One-dimensional phonon-coupled electron tunneling: A realistic model

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The transition probability for a one-dimensional tunneling electron coupled to acoustical phonons is calculated, with the Feynman path-integral method. We considered a realistic electron-phonon interaction (deformation potential, piezoelectric), making use of slowness of the phonon system compared to electron tunneling. We show that the problem of the complex nonlinear coupling of a tunneling electron to the zero-point fluctuations of a phonon field is equivalent to that of an electron tunneling through a slow fluctuating spatially uniform barrier, thus resulting in an increase of the tunneling probability due to electron coupling with zero-point phonon oscillations. We calculated also the energy change of the tunneling electron due to phonon emission. [S0163-1829(99)09423-0]

I. INTRODUCTION

Tunneling, being one of the most remarkable nonclassical manifestations of quantum dynamics, has been largely investigated. One of the major issues in the field is the understanding of the properties of tunneling particles coupled to degrees of freedom representing the environment. The case of a particle or macroscopic degree of freedom tunneling out of a metastable state in the presence of arbitrary linear dissipation mechanism, has been extensively studied in a series of papers by Caldeira and Leggett[1] and other groups.[2] Two state systems coupled to a dissipative environment have been studied in depth by a large number of groups,[3] in the last two decades.

The problem that we address in the present paper is the tunneling of an electron with a given energy E across a rectangular barrier where it is coupled with phonons. We calculate the change of the tunneling probability due to this coupling and the average energy loss due to phonon emission of tunneled electrons. In this paper, we consider only a one-dimensional problem that can be realized as a quantum wire, or in narrow constrictions.

This problem, finding the transmission probability and spectrum of a tunneling electron coupled to phonons is of fundamental interest as well as being potentially of great technological importance. Examples are tunneling through Josephson junctions,[4] bit errors in mesoscopic logic, and memory circuits,[5] as well as quantum cascade lasers,[6] and of course, scanning tunneling microscopy.[7] There are even some recent examples of the use of the transmission spectrum to define an experimental test between quantum mechanics and a class of alternative theories.[8] Also, recent development of nanostructure technology makes it possible to check experimentally the effect of coupling with the environment on the dependence of the tunneling probability on the width and the height of the barrier.

Typically the coupling between the tunneling particle and the environment is assumed to be linear with respect to particle coordinate. This assumption may be justified for tunneling of heavy atoms or macroscopic degrees of freedom but it is not realistic for electrons. A nonlinear coupling with phonons was considered by Bruinsma and Bak.[9] But they considered only the case when the coupling between the tunneling particle and each phonon degree of freedom is the same, which is not realistic in a regular lattice. Due to this the result of Bruinsma and Bak contains a cutoff frequency. In our realistic treatment of electron-phonon coupling a characteristic frequency naturally arises in the theory. Since the only length scale in the problem is the barrier length and from it a typical time scale emerges.

A recent treatment of the problem was given by Ueda,[10] who used the effective action technique and got analytic results, for some cases of the spectral density function of the phonon bath. Whereas Bruinsma and Bak[9] calculated the transmission spectrum, we show that the main effect, on the electron transition probability, is static, i.e., a static effective lowering of the barrier by phonons. Such an effect, a static lowering of the barrier due to coupling of the tunneling electron to zero-point fluctuations, was also discussed in two papers by Ueda and Ando[11] although they studied a different physical problem, the coupling of the tunneling electron to electromagnetic modes (in their paper this was referred to as the dynamic limit).

A deformation potential coupling of tunneling electrons with phonons was also studied by Gelfand *et al.*[12] However, they considered only an infinitesimally thin barrier.

