Symmetry-breaking transition in a two-level system coupled to an Ohmic bath: A squeezed-state approach

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Displaced squeezed states are proposed as variational ground states for phonons (Bose fields) coupled to two-level systems (spin systems). We have investigated the zero-temperature phase diagram for the localization-delocalization transition of a tunneling particle interacting with an Ohmic heat bath. Our results are compared with known existing approximate treatments. A modified phase diagram using the displaced squeezed state is presented.

Introduction. Quantum-mechanical-tunneling systems (e.g., two-level systems) subject to many-particle interactions (e.g., when interacting with their surroundings) have been studied in various branches of condensed-matter physics and it still continues to attract a great deal of attention.[1] These studies include the relaxation and tunneling of atoms or groups of atoms in glasses[2,3] which plays an important role in the low-temperature properties, defect motions in alkali halides,[4] charged-particle motion in metals,[5,6] and molecular transitions in liquids.[7] Pfeifer[8] has explained the existence of chiral molecules by a superselection rule which originates from the ever-present coupling of the molecule to the radiation field. Here the two states are nothing but the left-handed and right-handed configurations of molecules. In recent years these models have been applied extensively to the macroscopic quantum tunneling of quantized magnetic flux through superconducting quantum interference devices.[9] In all of these systems it is now well established that the coupling of phonons to a tunneling system causes the tunneling motion to occur less frequently, i.e., it reduces the effective tunneling matrix element, sometimes termed the Debye-Waller factor. This reduction stems from the orthogonal properties of many-particle wave functions with different local potentials and is known as the Anderson orthogonality theorem.[10]

Hamiltonian. In this paper we confine ourselves to the study of the ground-state properties of a two-level system coupled to a phonon bath. The Ohmic dissipation case has been considered here. We examine a model in which the particle is tunneling between two equivalent minima. Such a model can be represented by a two-level system coupled linearly to a phonon coordinate. The Hamiltonian for the system takes the form ($\hbar=1$)

$$\mathcal{H}=-\Delta_0(C_1^\dagger C_2+C_2^\dagger C_1)+\sum_k \omega_k b_k^\dagger b_k + \sum_k g_k(C_1^\dagger C_1 - C_2^\dagger C_2)(b_k^\dagger + b_k) \; . \qquad (2.1)$$

The coefficient $\Delta_0(>0)$ in (2.1) represents the bare tunneling matrix element, g_k the coupling constant, and ω_k the phonon frequency. C_i and $C_i^\dagger$ with $i=1,2$ are the annihilation and creation operators for the tunneling particle to be at position i; b_k and $b_k^\dagger$ are the annihilation and creation operators representing the phonon mode. Since we are dealing with a single tunneling particle here it does not matter whether it is a boson or a fermion. Although the Hamiltonian (2.1) itself is quite general, we restrict ourselves to an Ohmic dissipative bath, i.e., one for which the spectral density $S(\omega)$ is assumed to be proportional to the excitation energy,[1]

$$S(\omega)=\sum_k g_k^2 \delta(\omega-\omega_k)=\tfrac{1}{2}\alpha\omega, \quad \text{for } \omega\to 0 \; , \qquad (2.2)$$

where α is the dimensionless dissipation parameter.

Using the renormalization-group procedure it has been shown[1] that for the Ohmic dissipation case at zero temperature, a tunneling particle undergoes a sharp transition from a delocalized state to a localized state as the dissipation parameter α is monotonically increased. This is a symmetry-breaking transition. This localization phenomenon is associated with the infrared divergence induced by low-energy phonons, i.e., the phonon field keeps the particle localized at the expense of generating an infinite number of low-energy phonons. It has also been shown that when the tunneling matrix element Δ_0 is small compared to the upper phonon cutoff frequency ω_c, the effective tunneling matrix element is given by[1] $\Delta_{\text{eff}}=\Delta_0(2e\Delta_0/\omega_c)^{\alpha/(1-\alpha)}$. At $\alpha=1$ there is a transition to a localized state. The renormalization-group results have been obtained based mainly on the assumption of a dilute instanton gas or the dilute flip-gas approximation. In recent studies on dissipative quantum tunneling out of metastable states it has been shown that this approximation breaks down due to the condensation of the instanton gas.[11]

