Variational approach for tunneling diffusion of a particle interacting with phonons

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Displaced-squeezed states are proposed as the variational ground states of phonons coupled with a particle moving in a tight-binding band. The narrowing effect of the phonon overlapping integral on the renormalized bandwidth of the tunneling particle is investigated. We find that for Ohmic dissipation the conditions for the localization-delocalization transition of the tunneling particle are modified compared with the previous studies.

The problem of a quantum tunneling system interacting with a dissipative environment has recently attracted a great deal of attention, e.g., the dissipative two-state system[1-3] and dissipative tunneling diffusion problem.[4-9] Renormalization-group analysis shows that there exists a sharp localization-delocalization transition in the dissipative two-state system[2,3] and dissipative tunneling diffusion problem.[6-8] It is believed that such a transition is the result of infrared divergence stemming from the low-frequency phonons (or excitations) of the environment, thus it depends strongly on the ground states of phonons under coupling with a tunneling system. Unfortunately, there are few discussions about these states. Only displaced states were proposed as the variational ground states of phonons in the dissipative two-state system[10-12] and dissipative tunneling diffusion problem.[9,13] However, it can be physically understood that the coupling with a tunneling system may have two different influences, displacement and deformation, on the phonon wave functions depending upon the phonon frequency and coupling strength. For high phonon frequency and weak coupling the displacement will be dominant, while for low phonon frequency and strong coupling one must take into account both displacement and deformation effects.[14] The displaced state approximation only considers the former and omits the latter; therefore, it is desirable to find an appropriate description of the deformation effect on the ground states of phonons. Recently we proposed displaced-squeezed states as the variational ground states of phonons coupled with a two-state system,[15] which contain both displacement and deformation effects. The main purpose of this paper is to apply the displaced-squeezed states to the system of a particle moving in a tight-binding band and coupled with phonons.

The model Hamiltonian is as follows:[5,6]

$$H=-\sum_n \Delta_0 C_n^\dagger C_{n+1}+\text{H.c.}+\sum_k \hbar\omega_k b_k^\dagger b_k + \left(\sum_n nC_n^\dagger C_n\right)\left(\sum_k g_k(b_k^\dagger+b_k)\right) + \left(\sum_n nC_n^\dagger C_n\right)^2\sum_k \frac{g_k^2}{\hbar\omega_k}\,, \tag{1}$$

where $C_n^\dagger$ and C_n are operators for the particle, $\sum_n nC_n^\dagger C_n$ is the position operator for the particle in the tight-binding basis, $2\Delta_0$ is the bare bandwidth of the particle, $b_k^\dagger$ and b_k are operators for phonons with frequency ω_k, and g_k is the coupling coefficient. Applying the usual canonical transformation

$$U_1=\exp\left[\left(\sum_n nC_n^\dagger C_n\right)\left(\sum_k \frac{g_k}{\hbar\omega_k}(b_k^\dagger-b_k)\right)\right] \tag{2}$$

to Hamiltonian (1), we obtain

$$\bar H = U_1^\dagger H U_1 = -\sum_n \Delta_0 C_n^\dagger C_{n+1}\exp\left(\sum_k \frac{g_k}{\hbar\omega_k}(b_k^\dagger-b_k)\right) + \text{H.c.}+\sum_k \hbar\omega_k b_k^\dagger b_k\,. \tag{3}$$

A term concerning the interaction of two particles has been omitted, since we assume that there is only one particle in the system. It is useful to rewrite the particle operators at site n in the momentum space:

$$C_n=\frac{1}{\sqrt N}\sum_q e^{iqn}C_q\,, \tag{4a}$$

$$C_n^\dagger=\frac{1}{\sqrt N}\sum_q e^{-iqn}C_q^\dagger\,. \tag{4b}$$

Hamiltonian (3) then becomes

$$\bar H=-\sum_q \Delta_0 C_q^\dagger C_q \exp\left(iq+\sum_k \frac{g_k}{\hbar\omega_k}(b_k^\dagger-b_k)\right) + \text{H.c.}+\sum_k \hbar\omega_k b_k^\dagger b_k\,, \tag{5}$$

where $\bar H$ is diagonal in the particle operators and nondiagonal in the phonon operators. More importantly, it shows that linear coupling with the tunneling particle induces nonlinear interaction between phonons not only in the same modes but also in different modes.[15] Thus it is difficult to find an exact solution, and one has to look for approximations.