We consider interaction of tunneling electron with acoustic phonons via realistic coupling mechanisms: deformation potential or piezoelectric. Coupling with optical phonons is neglected for the following reasons. The amplitude for zero-point fluctuations for optical phonons, for a given frequency is proportional to one over the square root of the frequency. Since the optical frequencies are large compared to those of acoustic phonons we consider their zero-point fluctuations as negligible. Also the coupling constant with optical phonons in III-V materials[13] is not very large giving a further justification for neglecting the effect of optical phonons. Concerning optical phonon emission and absorption we study the low-temperature case and assume that electron energy and temperature are much smaller than the energy of the optical phonons so that emission and absorption can be neglected.

The coupling with acoustic phonons leads to a modulation of the barrier. This effect exists even at zero temperature when the modulation is controlled by zero-point phonon vibrations. In other words, as a result of coupling with phonons

the height of the potential barrier is not any more a classical parameter determined by fabrication of the structure but a quantum-mechanical dynamical variable that is characterized by a wave function. Thus, the complex nonlinear problem of a tunneling electron coupled to a phonon field is transformed to a that of an electron tunneling through an effective potential barrier where the barrier height fluctuates.

The paper is composed in the following way. In Sec. II, we formulate the model. In Sec. III we introduce two main approximations, which we use to facilitate the calculation of the tunneling probability. Both coupling mechanisms that we consider are nonlinear with respect to the electron coordinate. This nonlinearity makes the application of generally used instanton method difficult and to solve the problem we developed an expansion on some small parameters. First, it appears that frequencies of typical phonons interacting with a tunneling electron are so small that the phonon system can be considered slow compared to the electron. Second, we use the WKB approximation. The slowness of the phonon system allows us in the first approximation to neglect phonon dynamics and to consider their potential as time independent which dramatically simplifies the calculation (the calculation without this approximation appears in the Appendix). The corresponding calculation of the transmission coefficient are carried out in Sec. IV. The static approximation, however, does not include phonon emission and resulted energy loss. To calculate it a more general approach is necessary. In Sec. V, again making use of the slowness of the phonon system we go beyond the static approximation and calculate the average energy loss of tunneled electrons.

II. GENERAL FORMULATION OF THE PROBLEM

A. The model

We treat the problem of a one-dimensional electron coupled to acoustic phonons while tunneling through a rectangular barrier, of length L. The potentials restricting the electron's movement do not effect phonons, which move freely through the bulk and thus are treated as three dimensional. Being interested in the effect of the zero-point fluctuations of the phonon field on the electron tunneling probability, we consider the system at zero temperature. Practically, it means that temperature is low enough and this condition as well as the finite temperature case are discussed in the Appendix. Coupling the electron to the phonon field transforms the problem from a low-dimensional quantum problem to a field theory problem. A convenient way to approach such a field theory problem is via the formalism of path integrals.[14]

The first stage in the calculation of the transition probability for the tunneling process is the calculation of the retarded Green function. We express the energy-dependent retarded Green function as the Fourier transform of the time-dependent propagator,

$$K(x_b,u_{\mathbf{q}f},E|x_a,u_{\mathbf{q}i}) = \int_0^\infty K(x_b,u_{\mathbf{q}f},T|x_a,u_{\mathbf{q}i})\exp\left(\frac{\imath E\cdot T}{\hbar}\right)dT, \tag{2.1}$$

that can be written as the combined path integral of the electron and phonons

$$K(x_b,u_{\mathbf{q}f},T|x_a,u_{\mathbf{q}i}) = \int \mathcal{D}x \int \mathcal{D}u_{\mathbf{q}} \exp\left\{\frac{\imath}{\hbar}[\mathcal{S}_{el}(x) + \mathcal{S}_{ph}(u_{\mathbf{q}}) + \mathcal{S}_{int}(u_{\mathbf{q}},x)]\right\}, \tag{2.2}$$

where x is the electron coordinate, $u_{\mathbf{q}}$ are the Fourier coefficients of $u(x,t)$, which is the displacement vector, and $x_a,u_{\mathbf{q}i}$; $x_b,u_{\mathbf{q}f}$ are the initial and final coordinates of the electron and phonons, respectively. The limits over the energy Fourier transform result from the fact that we are calculating the retarded Green function. $\mathcal{S}_{el}$ is the action of the electron in the absence of phonons, given by