It has been rigorously shown that the ground-state properties of two-level systems coupled to Ohmic baths can be mapped onto the one-dimensional Ising model with a $1/r^2$ interaction.[12,13] In particular the delocalization-localization transition is related to the existence of a ferromagnetic phase transition. In the Ising case it is known that the spontaneous magnetization jumps at the critical point. However, since the correlation length diverges, the transition is not first order. On translating this observation back to the two-level system we should expect a discontinuous jump in the effective tunneling matrix element at the critical value of $\alpha=\alpha_c$. Moreover, provided that $\sum(g_k^2)$ is finite, in the limit $\Delta_0 \rightarrow 0$, α_c is bounded between 1 and 2 and α_c increases, as Δ_0 increases, i.e., α_c is a monotonic function of Δ_0. However no such discontinuous behavior has been shown in theoretical studies on two-level systems. Silbey and Harris[14] and independently Tanaka and Sakurai[15] have succeeded in rederiving the renormalization-group results by a simple variational procedure which amounts to a kind of mean-field theory.

Variational wave functions. Let us initially consider the simplest case when $\Delta_0=0$, i.e., when the system is just an oscillator. Since the net effect of the tunneling system being in one of the two levels amounts to the oscillator being displaced in a particular direction (and the effect of it occupying the other level results in the oscillator getting displaced in the opposite direction), the ground state of the many-boson system can be represented by a product of independent wave functions of displaced oscillators as

$$\phi_{gi}=\prod_k \exp\left[-\frac{1}{2}\frac{g_k^2}{\omega_k^2}\right]\exp\left\{(-1)^i\frac{g_k}{\omega_k}b_k^\dagger\right\}|0\rangle,\ i=1,2\ . \tag{3.1}$$

Here $|0\rangle$ represents the vacuum state. This wave function is localized. In the other case when the coupling constant $g_k=0$ (i.e., when the tunneling system and the phonon modes are decoupled) the eigenstates of the tunneling particle are given by the symmetric and antisymmetric combinations of the two-level states, the symmetric combination being the ground state. These two cases show that in general (for arbitrary parameters) the system exhibits a competition between the localization resulting from the phonon mode and the delocalization due to the tunneling. Motivated by these facts Tanaka and Sakurai[15] and independently Silbey and Harris[14] have constructed a variational wave function for the ground state of the coupled system, namely

$$\Psi(u_k)=\frac{1}{\sqrt{2}}\left[\prod_k \exp(-\tfrac{1}{2}|u_k^2|)\exp(-u_k b_k^\dagger)C_1^\dagger + \prod_k \exp(-\tfrac{1}{2}|u_k^2|)\exp(u_k b_k^\dagger)C_2^\dagger\right]|0\rangle\ , \tag{3.2}$$

where u_k is a set of variational parameters. For a choice of $u_k=-g_k/\omega_k$, (3.2) describes a linear combination of two degenerate ground states.

It should be noted that when a particle tunnels from one state to another it has two distinct effects on the phonon wave function; one is that of displacement and the other is of deformation. High-frequency phonons ($\omega>\Delta_0$) follow the tunneling particle adiabatically. Hence the displaced-phonon approximation gives the correct result. However, in the case of low-frequency phonons nonadiabatic effects dominate, which in turn (apart from displacement) produce strong deformations in the phonon wave function. The variational wave function in Eq. (3.2) treats the displacement effect in the wave function correctly but completely ignores the deformation aspect. To include the phonon wave-function deformation effects, Chen and co-workers proposed a displaced squeezed variational wave function[16–18]

$$\Psi(\gamma_k)=\frac{1}{\sqrt{2}}\left\{\prod_k \exp\left[-\frac{1}{2}\left[\frac{g_k}{\omega_k}\right]^2\right]\exp\left[-\frac{g_k}{\omega_k}b_k^\dagger\right]\times\exp[-\gamma_k(b_kb_k-b_k^\dagger b_k^\dagger)]C_1^\dagger + \prod_k \exp\left[-\frac{1}{2}\left[\frac{g_k}{\omega_k}\right]^2\right]\exp\left[\frac{g_k}{\omega_k}b_k^\dagger\right]\times\exp[-\gamma_k(b_kb_k-b_k^\dagger b_k^\dagger)]C_2^\dagger\right\}|0\rangle\ , \tag{3.3}$$

where γ_k is a variational parameter. When the parameter γ_k takes a finite nonzero value then the corresponding phonon state (or a two-photon or two-boson state) is squeezed.[19,20] The squeezed state represents a nonclassical state which has an uncertainty less than that of the coherent state in one of the quadrature phases. Moreover, the uncertainty product of the two quadrature phase fluctuations (variances) takes on a minimum value given by the Heisenberg uncertainty relation. For a finite nonzero γ_k the uncertainty in one of its quadrature components is given by $\exp(-\gamma_k)/2$ and in the other by $\exp(\gamma_k)/2$, which means that one of the quadrature phases is squeezed at the expense of the other.

