Correlated-squeezed-state approach for phonon coupling in a tunneling system

C. F. Lo and R. Sollie
Department of Physics, Florida State University, Tallahassee, Florida 32306
(Received 4 April 1991)

A variational study of a tunneling particle coupled to phonons is presented. The trial wave function has built in the correlation between different modes and thereby goes beyond earlier variational treatments. This leads to a significant improvement of the energy and therefore a better representation of the ground state. The condition for the localization-delocalization transition of the tunneling particle is modified in the correlated squeezed state compared to previous studies.

In recent years much attention has been paid to the study of quantum tunneling effects of a two-state system coupled linearly to a boson field (phonons).[1] 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, each of the variational trial wave functions for the ground state of the two-state system is uncorrelated and takes into account the nonlinear interaction between phonons in different modes within the framework of the Hartree approximation only. It is therefore the purpose of this paper to present a simple variational study based on a correlated trial wave function for the ground state of the two-level model. For the sake of simplicity, we treat here a two-state system coupled to two phonon modes only. This is the simplest, nontrivial model that includes the nonlinear interaction between phonons, not only in the same mode, but also in different modes. Generalization to coupling with many phonons is straightforward and will be published elsewhere. We show that our variational wave function leads to a better ground-state energy than the earlier treatments based on a variational formulation.

The two-state system coupled linearly to two phonons is described by the Hamiltonian

$$H=-\Delta_0\sigma_x+\sum_{i=1}^{2}\hbar\omega_i b_i^\dagger b_i+\sum_{i=1}^{2}g_i(b_i^\dagger+b_i)\sigma_z, \qquad (1)$$

where b_i and $b_i^\dagger$ 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_i the coupling constant to the ith phonon mode. When $\Delta_0=0$, the system consists of two 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 $E=-\sum_i g_i^2(\hbar\omega_i)^{-1}$. On the other hand, when $g_i=0$, 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 thus damp the oscillations. Motivated by these facts, Tanaka and Sakurai[2] as well as, separately, Silbey and Harris[3] suggested a two-mode coherent state as the trial ground-state wave function for the Hamiltonian H:

$$|G\rangle=\exp\left[\sigma_z\sum_{i=1}^{2}\frac{f_i}{\hbar\omega_i}(b_i^\dagger-b_i)\right]|\mathrm{vac}\rangle\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}, \qquad (2)$$

where $|\mathrm{vac}\rangle$ is the vacuum state of modes 1 and 2, and f_1 and f_2 are the variational parameters. Recently, to account for the anharmonicity of each phonon mode, Chen, Zhang, and Wu[4] proposed a modification of the above ansatz by replacing the coherent state of each mode by a squeezed state,[6] i.e.,

$$|G\rangle=\exp\left[\sigma_z\sum_{i=1}^{2}-\frac{g_i}{\hbar\omega_i}(b_i^\dagger-b_i)\right]\times\exp\left[\sum_{i=1}^{2}\gamma_i(b_i^\dagger b_i^\dagger-b_ib_i)\right]|\mathrm{vac}\rangle\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}, \qquad (3)$$

where γ_1 and γ_2 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. Both of these trial wave functions are within the Hartree approximation and thus uncorrelated. To go beyond the Hartree approximation, we propose here the following simple correlated trial wave function for the ground state of H:

$$|G\rangle = \exp\left[\sigma_z \sum_{i=1}^{2} \frac{f_i}{\hbar\omega_i}(b_i^\dagger - b_i)\right] \times \exp\left[\sum_{i=1}^{2} \gamma_i (b_i^\dagger b_i^\dagger - b_i b_i)\right] \times \exp[\alpha(b_1^\dagger b_2^\dagger - b_1 b_2)]|\mathrm{vac}\rangle \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} , \quad (4)$$

where f_i, γ_i, and α are the variational parameters. The unitary two-mode squeeze operator[6]