$$\mathcal{S}_{el} = \int_0^T dt\left(\frac{m}{2}\dot{x}^2 - V\right), \tag{2.3}$$

where m is the effective electron mass, and V is the constant potential height of the rectangular barrier. $\mathcal{S}_{ph}$ is the action of the uncoupled phonon field

$$\mathcal{S}_{ph} = \int_0^T dt \sum_q \left(\frac{\rho}{2}|\dot{u}_{\mathbf{q}}|^2 - \frac{\rho}{2}\cdot\omega_q^2|u_{\mathbf{q}}|^2\right), \tag{2.4}$$

where ρ is the crystal density and $u_{-\mathbf{q}} = u_{\mathbf{q}}^*$. Since we are treating acoustic phonons $\omega_q = q\cdot s$, s being the phonon velocity. $\mathcal{S}_{int}$ is the action associated with the interaction between the electron and the phonon environment

$$\mathcal{S}_{int} = -\int_0^T dt V_{int}. \tag{2.5}$$

We will treat two electron-phonon coupling mechanisms, piezoelectric and deformation potential, and consider crystals of cubic symmetry. We consider this symmetry as the most important because most of III-V compounds belong to this class.[13] So for the piezoelectric coupling

$$V_{int}^{piezo} = \frac{1}{\sqrt{V_{vol}}}\sum_{\mathbf{q}\nu} \Xi_{\mathbf{q}\nu}u_{\mathbf{q}\nu}M_{\mathbf{q}_\perp}\exp(iq_x x), \tag{2.6}$$

where

$$\Xi_{\mathbf{q}\nu} = \frac{4\pi e}{\epsilon q^2}\beta_{ijk}q_i q_j e_k^\nu \tag{2.7}$$

β_{ijk} is the piezoelectric modules, e is the electron charge, ϵ is the dielectric constant, e_k^ν is the polarization vector of the νth phonon branch, and V_{vol} is the normalization volume. $M_{\mathbf{q}_\perp}$ is the matrix element of the phonon exponent, $\exp(i\mathbf{q}_\perp\mathbf{r}_\perp)$, between the wave functions describing the electron quantization in the cross section of the wire, $\mathbf{q}_\perp$ and $\mathbf{r}_\perp$ are the phonon wave vector and electron radius vector in the cross section plane. In cubic crystals the only nonzero components of the piezoelectric module are $\beta_{xyz}=\beta_{yxz}$ and all other permutations.[15] They are equal and we will designate them as β.

The deformation potential couples electrons only with the longitudinal phonon mode and

$$V_{int}^{def}=\frac{1}{\sqrt{V_{vol}}}\sum_{q} i\Lambda|q|u_{\mathbf{q}i}M_{\mathbf{q}_\perp}\exp(iq_x x). \tag{2.8}$$

Here, Λ is the deformation potential constant.

We neglect the screening of V_{int}. Underneath the potential barrier there are no electrons and the screening by remote electrons is small.

B. Transition amplitude and transition probability

We can now define the transition amplitude through the use of the retarded Green function (2.2). $K(x_b,u_{\mathbf{q}f},E|x_a,u_{\mathbf{q}i})$ is the amplitude to go from initial phonon coordinate $u_{\mathbf{q}i}$ to final coordinate $u_{\mathbf{q}f}$ and from electron coordinate x_a to x_b, for a given energy E, of the joint system. (In all intermediate calculation we suppress the index of the phonon branch to simplify the notations.) The transition amplitude for the joint system to go from a phonon state designated by $\psi_0(u_{\mathbf{q}i})$ to a state $\psi_n(u_{\mathbf{q}f})$ is expressed by $K(x_b,u_{\mathbf{q}f},E|x_a,u_{\mathbf{q}i})$ in the following manner

$$A_{nb,0a}=\int du_{\mathbf{q}i}du_{\mathbf{q}f}\psi_n^*(u_{\mathbf{q}f})K(x_b,u_{\mathbf{q}f},E|x_a,u_{\mathbf{q}i})\psi_0(u_{\mathbf{q}i}). \tag{2.9}$$

We treat the problem with the temperature equal to zero, therefore, phonons are assumed to be initially in the ground state: $\psi_0(u_{\mathbf{q}i})$.

