Tunneling and localization in a two-state system interacting with a phonon bath

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A variational ground-state wave vector for a tunneling system coupled to a phonon bath is proposed taking into account the possibility of a symmetry breaking in the initial state of a two-state system. A best upper bound to the ground-state energy is found showing the impossibility of localization due to interaction with a phonon bath.

During the last few years there has been considerable interest in the theoretical investigation of the ground-state properties of a two-state system (particle) coupled to a phonon bath.[1] The most exciting property found for this system was the possibility of localization[2] in one of the states due to interaction with a bath in the case of Ohmic dissipation. In a variational approach,[3,4] the localization was manifested by a zero probability of interstate transitions[5,6] and was related to the one taking place in the quantum tunneling of magnetic flux in superconducting quantum interference device.[4,7]

In the variational approach,[3–6] the conclusion about localization of the particle due to its interaction to the Ohmic phonon bath was made on the ground of the specific behavior of the tunneling reduction factor which was found to be zero in the region of supposed localization. The main result which is reported in this paper is to show that actually variational methods used before are not suitable to describe the localization region. The reason is that variational ground-state wave vectors (GSWV) proposed in Refs. [3–6], working perfectly in the tunneling region, do not take into account the adiabatic symmetry breaking in the two-state system. We will show that this effect, being negligible for tunneling, becomes extremely important in the region of supposed localization. Adiabatic symmetry breaking leads to the onset of spontaneous magnetization and to the phase transition in the studied model.[8] At the same time, the adiabatic symmetry breaking gives a nonzero tunneling reduction factor in the same region of parameters making impossible the localization in this type of tunneling system. The phase transition is related to the symmetry breaking between potential wells but not to localization as it was supposed before.

A great deal of interest was also related to the quality of the approximation used in a variational approach.[3,4] It was related to the understanding of the effect of squeezing of the phonon modes on the ground-state properties of the model.[5,6,9,10] It was found that for definite values of the model parameters the phonon field is squeezed[6] in its ground state. This conclusion is not a universal one because there are cases when the original GSWV built with a help of the unitary operator generating the operator displacement of the boson modes[3,4] is more stable, providing a better upper bound to the ground-state energy (GSE).[6] It is only the combination of these two approaches that provides better estimates for all values of parameters.[5] This approach reveals a dependence of the upper bound to the GSE on the index λ of the coupling strength. Generally, the squeezing in the GSWV modifies slightly the localization conditions of the usual variational approach.

In this paper we show that localization is actually a very subtle and problematic property of a two-state system interacting with a phonon bath when it is studied in a variational approach. This notion was made in Ref. 11 where the GSWV was presented which always corresponds to *tunneling without localization* in the system. It provides a better upper bound to the GSE with a corresponding reduction factor which is nonzero everywhere.

We propose a trial GSWV taking into account both the delocalization at the small values of the tunneling matrix element[11] and the squeezing of the phonon modes.[5,6] This GSWV, when it is used in the Ritz variational method, gives the best known upper bound to the GSE of a model with a nonzero reduction factor. This means that the ground state found in Refs. 4 and 5 is unstable and there is no localization in the system.

The effectively two-state system (particle) linearly coupled to a phonon field is described by the Hamiltonian[4–6]

$$\mathcal{H} = -W\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \sigma_z \sum_k g_k (b_k^\dagger + b_k) , \qquad (1)$$

where W is the splitting parameter (tunneling matrix element) of the two-state system which is defined in terms of the Pauli spin matrices, g_k is the coupling strength, and ω_k is the frequency of a phonon of a mode k. The annihilation b_k and creation $b_q^\dagger$ operators of the phonon field satisfy the usual Bose commutation relations $[b_k, b_q^\dagger] = \delta_{kq}$. The summation in (1) is taken over all modes k of the field.

The Hamiltonian (1) is widely used in the literature to investigate a wide range of physical phenomena when an effectively two-state system interacts with its surroundings described in terms of elementary Bose excitations[1] The competition between localization of a particle due to

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its interaction with a phonon bath and delocalization inherent in tunneling is the main feature of the model (1).