$$S_{12} = \exp[\alpha(b_1^\dagger b_2^\dagger - b_1 b_2)] , \quad (5)$$

when applied to the vacuum state, generates a two-mode squeezed vacuum state for the two phonon modes. The two-mode squeezed state is a highly correlated state of the two phonon modes that exhibits reduced quadrature noise in linear combinations of variables of both modes; however, squeezing is not observed in the fluctuations of individual modes. Thus the two-mode squeeze operator is introduced here in order to account for the strong correlation and anharmonicity of the interaction between the two phonon modes. This correlated squeezed-state approach has been applied earlier[7] to the linear E-e Jahn-Teller effect, in which an electronic doublet interacts with a doubly degenerate vibration. The expectation value E of H in the correlated trial ground state of (4) is given by

$$E = \sum_{i=1}^{2} \frac{f_i^2 + 2f_i g_i}{\hbar\omega_i} + \frac{1}{2}\sum_{i=1}^{2} \hbar\omega_i(\cosh 4\gamma_i \cosh 2\alpha - 1) - \Delta_0 \exp\{-\tfrac{1}{2}[(A_1^2 + A_2^2)\cosh 2\alpha - 2A_1 A_2 \sinh 2\alpha]\} , \quad (6)$$

with $A_i = 2f_i \exp(-2\gamma_i)/\hbar\omega_i$. The optimum values of f_i, γ_i and α are determined by the variational approach, that is, when E arrives at its stable minimum.

To illustrate the correlation effect between the phonon modes, we shall confine ourselves to the special case in which the tunneling system is coupled to two identical phonon modes ($\hbar\omega_1 = \hbar\omega_2$ and $g_1 = g_2$). Thus we are left with only three variational parameters f, α, and γ. The total energy E in (6) can then be written as

$$E = 2f(f + 2g) + (\cosh 4\gamma \cosh 2\alpha - 1) - \Delta_0 \exp[-4f^2 \exp(-4\gamma)\exp(-2\alpha)] , \quad (7)$$

where we 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 to values 0.01, 1, and 100, 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 (7) 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. For all parameters we see a transition between the two extreme limits at $2g^2 \approx \Delta_0$, where all three terms in (7) 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 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 energy. Second, we put α equal to zero and vary both f and γ. This lowers the energy. And as shown in Fig. 2, the ener-

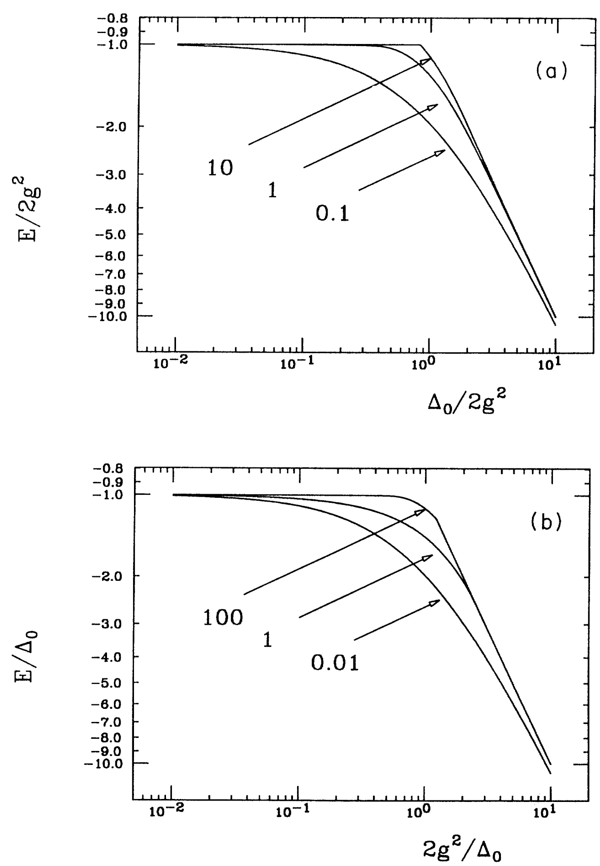

FIG. 1. Minimum energy vs (a) Δ_0 for g at the values of 0.1, 1, and 10, and (b) $2g^2$ for Δ_0 at the values of 0.01, 1, and 100.