The transition probability is the absolute value squared of the transition-matrix element. Since we are not interested in the final phonon configuration, final phonon states are summed over. From the completeness relation we get the following delta function: $\delta(u_{\mathbf{q}f}-\tilde{u}_{\mathbf{q}f})$. We end up with the following expression for the electron transmission probability

$$\begin{aligned}P_{b,a}&=\sum_n |A_{nb,0a}|^2\\&=\int du_{\mathbf{q}i}d\tilde{u}_{\mathbf{q}i}du_{\mathbf{q}f}\psi_0^*(\tilde{u}_{\mathbf{q}i})K(x_b,u_{\mathbf{q}f},E|x_a u_{\mathbf{q}i})\\&\quad\times\tilde{K}^*(x_b,u_{\mathbf{q}f},E|x_a\tilde{u}_{\mathbf{q}i})\psi_0(u_{\mathbf{q}i}).\end{aligned} \tag{2.10}$$

This equation defines the transmission coefficient.

III. MAIN APPROXIMATIONS

The usual approach to the calculation of the functional integral in Eq. (2.2) that has been started by Caldeira and Leggett[1] is the integration out the phonon degrees of freedom. This can be done exactly because the action is quadratic in $u_{\mathbf{q}}$. In the realistic electron-phonon coupling, this results in a complicated electron-electron effective potential, since the coupling mechanism is nonlinear in the electron coordinate, thus, a simpler approach is needed.

We use the following approach. We consider the situation (which is typical experimentally) when (i) the barrier is so high that the tunneling can be considered semiclassically and (ii) the interaction energy between electrons and phonons is small compared to the height of the barrier. The first point allows us to make use of the semiclassical approximation to integrate with respect to all electron paths. The main contribution to this integral comes from only one optimal trajectory that satisfies the equation

$$m\ddot{x}=-\frac{\partial V_{int}}{\partial x}, \tag{3.1}$$

(for a rectangular barrier $\partial V/\partial x=0$). This equation has to be solved for given $u(x,t)$. The second point allows us to consider V_{int} in Eq. (3.1) as a small perturbation and thus, it can be neglected. As usual in tunneling problems,[16,17] we change the time t to $-it$ (and T to iT) so that the first integral of Eq. (3.1) has the form

$$\frac{m\dot{x}^2}{2}=V-E'. \tag{3.2}$$

Here, E' is the integration constant that can be considered as the electron energy. The value of E' is determined from the boundary conditions $x(0)=x_a$ and $x(T)=x_b$. For a rectangular barrier when x_a and x_b are fixed E' is a function of T only. Without phonon emission E' eventually appears equal to the energy of the incident electron E that is also the total energy. If during tunneling phonons are emitted then the electron energy E' appears smaller than the total energy.

Thus in the tunneling problem an important parameter appears the electron velocity $v=\sqrt{2(V-E')/m}$. If $V-E'$ is around 10 meV or larger than in GaAs where $m=0.067m_0$ (m_0 is the free-electron mass) v is around or larger than 2×10^7 cm/s. This velocity is larger than the sound velocity s by about two orders of magnitude. That means that frequencies of phonons with the wave length around the length of the barrier L are much smaller than the inverse time necessary for an electron to traverse the barrier. Actually, the wave length of a typical phonon interacting with the tunneling electron is limited not by the length of the barrier but by the width of the constriction a that is smaller than L. However, practically the ratio a/L for a constriction where tunneling is still measurable is not very small and the assumption that the typical phonon frequencies are much smaller than the inverse traverse time is justified. This assumption means that during the traverse time (L/v) the phonon potential nearly does not change. In the extreme case we can consider it constant. We call this case the static approximation. A similar approximation was used by Flynn and Stoneham[18] and later by Kagan and Klinger[19] treating the problem of quantum diffusion of atomic particles.