The variational wave function given in Eq. (3.3) is found to be more stable (i.e., energetically favorable) when compared to the variational wave function in Eq. (3.2). For an Ohmic bath g_k can take either of the forms (i) $g_k=\hbar\sqrt{\omega_c\omega_k}$ or (ii) $g_k=\hbar\omega_c\sqrt{\omega_c/\omega_k}$. The delocalization-localization transition is predicted to occur at a value of $\alpha_c=2$ in case (i) and $\alpha_c=4$ in case (ii), respectively.[16–18] When $(\Delta_0/\omega_c)\ll 1$, the expressions for the effective tunneling matrix elements are $\Delta_{\rm eff}=(\Delta_0/\omega_c)^{\alpha/(\alpha-2)}$ and $\Delta_{\rm eff}=(\Delta_0/\omega_c)^{\alpha/(\alpha-4)}$ for $g_k\approx\sqrt{\omega_k}$ and $g_k\approx 1/\sqrt{\omega_k}$, respectively. In both these cases ω_c is the upper cutoff frequency of the boson excitations. α is the exponent of the overlap integral of the wave functions of the tunneling particle centered at two different sites. It appears as a reduction factor in the expression for $\Delta_{\rm eff}$. Since the width of the displaced squeezed phonon state is much larger than the width of the displaced-phonon state, the value of $\Delta_{\rm eff}$ is enhanced (favoring tunneling) and this in turn contributes to the enhancement of α_c beyond unity.

Although the variational wave function in Eq. (3.3) treats the deformation part of the phonon wave function correctly, it also assumes at the same time that phonons of all frequencies are displaced by an amount proportional to g_k/ω_k. This is true only for high-frequency phonons, i.e., $g_k/\omega_k>1$, while for low-frequency phonons this assumption breaks down. Hence to account for this fact we propose the following variational wave function[21]

$$\Psi(u_k,\gamma_k)=\frac{1}{\sqrt{2}}\Bigg\{\prod_k \exp[-\tfrac{1}{2}|u_k|^2]\exp[-u_k b_k^\dagger]\exp[-\gamma_k(b_k b_k - b_k^\dagger b_k^\dagger)]C_1^\dagger + \prod_k \exp[-\tfrac{1}{2}|u_k|^2]\exp[u_k b_k^\dagger]\exp[-\gamma_k(b_k b_k - b_k^\dagger b_k^\dagger)]C_2^\dagger\Bigg\}|0\rangle , \quad (3.4)$$

where γ_k and u_k are both treated as variational parameters. This variational wave function[21] has a ground-state energy that is lower than the ones obtained by using the wave functions in Eqs. (3.2) and (3.3). By setting the variational parameter $\gamma_k=0$ in Eq. (3.4) we can recover Eq. (3.2). Similarly by setting the variational parameter u_k equal to a constant (i.e., equal to $-g_k/\omega_k$), we can recover Eq. (3.3). Using the properties of squeezed states and Bose operators[19–21] we can readily evaluate the expectation value of the total ground-state energy. Using the Hamiltonian in Eq. (2.1) and the variational wave function in Eq. (3.4) we obtain[21]

$$E(u_k,\gamma_k)=-\Delta_0\exp\sum_k[(-2u_k^2)\exp(-\gamma_k)] + \sum_k\omega_k[u_k^2+(\sinh 2\gamma_k)^2]+\sum_k 2g_k u_k . \quad (3.5)$$

