Tunneling with "dissipation"

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A general approach to the problem of tunneling in the case of an interaction with the medium is examined. This approach is based on a direct determination of the overlap integral of the wave functions of the system. The two-well problem and the problem of a one–dimensional crystal in the case of an interaction with phonons are analyzed.

1. The problem of the tunneling of a particle which also interacts with excitations of the medium has recently attracted considerable interest. The solution method has usually been based on a functional-integration technique, with a special choice of the interaction Hamiltonian.[1–3] There is an alternative approach, based on a direct determination of the overlap integral of the many-particle wave functions of the system which are formed in the absence of a tunneling channel.[4] This approach makes it possible to take into account the fluctuational changes in the barrier[5] (these changes drop out of the picture when a model spin Hamiltonian is used[6–8]), to avoid a special choice of interaction, to directly single out coherent tunneling (without any real excitation of the medium), and to find the quantum-mechanical diffusion coefficient D in the transition to a crystal. Below we take this approach to deal with the problem of tunneling in an interaction with phonons.

2. Let us examine the problem of a tunneling between two wells whose lower levels are separated by an amount ξ. We assume that the effective tunneling amplitude $\tilde{\Delta}_0$, like ξ, is small in comparison with the distance to the next level of the particle in

the well, ω_0, and also in comparison with the characteristic excitation frequency of the medium, ω_D:

$$\tilde{\Delta}_0, \xi \ll \omega_0, \omega_D . \tag{1}$$

We further assume $T \ll \omega_0$ and that the transition occurs only through the lower level.

The particle spends a time $\tau \gg \tilde{\Delta}_0^{-1}$ in a well. Over this time, the overwhelming majority of excitations with energy $\omega > \tau^{-1}$ adapt to the single-well situation, with the respect that a single-well wave function of the system is formed: $\psi^{(i)}(r, x)$, where r is the coordinate of the particle, $i = 1,2$ specifies the well. In the initial potential relief for the particle, we single out one well, $U^{(i)}(r)$, and we continue its "banks" in the usual way. We denote by $H_1(r)$ the difference between the actual potential relief and the nondecaying well which we have singled out. We then have the following expression for the matrix element for a transition of the particle from one well to the other:

$$M_{\nu\nu'} = \langle \psi_\nu^{(2)}(r, x) \mid H_1(r) \mid \psi_{\nu'}^{(1)}(r, x) \rangle . \tag{2}$$

Once we know a matrix element in (2), which is not diagonal in the state of the medium, ν, and also a matrix element, which is diagonal in this state, we have completely solved the problem of tunneling in the case of an interaction with the medium, including the problem of a coherent transition accompanied by the formation of a band ($\nu' = \nu$) if we are dealing with a crystal.

3. The excitations of the medium can be classified as "fast," with frequencies $\omega > \omega_0$, and "slow," with $\omega < \omega_0$. The former adjust to the motion of the particle in the well, giving rise to a "screening" and thereby a renormalization of the potential $U^{(i)}$; to a slight extent, they impart a mass to the particle. The latter excitations, on the contrary, do not follow the particle, and the modified wave function of the medium which corresponds to these excitations turns out to be oriented toward the center of the potential well. These excitations have the decisive effect on the tunneling. This distinction between different types of excitations has been followed explicitly in the case of an interaction with an electron fluid.[4] In the present letter we examine an interaction with phonons, using the notation $\omega_c = (\omega_0, \omega_D)_{\min}$.

The Hamiltonian of the single-well problem can be written

$$H^{(i)} = H_p^{(i)} + H_{ph} + V^{(i)}(r, x), \tag{3}$$

where H_p is the Hamiltonian of a particle in the renormalized potential relief, and $V(r, x)$ is the interaction of the particle with the slow excitations.