It should be mentioned that the physical significance of the parameter ωt_0, ω being the phonon frequency, t_0 the tunneling time as defined by Büttiker and Landauer,[20] $t_0=L/v$ (in our case of a rectangular barrier) was also noted in the two papers of Ueda and Ando,[11] but in their problem the typical frequency ω was a tunable parameter defined by the properties of the electric circuit.

In the static approximation the problem is dramatically simplified because we need to consider electron motion in a static potential and the stationary Schrödinger equation is enough for this. The integration with respect to phonon coordinates is reduced to the integration only with respect to $u_{\mathbf{q}i}$. The derivation of the corresponding expression for the transmission coefficient in the static approximation from Eq. (2.10) with the help of the expansion in s/v is given in the Appendix.

In the static approximation we can add also $V_{int}^{stat}=V_{int}(u_{\mathbf{q}i})$ to the rhs of Eq. (3.2). That immediately shows that the small parameter characterizing the interaction with phonons is $V_{int}/(V-E)$. In the calculation of the transmission coefficient we take into account only terms of the first order in this parameter. So we ignore corrections to the trajectory $x=vt$ coming from the interaction with phonons. It is obvious in the calculation of V_{int} and this is also true for $\mathcal{S}_{el}$. Indeed, the trajectory $x=vt$ is found from the minimization of $\mathcal{S}_{el}$ and any correction to this functional contains a correction to the trajectory squared. Such an approximation means, in particular, that we neglect all polaron effects. The physical meaning of the phonon effect in this approximation is that different phonon configurations change the barrier and the main contribution to the transmission comes from the configurations corresponding to the barrier being a bit lower in average, so that the tunneling probability is higher. It is worthwhile to note that the average (over configurations) height of the barrier does not change because $\langle V_{int}\rangle=0$ but nevertheless the average of the tunneling exponent is modified due to V_{int} (similar to, e.g., $\langle\exp(V_{int})\rangle>1$).

The tunneling across a static barrier is an elastic process and the energy of the incident electron and the tunneled one is the same. Phonon emission and the corresponding change of the electron energy come about only in the first approximation in s/v when the phonon dynamics is taken into account. The calculation of the dynamic correction to the transmission coefficient that requires a more complete treatment of the modes presented in the previous section is given in Sec. V.

IV. STATIC APPROXIMATION

In the static approximation the problem of tunneling can be formulated in a very simple way, without making use of Eq. (2.2). First, we can find the transmission probability for a given static phonon field. The regular WKB approximation gives for it

$$D(E;u_{\mathbf{q}i})=\sqrt{\frac{m}{4(V+V_{int}^{stat}-E)}}\times\exp\left\{-\frac{2}{\hbar}\int_0^L\sqrt{2m(V+V_{int}^{stat}-E)}dx\right\}. \tag{4.1}$$

The calculation of the electron transmission coefficient in the case when phonon field is initially at the ground state is reduced now to the integration of $D(E;u_{\mathbf{q}i})$ multiplied by the ground state phonon wave function squared with respect to $u_{\mathbf{q}i}$,

$$P(E)=C^2\int D(E;u_{\mathbf{q}i})\exp\left(-\frac{1}{\hbar}\sum_q\rho qs|u_{\mathbf{q}i}|^2\right)du_{\mathbf{q}i} \tag{4.2}$$