The most well-known variational ansatz for the trial GSWV of the system (1) is given by the theory of localization-delocalization phase transition[3,4] and can be considered as a unitary reconstruction of the first-order perturbation theory,

$$|\psi_U\rangle = \mathbf{U}|0\rangle|\pi/4\rangle \ , \tag{2}$$

where the (operator) displacement unitary operator

$$\mathbf{U} = \exp\left\{\sigma_z \sum_k u_k (b_k^\dagger - b_k)\right\} \tag{3}$$

acts on the direct product of the phonon vacuum $|0\rangle$ and the symmetric spin state

$$|\pi/4\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} .$$

The state $|\pi/4\rangle$ describes tunneling in a free two-state system when it can be found with equal probability in either of its two symmetric states. A quantum particle is tunneling in its ground state between two wells through the finite barrier of a double-well potential.

A general wave vector of a two-state system has the form

$$|\varphi\rangle = \begin{bmatrix}\cos\varphi\\ \sin\varphi\end{bmatrix} .$$

The symmetry between "left" and "right" wells is broken in $|\varphi\rangle$. In other words, the probabilities to find a particle in these two wells are different, but nevertheless the particle is tunneling between two wells in the same sense as in the state $|\pi/4\rangle$.

The tunneling reduction factor of a free two-state system $\langle\varphi|\sigma_x|\varphi\rangle = \sin 2\varphi$ is proportional to the product of two probabilities. The reduction factor z becomes zero only in the localized states $|+\rangle$ and $|-\rangle$. The tunneling reduction factor calculated for the ground state of interacting systems is used as the order parameter in a variational approach[3-6] to the problem.

The upper bound E_U to the GSE of the system (1) found with the help of the GSWV (2) was investigated in Ref. 4, where the possibility of localization was deduced.

The squeezed state approach developed in Refs. 5 and 6 is centered around the GSWV,

$$|\psi_{UG}\rangle = \mathbf{UG}|0\rangle|\pi/4\rangle \ , \tag{4}$$

where the unitary operator

$$\mathbf{G} = \exp\left\{\sum_k \frac{\gamma_k}{2}(b_k^{\dagger 2} - b_k^2)\right\} \tag{5}$$

generates the Bogolubov transformation[12]

$$\mathbf{G}^\dagger b_k \mathbf{G} = b_k \cosh\gamma_k + b_k^\dagger \sinh\gamma_k$$

of the Bose operators. The squeezed GSWV with the fixed displacement,[6] $u_k = -g_k/\omega_k$, does not always provide a better upper bound than the purely displaced GSWV (2). The simultaneous minimization with respect to u_k and γ_k of the GSE obtained with the help of (4) has been done in Ref. 5. As for the GSWV (2), this approach leads to the symmetry-breaking phase transition from the tunneling to the localized state. As a consequence of additional squeezing, the phase boundary between these two states reveals dependence on the index of the coupling strength.

It was found in Ref. 11 that in the adiabatic approximation, which is the most relevant for small values of the tunneling matrix element, the GSWV converges to a direct product of independent vectors describing the tunneling particle and a field. The GSWV

$$|\psi_{UV\Phi}\rangle = \mathbf{UV\Phi}|0\rangle|+\rangle \tag{6}$$

was proposed, where

$$\mathbf{V} = \exp\left\{\sum_k v_k (b_k^\dagger - b_k)\right\} , \tag{7}$$

$$\mathbf{\Phi} = \exp\{-i\varphi\sigma_y\} , \tag{8}$$

$$|+\rangle = \begin{bmatrix}1\\0\end{bmatrix} . \tag{9}$$

Unlike the operator $\mathbf{U}$, the unitary operator $\mathbf{V}$ generates a c-number displacement of the Bose operators, while $\mathbf{\Phi}$, taken at an angle $\varphi \neq \pi/4$, breaks the symmetry between two initial states of a free tunneling particle. Taken independently in addition to the operator $\mathbf{U}$, the operators $\mathbf{V}$ and $\mathbf{\Phi}$ do not contribute to the GSE of the system, while together they improve the upper bound in the most interesting region of small W and large enough interaction strengths where the localization was found previously. The state (6) is more stable than (2) everywhere and gives a nonzero reduction factor corresponding to the tunneling particle without localization.[11]

We use Eqs. (4) and (6) to propose the trial GSWV,

$$|\psi_0\rangle = \mathbf{UVG\Phi}|0\rangle|+\rangle \ , \tag{10}$$

which takes into account both the deformation of the phonon bath through squeezing together with displacement of the boson modes and delocalization appropriate to (6).