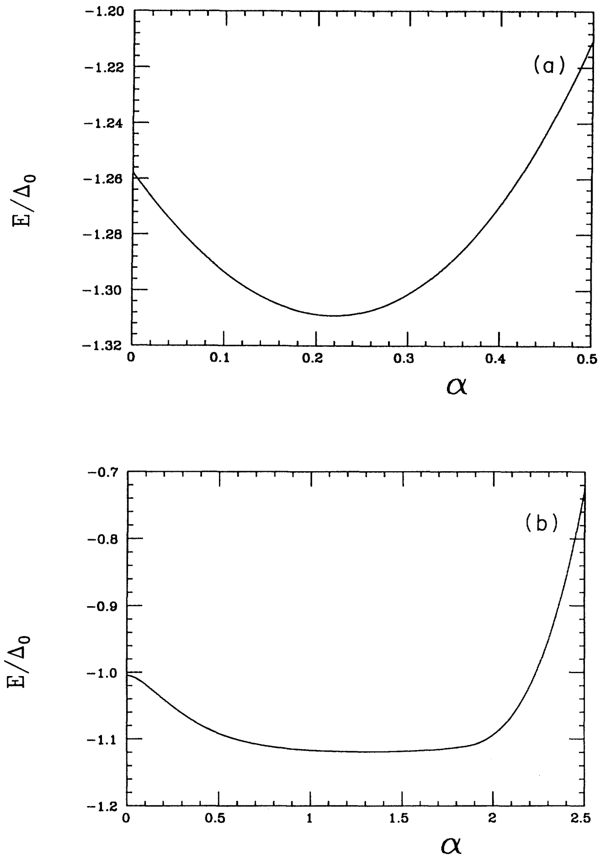

FIG. 2. Minimum energy vs α for (a) $g=1$ and (b) $g=10$ at the transition $\Delta_0=2g^2$.

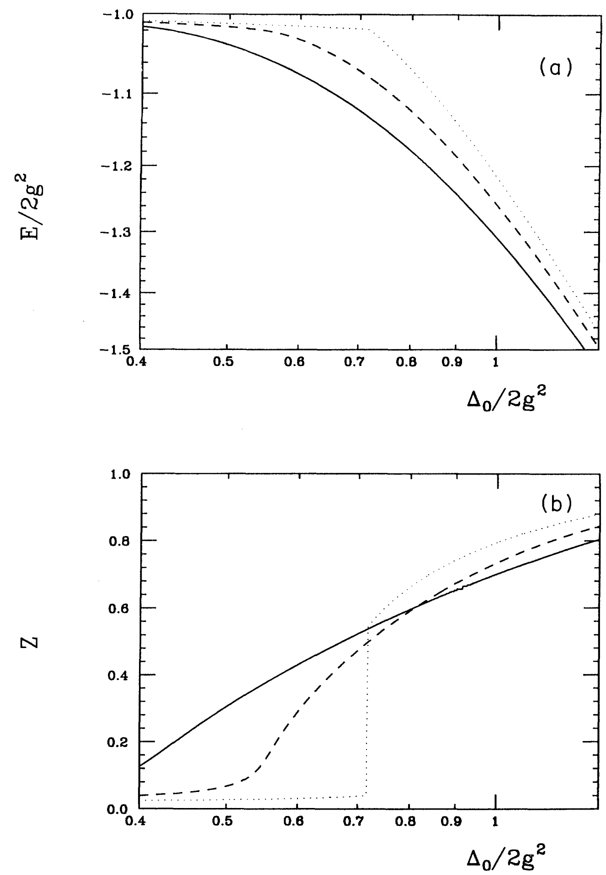

FIG. 3. (a) Minimum energy E and (b) reduction factor Z in the transition region. Solid line represents our result. Dashed line refers to the case $\gamma=0$ (i.e., no correlation) and dotted line to the case $\alpha=\gamma=0$ (i.e., only displacement) ($g=1$).

gy 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. Note the sudden jump in the reduction factor for the variational wave function consisting only of displacement. 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.

In conclusion, we have studied the effects of squeezing and correlation in the case of a quantum-mechanical two-level system coupled to phonons. The correlation among the phonons leads to a significant improvement of the energy and thereby a better representation of the ground state. Hence the condition for the localization-delocalization transition of the tunneling particle is modified in the correlated squeezed state compared with previous studies.

We acknowledge support for C. F. Lo by the DARPA sponsored Florida Initiative in Advanced Microelectronics and Materials under Contract No. MDA972-88-J-1006 and for R. Sollie by the Royal Norwegian Council for Scientific and Industrial Research (NTNF).

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