(C is a normalizing constant). The expansion in V_{int} gives

$$P(E)=P_0(E)C^2\int\times\exp\left\{-\sqrt{\frac{2m}{\hbar\sqrt{V-E}}}\int_0^L V_{int}^{stat}dx-\frac{\rho s}{\hbar}\times\sum_q q|u_{\mathbf{q}i}|^2\right\}du_{\mathbf{q}i}, \tag{4.3}$$

where

$$P_0(E)=\frac{\sqrt{m}}{2\sqrt{V-E}}\exp\left\{-\frac{2L}{\hbar}\sqrt{2m(V-E)}\right\}. \tag{4.4}$$

is the transmission coefficient without interaction with phonons. Equation (4.3) can be obtained directly from Eq. (2.10) (see Appendix). The result can be written in the form,

$$P(E)=P_0(E)\exp\left\{\frac{2}{\hbar}\Phi_{stat}(E)\right\}. \tag{4.5}$$

For the deformation potential

$$\Phi_{stat}(E)=\frac{\Lambda^2L}{8\pi^2\rho s_l v^2}\int|M_{\mathbf{q}_\perp}|^2q_\perp d^2\mathbf{q}_\perp, \tag{4.6}$$

where s_l is the longitudinal phonon velocity.

For the piezoelectric coupling

$$\Phi_{stat}(E)=\frac{1}{2\pi^3\rho v^2}\int_0^\infty dq_x\frac{\sin^2(q_xL/2)}{q_x^2}\times\sum_\nu\frac{1}{s_\nu}\int|\Xi_{\mathbf{q}\nu}|^2|M_{\mathbf{q}_\perp}|^2\frac{d^2\mathbf{q}_\perp}{q}. \tag{4.7}$$

Because of the anisotropy the result depends on the tunneling direction with respect to crystalographic axes. For the tunneling in [100] the contribution of the longitudinal phonons in Φ_{stat} is small compared to that of transverse ones in a/L and

$$\Phi_{stat}(E)=\frac{8\beta^2e^2L}{\rho v^2\epsilon^2 s_t}\int|M_{\mathbf{q}_\perp}|^2\frac{q_y^2q_z^2}{q_\perp^5}d^2\mathbf{q}_\perp, \tag{4.8}$$

where s_t is the velocity of the transverse phonons. For the tunneling in [110] direction the contributions of both longitudinal and transverse phonons are of the same order,

$$\Phi_{stat}(E)=\frac{2\beta^2e^2L}{\rho v^2\epsilon^2}\int|M_{\mathbf{q}_\perp}|^2\times\left[\frac{q_y^4+4q_y^2q_z^2}{s_tq_\perp^4}-\left(\frac{1}{s_t}-\frac{1}{s_l}\right)\frac{9q_y^4q_z^2}{q_\perp^6}\right]\frac{d^2\mathbf{q}_\perp}{q_\perp}. \tag{4.9}$$

As can be seen the typical phonon wave numbers with which the electron interacts are fixed through the length scales of the problem, the barrier length L and the width of the constriction a. It is important to note that, the static correction, in the exponent is positive, therefore static phonons reduce the effective potential barrier height, enhancing electron tunneling probability. The electron, due to coupling to

the zero-point fluctuations of the phonon field, tunnels through an effectively lower potential barrier.

V. DYNAMIC CORRECTIONS AND ENERGY LOSS

To get the electron's energy loss due to phonon emission during the tunneling process, one needs to go beyond the static approximation. As the first step we make use of the WKB approximation to simplify the expression for the propagator $K(x_b,u_{\mathbf{q}f},T|x_a,u_{\mathbf{q}i})$ (2.2). In this approximation the main contribution to the integral with respect to $x(t)$ comes from the saddle point trajectory that in the first approximation in $V_{int}/(V-E)$ is determined by Eq. (3.2), As a result the propagator is factorized. In Eq. (3.2), we passed to the imaginary time so the trajectory is $x_0(t)=vt$ where $v=\sqrt{2(V-E')/m}$, thus the propagator can be expressed as

$$K(x_b,u_{\mathbf{q}f},-iT|x_a,u_{\mathbf{q}i})=K_0(x_b,T|x_a)K_{ph}(u_{\mathbf{q}f},T|u_{\mathbf{q}i}). \tag{5.1}$$