Generally, the ground state of Hamiltonian (5) may be assumed to be written approximately as a product of two parts

$$|\psi\rangle = |\psi_B\rangle |\psi_p\rangle , \quad (6)$$

where $|\psi_p\rangle$ is the ground state of the tunneling particle and $|\psi_B\rangle$ is the ground state of phonons under coupling with the tunneling particle. From Hamiltonian (5), $|\psi_p\rangle$ is easily determined to be a single-particle state with zero momentum $|q=0\rangle$. Then

$$\begin{aligned}\bar{H}_{\text{ph}} &= \langle \psi_p | \bar{H} | \psi_p \rangle \\ &= -2\Delta_0 \cosh\left[\sum_k \frac{g_k}{\hbar\omega_k}(b_k^\dagger - b_k)\right] + \sum_k \hbar\omega_k b_k^\dagger b_k \end{aligned} \quad (7)$$

gives an effective Hamiltonian for the phonon subsystem. To zero order of $g_k/\hbar\omega_k$, the ground state of $\bar{H}_{\text{ph}}$ is a vacuum state, or a displaced state in its original space. Up to $(g_k/\hbar\omega_k)^2$, the ground state may be described by a squeezed state, or a displaced-squeezed state in its original space.[14,15] In the following, we propose the displaced-squeezed state

$$|\psi_B\rangle = U_2 |\text{vac}\rangle \quad (8)$$

with

$$U_2 = \exp\left[\sum_k \gamma_k (b_k^{+2} - b_k^2)\right] \quad (9)$$

as the variational ground state of phonons, where γ_k's are variational parameters. If $\gamma_k = 0$, $|\psi_B\rangle$ return to the displaced states. With the aid of the following identities

$$U_2^\dagger b_k U_2 = b_k \cosh 2\gamma_k + b_k^\dagger \sinh 2\gamma_k , \quad (10a)$$

$$U_2^\dagger b_k^\dagger U_2 = b_k^\dagger \cosh 2\gamma_k + b_k \sinh 2\gamma_k , \quad (10b)$$

the ground-state energy is derived,

$$\begin{aligned} E_g &= \langle \psi_B | \bar{H}_{\text{ph}} | \psi_B \rangle \\ &= -2\Delta_0 \exp\left[-\frac{1}{2}\sum_k \left(\frac{g_k}{\hbar\omega_k}\right)^2 e^{-4\gamma_k}\right] \\ &\quad + \sum_k \hbar\omega_k \sinh^2 2\gamma_k . \end{aligned} \quad (11)$$

For mathematical simplicity, we choose the power law for the coupling strength and phonon frequency[8]

$$g_k = g_0 (ka)^\lambda, \quad \omega_k = \omega_0 (ka)^\nu , \quad (12)$$

where ω_0 is the cutoff frequency, g_0 is a proportional constant, $0 < (ka) < 1$, and $\nu > 1$. In order to explore the influence of the phonon ground states on the tunneling particle, it is necessary to introduce a renormalized bandwidth of the tunneling particle

$$W_y = 2\Delta_0 K , \quad (13)$$

where K is just the phonon overlapping integral and can be defined from (11),

$$K = \exp\left[-\sum_k \frac{1}{2}\left(\frac{g_k}{\hbar\omega_k}\right)^2 e^{-4\gamma_k}\right] . \quad (14)$$

Minimizing the energy (11) leads to the equation for γ_k

$$e^{8\gamma_k} = 1 + \frac{K}{B}(ka)^{2\lambda - 3\nu} \quad (15)$$

and

$$K = \exp\left[-\frac{1}{4\pi}\left(\frac{g_0}{\hbar\omega_0}\right)^2 \int_0^1 dx\, x^{2\lambda - 2\nu}\left(1 + \frac{K}{B}x^{2\lambda - 3\nu}\right)^{-1/2}\right] \quad (16)$$

with

$$B = \frac{(\hbar\omega_0)^3}{4\Delta_0 g_0^2} . \quad (17)$$

From the self-consistent Eq. (16), the static properties of the tunneling particle may be derived. For example, the localization happens as K vanishes. Since the integral in (16) is very sensitive to the two indices (λ, ν), it is usually divided into three cases:[1] super-Ohmic $(2\lambda - 2\nu + 1 > 0)$, sub-Ohmic $(2\lambda - 2\nu + 1 < 0)$, and Ohmic dissipation $(2\lambda - 2\nu + 1 = 0)$. The present paper only deals with the most important and fascinating case, Ohmic dissipation, the other two cases will be discussed in separate papers. Then Eq. (16) is simplified,

$$K = \exp\left[-\frac{1}{4\pi}\left(\frac{g_0}{\hbar\omega_0}\right)^2 \int_0^1 dx\, x^{-1}\left(1 + \frac{K}{B}x^{-\nu - 1}\right)^{-1/2}\right] . \quad (18)$$