The eigenstates of Hamiltonian (3), which appear in definition (2), can be found in the ordinary adiabatic approximation,

$$\psi_\nu^{(i)}(r, x) = \varphi_0^{(i)}(r, x)\Phi_\nu^{(i)}(x), \tag{4}$$

where the wave functions φ_0 and Φ_ν are the solution of the equations

$$[H_p^{(i)} + V^{(i)}(r, x)]\varphi_0^{(i)}(r, x) = \epsilon_0^{(i)}(x)\varphi_0^{(i)}(r, x), \quad [H_{ph} + \epsilon_0^{(i)}(x)]\Phi_\nu^{(i)}(x) = E_\nu^{(i)}\Phi_\nu^{(i)}(x).$$

We expand $\epsilon_0(x)$ in a series in displacements of the atoms of the medium, expressed in terms of the normal phonon coordinates x_β:

$$\epsilon_0^{(i)}(x) - \epsilon_0^{(i)}(0) = \sum_\beta \gamma_\beta^{(i)} x_\beta + {}^1/_2 \sum_{\beta\beta'} \gamma_{\beta\beta'}^{(i)} x_\beta x_{\beta'} .$$

In the present letter we retain only the first term of the expansion, although the problem can be solved when the quadratic term is also retained. For $\Phi_\nu^{(i)}$ we then find the well-known solution corresponding to a shift of normal oscillators:

$$\Phi_\nu^{(i)}(x) = \prod_\beta \Phi_\beta^{(0)}(x_\beta - x_\beta^{(i)}), \qquad x_\beta^{(i)} = \gamma_\beta^{(i)} / \omega_\beta^2 , \tag{5}$$

where $\Phi_\beta^{(0)}$ is the wave function unperturbed by the particle. Transition matrix element (2) takes the following form when we use (4) and (5):

$$M_{\nu\nu'} = \langle \Phi_\nu^{(2)}(x) | J(x) | \Phi_{\nu'}^{(1)}(x) \rangle ,$$

$$J(x) = \langle \varphi_0^{(2)}(r, x) | H_1(r) | \varphi_0^{(1)}(r, x) \rangle \equiv \Delta_0 e^{-\Delta B(x)} ,$$

where $\Delta B(x) = B(x) - B(0)$. Restricting the discussion to the linear expansion, $\Delta B(x) = \Delta B(\bar{x}) + \Sigma_\beta B_\beta (x_\beta - \bar{x}_\beta)$, and using the results of Ref. 5, we find

$$M_{\nu\nu'} = J(T) \langle \Phi_\nu^{(2)}(x) | \Phi_{\nu'}^{(1)}(x) \rangle , \qquad J(T) = \Delta_0 \exp(-\Delta B(\bar{x}) + G(T)). \tag{6}$$

The expression for $J(T)$ reflects the dependence of the transition amplitude on the maximum possible change in the barrier structure. Important in this situation are both the relaxation of the surrounding atoms ($\bar{x}_\beta = (x_\beta^{(1)} + x_\beta^{(2)})/2$) and the "fluctuational preparation of the barrier,"[5] $G(T) = \Sigma_\beta |B_\beta|^2 \left(4\omega_\beta \tanh\left(\frac{\omega_\beta}{2T}\right)\right)^{-1}$, whose role increases with increasing T.

4. We assume $|\xi| \gg \Delta_0$. Using (5) and (6), we can then solve the problem for the tunneling probability W_{12} exactly:

$$W_{12} = J^2(T) \int_{-\infty}^{+\infty} dt \exp(i\xi_{12} t - \chi(t)) . \tag{7}$$

The function $\chi(t)$ has the form characteristic of the theory of a small-radius polaron:

$$\chi(t) = 2 \int_0^{\omega_c} \frac{d\omega}{\omega} \left[(1 - \cos\omega t) \coth {}^{\omega}/_{2T} - i \sin\omega t \right] f(\omega) , \tag{8}$$

$$f(\omega) = \sum_\beta \frac{|c_\beta^{(1)} - c_\beta^{(2)}|^2}{2\omega_\beta} \delta(\omega - \omega_\beta) . \tag{9}$$

For small wave vectors $\mathbf{q}$ ($\beta \equiv \mathbf{q}$, ξ, where ξ specifies the branch) we have

$$c_\beta^{(i)} = (\gamma_\beta^{(i)} (2\omega_\beta)^{-1/2}) e^{i\mathbf{q}\mathbf{R}_i} = c_\xi^{(i)} \left(\frac{\omega_\xi(\mathbf{q})\omega_D}{N}\right)^{1/2} e^{i\mathbf{q}\mathbf{R}_i} . \tag{10}$$

In the limit $\omega \to 0$, we have $f(\omega) \sim \omega^{d-1+(2)}$. The 2 in parentheses means that the two wells are identical if $c_\xi^{(1)} = c_\xi^{(2)}$. The integral in (8) has a singular behavior in the limit $\omega \to 0$ with $f(0) = b = \text{const}$. The problem of "tunneling with friction,"[1-3,6-8] assumes that specifically this relation holds. It follows from the results above that *this requires, in addition to a one-dimensional nature (d=1), that the wells not be identical.*

