

## Non-Markovian theory of tunneling in dissipative media

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Tunneling between two wells in the dissipative medium is considered in the framework of a spin-boson Hamiltonian. It is shown that, when the interaction energy between the two wells (characterizing the barrier between the wells),  $v$  is lower than certain critical energy  $v_c$ , determined by the interaction with bosons, the tunneling friction vanishes. This *supertunneling* phenomenon is considered in both the weak- and strong-coupling cases.

### I. INTRODUCTION

The problem of the tunneling of a particle that also interacts with excitations of the medium has recently attracted considerable interest.<sup>1-8</sup> Tunneling developed into an important field in solid-state physics, elucidated in the extensive early review by Duke.<sup>9</sup>

The simplest tunneling process in a dissipative medium is a transition between two approximate ground states of a two-well potential in the presence of phonons. Such a process can be described by a two-state system interacting with a harmonic solid.<sup>10-17</sup> This problem is isomorphous to that of energy transfer between localized electronic states in crystal.<sup>18,19(a)</sup>

As is known, interaction with the phonons of the medium to the decay of quantum beats two wells: "tunneling friction." The aim of this paper is to show that under certain conditions, when the interaction energy  $v$  between two wells is lower than critical energy  $v_c$ , determined by interaction with phonons, the tunneling friction vanishes. This phenomenon is called *supertunneling*.<sup>19(b)</sup>

The origin of this unusual behavior is connected with the appearance of discrete bound states in the spectrum of the two-state system interacting with phonons. It has to be noticed that existence of local states and local modes in the dissipative system interacting with some kind of impurity has been known for a long time. Rayleigh<sup>20</sup> found local modes in the chain of interacting oscillators in the framework of classical theory. The quantum one-level system interacting with the continuum of states has been considered by Rice<sup>21,22</sup> and Fano.<sup>23</sup> Riess,<sup>24</sup> Rosenfeld *et al.*,<sup>25</sup> and Gelbart and Jortner<sup>26</sup> have shown that discrete local states may exist in such systems provided certain conditions are satisfied. Cukier and Mazur<sup>27</sup> have proved that the existence of local modes in a harmonic-oscillator chain with an impurity, leads to the violation of the ergodic properties of the system. Similarly, the existence of bound discrete states in a spectrum of a two-level system interacting with bosons leads to a qualitative modification of the process of spontaneous emission of bosons.<sup>28,29</sup> (The probability to remain in the excited states does not tend to zero when  $t \rightarrow \infty$ .) But the most striking example of the influence of bound states on the properties of the system with the continuum of states is the superconductivity phenomenon.

Of course, the supertunneling phenomenon has nothing to do with the superconductivity.

The existence of isolated modes and bound states in dissipative systems has been extensively studied for many years. The novelty of the present work is the implication of the existence of local states to tunneling in a dissipative medium.

The material is organized as follows. Section II recalls the model in which tunneling in the condensed medium is reduced to a two-state system interacting with phonons. Section III is devoted to a general quantum-mechanical description of time development of the density matrix. In this section we do not use any specific approximations.

On the other hand, in Secs. IV and V the one-boson approximation is used. It is shown that this approximation is valid in the case of weak spin-phonon coupling. In Sec. VI the time development of tunneling system in the dissipative medium is obtained in the strong-coupling case.

The weak-coupling case is based on the exact non-Markovian solution for the relaxation via the spontaneous emission of bosons,<sup>28</sup> while the strong-coupling case uses the exact solution for the degenerate spin-boson system.<sup>29</sup> (See also Ref. 30.) Considering processes connected with the spontaneous emission of phonons, we restrict ourselves to the zero-temperature calculations.

### II. THE MODEL

We consider a quite general model<sup>31,13,32</sup> which may be appropriate for the description of nuclear group transfer, electron transfer accompanied by the transfer of nuclear groups, or a transition between two stable configurations of a molecule embedded in the condensed medium. We assume that all these processes occur in a single electronic state, i.e., we consider adiabatic transitions. In the Born-Oppenheimer approximation, such a system may be presented by the Hamiltonian

$$\mathcal{H} = T + U(Q) + \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 q_k^2) - \sum_k A_k(Q) q_k. \quad (2.1)$$

Here  $Q$  is the set of coordinates of singled-out nuclear modes describing the nuclear subsystem (molecule) interacting with its surrounding a condensed medium.  $T$  and  $U$  are the kinetic and potential energy of the nuclear subsystem; the third term in the Hamiltonian (2.1) de-

scribes the condensed medium in the harmonic approximation as a phonon bath, and the last term is the interaction energy between the nuclear subsystem and condensed medium. The only assumption about this interaction is that it is linear in the coordinates  $q_k$ , i.e., the excitations of the surrounding condensed medium are small enough.

The potential energy  $U$  is supposed to have two minima corresponding to two quasistable configurations of the nuclear subsystem. We assume that these two minima (potential wells) are divided by a barrier which is sufficiently large so that tunneling through this barrier may be considered as a small perturbation.

Let us consider the Hamiltonian of the isolated molecule

$$E = T + U(Q). \quad (2.2)$$

We assume that only two low-lying energy levels of this Hamiltonian are essential, i.e., that these two levels are separated from others so that it is possible to neglect excitations to other levels. Employing the assumption about the smallness of the tunneling, we can introduce the eigenfunctions  $|L\rangle$  and  $|R\rangle$  with eigenvalues  $E_L$  and  $E_R$  which are approximate stationary states (without taking into account the penetration through the barrier). These states are localized in the left and right wells, respectively.

Thus, we are dealing with a two-state system and the Hamiltonian of the molecule may be represented as

$$E = n_L E_L + n_R E_R + r_+ v_{LR} + r_- v_{RL}. \quad (2.3)$$

Here  $n_L = \frac{1}{2} + r_1$ ,  $n_R = \frac{1}{2} - r_1$ ,  $r_{\pm} = r_3 \pm ir_2$ ,  $r_1$ ,  $r_2$ , and  $r_3$  are components of the effective spin<sup>33</sup> describing the two-state systems

$$\begin{aligned} [r_1, r_2] &= ir_3, \\ [r_2, r_3] &= ir_1, \\ [r_3, r_1] &= ir_2, \\ r_j^2 &= \frac{1}{4}, \end{aligned} \quad (2.4)$$

and  $v$  is the matrix of the effective perturbation energy corresponding to the tunneling between the states  $|L\rangle$  and  $|R\rangle$ . It is reasonable to assume that this matrix element has the form

$$v_{LR} = v_{RL} = v = \hbar\omega e^{-\lambda}, \quad (2.5)$$

where the effective parameter  $\hbar\omega$  has the order of the characteristic energy difference in one well and  $\lambda$  is much larger than unity. For the one-dimensional case in the semiclassical approximation,<sup>34</sup>

$$\lambda = \frac{1}{\hbar} \int_b^a |P| dQ, \quad (2.6)$$

where  $a$  and  $b$  are the classical turning points, and  $P$  is the (imaginary) momentum inside the barrier. Now taking into account only two levels  $E_L$  and  $E_R$  of the molecule, the Hamiltonian (2.1) of the whole system can be presented in the form

$$\mathcal{H} = n_L \mathcal{H}_{LL} + n_R \mathcal{H}_{RR} + r_+ \mathcal{H}_{LR} + r_- \mathcal{H}_{RL}, \quad (2.7)$$

where the matrix elements are taken with the aid of the eigenfunctions  $|L\rangle$  and  $|R\rangle$ .

Thus, the effective Hamiltonian takes the form

$$\begin{aligned} \mathcal{H} &= n_L E_L + n_R E_R + \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 q_k^2) - n_R \sum_k \omega_k^2 q_{Rk} q_k \\ &\quad - n_L \sum_k \omega_k^2 q_{Lk}^2 q_k - r_+ \left[ v + \sum_k V_{LRk} q_k \right] \\ &\quad + r_- \left[ v + \sum_k V_{RLk} q_k \right], \end{aligned} \quad (2.8)$$

where

$$\omega_k^2 q_{Lk} = \langle L | A_k(Q) | L \rangle, \omega_k^2 q_{Rk} = \langle R | A_k(Q) | R \rangle, \quad (2.9)$$

$$V_{RLk} = V_{LRk}^* = \langle R | A_k(Q) | L \rangle.$$

Considering terms proportional to  $q_k$ , one can neglect terms containing the overlap integrals  $V_{RLk}$ . They have exponentially small factors of (2.5) type. Without the terms  $V_{RLk}$  and  $V_{LRk}$ , the Hamiltonian (1.8) is isomorphous to that describing a widely used model<sup>35-39</sup> in which the electron-nuclear system is represented by two intersecting electronic parabolas plus a perturbation causing transitions between these electronic states. A review of Silbey<sup>40</sup> is relevant to the problem. The generalization to the case of intersecting electronic energy hyperparabolas with a continuum of degrees of freedom was also considered in Refs. 41, 42, 31, and 32.

