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Correlated squeezed-state approach for a dissipative two-state system

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We propose a correlated squeezed-state approach to study the dissipative two-state system at zero temperature. We have found that the ground state of this system can be better described by the correlated squeezed-state ansatz than those given in earlier variational treatments. In this new ground state the suppression effect of the phonon overlapping integral on the renormalized tunneling parameter is much more alleviated. Thus, the condition for the localization-delocalization transition of the two-state system is significantly modified in this correlated squeezed state, when compared with previous studies.

I. INTRODUCTION

Recently much attention has been paid to the study of the influence of a phonon bath on a quantum-tunneling system.[1] For a particle with small tunneling probability, the system may be approximated as a dissipative two-state system. In terms of pseudospin formalism, the Hamiltonian of a two-state system coupled linearly to a phonon bath can be written as

$$H=-\Delta_0\sigma_x+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+\sum_{\mathbf{k}}g_{\mathbf{k}}(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}})\sigma_z\ , \qquad (1)$$

where $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^{\dagger}$ are boson annihilation and creation operators, and σ_x and σ_z are usual Pauli matrices. In this Hamiltonian Δ_0 represents the bare tunneling matrix element and $g_{\mathbf{k}}$ the coupling constant to the phonon mode $\mathbf{k}$. When $\Delta_0=0$, the system consists of a set of oscillators, displaced in one direction when the tunneling system is in one of the two levels and displaced in the other direction when the tunneling system is in the other of the two levels. Thus there is a twofold degenerate localized ground state with energy $E=-\sum_{\mathbf{k}}g_{\mathbf{k}}^2(\hbar\omega_{\mathbf{k}})^{-1}$. On the other hand, when $g_{\mathbf{k}}=0$, the eigenstates of the system are the symmetric and antisymmetric combinations of the spin states with energies $E=\pm\Delta_0$ Thus this two-state system exhibits a competition between the localization inherent in the interaction with the phonons and the delocalization inherent in the tunneling. In the intermediate regime, the effect of the phonons is to modify the tunneling matrix element and damp the oscillations.

This rather simple two-level model has long been a research area of considerable interest because of its extensive applicability in various fields of physics, such as molecular and solid-state physics, quantum optics, quantum dissipation, and quantum chaos. For instance, the model has been used to study the physics of polaron formation, molecular polarons, atoms in a cavity with a radiating field, defects in insulators, exciton motion, chaos in quantum systems, paraelastic defects in solids, diffusion of impurities, spin-phonon relaxation, sound attenuation in glasses, Kondo effect in metallic alloys, etc. Despite the relatively large amount of work found in the literature, no exact solution to the problem is yet available. Even for the simplest form of the model, namely, a two-state system coupled to a single mode, the eigenstates and eigenvalues are not known analytically in general. There do exist, however, analytic treatments of the model based on the variational principle.[2-5] So far the conventional approach to the dissipative two-state system works on an adiabatic (Born-Oppenheimer) type of approximation. According to the adiabatic approximation, the tunneling particle moves slowly and the phonon variables always instantaneously follow its motion; therefore, when the particle is in the state of $\sigma_z=\pm1$, the phonon operator $b_{\mathbf{k}}$ will be displaced to $b_{\mathbf{k}}\pm g_{\mathbf{k}}(\hbar\omega_{\mathbf{k}})^{-1}$. Motivated from these facts Tanaka and Sakurai[2] as well as separately Silbey and Harris[3] suggested a multimode coherent state as the approximate ground-state wave function for the system:

$$|G\rangle=\exp\left\{\sigma_z\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}(b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}})\right\}|\mathrm{vac}\rangle\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}\ , \qquad (2)$$

where $|\mathrm{vac}\rangle$ is the vacuum state of the phonon bath and $\{f_{\mathbf{k}}\}$ are the variational parameters. The expectation value of H in this multimode coherent state is given by

$$E=-\Delta_0K+\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}^2+2f_{\mathbf{k}}g_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}\ , \qquad (3)$$

where $K=\exp\{-\sum_{\mathbf{k}}2f_{\mathbf{k}}^2(\hbar\omega_{\mathbf{k}})^{-2}\}$ is the phonon overlapping integral. It is clear that the tunneling parameter endures serious suppression by the phonon overlapping integral. However, as pointed out by Sethna,[6] the application of these results to the atomic tunneling process in solids induces substantial difficulty.

In a recent paper Chen, Zhang, and Wu[4] proposed a squeezed-state approach to study the dissipative two-state system. To account for the anharmonicity of each phonon mode induced by coupling with the tunneling particle, they suggested a modification of the ansatz given in the adiabatic approximation by replacing the coherent state of each mode by a squeezed state,[7] i.e.,

$$|G\rangle = \exp\left\{-\sigma_z \sum_{\mathbf{k}} \frac{g_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})\right\} \times \exp\left\{\sum_{\mathbf{k}} \gamma_{\mathbf{k}}[(b_{\mathbf{k}}^\dagger)^2 - b_{\mathbf{k}}^2]\right\}|\text{vac}\rangle \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} , \quad (4)$$

where $\{\gamma_{\mathbf{k}}\}$ are the variational parameters. The squeezed state is a nonclassical state characterized by a reduction in one of the two quadrature components of the phonon mode, when compared with the coherent state. Their results show that the ground state of the system can be better described by this new ansatz, which by construction gives an estimate of the ground-state energy lower than that of the adiabatic approximation:

$$E = -\Delta_0 \tilde{K} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \sinh^2(2\gamma_{\mathbf{k}}) - \sum_{\mathbf{k}} \frac{g_{\mathbf{k}}^2}{\hbar\omega_{\mathbf{k}}} , \quad (5)$$

where $\tilde{K} = \exp\{-\sum_{\mathbf{k}} 2g_{\mathbf{k}}^2(\hbar\omega_{\mathbf{k}})^2 \exp(-4\gamma_{\mathbf{k}})\}$ is the phonon overlapping integral in this squeezed-state ansatz. It is evident that in this new approximate ground state not only the suppression effect of the phonon overlapping integral on the renormalized tunneling parameter is more alleviated than that in the adiabatic approximation, but also the condition for the localization-delocalization transition of the tunneling particle is modified compared with the previous studies.

