Squeezed-state approach for phonon coupling in tunneling systems at zero temperature

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In this paper we propose a new method to study tunneling problems in the presence of phonons at zero temperature. We have found that, by taking account of the nonadiabatic effect induced by coupling with a tunneling particle, the ground states of phonons can be described by displaced squeezed states, instead of by the displaced oscillator states given in the adiabatic approximation. On one hand, in these new ground states the suppression effect of the phonon overlapping integral on the renormalized tunneling parameter is more alleviated than that in displaced oscillator states. On the other hand, the condition for the localization-dislocalization transition of the tunneling particle is modified in the displaced squeezed states compared with the previous studies.

I. INTRODUCTION

Quantum-tunneling effects are studied in many various branches of solid-state physics. Recently, the influence of a phonon bath on the quantum-tunneling system has received considerable attention in the literature.¹ The Hamiltonian of a tunneling particle coupling linearly with a phonon bath takes the form

$$H = \frac{p^2}{2m} + V(Q) + \sum_k \hbar \omega_k b_k^{\dagger} b_k + \sum_k g_k (b_k + b_k^{\dagger}) , \quad (1)$$

where *m* is the mass of the particle, V(Q) the symmetric double-well potential with minima $\pm \frac{1}{2}Q_0$, b_k^{\dagger} and b_k the phonon operators, and g_k the coupling coefficient. For a system described by Hamiltonian (1), a problem of general concern is how to evaluate the renormalized tunneling parameter at 0 K. The conventional procedure works on the truncation approximation,² taking the wave function of the whole system as a simple product of those of the phonon bath and the particle. If the double-well potential is sufficiently steep as to split the motion of the particle into two minimum states ψ_+ and ψ_- , the renormalized tunneling parameter at 0 K can be expressed as

$$\Delta = \langle \psi_+ \phi_+ | H_t | \psi_- \phi_- \rangle = \Delta_0 \langle \phi_+ | \phi_- \rangle , \qquad (2)$$

where H_i is the Hamiltonian for the particle with the bare tunneling parameter Δ_0 . Hence, Δ can be calculated once we know the phonon ground states ϕ_+ and ϕ_- .

For a particle with small tunneling probability, the system may be regarded as a two-level system. In terms of pseudospin formalism, the Hamiltonian (1) can be rewritten as

$$H = -\Delta_0 \sigma_x + \sum_k \hbar \omega_k b_k^{\dagger} b_k + \sum_k g_k (b_k + b_k^{\dagger}) \sigma_z , \quad (3)$$

where σ 's are Pauli matrices. The above expression can be set into quadrature as

$$H = -\Delta_0 \sigma_x + \sum_k \hbar \omega_k \left[b_k^{\dagger} + \frac{g_k}{\hbar \omega_k} \sigma_z \right] \left[b_k + \frac{g_k}{\hbar \omega_k} \sigma_z \right] - \sum_k \left(g_k^2 / \hbar \omega_k \right) .$$
(4)

According to the adiabatic approximation, the phonon variables always instantaneously follow the motion of the particle; therefore when the particle is located at $\pm \frac{1}{2}Q_0$ ($\sigma_z = \pm 1$), the phonon operator b_k will be displaced to $b_k \pm g_k / \hbar \omega_k$, the corresponding phonon ground states are are

$$\phi_{\pm} = \prod_{k} \exp[\mp (g_k / \hbar \omega_k) (b_k^{\dagger} - b_k)] \phi_{\text{vac}} , \qquad (5)$$

where ϕ_{vac} is the usual vacuum state. The tunneling parameter (2) now becomes

$$\Delta = \Delta_0 \prod_k \langle e^{(g_k/\hbar\omega_k)(b_k^{\dagger} - b_k)} \phi_{\text{vac}} | e^{-(g_k/\hbar\omega_k)(b_k^{\dagger} - b_k)} \phi_{\text{vac}} \rangle$$
$$= \Delta_0 e^{-W} \tag{6}$$

with the Franck-Condon (or Debye-Waller) factor

$$W = \sum_{k} \left[2g_k^2 / (\hbar \omega_k)^2 \right] \,. \tag{7}$$

The energy of the whole system in this displacedoscillator state is

$$E = \frac{1}{2} \langle \psi_{+} \phi_{+} + \psi_{-} \phi_{-} | H | \psi_{+} \phi_{+} + \psi_{-} \phi_{-} \rangle$$
$$= -\Delta_{0} e^{-W} - \sum_{k} \left(g_{k}^{2} / \hbar \omega_{k} \right) . \tag{8}$$