The variational conditions $\partial E/\partial u_k=0$ and $\partial E/\partial\gamma_k=0$, determine the variational parameters, namely,

$$u_k=-g_k(2\Delta_0\exp\{-2u_k^2[\exp(-4\gamma_k)]\}\times\exp(-4\gamma_k)+\omega_k)^{-1} ,$$

$$e^{8\gamma_k}=1+(8\Delta_0\exp[-2u_k^2\{\exp(-4\gamma_k)\}]) . \quad (3.6)$$

We identify the factor multiplying the tunneling matrix element Δ_0 as the tunneling reduction factor (or Debye-Waller factor) Z, which is given by the expression

$$Z=\exp\sum_k\{-2u_k^2\exp(-4\gamma_k)\} .$$

The reduction factor Z has to be evaluated self-consistently using Eq. (3.6). In our analysis we restrict ourselves to the case of Ohmic dissipation,[1] for which

$$\sum_k g_k^2 f(\omega_k)=\int_0^{\omega_c}\sum_k g_k^2\delta(\omega-\omega_k)f(\omega)d\omega = \frac{\alpha}{2}\int_0^{\omega_c}\omega f(\omega)d\omega . \quad (3.7)$$

This can be used in evaluating summations of arbitrary functions $f(\omega_k)$ over many modes multiplied by the square of the coupling constant g_k. ω_c is the upper cutoff frequency of the boson excitations. The proportionality constant α is of the second order in the coupling constant g_k and also reflects the density of low-energy excitations. Here α is a dimensionless coupling constant representing the strength of Ohmic dissipation. In our treatment the effective tunneling parameter Z is very sensitive to the frequency dependence of the coupling constant g_k.[18] To this end we restrict ourselves to the two special cases referred to earlier, viz.:

$$\text{(i) } g_k=\hbar\omega_c(\omega_k/\omega_c)^{1/2} , \qquad \text{(ii) } g_k=\hbar\omega_c(\omega_c/\omega_k)^{1/2} . \quad (3.8)$$

Numerical studies. In this section we outline the numerical technique used to investigate the behavior of the reduction factor Z as a function of the parameter α and the bare tunneling matrix element Δ_0. The effective or renormalized tunneling parameter is given by the expression $\Delta_{\text{eff}}=\Delta_0 Z$. For a displaced squeezed state this can be rewritten as

$$\ln\Delta_{\text{eff}}=\ln\Delta_0-\sum_k\{2g_k^2 e^{-4\gamma_k}(2\Delta_0 Z e^{-4\gamma_k}+\omega_k)^{-2}\} . \quad (4.1)$$

Using Eq. (37) ln Z is evaluated to be

$$\ln Z=-\alpha\int_0^1\frac{x\Gamma}{(2\Delta Z\Gamma+x)^2}dx , \quad (4.2)$$

where $x=\omega/\omega_c$, $\Delta=\Delta_0/\omega_c$, and $\hbar=1$. In the process of evaluating the summation in (4.1), the variational parameter $e^{-4\gamma_k}$ is replaced by the variable Γ. An iterative scheme may now be employed to calculate ln Z in a self-consistent manner.

For case (i) mentioned above we have chosen $g_k=\sqrt{\omega_k\omega_c}$. Using (3.6), which determines the variational parameters, and making the identifications $u_k\mapsto\mathcal{V}_n$, $e^{4\gamma_k}\mapsto\mathcal{A}_n$, we arrive at the set of self-consistent equations

$$\mathcal{V}_n=\frac{-1}{2\Delta Z\mathcal{A}_{n-1}+x},\quad \mathcal{A}_n=(1+8\Delta Z\mathcal{V}_n^2)^{-1/2} . \quad (4.3)$$

These may be iterated and then finally integrated to yield

$$\ln Z_n=-\alpha\int_0^1\frac{x\mathcal{A}_n}{(2\Delta Z\mathcal{A}_n+x)^2}dx , \quad (4.4)$$

with the initial conditions $\mathcal{A}_0=1$ and $\mathcal{V}_0=0$. The corresponding self-consistent set of equations for case (ii) are

$$\mathcal{A}_{n-1}=\frac{x}{\sqrt{x^2+8\Delta Z\mathcal{V}_{n-1}^2}},\quad \mathcal{V}_n=-\frac{1}{2\Delta Z\mathcal{A}_{n-1}+x} ,$$
$$\mathcal{J}_n=\frac{\sqrt{x^2+8\Delta Z\mathcal{V}_n^2}}{(2\Delta Z+\sqrt{x^2+8\Delta Z\mathcal{V}_n^2})^{-2}},\quad \ln Z_n=-\alpha\int_0^1\mathcal{J}_n dx , \quad (4.5)$$

with initial conditions identical to those for case (i). The criterion used to decide the order up to which the self-consistent set of equations should be iterated is determined by demanding that $\ln(Z_{n+1}/Z_n)\ll 10^{-5}$.