Nevertheless, both of the above trial wave functions for the ground state of the tunneling system are within the Hartree approximation and thus uncorrelated. In order to account for the strong correlation and anharmonicity of the interaction between different phonon modes induced by the linear coupling with the tunneling particle, one needs to go beyond the Hartree approximation. In this paper we shall introduce the correlated squeezed-state ansatz as a new candidate of the ground state of the dissipative tunneling system. The correlated squeezed state is a highly correlated state of the phonon modes that exhibits reduced quadrature noise in linear combinations of variables of the phonon modes.[8] This correlated squeezed-state approach has been applied earlier to the linear E-e Jahn-Teller effect, a tunneling particle coupled to phonons, the large polarons, and some interacting electron-phonon systems.[9–14] In the next section we shall apply the correlated squeezed state as the variational trial wave function for the ground state of the dissipative two-state system. Numerical results for two special cases—(i) a two-state system coupled to two identical phonon modes, and (ii) a two-state system coupled to a dispersionless phonon bath—will be discussed in detail as examples showing the significance of the correlation effect between the phonon modes. Finally, the conclusion will be presented in Sec. III.

II. GROUND STATE OF THE DISSIPATIVE TUNNELING SYSTEM

In this section we shall apply the correlated squeezed-state approach to the problem of a tunneling particle coupled linearly to a phonon bath. Applying the unitary displacement transformation

$$D = \exp\left\{\sigma_z \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})\right\} \quad (6)$$

to the Hamiltonian in Eq. (1), we obtain

$$\tilde{H} \equiv D^\dagger H D \equiv \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}^2 + 2f_{\mathbf{k}}g_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sigma_z \sum_{\mathbf{k}} (f_{\mathbf{k}} + g_{\mathbf{k}})(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) - \Delta_0 \sigma_x \cosh\left[\sum_{\mathbf{k}} \frac{2f_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})\right] + i\Delta_0 \sigma_y \sinh\left[\sum_{\mathbf{k}} \frac{2f_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}(b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})\right] . \quad (7)$$

This shows that the linear coupling with the tunneling particle induces nonlinear interactions between phonons not only in the same mode, but also in different modes. To zeroth order of $g_{\mathbf{k}}$ in the weak-coupling limit, the Hamiltonian $\tilde{H}$ is already diagonal provided that $f_{\mathbf{k}} = -g_{\mathbf{k}}$. It is quite obvious that the Hamiltonian $\tilde{H}$ cannot be solved exactly, so we shall tackle it approximately by the variational approach. Taking into account the anharmonicity and correlation of the phonon modes, we now propose a generalized multimode squeezed vacuum state as the trial wave function for the ground state of the system:[8]

$$|G\rangle = \exp\left\{\frac{1}{2} \sum_{\mathbf{k},\mathbf{k}'} \alpha_{\mathbf{k},\mathbf{k}'}(b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger - b_{\mathbf{k}} b_{\mathbf{k}'})\right\}|\text{vac}\rangle \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} , \quad (8)$$

where $\alpha_{\mathbf{k},\mathbf{k}'} = \alpha_{\mathbf{k}',\mathbf{k}}$. The generalized multimode squeeze operator $\tilde{S}(\{\alpha_{\mathbf{k},\mathbf{k}'}\})$ transforms the annihilation and creation operators as follows:

$$\tilde{S}^\dagger \mathbf{a} \tilde{S} = \cosh(|\boldsymbol{\alpha}|)\mathbf{a} + \sinh(|\boldsymbol{\alpha}|)|\boldsymbol{\alpha}|^{-1}\boldsymbol{\alpha} a^\dagger , \quad (9)$$

$$\tilde{S}^\dagger \mathbf{a}^\dagger \tilde{S} = \cosh(|\boldsymbol{\alpha}|^T)\mathbf{a}^\dagger + \sinh(|\boldsymbol{\alpha}|^T)(|\boldsymbol{\alpha}|^T)^{-1}\boldsymbol{\alpha}^* \mathbf{a} , \quad (10)$$

where $|\boldsymbol{\alpha}|^T$ is the transpose of $|\boldsymbol{\alpha}|$, i.e., $(|\boldsymbol{\alpha}|^T)_{\mathbf{k},\mathbf{k}'} = |\boldsymbol{\alpha}|_{\mathbf{k}',\mathbf{k}}$, and $\mathbf{a}$ is the column vector consisting of annihilation operators $a_{\mathbf{k}}$, and $\mathbf{a}^\dagger$ is the vector of creation operators. Here the matrices $|\boldsymbol{\alpha}|$ and $|\boldsymbol{\alpha}|^{-1}$ are defined in the following way:

$$(|\boldsymbol{\alpha}|^2)_{\mathbf{k},\mathbf{k}'}=\sum_{\mathbf{q}}(|\boldsymbol{\alpha}|)_{\mathbf{k},\mathbf{q}}(|\boldsymbol{\alpha}|)_{\mathbf{q},\mathbf{k}'}=\sum_{\mathbf{q}}\alpha_{\mathbf{k},\mathbf{q}}\alpha^*_{\mathbf{q},\mathbf{k}'}\ , \tag{11}$$