Using definitions of operators  $n_L, n_R$ , we can rewrite the Hamiltonian (1.8) (without the terms with  $V_{RLk}, V_{LRk}$ ) in the form

$$\begin{aligned} \mathcal{H} &= r_1 (E_L - E_R) + 2r_3 v + \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 q_k^2) \\ &\quad - r_1 \sum_k \omega_k^2 (q_{Lk} - q_{Rk}) q_k - \frac{1}{2} \sum_k \omega_k^2 (q_{Lk} + q_{Rk}) q_k. \end{aligned} \quad (2.10)$$

Here we have dropped terms which do not depend on the system's variables  $q_k, p_k, r_1, r_2$ , and  $r_3$ . Performing the unitary transformation

$$q_k \rightarrow q_k - \frac{1}{2} (q_{Lk} + q_{Rk}), \quad (2.11)$$

we get (again dropping the constant terms)

$$\begin{aligned} \mathcal{H} &= r_1 (E_L - E_R) + 2r_3 v + \frac{1}{2} \sum_k (p_k^2 + \omega_k^2 q_k^2) \\ &\quad - r_1 \sum_k \omega_k^2 (q_{Lk} - q_{Rk}) q_k \\ &\quad - \frac{1}{2} r_1 \sum_k \omega_k^2 (q_{Lk}^2 - q_{Rk}^2). \end{aligned} \quad (2.12)$$

For the symmetrical two-well potential

$$E_L = E_R, \quad q_{Lk} = -q_{Rk} = q_k^0, \quad (2.13)$$

one can rewrite the Hamiltonian (2.12) in the form

$$\mathcal{H} = (r_3 + \frac{1}{2})\hbar\omega_0 + \frac{1}{2} \sum_k [(p_k^2 + w_k^2 q_k^2) - \hbar\omega_k] - 2r_1 \sum_k \omega_k^2 q_k^0 q_k \quad (2.14)$$

or

$$\mathcal{H} = (r_3 + \frac{1}{2})\hbar\omega_0 + \frac{1}{2} \sum_k a_k^\dagger a_k \hbar\omega_k - (r_+ + r_-) \sum_k B_k (a_k^\dagger + a_k) . \quad (2.15)$$

In the later relation  $r_\pm = r_1 \pm ir_2$ ,

$$q_k^0 = \left[ \frac{2}{\hbar\omega_k^3} \right]^{1/2} B_k \quad (2.15')$$

and  $a_k^\dagger, a_k$  are the creation and annihilation operators of phonons. The frequency  $\omega_0$  is expressed through the matrix element  $v$ ,

$$\hbar\omega_0 = 2v . \quad (2.16)$$

Parameters  $B_k$  describe an interaction between the tunneling system and phonons. A localization in the potential wells is described by the operator  $r_1$ . The localization in the left well corresponds to  $r_1 = \frac{1}{2}$ ,  $n_L = 1$ ,  $n_R = 0$ , while  $r_1 = -\frac{1}{2}$  corresponds to the localization in the second well:  $n_R = 1$ ,  $n_L = 0$ .

Two forms of the spin-boson Hamiltonian (2.14) and (2.15) are convenient for two different approximations. For the weak-coupling approximation, we divide the Hamiltonian into two parts:

$$\mathcal{H}_0 = (r_3 + \frac{1}{2})\hbar\omega_0 + \frac{1}{2} \sum_k a_k^\dagger a_k \hbar\omega_k - \sum_k B_k (r_+ a_k + r_- a_k^\dagger) \quad (2.17)$$

and

$$V = - \sum_k B_k (r_+ a_k^\dagger + r_- a_k) . \quad (2.18)$$

In the case of strong coupling, the perturbation energy is

$$V' = (r_3 + \frac{1}{2})\hbar\omega_0 , \quad (2.19)$$

while the unperturbed Hamiltonian is

$$\mathcal{H}'_0 = \frac{1}{2} \sum_k [(p_k^2 + \omega_k^2 q_k^2) - \hbar\omega_k] - 2r_1 \sum_k \omega_k^2 q_k^0 q_k . \quad (2.20)$$

The exact solution for the unperturbed Hamiltonian (2.17) has been presented in a previous paper,<sup>28</sup> while the exact solution for the Hamiltonian (2.20) has been found in Ref. 29. In this paper we will consider both the weak- and strong-coupling cases.

### III. TIME DEVELOPMENT OF THE SYSTEM: GENERAL RELATIONS

We consider a system described by the Hamiltonian

$$H = H_0 + V , \quad (3.1)$$

where the energy spectrum of the unperturbed Hamiltonian  $H_0$  contains discrete and continuous energy levels

and  $V$  is the interaction energy. Let  $S$  be a unitary matrix transformation which connects eigenstates of the Hamiltonian  $H$  with eigenstates of the Hamiltonian  $H_0$

$$\psi'_L = \sum_v S_{vL} \psi_v \quad (3.2)$$

or, equivalently,

$$S_{vL} = \langle \psi_v | \psi'_L \rangle . \quad (3.3)$$

The unitary matrix  $S$  connects the density matrix in the  $H_0$  representation with the density matrix  $\rho$  in  $H$  representation

$$\rho' = S^{-1} \rho S . \quad (3.4)$$

In the new representation, the von Neumann equation for the density matrix has the form

$$\dot{\rho}'_{LM} = -i\omega'_{LM} \rho'_{LM} \quad (3.5)$$

or

$$\rho'_{LM}(t) = \rho'_{LM}(0) e^{-i\omega'_{LM} t} ,$$

where

$$\hbar\omega'_{LM} = E'_L - E'_M \quad (3.6)$$

and  $E'_L, E'_M$  are eigenvalues of the Hamiltonian (3.1). We will be interested in the time development of the density matrix in the representation of the unperturbed states  $\psi_v$ . In particular, we will be interested in the time dependence of the probability of the localization in one of the wells. For this purpose we can use a relation inverse to (3.4)

$$\rho = S \rho' S^{-1} . \quad (3.7)$$

We find, from (3.7) and (3.5),

$$\rho_{uv}^{(t)} = \sum_{LM} S_{uL} \rho'_{LM}(0) S_{vM}^* e^{-i\omega'_{LM} t} . \quad (3.8)$$

To express  $\rho'_{LM}(0)$  through the initial conditions for the unperturbed density matrix  $\rho(0)$ , we use the relation (3.4)

$$\rho'_{LM}(0) = \sum_{u',v'} S_{u'L}^* \rho_{u'v'}(0) S_{v'M} . \quad (3.9)$$

Substituting relation (3.9) into (3.8), we get

$$\rho_{uv}(t) = \sum_{L,M,u',v'} S_{uL} S_{u'L}^* \rho_{u'v'}(0) S_{v'M} S_{vM}^* e^{-i\omega'_{LM} t} . \quad (3.10)$$

On the other hand, in many applications it is assumed that the time development can be described by the master equation

$$\dot{P}_n^{\text{cl}} = - \sum_k (W_{nk} P_n - W_{kn} P_L) . \quad (3.11)$$

Here,  $P_n$  is the probability that the system is in the state  $n$ , once  $W_{nk}$  is a probability of transition (per unit time) from state  $n$  to state  $k$ . This equation is derived in the Markovian approximation. The necessary condition of this approximation is that the eigenfrequency  $\omega_{mn}$  has to be much larger than the transition rate  $W_{mn}$

$$W_{mn}/|\omega_{mn}| \ll 1. \quad (3.12)$$

In previous papers<sup>28,29</sup> it has been shown that there is another necessary condition of the Markovian approximation. The exact spectrum of the whole system should not contain nondissipative discrete levels (apart from the ground state of the system). It will be shown below that the existence of the nondissipative discrete states leads to the crucial change in the time development of the system, which cannot be described by the Markovian approximation.

#### IV. UNITARY MATRIX IN THE WEAK-COUPLING CASE

To find a time development using expression (3.10), we have to find matrix elements  $S_{uL}$  of the unitary matrix. We will choose indices  $u$  as corresponding to the eigenfunctions of the Hamiltonian

$$H_0 = \hbar\omega_0(r_3 + \frac{1}{2}) + \sum_k a_k^\dagger a_k \hbar\omega_k. \quad (4.1)$$

These eigenfunctions have the form

$$\psi_{\pm 1/2, \{n_k\}} = \Phi_{\pm 1/2} \prod_k \Phi_{n_k}(q_k), \quad (4.2)$$

where  $\Phi_{n_k}$  are eigenfunctions of the harmonic-oscillator Hamiltonian

$$a_k^\dagger a_k \Phi_{n_k}(q_k) = n_k \Phi_{n_k}(q_k) \quad (4.3)$$

and

$$r_3 \Phi_{\pm 1/2} = \pm \frac{1}{2} \Phi_{\pm 1/2}. \quad (4.4)$$

In this paper we consider processes taking place at zero temperature. Therefore, we will analyze expansions (3.2) containing the phonon vacuum states:

$$\begin{aligned} \psi'_{L_1} = & S_{-1/2, L_1} \psi_{-1/2, 0} + \sum_\lambda S_{1/2, 1_\lambda; L_1} \psi_{1/2, 1_\lambda} \\ & + \sum_{\lambda_1, \lambda_2} S_{-1/2, 1_{\lambda_1}, 1_{\lambda_2}; L_1} \psi_{-1/2, 1_{\lambda_1}, 1_{\lambda_2}} + \dots, \end{aligned} \quad (4.5)$$

$$\begin{aligned} \psi_{L_2} = & S_{1/2, L_2} \psi_{1/2, 0} + \sum_\lambda S_{-1/2, 1_\lambda; L_2} \psi_{-1/2, 1_\lambda} \\ & + \sum_{\lambda_1, \lambda_2} S_{1/2, 1_{\lambda_1}, 1_{\lambda_2}; L_2} \psi_{1/2, 1_{\lambda_1}, 1_{\lambda_2}} + \dots. \end{aligned} \quad (4.6)$$

Here

$$\begin{aligned} \psi_{\pm 1/2} = & \Phi_{\pm 1/2} \prod_k \Phi_0(q_k), \\ \psi_{\pm 1/2, 1_\lambda} = & \Phi_{\pm 1/2} \Phi_1(q_\lambda) \prod_{k(\neq \lambda)} \Phi_0(q_k), \\ \psi_{\pm 1/2, 1_{\lambda_1}, 1_{\lambda_2}} = & \Phi_{\pm 1/2} \Phi_1(q_{\lambda_1}) \Phi_1(q_{\lambda_2}) \\ & \times \prod_{k(\neq \lambda_1, \lambda_2)} \Phi_0(q_k), \dots \end{aligned} \quad (4.7)$$

We substitute eigenfunctions (4.7) into the Schrödinger equation

$$(H_0 + V - E)\psi_L = 0, \quad (4.8)$$

where  $H_0$  is determined by Eq. (4.1) and

$$V = -(r_+ + r_-) \sum_k B_k (a_k^\dagger + a_k), \quad r_\pm = r_l \pm i r_2. \quad (4.9)$$

