z\,, \tag{1}$$

where Δ is the bare tunneling parameter, σ's the Pauli matrices, $b^\dagger$ and b the phonon operators, and g the coupling coefficient. Applying, as usual, the unitary transformation

$$S=\exp[\sigma_z(g/\omega)(b^\dagger-b)] \tag{2}$$

to (1), and then for the two-state system in its ground state ($\sigma_x=1$), we have an effective Hamiltonian for phonon subsystem[11]

$$H_{\rm ph}^{\rm eff}=\omega b^\dagger b-\Delta\cosh[(2g/\omega)(b^\dagger-b)]-g^2/\omega\,. \tag{3}$$

Because of the nonlinear interaction in $H_{\rm ph}^{\rm eff}$, it is difficult to find an exact solution, and one must look for approximations. To zero order in g, the ground state of $H_{\rm ph}^{\rm eff}$ is a vacuum state, or a displaced state in its original base. Up to g^2, the ground state is a squeezed state, or displaced-squeezed state in its original base. In the following, we will use both the displaced state and the displaced-squeezed state as variational ground states to calculate the ground-state energy of the Hamiltonian (1).

The variational displaced state has the form[9]

$$\phi_1=\exp[-\lambda\sigma_z(b^\dagger-b)]\phi_{\rm vac}\,, \tag{4}$$

where $\phi_{\rm vac}$ denotes both the vacuum state for phonons and the symmetric state for the two-state system ($\sigma_x\phi_{\rm vac}$

$=\phi_{vac}$). The energy of ϕ_1 is

$$E_1=\langle\phi_1|H|\phi_1\rangle=-\Delta\kappa_1+\omega\lambda^2-2g\lambda\ , \tag{5}$$

with

$$\kappa_1=\exp(-2\lambda^2)\ . \tag{6}$$

The condition $\partial E_1/\sigma\lambda=0$ determines the variational parameter λ as

$$\lambda=g/(\omega+2\Delta\kappa_1)\ . \tag{7}$$

Then (5) and (6) become

$$E_1=-\omega\left[\alpha\kappa_1+\beta\frac{1+4\alpha\kappa_1}{(1+2\alpha\kappa_1)^2}\right]\ , \tag{8}$$

$$\kappa_1=\exp[-2\beta/(1+2\alpha\kappa_1)^2]\ , \tag{9}$$

with $\alpha=\Delta/\omega$, $\beta=(g/\omega)^2$.

The variational displaced-squeezed state is[11]

$$\phi_2=\exp[-\sigma_z(g/\omega)(b^\dagger-b)]\exp[-\gamma(b^2-b^{+2})]\phi_{vac}\ . \tag{10}$$

Using the properties of the unitary transformation $R=\exp[\gamma(b^2-b^{+2})]$, we can calculate the energy of ϕ_2:

$$E_2=\langle\phi_2|H|\phi_2\rangle=-\omega(\alpha\kappa_2+\beta-\sinh^2 2\gamma)\ , \tag{11}$$

with

$$\kappa_2=\exp(-2\beta e^{-4\gamma})\ . \tag{12}$$

Minimizing E_2 leads to the equation for variational parameter γ

$$\gamma=\tfrac{1}{8}\ln(1+8\alpha\beta\kappa_2)\ , \tag{13}$$

and then

$$E_2=-\omega[\alpha\kappa_2+\beta+\tfrac{1}{2}-\tfrac{1}{4}(1+8\alpha\beta\kappa_2)^{1/2}-\tfrac{1}{4}(1+8\alpha\beta\kappa_2)^{-1/2}]\ , \tag{14}$$

$$\kappa_2=\exp[-2\beta/(1+8\alpha\beta\kappa_2)^{1/2}]\ . \tag{15}$$

Now we want to compare E_1 with E_2 in the limit $\alpha=\Delta/\omega\ll 1$, where the usual adiabatic approximation works.[1] It can be proved $\beta\kappa_i<1/2e$ $(i=1,2)$ for $\alpha\ll 1$. Then (8) and (14) can be approximated as

$$E_1=-\omega(\alpha\kappa_1+\beta)+O(\alpha^2)\ , \tag{16}$$

$$E_2=-\omega(\alpha\kappa_2+\beta)+O(\alpha^2)\ . \tag{17}$$

Based on (9) and (15)–(17), we have a characteristic value β_c satisfied for $\kappa_1>\kappa_2$ and $E_1<E_2$ for $\beta<\beta_c$; $\kappa_1<\kappa_2$ and $E_1>E_2$ for $\beta>\beta_c$. β_c is determined by $\kappa_1=\kappa_2$ (or $E_1=E_2$), then combining (9) and (15) gives

$$(1+2\alpha\kappa_1)^2=(1+8\alpha\beta_c\kappa_1)^{1/2}\ .$$

Taking into consideration $\alpha\ll 1$ and $\kappa_1<1$, we have $\beta_c=(g/\omega)^2=1+O(\alpha^2)$. Namely, the displaced state (4) is more stable for $(g/\omega)<1$ and the displaced-squeezed state (10) is more stable for $(g/\omega)>1$.

In conclusion, our study shows that the interaction with a two-state system has two different effects on phonon states: the displacement and the deformation. For high-frequency phonons and weak coupling, the displacement is dominant and the displaced state is more stable. While for low-frequency phonons and strong coupling, one must take account of both effects and the displaced-squeezed state is preferable.

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