$$\delta_{\mathbf{k},\mathbf{k}'}=\sum_{\mathbf{q}}(|\boldsymbol{\alpha}|^{-1})_{\mathbf{k},\mathbf{q}}(|\boldsymbol{\alpha}|)_{\mathbf{q},\mathbf{k}'}\ , \tag{12}$$

so that

$$[\cosh(|\boldsymbol{\alpha}|)]_{\mathbf{k},\mathbf{k}'}=\delta_{\mathbf{k},\mathbf{k}'}+\frac{1}{2!}\sum_{\mathbf{q}}\alpha_{\mathbf{k},\mathbf{q}}\alpha^*_{\mathbf{q},\mathbf{k}'}+\frac{1}{4!}\sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''}\alpha_{\mathbf{k},\mathbf{q}}\alpha^*_{\mathbf{q},\mathbf{q}'}\alpha_{\mathbf{q}',\mathbf{q}''}\alpha^*_{\mathbf{q}'',\mathbf{k}'}+\cdots\ , \tag{13}$$

$$\begin{aligned}[\sinh(|\boldsymbol{\alpha}|)|\boldsymbol{\alpha}|^{-1}\boldsymbol{\alpha}]_{\mathbf{k},\mathbf{k}'}&=\sum_{\mathbf{q},\mathbf{q}'}[\sinh(|\boldsymbol{\alpha}|)]_{\mathbf{k},\mathbf{q}}(|\boldsymbol{\alpha}|^{-1})_{\mathbf{q},\mathbf{q}'}(\boldsymbol{\alpha})_{\mathbf{q}',\mathbf{k}'}\\&=\frac{1}{1!}\alpha_{\mathbf{k},\mathbf{k}'}+\frac{1}{3!}\sum_{\mathbf{q},\mathbf{q}'}\alpha_{\mathbf{k},\mathbf{q}}\alpha^*_{\mathbf{q},\mathbf{q}'}\alpha_{\mathbf{q}',\mathbf{k}'}+\frac{1}{5!}\sum_{\mathbf{q},\mathbf{q}',\mathbf{q}'',\mathbf{q}'''}\alpha_{\mathbf{k},\mathbf{q}}\alpha^*_{\mathbf{q},\mathbf{q}'}\alpha_{\mathbf{q}',\mathbf{q}''}\alpha^*_{\mathbf{q}'',\mathbf{q}'''}\alpha_{\mathbf{q}''',\mathbf{k}'}+\cdots\ .\end{aligned} \tag{14}$$

Provided the matrix $\boldsymbol{\alpha}$ is real, the generalized multimode squeezed state is a multimode minimum-uncertainty state, which exhibits generalized multimode squeezing in the fluctuations of the phonon modes. Then the expectation value of the Hamiltonian is given by

$$\begin{aligned}E&\equiv\langle G|\tilde{H}|G\rangle\\&=\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}^2+2f_{\mathbf{k}}g_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}-\frac{1}{2}\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}+\frac{1}{4}\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}[\exp(2\boldsymbol{\alpha})]_{\mathbf{k},\mathbf{k}}\\&\quad+\frac{1}{4}\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}[\exp(-2\boldsymbol{\alpha})]_{\mathbf{k},\mathbf{k}}-\Delta_0 Z\ ,\end{aligned} \tag{15}$$

where

$$Z=\exp\left\{-2\sum_{\mathbf{k},\mathbf{k}'}\frac{f_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}[\exp(-2\boldsymbol{\alpha})]_{\mathbf{k},\mathbf{k}'}\frac{f_{\mathbf{k}'}}{\hbar\omega_{\mathbf{k}'}}\right\} \tag{16}$$

is the phonon overlapping integral in this correlated squeezed-state ansatz. The optimal values of $f_{\mathbf{k}}$ and $\alpha_{\mathbf{k},\mathbf{k}'}$ are determined by the variational approach, that is, when E arrives at its stable minimum. It is important to note that the energy E in Eq. (15) with optimal values of $f_{\mathbf{k}}$ and $\alpha_{\mathbf{k},\mathbf{k}'}$ is by construction lower than those of the earlier studies mentioned in Sec. I. This means that the correlated squeezed-state ansatz is more stable as the ground state of the system. Also, in this new approximate ground state the suppression effect of the phonon overlapping integral on the renormalized tunneling parameter is more alleviated than that in the adiabatic approximation. Hence the condition for the localization-delocalization transition of the tunneling system is modified in comparison with the earlier studies.

Now minimizing E by varying $A_{\mathbf{k}}\equiv f_{\mathbf{k}}/(\hbar\omega_{\mathbf{k}})$ and $(e^{2\alpha})_{\mathbf{k},\mathbf{k}'}$, we obtain two coupled transcendental equations:

$$0=A_{\mathbf{k}}+\frac{g_{\mathbf{k}}}{\hbar\omega_{\mathbf{k}}}+\frac{2\Delta_0 Z}{\hbar\omega_{\mathbf{k}}}\sum_{\mathbf{q}}A_{\mathbf{q}}(e^{-2\alpha})_{\mathbf{q},\mathbf{k}}\ , \tag{17}$$