After usual operations, we get

$$(E_{1/2, 0} - E'_{L_2}) S_{1/2, L_2} + \sum_\lambda V_{1/2, 0; -1/2, 1_\lambda} S_{-1/2, 1_\lambda; L_2} = 0, \quad (4.10)$$

$$(E_{-1/2, 1_\lambda} - E'_{L_2}) S_{-1/2, 1_\lambda; L_2} + V_{-1/2, 1_\lambda; 1/2, 0} S_{1/2, L_2} + \sum_{\lambda'(\neq \lambda)} V_{-1/2, 1_\lambda, 0_{\lambda'}; 1/2, 1_{\lambda'}} S_{1/2, 1_{\lambda'}; L_2} = 0, \quad (4.11)$$

$$\begin{aligned} (E_{1/2, 1_\lambda, 1_{\lambda'}} - E'_{L_2}) S_{1/2, 1_\lambda, 1_{\lambda'}; L_2} + V_{1/2, 1_\lambda, 1_{\lambda'}; -1/2, 1_\lambda, 0_{\lambda'}} S_{-1/2, 1_\lambda; L_2} \\ + V_{1/2, 1_\lambda, 1_{\lambda'}; -1/2, 0_{\lambda'}, 1_{\lambda'}} S_{-1/2, 1_\lambda; L_2} + \sum_{k(\neq \lambda, \lambda')} V_{1/2, 1_\lambda, 1_{\lambda'}, 0_k; -1/2, 1_\lambda, 1_{\lambda'}, 1_k} S_{-1/2, 1_\lambda, 1_{\lambda'}, 1_k; L_2} = 0, \end{aligned} \quad (4.12)$$

$$(E_{-1/2, 0} - E'_{L_1}) S_{-1/2, L_1} + \sum_\lambda V_{-1/2, 0; 1/2, 1_\lambda} S_{1/2, 1_\lambda; L_1} = 0, \quad (4.13)$$

$$(E_{1/2, 1_\lambda} - E'_{L_1}) S_{1/2, 1_\lambda; L_1} + V_{1/2, 1_\lambda; -1/2, 0} S_{-1/2, L_1} + \sum_{\lambda'(\neq \lambda)} V_{1/2, 1_\lambda, 0_{\lambda'}; -1/2, 1_{\lambda'}, 1_{\lambda'}} S_{-1/2, 1_{\lambda'}, 1_{\lambda'}; L_2} = 0, \quad (4.14)$$

$$\begin{aligned} (E_{-1/2, 1_\lambda, 1_{\lambda'}} - E'_{L_1}) S_{-1/2, 1_\lambda, 1_{\lambda'}; L_1} + V_{-1/2, 1_\lambda, 1_{\lambda'}; 1/2, 1_\lambda, 0_{\lambda'}} S_{1/2, 1_\lambda; L_1} \\ + V_{-1/2, 1_\lambda, 1_{\lambda'}; 1/2, 0_{\lambda'}, 1_{\lambda'}} S_{1/2, 1_\lambda; L_2} + \sum_{k(\neq \lambda, \lambda')} V_{-1/2, 1_\lambda, 1_{\lambda'}, 0_k; 1/2, 1_\lambda, 1_{\lambda'}, 1_k} S_{1/2, 1_\lambda, 1_{\lambda'}, 1_k; L_2} = 0. \end{aligned} \quad (4.15)$$

This infinite chain of coupled equations has been derived under the assumption that the boson system has a contin-

uum of modes, their number  $N \rightarrow \infty$ . The normalization condition of wave functions (4.5) and (4.6) provides the

following relations:

$$\begin{aligned} S_{\pm 1/2, L} &\propto (N^{-1})^0, \\ S_{\pm 1/2, 1_\lambda; L} &\propto (N^{-1})^{1/2}, \\ S_{\pm 1/2, 1_{\lambda_1}, 1_{\lambda_2}; L} &\propto (N^{-1}), \\ S_{\pm 1/2, 1_{\lambda_1}, 1_{\lambda_2}, 1_{\lambda_3}; L} &\propto (N^{-1})^{3/2}, \dots \end{aligned} \quad (4.16)$$

These relations enabled us not to include in Eqs. (4.10)–(4.15) terms of

$$V_{1/2, 1_\lambda; -1/2, 2_\lambda} S_{-1/2, 2_\lambda; L_1} \text{ type.}$$

The contribution of these terms vanishes in the continuum limit.

Now we will adopt a one-boson approximation. It means that we neglect terms having more than one boson: like  $S_{\pm 1/2, 1_\lambda, 1_{\lambda'}, \dots; L}$ . This also means that terms with a higher number of bosons can be neglected in comparison with terms containing a lower number of bosons. Conditions of the applicability of a one-boson approximation will be derived below.

In a one-boson approximation we have two systems of equations for the  $S$  matrix and for the eigenenergies which follow from the Hamiltonian (2.15)

$$(\hbar\omega_0 - E'_{L_2}) S_{1/2, L_2} - \sum_{\lambda} B_{\lambda} S_{-1/2, 1_\lambda; L_2} = 0, \quad (4.17)$$

$$(\hbar\omega_{\lambda} - E'_{L_2}) S_{-1/2, 1_\lambda; L_2} - B_{\lambda} S_{1/2, L_2} = 0, \quad (4.18)$$

$$\hbar\omega_0 - E'_{L_2} = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_{\lambda} - E'_{L_2}}, \quad (4.19)$$

$$E'_{L_1} S_{-1/2, L_1} + \sum_{\lambda} B_{\lambda} S_{1/2, 1_\lambda; L_1} = 0, \quad (4.20)$$

$$S_{1/2, 1_\lambda; L_1} (\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1}) - B_{\lambda} S_{-1/2, L_1} = 0, \quad (4.21)$$

$$E'_{L_1} = - \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1}}. \quad (4.22)$$

Equations (4.17)–(4.19) can be obtained as exact equations following from the Hamiltonian (2.17). This Hamiltonian is usually called a rotating-wave approximation Hamiltonian. Thus, the rotating-wave approximation leads to Eqs. (4.17)–(4.19). On the other hand, Eqs. (4.20)–(4.22) also describe one-boson states, but they follow from the counter-rotating part (2.18) of the interaction energy. Thus, strictly speaking, the rotating-wave approximation does not coincide with the one-boson approximation. The higher boson terms in Eqs. (4.10)–(4.15) are connected with both rotating and counter-rotating terms in the interaction energy (4.9).

Now we derive conditions of the one-boson approximation. Neglecting terms with more than the two bosons involved, we get, from (4.11), (4.12) and (4.14), (4.15),

$$S_{1/2, 1_\lambda, 1_{\lambda'}; L_2} = \frac{B_{\lambda'} S_{-1/2, 1_{\lambda'}; L_2} + B_{\lambda} S_{-1/2, 1_\lambda; L_2}}{\hbar\omega_0 + \hbar\omega_{\lambda} + \hbar\omega_{\lambda'} - E'_{L_1}}, \quad (4.23)$$

$$S_{-1/2, 1_\lambda; L_1} = \frac{B_{\lambda}}{\hbar\omega_{\lambda} - E'_{L_2}} S_{1/2, L_2},$$

$$S_{-1/2, 1_\lambda, 1_{\lambda'}; L_1} = \frac{B_{\lambda'} S_{1/2, 1_{\lambda'}; L_1} + B_{\lambda} S_{1/2, 1_\lambda; L_1}}{\hbar\omega_{\lambda} + \hbar\omega_{\lambda'} - E'_{L_1}}, \quad (4.24)$$

$$S_{1/2, 1_\lambda; L_1} = \frac{B_{\lambda}}{\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1}} S_{-1/2, L_1}.$$

Here we assume that higher boson contributions are much smaller than lower boson contributions. Taking into account one- and two-boson contributions, we can write the normalization conditions in the form

$$S_{1/2, L_2}^2 + \sum_{\lambda} S_{-1/2, 1_\lambda; L_2}^2 + \sum_{\lambda, \lambda'} S_{1/2, 1_\lambda, 1_{\lambda'}; L_2}^2 = 1, \quad (4.25)$$

$$S_{-1/2, L_1}^2 + \sum_{\lambda} S_{1/2, 1_\lambda; L_1}^2 + \sum_{\lambda, \lambda'} S_{-1/2, 1_\lambda, 1_{\lambda'}; L_1}^2 = 1. \quad (4.26)$$

Substituting Eqs. (4.23) and (4.24) into relations (4.25) and (4.26), respectively, one gets

$$S_{1/2, L_2}^2 \left[ 1 + \sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} - E'_{L_2})^2} + \sum_{\lambda, \lambda'} \frac{B_{\lambda}^2 B_{\lambda'}^2}{(\hbar\omega_{\lambda} + \hbar\omega_{\lambda'} - E'_{L_2})^2} \left( \frac{1}{\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1}} + \frac{1}{\hbar\omega_{\lambda'} - E'_{L_1}} \right)^2 \right] = 1, \quad (4.27)$$

$$S_{-1/2, L_1}^2 \left[ 1 + \sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1})^2} + \sum_{\lambda, \lambda'} \frac{B_{\lambda}^2 B_{\lambda'}^2}{(\hbar\omega_{\lambda} + \hbar\omega_{\lambda'} - E'_{L_1})^2} \left( \frac{1}{\hbar\omega_0 + \hbar\omega_{\lambda} - E'_{L_1}} + \frac{1}{\hbar\omega_0 + \hbar\omega_{\lambda'} - E'_{L_1}} \right) \right] = 1. \quad (4.28)$$

It is easy to see that the double sum in Eq. (4.27) has the order of the magnitude

$$\sum_{\lambda, \lambda'} \dots \lesssim \sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} - E'_{L_2})^2} \sum_{\lambda'} \frac{B_{\lambda'}^2}{(\hbar\omega_0 + \hbar\omega_{\lambda'})^2}. \quad (4.29)$$

It implies that one can use the one-boson approximation

provided

$$\sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_0 + \hbar\omega_{\lambda})^2} \ll 1, \quad (4.30)$$

or a more strict condition is fulfilled

$$\sum_{\lambda} \frac{B_{\lambda}^2}{\hbar^2 \omega_{\lambda}^2} \ll 1. \quad (4.31)$$

It can be shown that the same condition is sufficient in order to neglect the double sum in Eq. (4.28).

We will solve one-boson equations (4.17)–(4.19) and (4.20)–(4.22) separately. They generate two classes of one-boson eigenstates:

$$\psi'_{L_1} = S_{-1/2, L_1} \psi_{-1/2, 0} + \sum_{\lambda} S_{1/2, 1_{\lambda}; L_1} \psi_{1/2, 1_{\lambda}}, \quad (4.32)$$

$$\psi'_{L_2} = S_{1/2, L_2} \psi_{1/2, 0} + \sum_{\lambda} S_{-1/2, 1_{\lambda}; L_2} \psi_{-1/2, 1_{\lambda}}. \quad (4.33)$$

First we will consider Eqs. (4.17)–(4.19) and (4.33). These equations describe the interaction of one discrete state  $|\frac{1}{2}, 0\rangle$  with the continuum of states  $|\frac{1}{2}, 1_{\lambda}\rangle$ .