Here,

$$K_0(x_b,T|x_a)=\left[\frac{m}{4(V+V_{int}^{stat}-E)}\right]^{1/4}\exp\left(\frac{-E'T}{\hbar}\right)\times\exp\left(-\frac{1}{\hbar}\int_0^L dx\sqrt{2m(V-E')}\right) \tag{5.2}$$

is the electron propagator without interaction with phonons and

$$K_{ph}(u_{\mathbf{q}f},T|u_{\mathbf{q}i})=\int \mathcal{D}u_{\mathbf{q}}\exp\left\{-\frac{1}{\hbar}[\mathcal{S}_{ph}(u_{\mathbf{q}})+\mathcal{S}_{int}(u_{\mathbf{q}},x_0)]\right\} \tag{5.3}$$

is the phonon part of the propagator.

So as the electron trajectory is determined the phonon part of the propagator is the propagator of an ensemble of forced harmonic oscillators.[14] The integration with respect to $u_{\mathbf{q}}$ leads to

$$K_{ph}(u_{\mathbf{q}f},T|u_{\mathbf{q}i})=g(T)\exp\left[-\frac{1}{\hbar}\,\mathcal{S}_{cl}(u_{\mathbf{q}f},T|u_{\mathbf{q}i})\right], \tag{5.4}$$

where

$$g(T)=\prod_{\mathbf{q}}\sqrt{\frac{\rho\omega_q}{2\pi\hbar\sinh\omega_qT}}, \tag{5.5}$$

and

$$\begin{aligned}\mathcal{S}_{cl}(u_{\mathbf{q}f},T|u_{\mathbf{q}i})=\sum_q\frac{\rho\omega_q}{2\sinh(\omega_qT)}\Bigg\{&\cosh(\omega_qT)\\&\times(|u_{\mathbf{q}i}|^2+|u_{\mathbf{q}f}|^2)-(u_{\mathbf{q}i}u_{\mathbf{q}f}^*+u_{\mathbf{q}i}^*u_{\mathbf{q}f})\\&-u_{\mathbf{q}f}\left[\frac{1}{\rho\omega_qv}\int_0^L dx f_{\mathbf{q}}(x)\sinh\left(\frac{\omega_qx}{v}\right)\right]\\&-u_{\mathbf{q}i}\left[\frac{1}{\rho\omega_qv}\int_0^L dx f_{\mathbf{q}}(x)\sinh\left(\frac{\omega_q(L-x)}{v}\right)\right]\\&-u_{\mathbf{q}f}^*\left[\frac{1}{\rho\omega_qv}\int_0^L dt f_{\mathbf{q}}^*(x)\sinh\left(\frac{\omega_qx}{v}\right)\right]\\&-u_{\mathbf{q}i}^*\left[\frac{1}{\rho\omega_qv}\int_0^L dx f_{\mathbf{q}}^*(x)\sinh\left(\frac{\omega_q(L-x)}{v}\right)\right]\\&-\frac{2}{\rho^2\omega_q^2v^2}\int_0^L dx\int_0^x dy[f_{\mathbf{q}}(x)f_{\mathbf{q}}^*(y)\\&+f_{\mathbf{q}}^*(x)f_{\mathbf{q}}(y)]\sinh\left(\frac{\omega_qy}{v}\right)\sinh\left[\frac{\omega(L-x)}{v}\right]\Bigg\}.\end{aligned} \tag{5.6}$$

Here, according to Eqs. (2.8) and (2.6)

$$f_{\mathbf{q}}(x)=\frac{\Xi M_{\mathbf{q}_\perp}}{\sqrt{V_{vol}}}\,e^{iq_xx} \tag{5.7}$$

for the piezoelectric interaction and

$$f_{\mathbf{q}}(x)=i|q|\frac{\Lambda M_{\mathbf{q}_\perp}}{\sqrt{V_{vol}}}\,e^{iq_xx} \tag{5.8}$$

for the deformation potential interaction. One should note that in Eq. (5.6) we made a transformation of variables from t in the action, to $x=vt$.