$$\begin{aligned}0=\frac{1}{4}\hbar\omega_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}&+\frac{1}{4}\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}\{(e^{-2\alpha})^2_{\mathbf{q},\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}\\&-2(e^{-2\alpha})_{\mathbf{k},\mathbf{q}}(e^{-2\alpha})_{\mathbf{q},\mathbf{k}'}\}\\-\Delta_0 Z&\left\{-2\sum_{\mathbf{q},\mathbf{q}'}A_{\mathbf{q}}(e^{-2\alpha})_{\mathbf{q},\mathbf{k}}(e^{-2\alpha})_{\mathbf{k},\mathbf{q}'}A_{\mathbf{q}'}\delta_{\mathbf{k},\mathbf{k}'}\right.\\&\left.+4\sum_{\mathbf{q},\mathbf{q}'}A_{\mathbf{q}}(e^{-2\alpha})_{\mathbf{q},\mathbf{k}}(e^{-2\alpha})_{\mathbf{k}',\mathbf{q}'}A_{\mathbf{q}'}\right\}\ ,\end{aligned} \tag{18}$$

whose solution yields the optimal values of the variational parameters. In general, these equations must be solved by numerical methods. However, in order to obtain analytical results without loss of physical content, here we shall focus our attention to the following two particular cases, namely (i) a tunneling system coupled to two identical phonon modes, and (ii) a tunneling system coupled to a dispersionless phonon bath.

A. Tunneling system coupled to two identical phonon modes

To illustrate the correlation effect between the phonon modes more explicitly, we shall first confine ourselves to the special case in which the tunneling system is coupled to two identical phonon modes ($\hbar\omega_1=\hbar\omega_2\equiv\hbar\omega$ and $g_1=g_2\equiv g$). The correlated trial wave function for the ground state is given by

$$\begin{aligned}|G\rangle=\exp&\left\{\sigma_z\frac{f}{\hbar\omega}\sum_{i=1}^{2}(b_i^\dagger-b_i)\right\}\\&\times\exp\left\{\gamma\sum_{i=1}^{2}(b_i^{\dagger 2}-b_i^2)\right\}\\&\times\exp\{\alpha(b_1^\dagger b_2^\dagger-b_1b_2)\}|\text{vac}\rangle\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}\ ,\end{aligned} \tag{19}$$

where f, α, and γ are the variational parameters. Note that this trial ground state is chosen slightly different from the generalized two-mode squeezed state introduced above. [In quantum optics, the operators $\exp\{\alpha(b_i^{\dagger 2}-b_i^2)\}$ are called the single-mode squeeze operators which generate the single-mode squeezing,[15] whilst the operator $\exp\{\alpha(b_1^\dagger b_2^\dagger-b_1b_2)\}$ is the two-mode squeeze operator which is responsible for the two-mode squeezing.[16,17]] It is because in this way a clearer picture of the interplay of the anharmonicity and correlation of the phonon modes can be obtained. Here the modified adiabatic approximation corresponds to the special case in which both γ and α equal zero, whereas Chen *et al.*'s squeezed-state approach is the case with $\alpha=0$ and $f=-g$. The total energy E of the system can then be written as

$$\begin{aligned}E=2f(f+2g)&+[\cosh4\gamma\cosh2\alpha-1]\\&-\Delta_0\exp\{-4f^2\exp(-4\gamma)\exp(-2\alpha)\}\ .\end{aligned} \tag{20}$$

For simplicity, we have set the phonon energy equal to unity. We now minimize the energy with respect to the three variational parameters.

In Fig. 1 we show the minimum energy for two cases: in (a) we consider the coupling g fixed to values 0.1, 1, and 10, and let the Δ_0 vary. In (b) we let g vary, while Δ_0 is fixed. If Δ_0 is small, the first term in Eq. (20) dominates and the energy is $E \approx -2g^2$, whereas when Δ_0 is large, the energy is simply $E \approx -\Delta_0$. In these two extreme cases we expect neither the squeezing (controlled by γ) nor the correlation (controlled by α) to play any role. However, in the intermediate region we see a transition between the two extreme limits at $2g^2 \approx \Delta_0$, where all three terms in Eq. (20) are of the same magnitude. This is the interesting, nontrivial region which has been studied the most in the literature.

In Fig. 2 we show the effect of taking the correlation into account for two cases: (a) $g=1$ and (b) $g=10$. For every value of α, the two remaining parameters f and γ are varied so as to minimize the energy. We clearly see that keeping a finite α lowers the energy in both cases, and that the reduction is as much as 10% for $g=10$. Thus the correlation does play a significant role and has to be accounted for to obtain a good estimate of the ground-state energy.

In Fig. 3 we show how important the various terms in

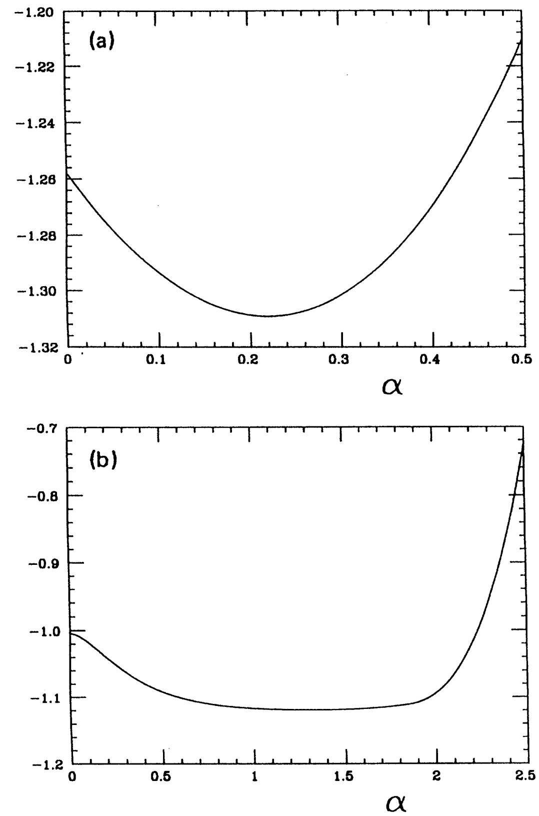

FIG. 2. Minimum energy versus α for (a) $g=1$ and (b) $g=10$, at the transition $\Delta_0=2g^2$.