Results and conclusions. For a given value of Δ expressed as a function of α we have observed that the effective tunneling parameter Z decreases monotonically and at a particular critical value of $\alpha=\alpha_c$ (depending on Δ) Z drops to zero discontinuously. The value of α_c signifies the transition from a delocalized state (tunneling state) to a localized state (broken symmetry state). For

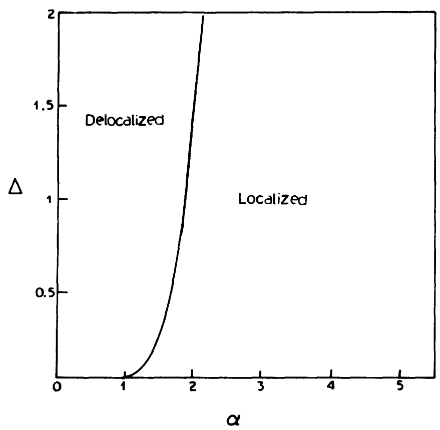

FIG. 1. Phase diagram for the delocalization-localization transition in a two-level system coupled to an Ohmic bath for case (i) where $g_k \approx \sqrt{\omega_k}$.

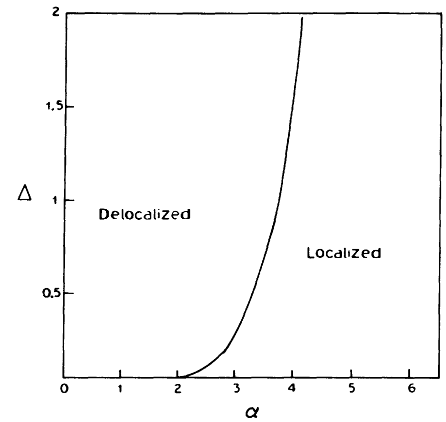

FIG. 2. Phase diagram for the delocalization-localization transition in a two-level system coupled to an Ohmic bath for case (ii) where $g_k \approx 1/\sqrt{\omega_k}$.

the case (i) Fig. 1 shows the phase boundary between the localized and delocalized states for various values of Δ. It should be noted that in the limit $\Delta \to 0^+$, the phase boundary is located at a value of $\alpha_c = 1$ and increases monotonically as a function of Δ. Our results for the phase boundary are quite different from the results obtained earlier. The results based on variational wave functions (3.2) and (3.3) predict the phase boundary, as $\Delta \to 0^+$, at values of $\alpha_c = 1$ and 2, respectively. In these cases, for small values of Δ, $\alpha_c(\Delta)$ is independent of Δ and the transition is continuous, in the sense that there is no discontinuity in Z across the phase boundary. We have observed discontinuous jumps in Z across the phase boundary for all values of Δ. This fact has not been observed in earlier studies. However, the magnitude of the discontinuity decreases monotonically to zero as we approach $\Delta \to 0^+$. Our results are consistent with the known results on the discontinuous nature of this transition.[12,13] Figure 2 shows the phase boundary for case (ii). Here again our results are different from those obtained earlier. Variational wave functions (3.2) and (3.3) predict $\alpha_c = 1$ and 4, respectively, for $\Delta \to 0^+$. For case (ii) we find that $\alpha_c = 2$ as $\Delta \to 0^+$.

In summary, we have obtained through a displaced-squeezed state variational wave-function treatment the phase boundary of the symmetry breaking transition in a two-level system coupled to boson excitations. For the Ohmic case we have shown that the nature of the phase boundary depends very crucially on the frequency dependence of g_k. In our treatment we have restricted ourselves to two specific cases, namely $g_k \approx \sqrt{\omega_k}$ and $g_k \approx 1/\sqrt{\omega_k}$. It would be interesting to study the tunneling reduction (or effective mass) factor in other physically relevant systems. In such cases one would have to choose the proper spectral function. This would include the sub-Ohmic and super-Ohmic frequency spectrums.[1]

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