Such a problem has been analyzed in Refs. 21–26 in the context of the configurational interaction. In the context of the spontaneous emission of bosons, this problem has been considered in a previous paper.<sup>28</sup> We will briefly review here the main results of the analysis. From the normalization condition for  $\psi'_{L_2}$  (4.33) and Eq. (4.18), it follows that

$$S_{1/2, L_2}^2 = \frac{1}{1 + \sum_{\lambda} [B_{\lambda}^2 / (\hbar\omega_{\lambda} - E'_{L_2})^2]}. \quad (4.34)$$

Now we will assume that spectrum of the boson energies

$$E_{\lambda} = \hbar\omega_{\lambda} \quad (4.35)$$

is spread from zero to

$$E_{\max} = \hbar\omega_{\max}. \quad (4.36)$$

Eigenvalues of  $E'_{L_2}$  may lie either in the continuum region

$$0 < E'_{L_2} < E_{\max} \quad (4.37)$$

or below zero and above  $E_{\max}$ . The latter belong to the discrete spectrum of the entire system (the tunneling subsystem coupling with the phonon bath) while the former belong to the continuum of the entire system. The existence of the discrete states in the context of the configuration interaction has been discussed by Riess,<sup>24</sup> Rosenfeld *et al.*,<sup>25</sup> and by Gelbart and Jortner.<sup>26</sup>

It is easy to see that the existence of excited discrete states  $|d\rangle$  leads to nondecaying harmonic terms in the time dependence of the density matrix (3.10). [The ground discrete state always exists and it is the solution of Eqs. (4.20)–(4.22) as will be shown below.] If  $E'_d$  are eigenenergies of the excited discrete states, then nondecaying harmonic terms in (3.10) emerge, provided

$$\lim_{N \rightarrow \infty} S_{ud} \neq 0, \quad (4.38)$$

otherwise these terms will give an infinitesimal contribution to the corresponding Fourier integral. This property (nonvanishing of  $S_{ud}$  for  $N \rightarrow \infty$ ) may serve as a definition of the discrete state. If  $E'_{L_2}$  lies in the region

(4.37), then it follows from (4.34) that  $S_{1/2, L_2} \rightarrow 0$  when  $N \rightarrow \infty$ . The only exception may be if  $B_{\lambda} \rightarrow 0$  at  $E'_{L_2} = \hbar\omega_{\lambda}$ . We do not consider this case. On the other hand, states lying beyond the continuum region (4.37) give finite contributions to the sum (3.10). In this case

$$(\hbar\omega_{\lambda} - E'_{L_2})^2 > 0 \quad (4.39)$$

and  $S_{1/2, L_2}^2$  is finite.

The onset of the continuum starts at the zero energy. Therefore, the state with negative energy

$$E'_d = -E_0, \quad E_0 > 0 \quad (4.40)$$

is the discrete state. We find from Eq. (4.19) that

$$\hbar\omega_0 + E_0 = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_{\lambda} + E_0}. \quad (4.41)$$

It is easy to see that the root  $E_0 > 0$  exists provided

$$\hbar\omega_0 < \hbar\omega_c = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_{\lambda}}. \quad (4.42)$$

By the same token there may exist a discrete level above  $E_{\max}$

$$E'_d = E_{\max} + \delta, \quad \delta > 0 \quad (4.43)$$

provided

$$E_{\max} - \hbar\omega_0 < \sum_{\lambda} \frac{B_{\lambda}^2}{E_{\max} - \hbar\omega_{\lambda}}. \quad (4.44)$$

Also in this case the sum in (4.34) does not contain the singularity, since condition (4.39) is fulfilled. Therefore, for discrete states  $E'_d, E'_{d'}$ , we get

$$S_{1/2, d}^2 = \frac{1}{1 + \sum_{\lambda} [B_{\lambda}^2 / (\hbar\omega_{\lambda} + E_0)^2]}, \quad (4.45)$$

$$S_{1/2, d'}^2 = \frac{1}{1 + \sum_{\lambda} [B_{\lambda}^2 / (E_{\max} - \hbar\omega_{\lambda} + \delta)^2]}. \quad (4.46)$$

For simplicity's sake, we will consider the case when condition (4.44) is not fulfilled. In this case,

$$S_{1/2, d'}^2 = 0 \quad (4.47)$$

while the value of  $S_{1/2, d}$  depends on parameter  $\omega_0$

$$S_{1/2, d}^2 = \begin{cases} \left[ 1 + \sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} + E_0)^2} \right]^{-1}, & \omega_0 < \omega_c = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar^2 \omega_{\lambda}}, \\ 0, & \omega_0 > \omega_c \end{cases} \quad (4.48)$$

The eigenfunction  $\psi'_d$  corresponding to the eigenvalue  $E'_d = -E_0$  has the form

$$\psi'_d = S_{1/2, d} \psi_{1/2, 0} + \sum_{\lambda} S_{-1/2, 1_{\lambda}; d} \psi_{-1/2, 1_{\lambda}}, \quad (4.49)$$

where  $S_{-1/2, 1_{\lambda}; d}$  can be found from (4.18):

$$S_{-1/2,1\lambda;d} = \frac{1}{\hbar\omega_\lambda + E_0} S_{1/2,d} . \quad (4.50)$$

Now we will consider the eigenstates  $\psi'_\alpha$  of the new continuum. First, we consider the case when eigenvalues  $E_\lambda = \hbar\omega_\lambda$  form an equidistant spectrum, being the difference between two neighboring energies,<sup>21,22</sup>  $\varepsilon$  tends to zero in the continuum limit  $N \rightarrow \infty$ . From Eq. (4.19) we have

$$\hbar\omega_0 - E'_\alpha = \sum_\lambda \frac{B_\lambda^2}{E_\lambda - E'_\alpha} . \quad (4.51)$$

All the contributions to the summation in this equation are of two kinds. There are contributions for which  $E_\lambda$  is very different from  $E'_\alpha$  and contributions from the region in which  $E_\lambda - E'_\alpha$  is of the order of  $\varepsilon$ . Let  $a_\alpha$  be the least positive value of  $E_\lambda - E'_\alpha$ , and let  $b_\alpha$  be

$$b_\alpha = a_\alpha - \varepsilon/2 . \quad (4.52)$$

It can be shown<sup>21,22</sup> that a contribution from the region where  $E_\lambda - E'_\alpha$  is of the order of  $\varepsilon$  takes the form

$$-B_\alpha^2 \frac{\pi}{\varepsilon} \tan(\pi b_\alpha / \varepsilon) , \quad (4.53)$$

where  $B_\alpha$  is the value of  $B_\lambda$  for very small  $E_\lambda - E'_\alpha$ . In the continuum limit  $N \rightarrow \infty$  when  $\varepsilon \rightarrow 0$ , the rest of the sum may be rewritten as an integral, and one gets

$$\hbar\omega_0 - E_\alpha + B_\alpha^2 \frac{\pi}{\varepsilon} \tan \frac{\pi b_\alpha}{\varepsilon} - \int_0^{E_{\max}} \frac{B_\gamma^2 / \varepsilon}{E_\gamma - E_\alpha} dE_\gamma = 0 . \quad (4.54)$$

Therefore,

$$B_\alpha^2 \frac{\pi}{\varepsilon} \tan \frac{\pi b_\alpha}{\varepsilon} = E_\alpha - E_+ , \quad (4.55)$$

where

$$E_+ = \hbar\omega_0 - \int_0^{E_{\max}} \frac{B_\gamma^2 / \varepsilon}{E_\gamma - E_\alpha} dE_\gamma . \quad (4.56)$$

Equation (4.55) determines  $\tan(\pi b_\alpha / \varepsilon)$  as a function of  $E_\alpha$  belonging to the unperturbed continuum. The eigenfunctions of the new continuum have the form

$$\psi'_\alpha = S_{1/2,\alpha} \psi_{1/2,0} + \sum_\lambda S_{-1/2,1\lambda;\alpha} \psi_{-1/2,1\lambda} . \quad (4.57)$$

From Eq. (4.18) and the normalization condition one gets

$$S_{-1/2,1\lambda;\alpha} = \frac{B_\lambda}{E_\lambda - E'_\alpha} S_{1/2,\alpha} , \quad (4.58)$$

$$S_{1/2,\alpha}^2 = \left[ 1 + \sum_\lambda \frac{B_\lambda^2}{(E_\lambda - E'_\alpha)^2} \right]^{-1} .$$

In the limit  $\varepsilon \rightarrow 0$ , one gets<sup>21,22</sup>

$$S_{1/2,\alpha}^2 = \left[ \frac{B_\alpha^2 \pi^2}{\varepsilon^2} \left[ 1 + \tan^2 \frac{\pi b_\alpha}{\varepsilon} \right] \right]^{-1} . \quad (4.59)$$

Now, substituting the value of  $\tan(\pi b_\alpha / \varepsilon)$  from Eq. (4.55), we obtain

$$S_{1/2,\alpha}^2 = B_\alpha^2 / \left[ \left[ \frac{B_\alpha^2 \pi}{\varepsilon} \right]^2 + (E_+ - E_\alpha)^2 \right] . \quad (4.60)$$

In general, when the continuum spectrum is not necessarily equidistant,  $\varepsilon^{-1}$  has to be substituted by the density of states  $\rho$  in the unit energy interval and one gets<sup>23</sup>

$$S_{1/2,\alpha}^2 = \frac{1}{\pi \rho(E_\alpha)} \frac{\hbar \gamma(E_\alpha)}{\hbar^2 \gamma^2(E_\alpha) + (E_+ - E_\alpha)^2} , \quad (4.61)$$

where

$$E_+(E_\alpha) = \hbar\omega_0 - \int_0^{E_{\max}} \frac{B_\lambda^2}{E_\lambda - E_\alpha} \rho(E_\lambda) dE_\lambda \quad (4.62)$$

and

$$\gamma(E_\alpha) = \frac{\pi}{\hbar} \rho(E_\alpha) B_\alpha^2 . \quad (4.63)$$

To analyze the function  $S_{1/2,\alpha}$ , we consider the roots of equation

$$E_+(\bar{E}) - \bar{E} = 0$$

or

$$\hbar\omega_0 - \int_0^{E_{\max}} \frac{B_\lambda^2}{E_\lambda - \bar{E}} \rho(E_\lambda) dE_\lambda - \bar{E} = \hbar\omega_0 - F(\bar{E}) - \bar{E} = 0 , \quad (4.64)$$

where

$$F(E) = \int_0^{E_{\max}} \frac{B_\lambda^2}{E_\lambda - E} \rho(E_\lambda) dE_\lambda = P \sum_\lambda \frac{B_\lambda^2}{\hbar\omega_\lambda - E} .$$

Here P designates a principal part of the corresponding integral.