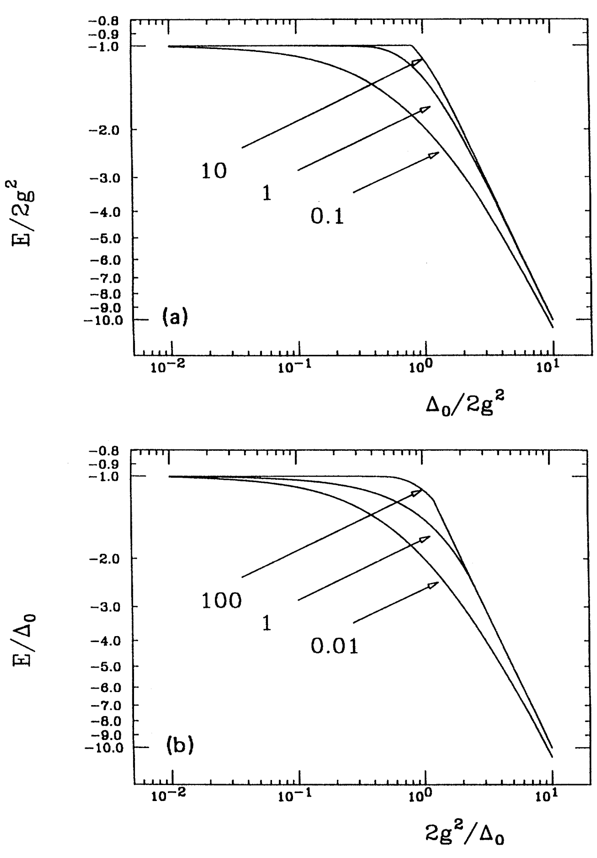

FIG. 1. Minimum energy versus (a) Δ_0 for g taking the values 0.1, 1, and 10, and (b) $2g^2$ for Δ_0 taking the values 0.01, 1, and 100.

the trial wave function are. We have done the calculation for three cases: first, we consider the displacement only and put both α and γ equal to zero. This corresponds to the case with the trial wave function given by Eq. (2), and necessarily gives the poorest estimate of the ground-state energy. Second, we put α equal to zero and vary both f and γ. This lowers the energy significantly. As shown in Fig. 2, the energy improves further when all three parameters are allowed to vary. Note that the improvement by taking proper care of the correlation is as large as the improvement obtained when squeezing was introduced. Therefore, the correlation is not just a marginal effect and cannot be neglected. In Fig. 3(b) we have plotted the tunneling reduction factor $Z=\exp[-4f^2\exp(-4\gamma-2\alpha)]$ for the same three cases. Notice that there appears a sudden jump in the reduction factor for the variational wave function consisting of displacement only. This was also pointed out by Tanaka and Sakurai (see Fig. 1 in Ref. 2). However, as shown in Fig. 3(b), this abrupt jump is just an artifact due to the inadequacy of the trial wave function to represent the true ground state. This is improved upon by introducing the squeezing, which smears the transition. Our results show an even smoother transition from the localized regime to the delocalized (tunneling) regime.

There are, however, regions in the parameter space (Δ_0, g) where this abrupt transition still persists, even for our improved trial wave function. This is shown explicitly in Fig. 4 where we have plotted the minimum energy E and reduction factor Z versus g for $\Delta_0=2$ in the transition region. The energy curves in Fig. 4(a) are no longer smooth and thus indicate a transition. The presence of a transition is more pronounced in Fig. 4(b), where we have plotted the tunneling reduction factor for the same three cases as in Fig. 3(b). The dotted line corresponds to the case with displacement transformation only and shows the most prominent transition. Introducing squeezing (dashed line) and subsequently correlation (solid line) helps alleviate the transition. Therefore, improving the wave function makes the localization-delocalization transition less pronounced, but it is still noticeable.

B. Tunneling system coupled to a dispersionless phonon bath

Now we consider the special case of point coupling with dispersionless optical phonons: $\omega_{\mathbf{k}}=\omega_0$ and $g_{\mathbf{k}}=\lambda\sqrt{\hbar/2NM\omega_{\mathbf{k}}}$. This is, in fact, the well-known molecular crystal model,[18,19] and is relevant for the study of small polaron dynamics.[20] This system has been recently studied by Ivić *et al.*[21] using the conventional modified adiabatic approximation, which is based on the multimode coherent-state ansatz in Eq. (2), and the conditions for its localization-delocalization transition were derived. Here we shall go beyond the conventional approximation and apply the correlated squeezed-state approach to investigate the ground-state properties of this system, especially its localization-delocalization transition. To begin with, let us choose the parameters $f_{\mathbf{k}}$ and $\alpha_{\mathbf{k},\mathbf{k}'}$ in Eq. (15) to be of the form $f_{\mathbf{k}}=\delta g_{\mathbf{k}}$ and $\alpha_{\mathbf{k},\mathbf{k}'}=2\alpha g_{\mathbf{k}} g_{\mathbf{k}'}/\sum_{\mathbf{q}} g_{\mathbf{q}}^2$; thus, we are left with two variational parameters α and δ only. For simplicity, we shall choose $\hbar\omega_0$ as the energy unit. Then the expression of the ground-state energy E in Eq. (15) becomes