Equation (6) shows that the tunneling parameter Δ endures serious suppression by the phonon overlapping integral. However, the application of the above results to the atomic tunneling process in solids induces substantial difficulty.²

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We believe the adiabatic approximation turns out to be inadequate physically when applied to the atomictunneling phenomena in solids. It is generally accepted that the atomic-tunneling state is in some extent related to the softening of local structures, for example, the atomic-tunneling states in glasses.³⁻⁵ The softening of local structures leads to strong coupling between the tunneling particle and the environmental lattice vibration as well as provides the phonon spectrum with an accentuated low-frequency regime. Both effects are unfavorable for application of the adiabatic approximation. To overcome this difficulty, Sethna^{2,6} attempted to apply the instanton approximation to the path integral in his studies on the influence of the phonon bath on the atomictunneling states. His results show, due to the coupling with the phonon bath, the tunneling particle not only moves in an adiabatic potential, but is also influenced by a retarded potential, which originates from the fact that the phonons are not always in equilibrium with the particle. The motion of the particle at time t disturbs the phonon state, which in turn acts on the motion of the particle at later time t', and the process then turns out to be nonmarkovian. In other words, the adiabatic approximation breaks down, and the displaced-oscillator state does not properly represent the real phonon ground state. Besides the microscopic atomic tunneling in solids, the lowfrequency phonon also plays an important role in dissipative macroscopic quantum-tunneling systems such as SQID. It is the infrared divergence induced by the lowfrequency phonon that leads to the localizationdislocalization transition in the system.¹

The question arises: How is the ground state of phonon, especially the low-frequency phonon, represented under the coupling with a tunneling particle? Unfortunately, this point has not been fully discussed in the literature. Recently in Refs. 7 and 8, the displaced squeezed-phonon state was proposed as the variational function to obtain a more stable approximate ground state in bipolaron systems. This new phonon ground state has also been applied to the valence-transition theory in heavy Fermi systems⁹ as well as to the theory of high- T_c superconductivity.¹⁰ In this paper we will introduce this displaced squeezed state to the dissipative tunneling systems as a new candidate of the phonon ground state to demonstrate the nonadiabatic aspect of the problem. We will also calculate the effect of the new ground state on the renormalized tunneling parameter. The arrangement of the paper is as follows. In the next section, we will investigate the influence of the tunneling particle to the phonon state and give a heuristic derivation to see under which conditions one can get a displaced squeezed state as the phonon ground state. In Sec. III we will use the displaced squeezed state as the variational trial function of phonon to treat the whole Hamiltonian of the system. Some concluding remarks will given in Sec. IV.

II. DISPLACED SQUEEZED STATE AS THE PHONON GROUND STATE

In this section, we want to study the problem of the tunneling particle coupling with one phonon mode. Coupling with many phonon modes will be investigated in the next section. For phonon mode k, the Hamiltonian (3) reduces to

$$H_k = -\Delta_0 \sigma_x + \hbar \omega_k b_k^{\dagger} b_k + g_k (b_k + b_k^{\dagger}) \sigma_z .$$
⁽⁹⁾

We apply as usual the unitary transformation

$$S_k = \exp[\sigma_z(g_k / \hbar \omega_k)(b_k^{\top} - b_k)]$$
(10)

to absorb the interaction term. Then

$$\begin{split} \tilde{H}_{k} &= S_{k} H_{k} S_{k}^{-1} \\ &= \hbar \omega_{k} b_{k}^{\dagger} b_{k} - (g_{k}^{2} / \hbar \omega_{k}) \\ &- \Delta_{0} \{ \cosh[(2g_{k} / \hbar \omega_{k})(b_{k}^{\dagger} - b_{k})] \} \sigma_{x} \\ &- \Delta_{0} \{ i \sinh[(2g_{k} / \hbar \omega_{k})(b_{k}^{\dagger} - b_{k})] \} \sigma_{y} \;. \end{split}$$
(11)