First, we consider the case when Eq. (4.64) has a negative root  $E$ . It is easy to verify that this root coincides with (4.40) and (4.41),

$$\bar{E} = E'_d = -E_0 . \quad (4.65)$$

As we know, this is the case when (4.42)

$$\omega_0 < \omega_c . \quad (4.66)$$

Now, having in mind the condition of the one-boson approximation (4.31), we get for the unitary matrix elements (4.48) and (4.61) the following expressions:

$$S_{1/2,d}^2 \approx 1 - \sum_\lambda \frac{B_\lambda^2}{E_\lambda^2} \approx 1, \quad E'_d \approx - \sum_\lambda \frac{B_\lambda^2}{E_\lambda} + \hbar\omega_0 , \quad (4.67)$$

$$S_{1/2,\lambda}^2 \approx \frac{B_\lambda^2}{E_\lambda^2} \approx 0 . \quad (4.68)$$

[It is also assumed that  $\hbar \gamma(E_\lambda) \ll (E_\lambda + E_0)$ .] On the other hand, in the case

$$\omega_0 > \omega_c = \sum_\lambda \frac{B_\lambda^2}{\hbar^2 \omega_\lambda} , \quad (4.69)$$

the excited discrete state does not exist and

$$S_{1/2,d}^2 = 0, \quad (4.70)$$

and  $S_{1/2,\alpha}^2$  is given by Eq. (4.61). Now let us consider the case when  $\gamma(E_\alpha)$  and  $E_+(E_\alpha)$  are smooth enough functions so that one can neglect the variations of  $\gamma(E)$  and  $E_+(E)$  near  $E = \bar{E}$ —the root of Eq. (4.64). This means that

$$\bar{\gamma} = \gamma(\bar{E}) \ll \omega^*, \quad \bar{E}/\hbar, \quad (4.71)$$

where  $\hbar\omega^*$  is a characteristic scale of the variation of functions  $\gamma(E)$  and  $E_+(E)$ . This approximation corresponds to the so-called pole approximation. In this approximation, Eq. (4.61) takes the form

$$S_{1/2,\alpha}^2 \approx \frac{1}{\pi\rho(E_\alpha)} \frac{\hbar\bar{\gamma}}{\hbar^2\bar{\gamma}^2 + (\bar{E} - E_\alpha)^2}. \quad (4.72)$$

The normalization condition

$$\sum_{\alpha} S_{1/2,\alpha}^2 = 1 \quad (4.73)$$

can be written as

$$\frac{1}{\pi} \int_0^{E_{\max}} \frac{\hbar\bar{\gamma} dE}{\hbar^2\bar{\gamma}^2 + (\bar{E} - E)^2} = \frac{1}{\pi} \int_{-\bar{E}}^{E_{\max} - \bar{E}} \frac{\hbar\bar{\gamma} dx}{\hbar^2\bar{\gamma}^2 + x^2}. \quad (4.74)$$

Using condition (4.71) and the additional condition

$$\hbar\bar{\gamma} \ll E_{\max} - \bar{E}, \quad (4.75)$$

we obtain the normalization condition in this approximation.

Using the same approximations, we get the solutions of Eqs. (4.20) and (4.21). For the ground state of the system we get

$$E_g = - \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_0 + \hbar\omega_{\lambda} - E_g} \approx - \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar\omega_0 + \hbar\omega_{\lambda}}, \quad (4.76)$$

$$S_{-1/2,g}^2 \approx 1 - \sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_0 + \hbar\omega_{\lambda})^2} \approx 1. \quad (4.77)$$

For the continuum states we get

$$S_{-1/2,\lambda}^2 \approx \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} + \hbar\omega_0)^2} \approx 0. \quad (4.78)$$

Thus, performing the consistent one-boson approximation (4.31), we have obtained all one-boson unitary matrix elements:  $S_{-1/2,\alpha}$  [(4.61), (4.72), and (4.68)],  $S_{-1/2,d}$  [(4.67) and (4.70)],  $S_{-1/2,g}$  [(4.77)], and  $S_{-1/2,\lambda}$  [(4.76)]. It is worthwhile to mention that only these approximate expressions are consistent. For example, expression (4.48) is the exact matrix element  $S_{2,d}$  for the truncated "rotating-wave" Hamiltonian (2.17). However, the one-boson approximation employed to the nontruncated Hamiltonian (2.15) leads to expression (4.67).

## V. TUNNELING FRICTION AND SUPERTUNNELING IN THE WEAK-COUPPLING CASE

Now we will be interested in the time development of the tunneling system interacting with the phonon bath. For this purpose we will use relation (3.10) and unitary matrix elements found in the preceding sections. These matrix elements use the basis eigenfunctions of the (4.2) type. They are eigenfunctions of the operator  $r_3$  and describe delocalized states, while the localization in one of the wells is described by the eigenfunctions of the operator  $r_1$  (see the beginning of Sec. II). To find the probability of the localization in one of the potential wells, we perform the unitary transformation to the localized states

$$\begin{aligned} \psi'_{1/2} &= \frac{1}{\sqrt{2}}(\psi_{-1/2} + \psi_{1/2}), \\ \psi'_{-1/2} &= \frac{1}{\sqrt{2}}(\psi_{-1/2} - \psi_{1/2}). \end{aligned} \quad (5.1)$$

Thus, the density matrix in the new representation can be expressed through the density matrix in the  $r_3$  representation

$$\rho'_{mn} = \sum_{k,l} U_{km}^* \rho_{kl} U_{ln}, \quad (5.2)$$

where

$$\psi'_n = \sum_m U_{mn} \psi_m \quad (5.3)$$

and

$$\begin{aligned} U_{1/2,1/2} &= U_{-1/2,1/2} \\ &= U_{-1/2,1/2} = -U_{1/2,-1/2} = \frac{1}{\sqrt{2}}. \end{aligned} \quad (5.4)$$

In particular, it follows from these relations that the probability to remain in the first well equals

$$P_1 = \rho'_{1/2,1/2} = \frac{1}{2} + \frac{1}{2}(\rho_{-1/2,1/2} + \rho_{1/2,-1/2}). \quad (5.5)$$

Therefore, using the unitary matrix  $S$  derived in the previous sections, it is enough to find

$$\rho_{-1/2,1/2} = \rho_{1/2,-1/2}^*. \quad (5.6)$$

We assume that initially ( $t=0$ ) the system was in the first well

$$\begin{aligned} \rho_{1/2,1/2}(0) &= \rho_{-1/2,-1/2}(0) \\ &= \rho_{-1/2,1/2}(0) = \rho_{1/2,-1/2}(0) = \frac{1}{2}. \end{aligned} \quad (5.7)$$

These initial conditions correspond to the zero temperature of the phonon bath. Using Eq. (3.9) and the initial conditions (5.7), we find

$$\rho_{uv} = \frac{1}{2} R_u R_v^*, \quad (5.8)$$

where

$$R_u = \sum_{u'L} S_{uL} S_{u'L}^* e^{-(i/\hbar)E_L' t}. \quad (5.9)$$

As in the previous section, we assume validity of the



one-boson approximation (4.31). We first consider the nonvanishing approximation in the parameter (4.31)

$$\sigma = \sum_{\lambda} \frac{B_{\lambda}^2}{E_{\lambda}^2}. \quad (5.10)$$

We start from the case (4.69)

$$\omega_0 > \omega_c = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar^2 \omega_{\lambda}}. \quad (5.11)$$

In this case, the discrete state  $E'_d$  does not exist and  $S_{1/2,d} = 0$ , (4.70). Then, using expression  $S_{1/2,\alpha}$ , (4.72), in the pole approximation, one gets, from relations (5.8), (5.9), (4.76), and (4.77),

$$\begin{aligned} R_{1/2} &= \sum_{\alpha} S_{1/2,\alpha}^2 e^{-(i/\hbar)E_{\alpha}t} \\ &\approx \frac{1}{\pi} \int_0^{E_{\max}} dE \frac{\hbar \bar{\gamma} e^{-(i/\hbar)\bar{E}t}}{\hbar^2 \bar{\gamma}^2 + (\bar{E} - E)^2} \\ &\approx \exp \left[ -\frac{i}{\hbar} \bar{E}t \right] e^{-\bar{\gamma}t}, \end{aligned} \quad (5.12)$$

$$\begin{aligned} R_{-1/2} &= e^{-(i/\hbar)E_g t}, \\ \bar{E} &\approx \hbar \omega_0 - \int_0^{E_{\max}} dE_{\lambda} \rho(E_{\lambda}) \frac{B_{\lambda}^2}{E_{\lambda} - \hbar \omega_0}, \end{aligned} \quad (5.13)$$

$$E_g \approx - \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar \omega_0 + \hbar \omega_{\lambda}}.$$

From these relations and (5.8) and (5.9), we find

$$\rho_{-1/2,1/2} = \rho_{1/2,-1/2}^*$$

and  $P_1$ ,

$$\begin{aligned} P_1 &= \frac{1}{2} \left[ 1 + \cos \left[ \frac{1}{\hbar} (\bar{E} - E_g) t \right] e^{-\gamma t} \right] \\ &\approx \frac{1}{2} (1 + \cos \omega_0 t e^{-\gamma t}). \end{aligned} \quad (5.14)$$

When the tunneling transition matrix element (2.16),  $v = (\hbar \omega_0 / 2)$ , does not satisfy condition (5.11) and the opposite condition

$$\omega_0 = \frac{2v}{\hbar} < \omega_c = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar^2 \omega_{\lambda}} \quad (5.15)$$

is satisfied, the tunneling friction vanishes and a super-tunneling regime emerges. Again, using relations (5.5), (5.8), and (5.9) and matrix elements (4.67) and (4.77), we get

$$\begin{aligned} P_1 &= \frac{1}{2} \left[ 1 + \cos \left[ \frac{1}{\hbar} (E'_d - E_g) t \right] \right] \\ &\approx \frac{1}{2} (1 + \cos \omega_0 t). \end{aligned} \quad (5.16)$$