$$E=\delta(\delta+2)\sum_{\mathbf{k}} g_{\mathbf{k}}^2+\frac{1}{4}(\tau+\tau^{-1}-2)-\Delta_0 Z\ , \tag{21}$$

where $\tau=\exp(-4\alpha)$ and $Z=\exp(-2\delta^2\tau\sum_{\mathbf{k}} g_{\mathbf{k}}^2)$. Besides, one can introduce the set of dimensionless parameters $B=2\Delta_0$ describing the adiabaticity and $S=\sum_{\mathbf{k}} g_{\mathbf{k}}^2$ giving the measure of the coupling strength, and rewrite Eq. (21) as

$$E=\delta(\delta+2)S+\frac{1}{4}(\tau+\tau^{-1}-2)-\Delta_0 Z\ , \tag{22}$$

with $Z=\exp(-2\delta^2\tau S)$. Minimizing E with respect to δ and α, we obtain two coupled algebraic equations:

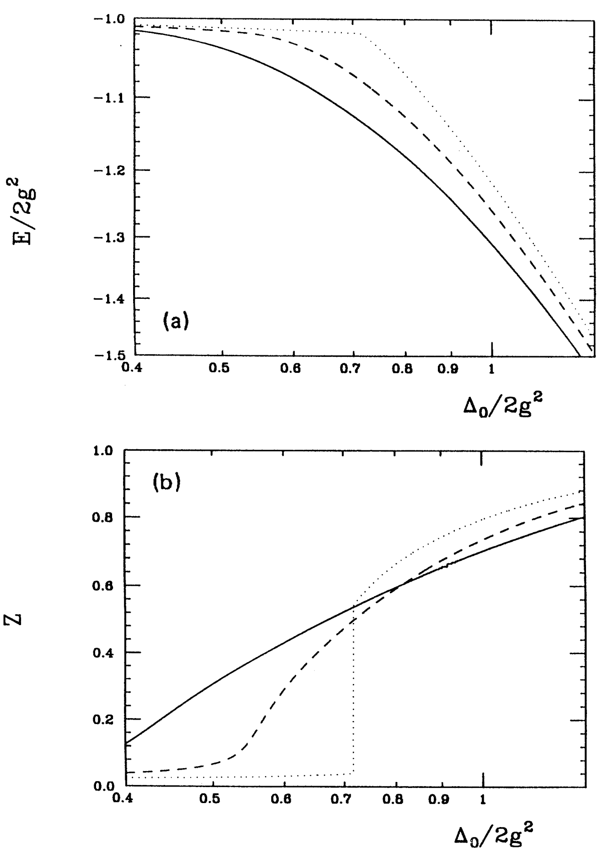

FIG. 3. (a) Minimum energy E and (b) reduction factor Z in the transition region for $g=1$. Solid line represents our result. Dashed line refers to the case $\gamma=0$ (i.e., no correlation), and dotted line the case $\alpha=\gamma=0$ (i.e., only displacement).

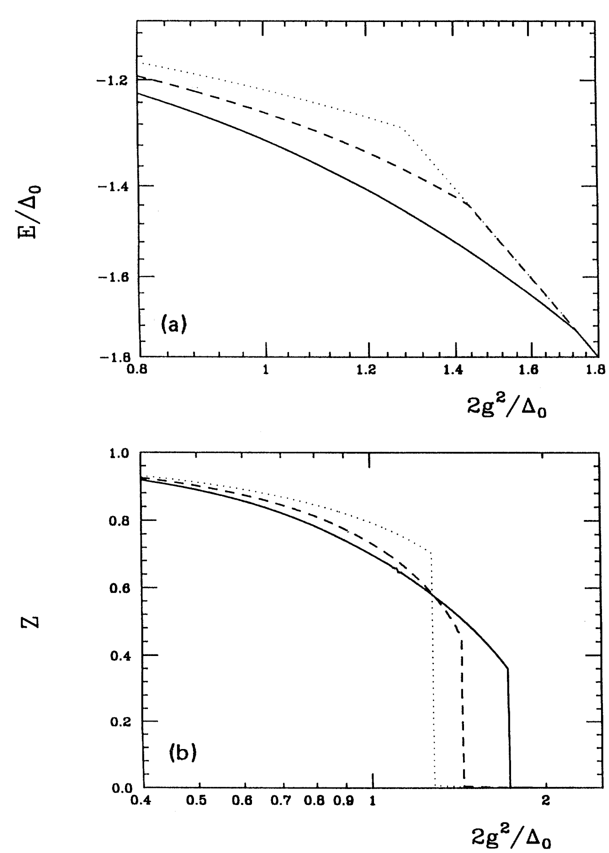

FIG. 4. (a) Minimum energy E and (b) reduction factor Z in the transition region for $\Delta_0=2$. Solid line represents our result. Dashed line refers to the case $\gamma=0$ (i.e., no correlation), and dotted line the case $\alpha=\gamma=0$ (i.e., only displacement).

$$1+\delta(1+BZ\tau)=0\ , \tag{23}$$

$$\frac{1}{4}(1-\tau^{-2})+BZ\delta^2\tau S=0 \Longrightarrow \tau^2-4\delta(\delta+1)S\tau-1=0\ . \tag{24}$$

The only admissible solution for τ in Eq. (24) is given by $\tau=2\delta(\delta+1)S+\sqrt{[2\delta(\delta+1)S]^2+1}$. With this given τ, we still need to solve Eq. (23) numerically to obtain δ. The optimal value of δ should give the minimum ground-state energy E. Furthermore, since B, τ, and Z are all non-negative numbers, δ must lie within the interval $[-1,0]$.