A direct integration of expression (7) under the condition $T \ll \omega_c$ in this case yields

$$W_{12} = 2\sqrt{\pi}\frac{\tilde{\Delta}_0^2(T)\Omega_T}{\xi_{12}^2 + \Omega_T^2}\frac{|\Gamma(1 + b + i\xi_{12}/2\pi T)|^2}{\Gamma(1+b)\Gamma(1/2 + b)}e^{\xi_{12}/2T} \tag{11}$$

$$\tilde{\Delta}_0(T) = \Delta_0 \exp(-\Delta B(\bar{x}) + G(T))\exp(-b\ln \omega_c/T), \quad \Omega_T = 2\pi bT. \tag{12}$$

In contrast with the result of Refs. 7 and 8, expressions (11) and (12) contain exponential factors which correspond to a fluctuational preparation of the barrier. The expression found in Refs. 7 and 8 for $\tilde{\Delta}_0(T)$, which corresponds to the last factor in (12), it is simply equal to the polaron overlap integral of the wave functions in (6).

Expression (11) remains valid as long as at least one of the conditions $|\xi| > \tilde{\Delta}_0$ and $\Omega_T > \tilde{\Delta}_0$ holds. Under the conditions $\xi = 0$ and $T, \Omega_T < \tilde{\Delta}_0(T)$ (we are assuming $b < 1$), the tunneling of the particle acquires a coherent, dissipationless nature, corresponding to a diagonal matrix element in (6). Its value is the same as (12) if we replace T by $\tilde{\Delta}_0$ in the argument of the natural logarithm, because the phonons with $\omega < \tilde{\Delta}_0$ do not have time to participate in the polaron effect during the time spent by the particle in the well. The coherent amplitude then takes on a T-independent value,

$$\tilde{\Delta}_0^* = J(0)(J(0)/\omega_c)^{b/1-b} \tag{13}$$

If we ignore inelastic processes, we find that the system has two eigenstates, separated by an interval $2\tilde{\Delta}_0^*$, and the probability for the particle to be in the second well if it was in the first well at $t = 0$ is of an oscillatory nature. Actually, even at $T = 0$ these oscillations decay over the time taken for transition from the upper level to the lower level:

$$\tau^{-1} = 2\pi b\tilde{\Delta}_0^*/(1 - \exp(-2\tilde{\Delta}_0^*/T)). \tag{14}$$

In the method used here, a direct transition can be made from the two-well problem to the crystal. At low temperatures the problem becomes equivalent to that of band motion in the strong-coupling approximation with a band width $\tilde{\Delta} \cong 4J(0)(4J(0)/\omega_c)^{b/1-b}$. The particles are scattered by phonons with frequencies $\omega_\beta < \tilde{\Delta}$, which do not participate in the polaron effect. The energy and momentum conservation laws can hold at $\tilde{\Delta} \ll \omega_D$ only if conditions repeat periodically through the crystal: $c^{(n)} \neq c^{(n+1)}$. The mean free time τ_p is then given by

$$1/\tau_p = \pi b(\epsilon_p - \epsilon_{p+\pi/a})/(1 - \exp((\epsilon_{p+\pi/a} - \epsilon_p)/T)). \tag{15}$$

At $T \sim \tilde{\Delta}$ the diffusion coefficient is

$$D \approx 1/8\tilde{\Delta}^2/\Omega_T. \tag{16}$$

At $T \ll \tilde{\Delta}$, the single-phonon scattering falls off exponentially, and the scattering in second order in the single-phonon interaction becomes important. For the latter type of scattering, the conservation laws are easily satisfied. Solving the kinetic equation, allowing for the transport effect $[(q/p)^2 \ll 1]$, we find

$$D = \frac{15a^2}{4\pi^7 b^2} \frac{\tilde{\Delta}^2 \omega_D^2}{T^3} . \qquad (17)$$

At $\Omega_T > \tilde{\Delta}$, there is a dynamic destruction of the zone, and the probability for a transition from well n to well $n+1$ is determined by the two-well expression in (11), which leads to a diffusion coefficient analogous to that in (16).

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