Thus, the main result of this section may be summarized by the formula expressing the transition to the supertunneling regime (in the one-boson approximation)

$$P_1 = \begin{cases} \frac{1}{2} \left[ 1 + \cos \frac{2v}{\hbar} t e^{-\gamma t} \right], & 2v > \hbar \omega_c = \sum_{\lambda} \frac{B_{\lambda}^2}{\hbar \omega_{\lambda}}, \\ \frac{1}{2} \left[ 1 + \cos \frac{2v}{\hbar} t \right], & 2v < \hbar \omega_c. \end{cases} \quad (5.17)$$

## VI. SUPERTUNNELING: STRONG COUPLING

In Refs. 29 and 30, exact solutions corresponding to the Hamiltonian (2.14) with  $\omega_0 = 0$  have been found. Discrete levels corresponding to such a Hamiltonian are degenerated. These solutions open the possibility of considering the case of very low frequencies  $\omega_0$ , considering  $\omega_0$  as a small perturbative parameter. This case may be called the strong-coupling case since there is no limitation on the strength of the spin-phonon coupling  $B_k$ . We will rewrite the Hamiltonian (2.14) in the form

$$\begin{aligned} \mathcal{H} &= \frac{1}{2} \sum_k [p_k^2 + \omega_k^2 (q_k - 2r_1 q_k^0)^2 - \hbar \omega_k] \\ &\quad - \sum_k \frac{B_k^2}{\hbar \omega_k} + (r_3 + \frac{1}{2}) \hbar \omega_0 = H_0 + V, \end{aligned} \quad (6.1)$$

where

$$q_k^0 = \left[ \frac{2}{\hbar \omega_k^3} \right]^{1/2} B_k. \quad (6.2)$$

The unperturbed Hamiltonian  $H_0$  has the form

$$H_0 = \frac{1}{2} \sum_k [p_k^2 + \omega_k^2 (q_k - 2r_1 q_k^0)^2 - \hbar \omega_k] - \sum_k \frac{B_k^2}{\hbar \omega_k}, \quad (6.3)$$

while the interaction Hamiltonian is

$$V = (r_3 + \frac{1}{2}) \hbar \omega_0. \quad (6.4)$$

The eigenfunctions and eigenvalues of the Hamiltonian  $H_0$  have the form

$$\psi_{r_1 = \pm 1/2, \{n\}} = \Phi'_{\pm 1/2} \prod_k \Phi_{n_k}(q_k \mp q_k^0), \quad (6.5)$$

$$E_{\pm 1/2, \{n\}} = \sum_k n_k \hbar \omega_k - \sum_k \frac{B_k^2}{\hbar \omega_k}, \quad (6.6)$$

and

$$\begin{aligned} r_1 \Phi'_{\pm 1/2} &= \pm \frac{1}{2} \Phi'_{\pm 1/2}, \\ \Phi'_{\pm 1/2} &= \frac{1}{\sqrt{2}} (\Phi_{-1/2} \pm \Phi_{1/2}), \end{aligned} \quad (6.7)$$

$$r_3 \Phi_{\pm 1/2} = \pm \frac{1}{2} \Phi_{\pm 1/2}.$$

The energy levels (6.6) are degenerate, therefore, the correct zeroth-order approximation eigenfunctions are

$$\begin{aligned} \psi_{1\{n\}} &= \frac{1}{\sqrt{2}} \left[ \Phi'_{1/2} \prod_k \Phi_{n_k}(q_k - q_k^0) \right. \\ &\quad \left. + \Phi'_{-1/2} \prod_k \Phi_{n_k}(q_k + q_k^0) \right], \end{aligned} \quad (6.8)$$

$$\psi_{2\{n\}} = \frac{1}{\sqrt{2}} \left[ \Phi'_{1/2} \prod_k \Phi_{n_k}(q_k - q_k^0) - \Phi'_{-1/2} \prod_k \Phi_{n_k}(q_k + q_k^0) \right]. \quad (6.9)$$

In the first approximation, the eigenenergies have the form

$$E_1 = \sum_k n_k \hbar \omega_k - \sum_k \frac{B_k^2}{\hbar \omega_k} + V_{11}, \quad (6.10)$$

$$E_2 = \sum_k n_k \hbar \omega_k - \sum_k \frac{B_k^2}{\hbar \omega_k} + V_{22},$$

where

$$V_{11} = \hbar \omega_0 \left( \frac{1}{2} + \langle \psi_{1\{n\}}, r_3 \psi_{1\{n\}} \rangle \right), \quad (6.11)$$

$$V_{22} = \hbar \omega_0 \left( \frac{1}{2} + \langle \psi_{2\{n\}}, r_3 \psi_{2\{n\}} \rangle \right).$$

Using (6.7)–(6.9), one finds

$$\langle \psi_{1\{n\}}, r_3 \psi_{1\{n\}} \rangle = -\frac{1}{2} \prod_k \langle n_k | e^{-(2i/\hbar)q_k^0 p_k} | n_k \rangle$$

$$= -\langle \psi_{2\{n_k\}}, r_3 \psi_{2\{n_k\}} \rangle. \quad (6.12)$$

Here

$$|n_k\rangle = \Phi_{n_k}(q_k). \quad (6.13)$$

Thus, the operator  $V$ , (6.4), removes the degeneracy of levels (6.6) and the new eigenvalues are

$$E_{1\{n\}} = \sum_k n_k \hbar \omega_k - \sum_k \frac{B_k^2}{\hbar \omega_k} + \frac{1}{2} \hbar \omega_0 (1 - \Pi_d), \quad (6.14)$$

$$E_{2\{n\}} = \sum_k n_k \hbar \omega_k - \sum_k \frac{B_k^2}{\hbar \omega_k} + \frac{1}{2} \hbar \omega_0 (1 + \Pi_d), \quad (6.15)$$

where

$$\Pi_d = \prod_k \langle n_k | e^{-(2/\hbar)q_k^0 p_k} | n_k \rangle. \quad (6.16)$$

When frequencies  $\omega_k$  form a quasicontinuum, and  $q_k^0 \propto N^{-1/2}$  (with  $N \rightarrow \infty$ , when approaching the continuum), we follow a conventional procedure and will expand exponents in (6.16) up to the terms of order  $N^{-1}$  in each mode  $k$  and present it in the form of the exponent

$$1 - O(N^{-1}) = e^{-O(N^{-1})}, \quad (6.17)$$

$$\Pi_d = \exp \left[ -\sum_k \frac{(q_k^0)^2 \omega_k}{\hbar} (2n_k + 1) \right]$$

$$= \exp \left[ -2 \sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} (2n_k + 1) \right]. \quad (6.18)$$

In order to estimate the approximation in which solutions (6.8), (6.9), (6.14), and (6.15) have been obtained, we will consider a second-order perturbation correction to the energy eigenvalues

$$E_n^{(2)} = \sum_{m(\neq n)} \frac{V_{nm} V_{mn}}{E_n^0 - E_m^0}. \quad (6.19)$$

We need to obtain expressions for off-diagonal matrix elements  $V_{nm}$ . For this purpose we use expressions for nonvanishing matrix elements of  $r_3$  over eigenfunctions  $\phi_{\pm 1/2}$ ,

$$\langle \frac{1}{2} | r_3 | -\frac{1}{2} \rangle = \langle -\frac{1}{2} | r_3 | \frac{1}{2} \rangle = -\frac{1}{2}. \quad (6.20)$$

Thus, we get from (6.8) and (6.9)

$$\langle 1\{n\} | V | 1\{n'\} \rangle = -\langle 2\{n\} | V | 2\{n'\} \rangle$$

$$= -\frac{\hbar \omega_0}{4} \left[ \prod_k \langle \Phi_{n_k}(q_k - q_k^0) \Phi_{n'_k}(q_k + q_k^0) \rangle + \prod_k \langle \Phi_{n_k}(q_k + q_k^0) \Phi_{n'_k}(q_k - q_k^0) \rangle \right],$$

$$\langle 1\{n\} | V | 2\{n'\} \rangle = \frac{\hbar \omega_0}{4} \left[ \prod_k \langle \Phi_{n_k}(q_k - q_k^0) \Phi_{n'_k}(q_k + q_k^0) \rangle - \prod_k \langle \Phi_{n_k}(q_k + q_k^0) \Phi_{n'_k}(q_k - q_k^0) \rangle \right].$$

These relations may be rewritten as follows:

$$\langle 1n | V | n \rangle = -\langle 2n | V | 2n' \rangle$$

$$= -\frac{\hbar \omega_0}{4} \left[ \prod_k \left\langle n_k \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| n'_k \right\rangle + \prod_k \left\langle n_k \left| \exp \left[ -\frac{2i}{\hbar} q_k^0 p_k \right] \right| n'_k \right\rangle \right], \quad (6.21)$$

$$\langle 1n | V | 2n' \rangle = \frac{\hbar \omega_0}{4} \left[ \prod_k \left\langle n_k \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| n'_k \right\rangle - \prod_k \left\langle n_k \left| \exp \left[ -\frac{2i}{\hbar} q_k^0 p_k \right] \right| n'_k \right\rangle \right].$$

In the continuum limit  $N \rightarrow \infty$ , one can easily obtain nonvanishing elements of these matrices. We will consider vacuum states  $|n=0\rangle = |\{0, 0, \dots, 0, \dots\}\rangle$  and one-phonon, two-phonon, etc., states  $|n'\rangle$ ;

$$|n'\rangle = |\{0\}\rangle,$$

$$|n'\rangle = |\{0, \dots, 1_\lambda, \dots, 0, \dots\}\rangle = |1_\lambda\rangle,$$

$$|n'\rangle = |\{0, \dots, 0, 1_{\lambda_1}, 0, \dots, 0, 1_{\lambda_2}, \dots\}\rangle = |1_{\lambda_1} 1_{\lambda_2}\rangle, \dots$$