When $\Delta_0 = 0$ (or at the strong-coupling limit) the Hamiltonian (11) is already diagonal. We will expand it with respect to $(g_k / \hbar \omega_k) (b_k^{\dagger} - b_k)$ in a weak-coupling meaning, however this is done to the renormalized coupling coefficient due to the rescaling of $b_k^{\dagger} - b_k$ in a special ground state, as will be shown below. From Hamiltonian (11), one can see there are two kinds of influence on the phonon system due to the coupling with the tunneling particle. The first is the term containing σ_x , giving the influence of the tunneling particle in its ground state $(\sigma_x = +1)$ or in its excited state $(\sigma_x = -1)$. The second is the term containing σ_y , representing the influence of the transition of the tunneling particle between its ground and excited states. Such transition needs the participation of phonons, then it will be important only for temperature $T > \Delta/k_B$. In the following we will neglect the term containing σ_{v} , since in this paper we are only interested in the case of zero temperature. When the tunneling particle in its ground state, Hamiltonian (11) becomes

$$\widetilde{H}_{k,g} = -\Delta_0 \cosh[(2g_k / \hbar \omega_k)(b_k^{\dagger} - b_k)] + \hbar \omega_k b_k^{\dagger} b_k - g_k^2 / \hbar \omega_k .$$
(12)

It represents a phonon system with nonlinear interaction. Such nonlinear interaction is the result of the nonadiabatic effect due to the coupling with the tunneling particle: The coupling not only leads to the rigid displacement, but also to the deformation of a phonon wave function.

To zeroth order of g_k , the ground state of Hamiltonian (12) is the vacuum state ϕ_{vac} , which gives the displaced oscillator state of the adiabatic approximation as the ground state of phonon in original base. Up to g_k^2 , Hamiltonian (12) can be approximated as

$$\tilde{H}_{k,g} \simeq -\Delta_0 + \hbar \omega_k \{ b_k^{\dagger} b_k - [2\Delta_0 g_k^2 (b_k^{\dagger} - b_k^{\dagger})^2 / (\hbar \omega_k^{\dagger})^3] \} - g_k^2 / \hbar \omega_k .$$
(13)

The term in the curly brackets is familiar in quantum optics; it can be expressed as the linear combination of three generators of SU(1,1) group, namely $\frac{1}{2}b^2$, $\frac{1}{2}b^{\dagger 2}$, and $\frac{1}{2}(b^{\dagger}b+\frac{1}{2})$. The ground state is the squeezed (or two-photon coherent) state.^{11,12} Direct inspection verifies that the following unitary transformation:

$$R_{k} = \exp[\gamma_{k}(b_{k}^{2} - b_{k}^{\dagger 2})]$$
(14)

diagonalizes $\widetilde{H}_{k,g}$ in (13) to

$$R_k \tilde{H}_{k,g} R_k^{-1} = e^{4\gamma_k} \hbar \omega_k b_k^{\dagger} b_k + E_{k,g}$$
⁽¹⁵⁾

with the ground-state energy

$$E_{k,g} = -\Delta_0 + \frac{1}{2} \hbar \omega_k (e^{4\gamma_k} - 1) - g_k^2 / \hbar \omega_k$$
(16)

and

$$\gamma_{k} = \frac{1}{8} \ln[1 + 8\Delta_{0}g_{k}^{2} / (\hbar\omega_{k})^{3}] .$$
(17)

In arriving to the above results, the following identities are useful:

$$e^{\gamma(b^2-b^{\dagger 2})}be^{-\gamma(b^2-b^{\dagger 2})}=b\cosh 2\gamma+b^{\dagger}\sinh 2\gamma$$
, (18a)

$$e^{\gamma(b^2-b^{\dagger 2})}b^{\dagger}e^{-\gamma(b^2-b^{\dagger 2})} = b^{\dagger}\cosh 2\gamma + b\sinh 2\gamma , \qquad (18b)$$

$$e^{\gamma(b^2-b^{\dagger}2)}(b^{\dagger}\pm b)e^{-\gamma(b^2-b^{\dagger}2)}=(b^{\dagger}\pm b)e^{\pm 2\gamma}$$
. (18c)