The upper bound to the GSE of the Hamiltonian (1),

$$E_0 \le \langle\psi_0|\mathcal{H}|\psi_0\rangle \ ,$$

is easily found with the help of Eqs. (3), (5), and (7)–(10),

$$E_0 \le \sum_k [\omega_k(u_k^2 + v_k^2 + \sinh^2\gamma_k) + 2g_k u_k + 2\cos 2\varphi(\omega_k u_k + g_k)v_k] - Wz \ , \tag{11}$$

where the notation

$$z = \sin 2\varphi \exp\left\{-2\sum_k u_k^2 \exp\{-2\gamma_k\}\right\} \tag{12}$$

has been introduced for the tunneling reduction factor

$$z = \langle\psi_0|\sigma_x|\psi_0\rangle .$$

The uniform squeezing approximation where $\gamma_k = \gamma$ for every field mode is used below. We will see that it suffices to provide better bounds to the GSE and clarify considerably our understanding of the localization-delocalization problem.

To proceed further, the dimensionless ground-state energy, normalized to the upper cutoff frequency Ω of excitations, $\mathcal{E}_0 = E_0/\Omega$, and the dimensionless tunneling matrix element $w = W/\Omega$ are introduced. We also use the standard for the Ohmic dissipation spectral density of energy excitations,[4-6]

$$S(\omega)=\sum_k g_k^2\delta(\omega-\omega_k)=\tfrac{1}{2}\alpha\omega\ ,$$

and convert in a usual way the summation over field modes into the integration over frequencies ω,

$$\sum_k g_k^2 f(\omega_k)=\int_0^{\Omega}S(\omega)f(\omega)d\omega\ .$$

As in the squeezed-state approach,[5] our upper bound is sensitive to the frequency dependence of the coupling strength which is specified by the index λ,

$$g_k=\Omega\left[\frac{\omega_k}{\Omega}\right]^{\lambda}.$$

Two major upper bounds for the normalized GSE $\mathcal{E}_0$ of the Hamiltonian (1) follow from (11). The first one is found after minimization on φ, v_k, and u_k and is given by

$$\mathcal{E}_0\le\mathcal{E}_{01}(\alpha,w)=\min_{\{\gamma\}}\epsilon_{01}(\alpha,w;\gamma)\ , \tag{13}$$

where

$$\epsilon_{01}(\alpha,w;\gamma)=-\frac{\alpha}{2}\left[1-\frac{\sinh^2\gamma}{3-2\lambda}\right]-\frac{(w\zeta)^2}{2\alpha-e^{2\gamma}}$$

and

$$\zeta=\sqrt{e}\left[\frac{2\alpha-e^{2\gamma}}{2\alpha}\right]^{\alpha e^{-2\gamma}}.$$

The uniform squeezing approximation gives a nonzero contribution for the indices of the coupling strength $\lambda<\frac{3}{2}$. Also there are limitations on the use of the bound (13) itself. First of all, it is valid for the coupling strengths

$$\alpha\ge\tfrac{1}{2}e^{2\gamma}\ . \tag{14}$$

In addition, minimization on φ of the GSE (11) can be done only if $|\sin 2\varphi|\le 1$. If this constraint is not fulfilled one must fix the best value of $\varphi=\pi/4$, as will be done for the second major upper bound $\mathcal{E}_{02}(\alpha,w)$. For the upper bound $\mathcal{E}_{01}(\alpha,w)$, the above constraint is equivalent to

$$w\le w^*=(2\alpha-e^{2\gamma})/2\zeta\ . \tag{15}$$

The tunneling reduction factor (12) corresponding to the bound (13) is given by

$$z=2w\zeta^2/(2\alpha-e^{2\gamma}) \tag{16}$$

and the only remaining variational parameter γ minimizing the function $\epsilon_{01}(\alpha,w;\gamma)$ is defined from the self-consistency equation

$$\alpha(2\alpha-e^{2\gamma})\sinh 2\gamma+8(3-2\lambda)(w\zeta)^2\ln\zeta=0\ .$$