We can easily find that the infrared divergence appearing in the renormalization-group analysis is, to an extent, deterred due to the last factor. Completing the integral, we obtain

$$K = \exp\left[-\frac{\alpha}{1-\alpha}\ln(\sqrt{B} + \sqrt{B+K})^2\right] . \quad (19)$$

The dimensionless coupling strength is

$$\alpha = \frac{1}{4\pi(\nu+1)}\left(\frac{g_0}{\hbar\omega_0}\right)^2 . \quad (20)$$

For $\alpha < 1$ there is always a nonzero solution of K, while for $\alpha > 1$ there exists a critical value B_c, leading to two nonzero solutions of K when $B < B_c$; only zero solution when $B > B_c$. B_c is determined by the following equation:

$$B_c = \frac{(\alpha-1)^{\alpha-1}}{(\alpha+1)^{\alpha+1}} , \quad (21)$$

or

$$\left(\frac{\hbar\omega_0}{\Delta_0}\right) = 16\pi(\nu+1)\frac{\alpha(\alpha-1)^{\alpha-1}}{(\alpha+1)^{\alpha+1}} . \quad (22)$$

When there are two nonzero solutions, detailed analysis of stability tells us that the large one corresponds to a minimum point and the small one to a saddle point. Thus we choose the large one as the stable solution. These results imply that a sharp localization-delocalization transition of the tunneling particle can be triggered with an increase in the dimensionless coupling strength.

The displaced states have been used as the variational

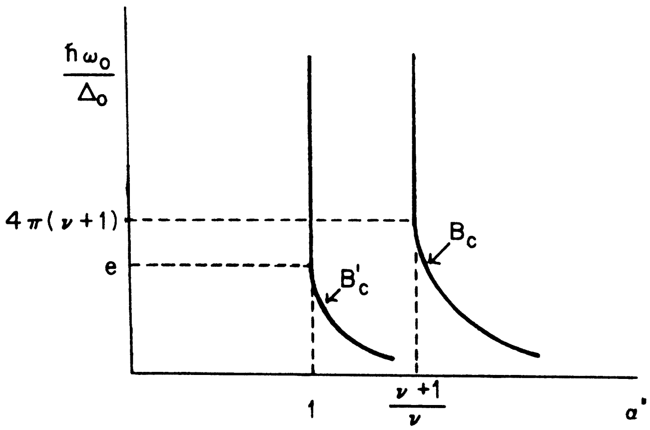

FIG. 1. Localization-delocalization transition given by the displaced state approximation (B_c') and by the displaced-squeezed state approximation (B_c).

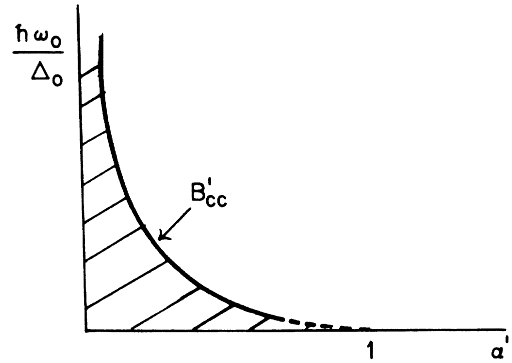

FIG. 2. Comparison of E_g and E_g'. The shaded area is $E_g > E_g'$ and the unshaded area is $E_g < E_g'$.

ground states of phonons in the dissipative tunneling diffusion problem.[9,13] In the following, we would like to give the results using the displaced states as the ground states of phonons in order to compare the different approaches. For the model Hamiltonian (1), it is convenient to assume the variational phonon wave function is

$$|\psi_B'\rangle = \exp\left[\left(\sum_n nC_n^\dagger C_n\right)\left(\sum_k \lambda_k (b_k^\dagger - b_k)\right)\right]. \tag{23}$$

Minimizing the ground-state energy

$$E_g' = -2\Delta_0 K' + \sum_k \left(\hbar\omega_k \lambda_k^2 - 2g_k\lambda_k + \frac{g_k^2}{\hbar\omega_k}\right) \tag{24}$$

leads to the following equations:

$$\lambda_k = \frac{g_k}{\hbar\omega_k + \Delta_0 K'}, \tag{25}$$

$$K' = \exp\left(-\sum_k \frac{\lambda_k^2}{2}\right) = \exp\left[-\frac{\alpha'}{1-\alpha'}\left(\ln(B'+K') - \frac{B'}{B'+K'}\right)\right], \tag{26}$$

with

$$\alpha' = \frac{1}{4\pi\nu}\left(\frac{g_0}{\hbar\omega_0}\right)^2, \quad B' = \left(\frac{\hbar\omega_0}{\Delta_0}\right). \tag{27}$$