Therefore the ground wave function of Hamiltonian (12), up to g_k^2 , takes the standard form of the squeezed state

$$\tilde{\phi}_{k} = R_{k}^{-1} \phi_{\text{vac}} = e^{-\gamma_{k} (b_{k}^{2} - b_{k}^{+2})} \phi_{\text{vac}} .$$
(19)

The fluctuations in ground state are readily evaluated as

$$\langle \, \tilde{\phi}_k \, | \, (b_k + b_k^{\dagger})^2 | \, \tilde{\phi}_k \, \rangle = e^{4\gamma_k} \, , \qquad (20a)$$

$$\langle \tilde{\phi}_k | (b_k - b_k^{\dagger}) / i j^2 | \tilde{\phi}_k \rangle = e^{-4\gamma_k}$$
 (20b)

We see one of the quadrature is squeezed at the expense of the other, at the same time, the Heisenberg uncertainty remains at minimum. According to Eq. (18c), the squeezed $b_k^{\dagger} - b_k$ now acquires a factor $\exp(-2\gamma_k)$, or in (12) the coupling coefficient g_k reduces to $g_k \exp(-2\gamma_k)$, which accounts for the expansion leading to (13).

Return to our original base with $\tilde{\phi}_k$ in (19), S_k in (10), and $\psi_S = 2^{-1/2}(\psi_+ + \psi_-)$, the ground wave function of the whole system now becomes

$$\Phi = S_k^{-1} \psi_S \tilde{\phi}_k = 2^{-1/2} (\psi_+ \phi_{kS,+} + \psi_- \phi_{kS,-}) , \qquad (21)$$

where the displaced phonon squeezed states are defined as

$$\phi_{kS,\pm} = \left[\exp \left[\mp \frac{g_k}{\hbar \omega_k} (b_k^{\dagger} - b_k) \right] \times \exp[-\gamma_k (b_k^2 - b_k^{\dagger 2})] \right] \phi_{\text{vac}} .$$
(22)

The two unitary transformations in (22) represent two different effects of the tunneling particle to the phonon state: displacement and deformation. Return to coordinate q_k representation, the two-phonon unitary transformation of (14) has the form as

$$R_{k} = \exp\left[\gamma_{k}\left[1 + 2q_{k}\frac{d}{dq_{k}}\right]\right].$$
(23)

For any function $f(q_k)$, we have

$$R_k^{-1} f(q_k) = e^{-\gamma_k} f(\tilde{q}_k)$$
(24)

with $\tilde{q}_k = e^{-2\gamma_k} q_k$. This means that, under the squeezed-state approach, the deformative effect of the tunneling particle to the phonon state is to rescale the phonon coordinate q_k . The phonon overlapping integrals in the displaced squeezed states is

$$\prod_{k} \langle \phi_{kS,-} | \phi_{kS,+} \rangle = \langle \phi_{vac} | e^{\gamma_{k} (b_{k}^{2} - b_{k}^{+2})} e^{-2g_{k} (b_{k}^{+} - b_{k})/\hbar\omega_{k}} e^{-\gamma_{k} (b_{k}^{2} - b_{k}^{+2})} | \phi_{vac} \rangle$$

$$= \langle \phi_{vac} | \exp[-(2g_{k}/\hbar\omega_{k}) e^{-2\gamma_{k}} (b_{k}^{+} - b_{k})] | \phi_{vac} \rangle = \exp\left[-\sum_{k} [2g_{k}^{2}/(\hbar\omega_{k})^{2}] e^{-4\gamma_{k}}\right].$$
(25)

Compared with the phonon overlapping integrals in (6) under the adiabatic approximation, we find that the contribution to the Franck-Condon factor W from each mode k is reduced by a factor $\exp(-4\gamma_k)$, hence the suppression of the tunneling parameter will be lifted very much provided $4\gamma_k >> 1$.