Another major upper bound is derived from (11) for the symmetric case of $\varphi=\pi/4$ and has the form

$$\mathcal{E}_0\le\mathcal{E}_{02}(\alpha,w)=\min_{\{\gamma\}}\epsilon_{02}(\alpha,w;\gamma)\ , \tag{17}$$

$$\epsilon_{02}(\alpha,w;\gamma)=\frac{\alpha}{2}\left[\frac{\sinh^2\gamma}{3-2\lambda}\right]-\frac{\alpha}{2}\frac{1}{1+2wze^{-2\gamma}}-wz\ ,$$

where now both reduction factor z and variational parameter γ are defined self-consistently from the equations

$$\ln z=-\alpha e^{-2\gamma}\left[\ln\left[1+\frac{1}{2wze^{-2\gamma}}\right]-\frac{1}{1+2wze^{-2\gamma}}\right]$$

and

$$e^{4\gamma}=1-(8wz/\alpha)e^{2\gamma}(3-2\lambda)\ln\zeta\ .$$

The full upper bound to the GSE of the model (1) is given by the inequality

$$\mathcal{E}_0\le\min[\mathcal{E}_{01}(\alpha,w),\mathcal{E}_{02}(\alpha,w)]\ . \tag{18}$$

For those values of α,w where no localization was found previously, the upper bound is given by $\mathcal{E}_{02}(\alpha,w)$. It follows from Eqs. (13), (17), and (18) that it is for the most interesting region of the possible "localization" the upper bound $\mathcal{E}_{01}(\alpha,w)$ becomes important. The ground state corresponding to this bound remains tunneling everywhere, inhibiting the localization.

As in Ref. 11, the bound $\mathcal{E}_{02}(\alpha,w)$ is not greater than $\mathcal{E}_{01}(\alpha,w)$ for values of the coupling parameter $\alpha\le 1/2$. Consequently, the upper bound has the form $\mathcal{E}_0\le\mathcal{E}_{02}(\alpha,w)$. The function $\mathcal{E}_{02}(\alpha,w)$ is analytical in w and the reduction factor $z_{02}(\alpha,w)$ is nonzero in this region.

The localization was found in Refs. 3 and 4 for $\alpha>\frac{1}{2}$ and small w. In Fig. 1 we compare our upper bound (18) with the upper bound $\mathcal{E}_U(\frac{3}{2},w)$ corresponding to the GSWV (2) (see Ref. 4 for details) for $\alpha=\frac{3}{2}$ and $\lambda=\frac{1}{2}$ (for $\lambda=\frac{3}{2}$ the effect of additional squeezing in the GSWV $|\psi_0\rangle$ becomes irrelevant). As shown in Fig. 1 there is no contribution of the tunneling part of the Hamiltonian (1) to the GSE $\mathcal{E}_U(\frac{3}{2},w)$ for $w\le w_c=0.4779$ (see Refs. 4 and 11), so that $\mathcal{E}_U(\frac{3}{2},w)=\text{const}$ and the corresponding reduction factor of tunneling $z_U(\frac{3}{2},w)$ is zero (see Fig. 2). The interstate transitions are inhibited and the particle is localized in one of its degenerate ground states.

For values of the coupling strength index $\lambda<\frac{3}{2}$, the contribution of squeezing of the phonon cloud surrounding the tunneling particle becomes important, so that $\mathcal{E}_{02}(\alpha,w)<\mathcal{E}_U(\alpha,w)$ and the GSWV $|\psi_0\rangle$ is more stable than $|\psi_U\rangle$. The similar upper bound has been studied in Refs. 5 and 6 with a confirmation of existence of localization and conclusion that the squeezing just modifies the phase boundary separating the localized and tunneling phases.

The situation is changed drastically for the full upper bound (18). In the region of $\alpha>\frac{1}{2}$ and $0\le w\le w^*=0.6603$ (the inequality $w_c<w^*$ always holds), the symmetry of the initial state $\Phi|+\rangle$ of the two-state system in (10) is broken ($\varphi\ne\pi/4$). Conditions (14) and (15) are also satisfied. Our GSWV $|\psi_0\rangle$ becomes more stable than the displaced state $|\psi_U\rangle$ and displaced squeezed state $|\psi_{UG}\rangle$ (see Fig. 1). The reduction factor (16) remains nonzero in this region, showing the *impossibility of localization* in the model (1) in general. The interaction of a two-state system with a phonon bath specified by the Hamiltonian (1) is only reducing the probability of interstate transitions and cannot cause the localization in one of the states.