Then we get

$$\begin{aligned} \langle 1,0|V|1,0\rangle &= -\frac{\hbar\omega_0}{4} \left[ \prod_k \left\langle 0 \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| 0 \right\rangle + \prod_k \left\langle 0 \left| \exp \left[ -\frac{2i}{\hbar} q_k^0 p_k \right] \right| 0 \right\rangle \right] \\ &= -\frac{\hbar\omega_0}{2} \Pi_d = -\frac{\hbar\omega_0}{2} \exp \left[ -2 \sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} \right], \\ \langle 10|V|11_\lambda\rangle &= -\frac{\hbar\omega_0}{4} \left\{ \left\langle 0 \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| 1_\lambda \right\rangle \prod_{k(\neq\lambda)} \left\langle 0 \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| 0 \right\rangle \right. \\ &\quad \left. + \left\langle 0 \left| \exp \left[ -\frac{2i}{\hbar} q_k^0 p_k \right] \right| 1_\lambda \right\rangle \prod_{k(\neq\lambda)} \left\langle 0 \left| \exp \left[ -\frac{2i}{\hbar} q_k^0 p_k \right] \right| 0 \right\rangle \right\} \\ &= -2 \frac{B_\lambda}{\hbar\omega_\lambda} \hbar\omega_0 \Pi_d. \end{aligned}$$

In the continuum limit matrix elements of type

$$\left\langle 0 \left| \exp \left[ \frac{2i}{\hbar} q_k^0 p_k \right] \right| 1_\lambda \right\rangle$$

can be calculated as

$$\left\langle 0 \left| \frac{2i}{\hbar} q_k^0 p_k \right| 1_\lambda \right\rangle,$$

all higher-order terms can be neglected in the limit  $N \rightarrow \infty$ . In the same way we get expressions for matrix elements for many-boson transitions:

$$\langle 1,0|V|1,1_{\lambda_1}, \dots, 1_{\lambda_{2n}}\rangle = -\langle 2,0|V|2,1_{\lambda_1}, \dots, 1_{\lambda_{2n}}\rangle = -2^{2n-1} \frac{B_{\lambda_1} \dots B_{\lambda_{2n}}}{\hbar\omega_{\lambda_1} \dots \hbar\omega_{\lambda_{2n}}} \hbar\omega_0 \Pi_d, \quad (6.22)$$

$$\langle 1,0|V|2,1_{\lambda_1}, \dots, 1_{\lambda_{2n-1}}\rangle = -2^{2n-2} \frac{B_{\lambda_1} \dots B_{\lambda_{2n-1}}}{\hbar\omega_{\lambda_1} \dots \hbar\omega_{\lambda_{2n-1}}} \hbar\omega_0 \Pi_d. \quad (6.23)$$

Using these matrix elements and formula (6.19), we get the second-order correction to the energy level of the system

$$\begin{aligned} E_{1,\{0\}}^{(2)} &= -(\hbar\omega_0)^2 \Pi_d^2 \left[ \frac{1}{2!} 2^2 \sum_{\lambda,\lambda'} \frac{\eta_\lambda^2 \eta_{\lambda'}^2}{\hbar\omega_\lambda + \hbar\omega_{\lambda'}} + \dots + \frac{2^{4n-2}}{(2n)!} \sum_{\lambda_1, \dots, \lambda_{2n}} \frac{\eta_{\lambda_1}^2 \dots \eta_{\lambda_{2n}}^2}{\hbar\omega_{\lambda_1} + \dots + \hbar\omega_{\lambda_{2n}}} \right. \\ &\quad \left. + \dots + \sum_{\lambda} \frac{\eta_\lambda^2}{\hbar\omega_0 \Pi_d + \hbar\omega_\lambda} + \dots + \sum_{\lambda_1, \dots, \lambda_{2n-1}} \frac{\eta_{\lambda_1}^2 \dots \eta_{\lambda_{2n-1}}^2}{\hbar\omega_0 \Pi_d + \hbar\omega_{\lambda_1} + \dots + \hbar\omega_{\lambda_{2n-1}}} + \dots \right], \quad (6.24) \end{aligned}$$

where

$$\eta_\lambda = \frac{B_\lambda}{\hbar\omega_\lambda}. \quad (6.25)$$

It is easy to get the following estimate for the large parentheses in (6.24):

$$\begin{aligned} [\dots] &\leq \left[ \sum_{\lambda} \frac{\eta_\lambda^2}{\hbar\omega_\lambda} \right] \left[ 1 + \frac{\eta}{2!} + \frac{\eta^2}{3!} + \dots \right] \\ &= \frac{1}{\eta} (e^\eta - 1) \sum_{\lambda} \frac{\eta_\lambda^2}{\hbar\omega_\lambda}, \quad (6.26) \end{aligned}$$

where

$$\eta = 2^2 \sum_{\lambda} \eta_\lambda^2. \quad (6.27)$$

The quantity  $\Pi_d$  (for  $n_k = 0$ ) (6.18) is expressed through  $\eta$ :

$$\Pi_d = e^{-\eta/2}. \quad (6.28)$$

Thus,

$$-E_{1,\{0\}}^{(2)} \lesssim e^{-\eta} (\hbar\omega_0)^2 (e^\eta - 1) / \eta. \quad (6.29)$$

The condition of smallness of the second-order correction in comparison with the energy difference (6.14) and (6.15), of the first order  $\hbar\omega_0 \Pi_d$  takes the form

$$\left[ \sum_{\lambda} \frac{\eta_\lambda^2}{\hbar\omega_\lambda} \right] \hbar\omega_0 \ll \frac{\eta e^{-\eta/2}}{(1 - e^{-\eta})}. \quad (6.30)$$

For the interaction with acoustic phonons  $\eta_\lambda \propto \omega_\lambda^{-1/2}$ , we

get, in the Debye model,

$$\omega_0 \ll \omega_D \frac{e^{-\eta/2}}{1-e^{-\eta}}. \quad (6.31)$$

For the weak coupling we get

$$\eta \ll 1, \quad \eta\omega_0 \ll \omega_D, \quad (6.32)$$

while for the strong coupling,

$$\omega_0 \ll \omega_D e^{-\eta/2}, \quad \eta \gtrsim 1. \quad (6.33)$$

Of course, in the case of weak coupling (the one-boson approximation),  $\omega_0$  should satisfy condition (5.15) as well. This later condition is compatible with condition (6.32).

Now we are ready to consider the time development of the tunneling system coupled with the phonon bath and described by the Hamiltonian (2.14) or its equivalent (6.1). In the strong-coupling case, the eigenfunctions are presented by formulas (6.8) and (6.9) while the eigenenergies have the form (6.14) and (6.15).

We again use relation (3.10) to determine the time development of the density matrix. Matrix elements of the unitary matrix connecting states

$$|\pm \frac{1}{2}, N\rangle = \Phi'_{\pm 1/2} \prod_k \Phi_{N_k}(q_k) \quad (6.34)$$

$$R_{1/2, N} = \frac{1}{2} \sum_{\{n_k\}} \prod_k \langle N_k \left| \exp \left[ -\frac{i}{\hbar} q_k^0 p_k \right] \right| n_k \rangle \langle 0 \left| \exp \left[ -\frac{i}{\hbar} q_k^0 p_k \right] \right| n_k \rangle e^{-in_k \omega_k t} (e^{-(i/\hbar)E_{1,t}} + e^{-(i/\hbar)E_{2,t}}), \quad (6.39)$$

where

$$E_{1,2} = -\sum_k \frac{B_k^2}{\hbar \omega_k} + \frac{1}{2} \hbar \omega_0 (1 \mp \Pi_d). \quad (6.40)$$

Using conventional transformations we get

$$R_{1/2, N} = \exp \left[ -\frac{i}{2} \omega_0 t - i \sum_k \frac{B_k}{\hbar^2 \omega_k} t \right] \left\langle N \left| \exp \left[ -\frac{i}{\hbar} \sum_k q_k^0 p_k(t) \right] \exp \left[ \frac{i}{\hbar} \sum_k q_k^0 p_k \right] \right| 0 \right\rangle \exp \left[ -i \sum_k N_k \omega_k t \right] \cos(\frac{1}{2} \omega_0 \Pi_d t), \quad (6.41)$$

where

$$p_k(t) = p_k \cos \omega_k t - \omega_k q_k \sin \omega_k t. \quad (6.42)$$

Now, using (6.17)-type transformations (for the continuum states), we obtain

$$\begin{aligned} \langle 0 \left| \exp \left[ -\frac{i}{\hbar} \sum_k q_k^0 p_k(t) \right] \exp \left[ \frac{i}{\hbar} \sum_k q_k^0 p_k \right] \right| 0 \rangle &= \exp \left[ -\sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} (1 - e^{-i\omega_k t}) \right] \equiv \langle 0|0 \rangle, \\ \langle 1_\lambda | \cdots | 0 \rangle &= \frac{B_\lambda}{\hbar \omega_\lambda} (e^{i\omega_\lambda t} - 1) \langle 0|0 \rangle, \end{aligned} \quad (6.43)$$

$$\langle 1_{\lambda_1}, 1_{\lambda_2} | \cdots | 0 \rangle = \frac{B_{\lambda_1}}{\hbar \omega_{\lambda_1}} \frac{B_{\lambda_2}}{\hbar \omega_{\lambda_2}} (e^{i\omega_{\lambda_1} t} - 1) (e^{i\omega_{\lambda_2} t} - 1) \langle 0|0 \rangle.$$

Substituting these relations into Eq. (6.41), we finally get

$$\begin{aligned} \rho'_{1/2, 1/2} &= \sum_N \rho'_{1/2, N; 1/2, N} = P_1(t) = \cos^2(\frac{1}{2} \omega_0 \Pi_d t) \\ &= \frac{1}{2} \left[ 1 + \cos \frac{2\bar{v}}{\hbar} t \right], \end{aligned} \quad (6.44)$$

with correct states of zero approximation (6.8) and (6.9) have the form

$$\begin{aligned} S_{(1/2)N; 1n} &= S_{(1/2)N; 2n} \\ &= \frac{1}{\sqrt{2}} \prod_k \langle N_k \left| \exp \left[ -\frac{i}{\hbar} q_k^0 p_k \right] \right| n_k \rangle, \\ S_{-(1/2)N; 1n} &= -S_{-(1/2)N; 2n} \\ &= \frac{1}{\sqrt{2}} \prod_k \langle N_k \left| \exp \left[ \frac{i}{\hbar} q_k^0 p_k \right] \right| n_k \rangle. \end{aligned} \quad (6.35)$$

Assuming that, at  $t=0$ ,

$$\rho'_{1/2, 0; 1/2, 0}(0) = 1, \quad (6.36)$$

we obtain from (3.10)

$$\rho'_{1/2, N; 1/2, N} = R_{1/2, N} R_{1/2, N}^*, \quad (6.37)$$

where

$$R_{1/2, N} = \sum_L S_{1/2, N; L} S_{1/2, 0; L}^* e^{-(i/\hbar)E_L' t}. \quad (6.38)$$

Substituting (6.35) into relation (6.38), one gets

where  $\bar{v}$  is a "dressed" matrix element of the transition between two symmetric wells

$$\bar{v} = v \exp \left[ -2 \sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} \right]. \quad (6.45)$$

It has to be stressed that solution (6.44) describes quan-

tum beats without friction, while the usual Markovian approach (see, e.g., Ref. 32) would give decaying quantum beats. In the case of weak coupling,

$$\sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} \ll 1,$$

expression (6.44) reduces to expression (5.17) in the supertunneling regime ( $2v < \hbar\omega_e$ ).