For $\alpha' < 1$ there is always a solution $K' \neq 0$, while for $\alpha' > 1$ the solutions K' depend on B': $K' \neq 0$ for $B' < B_c'$ and $K' = 0$ for $B' > B_c'$. The critical value B_c' is

$$B_c' = \left(\frac{\hbar\omega_0}{\Delta_0}\right) = [(\alpha')^{1/2} - 1]^{\alpha'-1}(\alpha')^{-\alpha'/2}\exp[(\alpha')^{1/2}]. \tag{28}$$

The condition of the localization-delocalization transition in the displaced state approximation is represented in Fig. 1. It is shown that the transition depends on the $\hbar\omega_0/\Delta_0$ and α'. For $(\hbar\omega_0/\Delta_0) < e$, α_c' increases as $\hbar\omega_0/\Delta_0$ decreases. Such behavior has occurred in the problem of a particle in a periodic potential with quasiparticle dissipation.[16,17] For $(\hbar\omega_0/\Delta_0) > e$, $\alpha_c' = 1$ is independent of $\hbar\omega_0/\Delta_0$. This result is precisely the same as that of the renormalization-group analysis.[5,9] It is worthwhile to point out that the results of the renormalization-group analysis are obtained mainly on the assumption of the dilute instanton gas or dilute flip gas, where only the close pair of instanton and anti-instanton or flip and flop are important[18] (noninteracting blip approximation[1]). Therefore, the displaced state approximation is equivalent to the noninteracting blip approximation.[19] Recently, it has been pointed out in the study of dissipative tunneling out of a metastable that there is the possibility of condensation of an instanton gas as the breakdown of the dilute gas approximation.[20] For convenience of comparison, the condition of the localization-delocalization transition in the displaced-squeezed state approximation is also shown in Fig. 1. It shows that the displaced-squeezed state approximation gives broader delocalization region than that of the displaced state approximation. Moreover, for $(\hbar\omega_0/\Delta_0) \gg 1$, the localization transition occurs at $\alpha_c' = 1 + (1/\nu)$ instead of $\alpha_c' = 1$. From the point of view of the ground states, it is crucially important to compare the energies between (10) and (24). For $(\hbar\omega_0/\Delta_0) \gg 1$, E_g and E_g' become

$$E_g = -2\Delta_0 K(1-\alpha), \tag{29}$$

$$E_g' = -2\Delta_0 K'(1-\alpha'). \tag{30}$$

The condition $E_g = E_g'$ determines a critical B_{cc}', leading to $E_g > E_g'$ for $B' < B_{cc}'$ and $E_g < E_g'$ for $B' > B_{cc}'$. The critical value

$$B_{cc}' = \left(\frac{\hbar\omega_0}{\Delta_0}\right) = \left(\frac{1-\alpha'}{1-[\nu/(\nu+1)]\alpha'}\right)^{[(\nu+1)/\alpha']\{1-[\nu/(\nu+1)]\alpha'\}(1-\alpha')} \exp((\nu+1)\{1-[\nu/(\nu+1)]\alpha'\})(4\pi\nu\alpha')^{-(1-\alpha')\nu} \tag{31}$$

is shown in Fig. 2. In the calculation of B'_{cc}, we have used the relations $\alpha = [\nu/(\nu+1)]\alpha'$ and $B = B'/16\pi\nu\alpha'$. When $\alpha' \geq (\nu+1)/\nu$ or $\alpha > 1$, we have $K = K' = 0$, then $E_g = E'_g = 0$ for $\hbar\omega_0/\Delta_0 \gg 1$. For $\alpha' \ll 1$, (31) gives $\alpha'_{cc} \approx (\hbar\omega_0/\Delta_0 e^{\nu+1})^{-1\nu}(4\pi\nu)^{-1} \ll 1$. This means that for $\hbar\omega_0/\Delta_0 \gg 1$ and $\alpha'_{cc} < \alpha' < \nu + 1/\nu$ the displaced-squeezed states are more stable than the displaced states. Therefore, we believe that our description of the localization-delocalization transition is more preferable at least in the view of ground-state energy.

In conclusion, we have developed a new theory to study the tunneling diffusion of a particle moving in a tight-binding band and coupled with phonons. The main feature of the theory is to use displaced-squeezed states as the variational ground states of phonons. The narrowing effect of the phonon-overlapping integral on the renormalized bandwidth of the tunneling particle is investigated. We find that for Ohmic dissipation the occurrence of the localization of the particle depends on $\hbar\omega_0/\Delta_0$ and the coupling strength. Moreover, the present theory gives a broader delocalization region compared with previous studies.

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