III. VARIATIONAL APPROACH

Now we consider the problem of the tunneling particle coupling with many phonon modes described by Hamiltonian (3). Applying the unitary transformation

$$S = \prod_{k} S_{k} = \exp\left[\sigma_{z} \sum_{k} (g_{k} / \hbar \omega_{k}) (b_{k}^{\dagger} - b_{k})\right]$$
(26)

to Hamiltonian (3), we get

$$\widetilde{H} = SHS^{-1}$$

$$= \sum_{k} \hbar \omega_{k} b_{k}^{\dagger} b_{k} - \sum_{k} (g_{k}^{2} / \hbar \omega_{k}) - \Delta_{0} \left[\cosh \left[\sum_{k} (2g_{k} / \hbar \omega_{k}) (b_{k}^{\dagger} - b_{k}) \right] \right] \sigma_{x}$$

$$- \Delta_{0} \left[i \sinh \left[\sum_{k} (2g_{k} / \hbar \omega_{k}) (b_{k}^{\dagger} - b_{k}) \right] \right] \sigma_{y} .$$
(27)

This shows that the linear coupling with the tunneling particle induces the nonlinear interaction between phonons not only in the same mode, but also in different modes. Although the Hamiltonian (27) cannot be solved exactly, we may attack it approximately by variational approach. Stimulated by the heuristic derivation in the last section, we adopt the trial function as a simple product of a spin state and squeezed-photon states. As it is easy to see that the matrix element of $\sinh[\sum_k (2g_k /\hbar\omega_k)(b_k^{\dagger} - b_k)]$ between any pair of squeezed states always vanishes, the last term in (27) containing σ_y has no contribution to the energy for this special trial wave function. Consequently the trial function for the ground state becomes

$$\Phi = \psi_{S} \exp\left[-\sum_{k} \gamma_{k} (b_{k}^{2} - b_{k}^{\dagger 2})\right] \phi_{\text{vac}} .$$
⁽²⁸⁾

With the aid of the identities (18), straightforward calculation leads to

$$E = \langle \Phi | \tilde{H} | \Phi \rangle$$

= $-\Delta_0 \exp\left[-\sum_k \left[2g_k^2/(\hbar\omega_k)^2\right]e^{-4\gamma_k}\right] + \sum_k (\sinh 2\gamma_k)^2 \hbar\omega_k - \sum_k \left(g_k^2/\hbar\omega_k\right).$ (29)

Now we change γ_k 's to minimize E, then γ_k 's must satisfy the following conditions:

$$e^{\delta \gamma_k} = 1 + 8\Delta_0 g_k^2 K / (\hbar \omega_k)^3 , \qquad (30)$$

where

$$K = \exp\left[-\sum_{k} \left[2g_{k}^{2}/(\hbar\omega_{k})^{2}\right]e^{-4\gamma_{k}}\right]$$
$$= \exp\left[-\sum_{k} \left[2g_{k}^{2}/(\hbar\omega_{k})^{2}\right]\left[1 + 8\Delta_{0}g_{k}^{2}K/(\hbar\omega_{k})^{3}\right]^{-1/2}\right]$$
(31)

is just the phonon overlapping integrals in the displaced squeezed states [see (25)]. It is to be solved from (31).

Compared with (8), we remark that the energy E in (29) with γ_k in (30) is by contruction lower than that of the adiabatic approximation, which simply corresponds to the case of $\gamma_k = 0$. This means that the displaced squeezed state is more stable than the displaced oscillator state or as the ground state of a phonon.

In displaced squeezed state, the renormalized tunneling parameter is $\Delta = \Delta_0 K$, then (31) gives

$$\ln\Delta = \ln\Delta_0 - \sum_{k} \left[\frac{2g_k^2 / (\hbar\omega_k)^2}{[1 + 8\Delta g_k^2 / (\hbar\omega_k)^3]^{1/2}} \right].$$
 (32)