## VII. DISCUSSION AND CONCLUSIONS

Tunneling between two potential wells in the dissipative medium has been considered in the framework of the spin-boson Hamiltonian (2.14) and (2.15). The time evolution of such a system can be described by the density matrix formalism. The time-dependent density matrix is presented by Eq. (3.10). This equation, which is exact, can describe two qualitatively different kinds of behaviors. In one case, the energy spectrum of the whole system, spin interacting with bosons, is continuous (besides the ground state). In this case the summation in (3.10) can be transformed into an integration. Corresponding Fourier integrals describe irreversible behavior—decaying quantum beats. Quite different behavior is predicted in the case when the whole system contains both discrete (besides the ground state) and continuous states. In this case, nondecaying quantum beats emerge. This analysis is model independent and is not connected with any specific approximation.

Now, assume that the spin-boson Hamiltonian has discrete states, e.g., ground and excited discrete states, while continuous states lie above these discrete states. The discrete states correspond to delocalized states in the two-well potential. If we are interested by the probability to remain in one of the wells, then the transformation to the site presentation has to be performed. In the model system described by the truncated Hamiltonian (2.17), the analysis has been performed exactly. When the interaction energy between the two wells characterizing the barrier between the wells,  $v$  is lower than critical energy  $v_c$ , then discrete levels in the whole system emerge. In this case,

$$v < v_c = \frac{1}{2} \sum_k \frac{B_k^2}{\hbar\omega_k} \quad (7.1)$$

and the tunneling friction vanishes. For the spin-boson Hamiltonian, the transformation to the site representation corresponds to the transformation to the basis of the  $r_1$  operator (5.1). It is worthwhile to stress again that both the general analysis and the application to the specific case of the truncated spin-boson Hamiltonian (2.17) are exact. The physical explanation for the prediction of the vanishing of the tunnel friction in case (7.1) is quite simple. The time development of the system with the discrete nondecaying states is described by the density matrix  $\rho'_{1/2,1/2}(t)$ , (5.5). This density matrix (in the site representation) is expressed through the off-diagonal matrix elements (in the energy representation) and therefore it contains nondecaying harmonic terms.

For more quantitative predictions certain approximations have been made. The use of the truncated rotating-wave Hamiltonian is justified if one can neglect many-boson contributions connected with those omitted in the (2.17) counter-rotating terms (2.18). It has been shown that many-boson contributions can be neglected provided the parameter  $\sigma$ , (5.10) and (4.31), is small

$$\sigma = \sum_k \frac{B_k^2}{\hbar^2 \omega_k^2} \ll 1. \quad (7.2)$$

On the other hand, the supertunneling regime emerges provided condition (7.1) is satisfied. Another condition which has to be satisfied is (4.71) and (4.75). This condition provides the applicability of the pole approximation used in the derivation of formula (5.17). This condition can be written in the form

$$\bar{\gamma} = \frac{\pi}{\hbar} \rho(\bar{E}) B_k^2(\bar{E}) \ll \omega_0. \quad (7.3)$$

(Here we assume that  $E_{\max} \gg \bar{E}$  and  $\bar{E} \approx \hbar\omega_0$ .) Of course, one has to verify the consistency of these three conditions (7.1)–(7.3). At first sight, condition (7.1) contradicts conditions (7.2) and (7.3): condition (7.1) requires  $B_k$  to be large enough, while conditions (7.2) and (7.3) require the smallness of  $B_k$ . Also, it has to be stressed that conditions (7.1) and (7.2) might not be satisfied for all dependencies  $B_k(E_k)$ . Particularly, the sum (7.2) may be divergent. To clarify conditions (7.1)–(7.3), we will consider here the deformation interaction of localized electrons with acoustic phonons<sup>43</sup>

$$\begin{aligned} B_k &= \left[ \frac{\hbar}{2MNu} \right]^{1/2} k^{1/2} E_{\text{def}} \\ &= \frac{1}{\sqrt{N}} \left[ \frac{\hbar}{2M\omega_D} \right]^{1/2} \frac{1}{a} \left[ \frac{\omega_k}{\omega_D} \right]^{1/2} E_{\text{def}}, \end{aligned} \quad (7.4)$$

where  $E_{\text{def}}$  is called a deformation energy,  $u$  is a sound velocity  $u = \omega_D/a$  with  $\omega_D$ ,  $a$ , and  $N$  being a Debye frequency, a lattice constant, and an effective number of vibrational degrees of freedom of the solid, respectively.

For our estimates we can use the density of states in the Debye model

$$\rho(\omega_k) = N \frac{3\omega_k^2}{\omega_D^3}. \quad (7.5)$$

Using these relations, transforming the summation (7.1) and (7.2) into the integration, we get the following expressions for  $\sigma$ ,  $v_c$ , and  $\gamma$ :

$$\sigma = \frac{3}{2} \frac{\hbar}{2M\omega_D} \frac{1}{a^2} \frac{E_{\text{def}}^2}{(\hbar\omega_D)^2}, \quad (7.6)$$

$$v_c = \frac{\hbar\omega_c}{2} = \frac{1}{3} \sigma \hbar\omega_D, \quad (7.7)$$

$$\bar{\gamma} = 2\pi\sigma \left[ \frac{\omega_0}{\omega_D} \right]^2 \omega_0. \quad (7.8)$$

We see that the condition of the one-phonon approxima-

tion (7.2), i.e., a smallness of the parameter  $\sigma$ , is satisfied provided a product of dimensionless parameters  $\hbar/2M\omega_D a^2$  and  $(E_{\text{def}}/\hbar\omega_D)^2$  is small enough.

Condition (7.3) may be rewritten in the form

$$\frac{\bar{\gamma}}{\omega_0} = 2\pi\sigma \left[ \frac{\omega_0}{\omega_D} \right]^2 \ll 1 \quad (7.9)$$

and is ensured by smallness of parameters  $\sigma$  and

$$\eta = \frac{\omega_0}{\omega_D} = \frac{2v}{\hbar\omega_D} \ll 1. \quad (7.10)$$

Using Eq. (7.7), one can express the parameter  $\sigma$  as

$$\sigma = \frac{3}{2} \frac{\omega_c}{\omega_D}.$$

Therefore, the condition of the one-phonon approximation together with condition (7.1) can be expressed in the forms

$$\omega_0 < \omega_c \ll \omega_D \quad (7.11)$$

or

$$\eta < \frac{2}{3}\sigma \ll 1. \quad (7.12)$$

Thus, we see that condition (7.1),  $\omega_c > \omega_0$ , is compatible with the one-phonon approximation, provided parameter  $\eta$ , (7.10), is smaller than  $\frac{2}{3}\sigma$ .

Several words have to be added about the weak-coupling case. It has to be stressed that it is not the usual perturbation theory using an expansion over powers of the interaction parameter  $B_k$ . Expression (4.72) for the unitary matrix element contains all powers of  $\bar{\gamma}$ , (7.3).

Let us consider a contribution of a certain separate level  $E_L$  to the unitary matrix element (4.34):

$$S_{1/2,L}^2 = \frac{1}{1 + \sum_{\lambda} [B_{\lambda}^2 / (\hbar\omega_{\lambda} - E_L')^2]}. \quad (7.13)$$

When  $E_L'$ , an energy of the whole system, lies in the continuum region, then the sum in the denominator tends to infinity (with  $N \rightarrow \infty$ )

$$\sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} - E_L')^2} \sim \frac{B_{\lambda}^2}{\varepsilon^2} \propto N, \quad B_{\lambda}^2 \propto N^{-1}, \quad \varepsilon \propto N^{-1}, \quad (7.14)$$

and  $S_{1/2,L}^2 \propto N^{-1} \rightarrow 0$ . This can also be explicitly evident from the expression (4.72). At resonance  $\bar{E} = E_a$ , expression (4.72) is proportional to  $1/\rho(\bar{E})\bar{\gamma}$  and cannot be obtained as an expansion over  $B_k^n$ . It has to be stressed that expression (4.72) takes place in the one-phonon approximation and it describes the usual tunneling friction.

When  $E_L'$  lies beyond the continuum region and has a negative value  $E_L' = -E_v$ , then the sum in the denominator of (7.13) is finite and equal to

$$\sum_{\lambda} \frac{B_{\lambda}^2}{(\hbar\omega_{\lambda} + E_0)^2} \approx \sigma \quad (7.15)$$

and

$$S_{1/2,d}^2 \approx 1 - \sigma \approx 1.$$

This happens when  $\omega_0 < \omega_c$ .

We see that so-called weak-coupling case (7.2) does not mean an expansion over the interaction parameter  $B_k$ . It means only that the ratio of the interaction constant to a certain quantity is small [see (7.6)]. At the same time, the ratio of  $B_{\lambda}^2$  to another quantity, like  $(\hbar\omega_{\lambda} - E_L')^2$  [see (7.14)] can be infinitely large.

We summarize the main results of the paper. A consistent analysis in the one-boson approximation shows that the tunneling friction vanishes when the interaction energy  $v = (\hbar\omega_c/2)$  between two wells is lower than the critical energy

$$v < v_c = \frac{1}{2} \sum_k \frac{B_k^2}{\hbar\omega_k}.$$

This supertunneling regime is connected with the existence of discrete states in the spectrum of combined spin-phonon system described by the Hamiltonian (2.14) and (2.15). It has been stressed in previous papers<sup>28,29</sup> that the existence of such states (except the ground state, which always exists) precludes the use of the conventional Markovian approach. It also means that the supertunneling phenomenon cannot be understood in the framework of the usual Bloch equations.

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