In Fig. 5(a) we plot the minimum energy against Δ_0 for different values of S, while Fig. 5(b) shows the minimum energy versus S for different values of Δ_0. If Δ_0 is small, the first term in Eq. (22) dominates and the energy is $E\approx -S$, whereas when Δ_0 is large, the energy is simply $E\approx -\Delta_0$. In these two extreme cases the generalized multimode squeezing (controlled by α) does not play any significant role. However, in the intermediate region we see a transition between these two extreme limits around $S\approx\Delta_0$, where all three terms in Eq. (22) are of the same magnitude.

In Fig. 6 we try to show how significant the effect of the generalized multimode squeezing is. First of all, we allow only the parameter δ to vary and put α equal to zero. In other words, we consider the displacement only and neglect the effect of the generalized multimode squeezing completely. This corresponds to the case with the trial wave function given by Eq. (2). Then we vary both α and δ, and this lowers the energy significantly. Therefore, the generalized multimode squeezing is not just a marginal effect and cannot be neglected. In Fig. 6(b) we have plotted the tunneling reduction factor Z for the same two cases. Notice that there is a sudden jump in the reduction factor for the variational wave function consisting of displacement only. This was also pointed out by Tanaka and Sakurai (see Fig. 1 in Ref. 2). However, as shown in Fig. 6(b), this abrupt jump disappears and we have a smooth transition from the localized regime to the delocalized (tunneling) regime when we introduce the generalized multimode squeezing effect in our approximation. Thus this implies the inadequacy of the trial wave function within the conventional adiabatic approximation.

As in the previous example, there are, however, regions in the parameter space (Δ_0,S) where this abrupt transition still persists, even for our improved trial wave function. This is shown explicitly in Fig. 7 where the minimum energy E and reduction factor Z for $\Delta_0=2$ in the transition region are plotted against S. The energy curves in Fig. 7(a) are no longer smooth and thus indicate

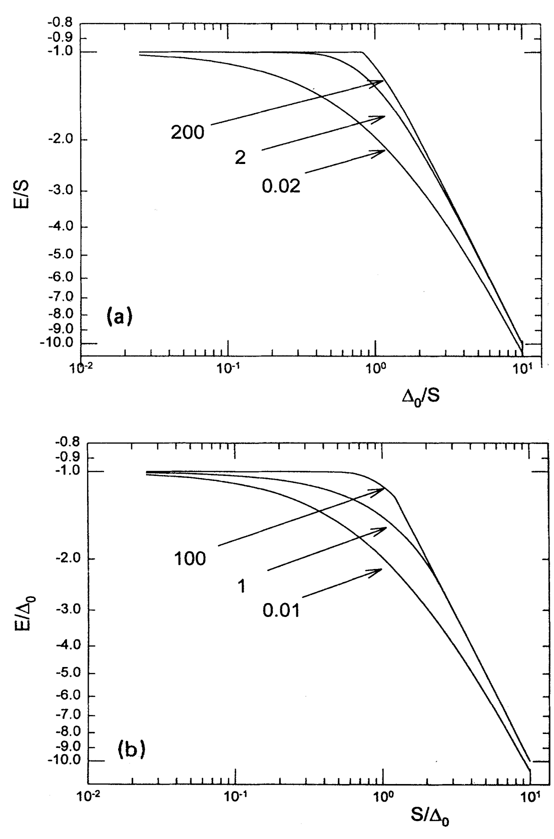

FIG. 5. Minimum energy versus (a) Δ_0 for S taking the values 0.02, 2, and 200, and (b) S for Δ_0 taking the values 0.01, 1, and 100.

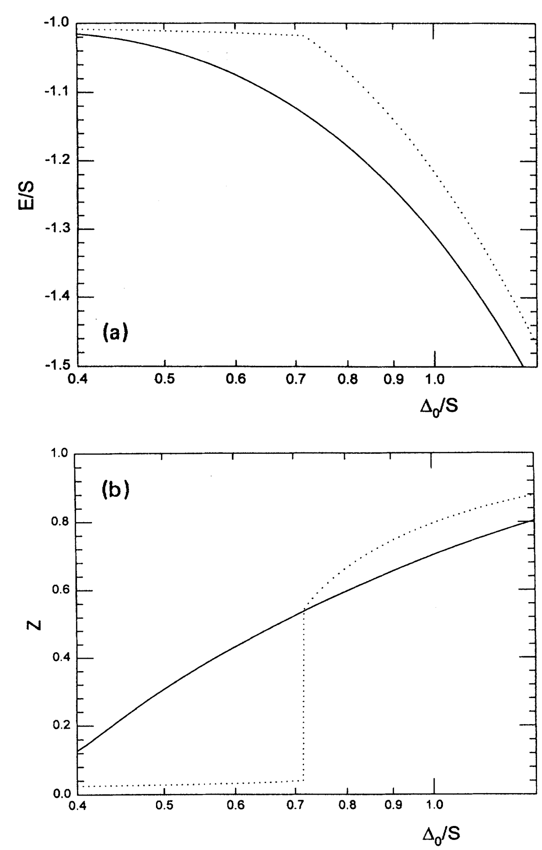

FIG. 6. (a) Minimum energy E and (b) reduction factor Z in the transition region for $S=2$. Solid line represents our result and dotted line refers to the case $\alpha=0$ (i.e., only displacement).

a transition. The presence of a transition is more pronounced in Fig. 7(b), where we have plotted the tunneling reduction factor versus S. The dotted line corresponds to the case with displacement transformation only and shows a prominent transition. Introducing the generalized multimode squeezing (solid line) helps alleviate the transition, but it is still noticeable. Therefore, improving the wave function makes the localization-delocalization transition less pronounced.