The tunneling parameter is very sensitive to the frequency dependence of the coupling coefficient g_k . In general it can be written as

$$g_k = \hbar \omega_c (\omega_k / \omega_c)^{n/2 - 1} , \qquad (33)$$

where ω_c is the highest frequency of the phonons coupled with the tunneling particle. For three-dimension phonon bath, we have

$$\sum_{k} g_{k}^{2} = 2\alpha \int \omega^{n} d\omega , \qquad (34)$$

where α is a constant independent of frequency. Substituting (33) and (34) into (32) leads to

$$\ln\Delta = \ln\Delta_0 - \frac{4\alpha}{\hbar^2} \int_0^{\omega_c} \frac{J(\omega)}{\omega^2} d\omega$$
(35)

with

$$U(\omega) = \omega^{n} / [1 + (8\Delta/\hbar\omega_{c}^{n-4})\omega^{n-5}]^{1/2} .$$
 (36)

If n < 5 the asymptotic behavior of $J(\omega)$ as $\omega \rightarrow 0$ is

$$J(\omega) \sim \omega^{(n+5)/2} . \tag{37}$$

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 $J(\omega)$ decreases more quickly than ω as $\omega \rightarrow 0$ provided n > -3, then the integral in (35) is convergent and it gives a nonzero value of Δ . However, recent study of the adiabatic approximation has shown¹ $\Delta=0$ for n < 1; $\Delta \neq 0$ for n > 1. When n = 1 (Ohmic dissipation), Δ depends on α with $\Delta=0$ for $\alpha > \hbar^2/4$ and $\Delta \neq 0$ for $\alpha < \hbar^2/4$. This phenomenon, also found by renormalization group method,^{13,14} is called localization-dislocalization transition. Our above result indicates that the condition for such transition is modified in the displaced squeezed state.

Another interesting case is n = 3, corresponding to atomic tunneling in solids.^{2,6} In this case we have

$$\sum_{k} 2g_{k}^{2} / (\hbar\omega_{k})^{2} = \frac{1}{t^{2}} \int \omega \, d\omega$$
(38)

with

$$t = (\pi^2 c^3 / V \omega_c)^{1/2} , \qquad (39)$$

where c is the velocity of phonon, V is the volume. Inserting (38) into (32) gives

$$\ln\Delta = \ln\Delta_{0} - W\tilde{\omega}_{c}^{-2} \int_{0}^{\bar{\omega}_{c}} \frac{x^{2} dx}{(1+x^{2})^{1/2}}$$

= $\ln\Delta_{0} - W\{\tilde{\omega}_{c}^{-1}(1+\tilde{\omega}_{c}^{2})^{1/2} - \tilde{\omega}_{c}^{2}\ln[\tilde{\omega}_{c} + (1+\tilde{\omega}_{c}^{2})^{1/2}]\},$ (40)

where W is Franck-Condon factor for n = 3, $\tilde{\omega}_c$ is the di-

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mensionless frequency

$$\widetilde{\omega}_c = \omega_c / \omega_0 \tag{41}$$

with

$$\omega_0 = (8\omega_c \Delta/\hbar)^{1/2} . \tag{42}$$

For $\tilde{\omega}_c \ll 1$, (40) leads to

$$\Delta \simeq \Delta_0 e^{-\tilde{\omega}_c W} = \Delta_0 e^{-\tilde{W}} .$$
(43)

This shows that the suppression of phonon overlapping integral to the tunneling parameter is reduced very much in displaced squeezed state due to the smaller effective Franck-Condon factor $\tilde{W} = \tilde{\omega}_c W \ll W$ compared with that of the adiabatic approximation. For $\tilde{\omega}_c \gg 1$, (40) gives

$$\Delta \simeq \Delta_0 e^{-W} \,, \tag{44}$$

which has the same form as that of the adiabatic approximation.

IV. CONCLUDING REMARKS

The main feature of the present theory is that there are two effects of coupling with a tunneling particle on a phonon state: one is displacement and the other is deformation. The conventional adiabatic approximation only considers the former and neglects the latter. By taking account of the nonadiabatic effect, we find in this paper that the ground state of the phonon can be described by a displaced squeezed state approximately. In this new ground state, the coordinate of the phonon is rescaled, on the one hand. On the other hand, the suppression of the phonon overlapping integral to renormalized tunneling parameter is much alleviated than that in a displacedoscillator state of the adiabatic approximation. Moreover the condition for localization-dislocalization transition is modified in a displaced squeezed state compared with the result of previous studies. We expect that the present theory may be useful for both macroscopic and microscopic tunneling systems coupled with a lowfrequency phonon bath.

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