A different way to study the tunneling problem has been chosen in Refs. 8, 13, and 14. It is based on the notion that it is possible to accept the correlator

$$m=\langle\psi_0|\sigma_z|\psi_0\rangle$$

as the order parameter of the problem. In distinction from z the order parameter m is zero in the pure tunneling state $|\pi/4\rangle$ and has its maximal absolute value in the

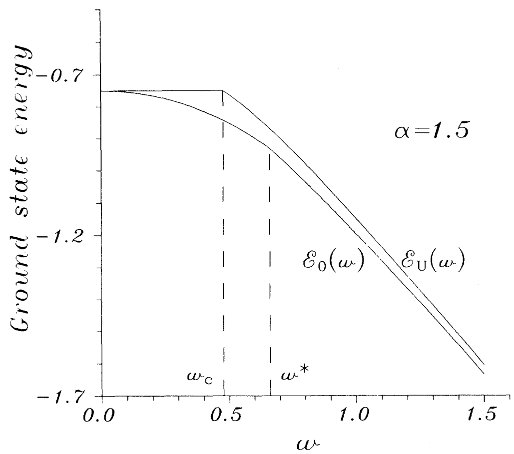

FIG. 1. Upper bound to the ground-state energy as a function of the normalized tunneling matrix element w. The bound $\mathscr{E}_U(w)$ has a plateau between 0 and w_c corresponding to "localization." Our upper bound $\mathscr{E}_0(w)$ is better than $\mathscr{E}_U(w)$ everywhere and corresponds to a tunneling system without localization. Two branches of the bound $\mathscr{E}_0(w)$ are merging at w^*.

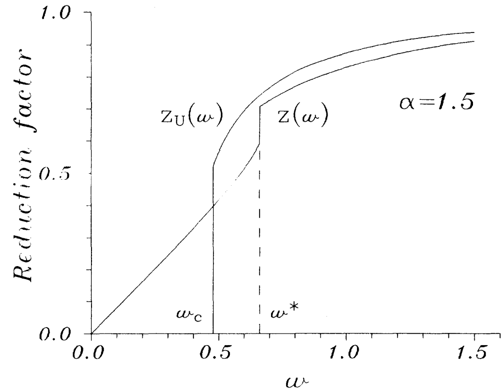

FIG. 2. Reduction factor as a function of the normalized tunneling matrix element w. The reduction factor $z_U(w)$ is zero in the "localized" state when w is smaller than w_c.

two maximally ordered localized states. A particle is equally likely in either of two wells if $m=0$, while $m \geq 0$ means that the particle is predominantly in the "right" well.[8] We should stress here that the condition $m \geq 0$ does not exclude at all the tunneling of the particle. For example, in the tunneling state $|\varphi\rangle$ both order parameters z and m are nonzero.

In the case of the model (1) the order parameter m is related[13] to the breaking of reflection symmetry $\sigma_z \rightarrow -\sigma_z, b_k \rightarrow -b_k$ of the Hamiltonian (1). The spontaneous breaking of reflection symmetry in the ground state of $\mathcal{H}$ associated with the onset of the nonzero spontaneous magnetization m was found in Ref. 8 and investigated in Refs. 8, 13, and 14.

The magnetization m has been never studied in the framework of the variational approach. The reason is very simple: it is equal to zero identically in any previous variational approach. Following the argumentation of Refs. 8, 13, and 14, this would mean the absence of localization for any interaction strength.

We have found that for the GSWV (6) the magnetization is given by the mean-field-type equation

$$m=\sqrt{1-(w/w^*)^2}\ , \qquad (19)$$

if $w \leq w^*$; otherwise, $m=0$ if $w > w^*$. In Eq. (19) the normalized tunneling matrix element plays the role of temperature in the usual theory of magnetic phase transition. The critical value w^* is given by (15).

Our Eq. (19) confirms variational results of Ref. 8 with a different value of w^* which depends on the ground-state choice. Although the model does exhibit the phase transition at the critical point w^*, its ground state remains tunneling because the tunneling reduction factor remains nonzero for $w \leq w^*$. The phase transition is associated with the discontinuity of the ground-state energy derivative at w^*. We can speak about the onset of magnetization but there is no reason to conclude that the particle is localized in the potential well. The magnetization is stressing the symmetry breaking between two states of the quantum particle and does not contradict its tunneling.

Although the variational method cannot be used for the rigorous proof of existence or absence of localization in the model with the Hamiltonian $\mathcal{H}$, it brings a lot of understanding of its main features. In this paper we were able to give the most stable GSWV of the model (1) corresponding to pure tunneling without localization which was found in the earlier variational study of the same model.

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