Finally, to exemplify the origin of the abrupt transition, we have plotted in Fig. 8 the optimal values of the variational parameters corresponding to Figs. 6 and 7. In the absence of the generalized multimode squeezing effect, the dotted curve in Fig. 8(a) representing the parameter δ has an optimal value about $\delta \approx -1$ for Δ_0 being very small, while for large Δ_0 the optimal value of δ is vanishingly small, i.e., $\delta \approx 0$. In between these two extreme limits, there exists a particular Δ_0 at which a discontinuous jump from $\delta \approx -1$ to 0 appears. This abrupt jump induces the cusp in the minimum energy curve (dotted curve) in Fig. 6(a). Since the reduction factor Z depends exponentially on the parameter δ, the sudden jump affects Z more dramatically, as shown in Fig. 6(b). Then, the inclusion of the generalized multimode squeezing smooths away the discontinuity as shown by the solid curve. However, in Fig. 8(b) it is shown that the discontinuous jump in the optimal values of δ still persists, even when the parameter α is allowed to vary. It is because the squeezing parameter α suffers from a similar discontinuity as well.

III. CONCLUSION

In this paper we propose a correlated squeezed-state approach to study the dissipative tunneling system at zero temperature. We have found that the ground state of the tunneling system can be better described by the correlated squeezed-state ansatz than those given in earlier variational treatments. Unlike the conventional adiabatic approximation, this new ansatz takes into account the nonlinear interactions between phonons not only in the same mode, but also in different modes. Thus this variational ansatz leads to a significant improvement of the ground-state energy and therefore a better representation of the ground state. In this new ground state the suppression effect of the phonon overlapping integral on the renormalized tunneling parameter is much more alleviated. As a result, the condition for the localization-delocalization transition of the tunneling particle is significantly modified in the correlated squeezed state, when compared with previous studies.

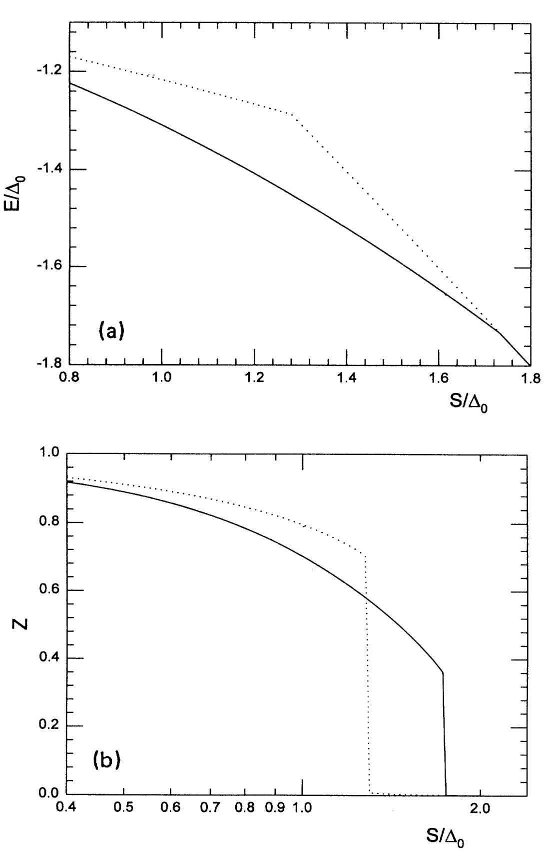

FIG. 7. (a) Minimum energy E and (b) reduction factor Z in the transition region for $\Delta_0=2$. Solid line represents our result and dotted line refers to the case $\alpha=0$ (i.e., only displacement).

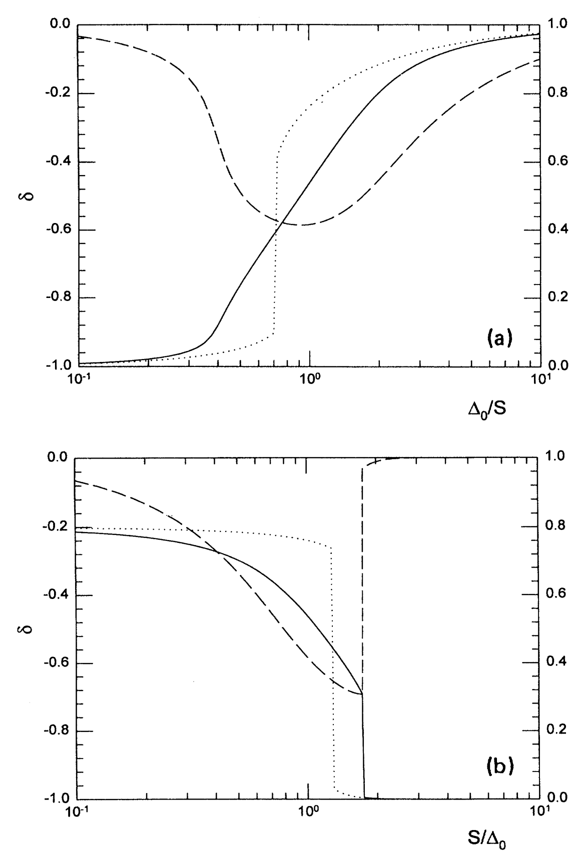

FIG. 8. Optimal values of the variational parameters δ and α versus (a) Δ_0 for $S=2$ and (b) S for $\Delta_0=2$. Solid lines represent our results for δ. Dotted lines refer to the special case $\alpha=0$ (i.e., displacement only). Dashed lines denote our results for τ.

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