Making use of the factorization (5.1) the expression for tunneling probability (2.10) can be written as

$$P(E)=\int dT\int d\tilde{T}K_0(x_b,T|x_a)K_0(x_b,\tilde{T}|x_a)\xi_{ph}(T;\tilde{T}), \tag{5.9}$$

where

$$\begin{aligned}\xi_{ph}(T;\tilde{T})=g(T)g(\tilde{T})&\\\times\int du_{\mathbf{q}i}\int du_{\mathbf{q}f}\int d\tilde{u}_{\mathbf{q}i}&\\\times\exp\Bigg[-\frac{1}{\hbar}\mathcal{S}_{cl}(u_{\mathbf{q}f},T|u_{\mathbf{q}i})&\\-\frac{1}{\hbar}\mathcal{S}_{cl}(u_{\mathbf{q}f},\tilde{T}|\tilde{u}_{\mathbf{q}i})\Bigg]\psi_0(u_{\mathbf{q}i})\psi_0^*(\tilde{u}_{\mathbf{q}i}),&\end{aligned} \tag{5.10}$$

and $\psi_0(u_{\mathbf{q}i})$ is the phonon ground state wave function. The integrals with respect to T and $\tilde{T}$ in Eq. (5.9) are calculated by the saddle-point method.[16] Due to the symmetry of $\xi_{ph}[T;\tilde{T}]$ with respect to the transposition of T and $\tilde{T}$ the saddle point values of these variables are identical. We are interested only in the exponential part of the transition probability and for this only $\xi_{ph}[T;T]$ is necessary. The result can be written in the form

$$\xi_{ph}(T;T)=A\exp\left[\frac{2}{\hbar}\Phi_{ph}(T)\right], \tag{5.11}$$

where $\Phi_{ph}(T)$ is calculated in the Appendix and the preexponential factor A, will not be calculated.

We now break $\Phi_{ph}(T)$ into a static part, Φ_{stat}, and a dynamical correction so that $\Phi_{ph}=\Phi_{stat}+\Phi_{dyn}$. As one can expect the static part is identical to $\Phi_{stat}(E')$ obtained in Sec. IV, Eq. (4.8), in a more simple way. The dynamical

correction, $\Phi_{dyn}(T,E')$, is obtained in the Appendix in the leading order in $s/v \ll 1$. Using these notations the saddle-point equation for time integration is given by

$$\left(\frac{\partial \Phi_{el}}{\partial E'} - \frac{\partial \Phi_{stat}}{\partial E'} - T \right) \frac{dE'}{dT} - \frac{d\Phi_{dyn}}{dT} + E - E' = 0, \tag{5.12}$$

where $\Phi_{el}(E') = L\sqrt{2m(V-E')}$.

According to Sec. IV, $\Phi_{el}(E') - \Phi_{stat}(E')$ is the electron action in the phonon static field at the trajectory with the energy E'. The derivative of the action with respect to the energy is the traveling time along the trajectory. The first term, $\partial \Phi_{el}/\partial E'$, has been defined by Büttiker and Landauer[20] as a semiclassical traverse time. The second term, $\partial \Phi_{stat}/\partial E'$, gives a phonon correction to the traverse time. The sum to the two terms equals T and the expression in the parentheses is identically zero. Then, Eq. (5.12) can be written in the form

$$E - E' = -\frac{\partial \Phi_{dyn}}{\partial v} \frac{v^2}{L}. \tag{5.13}$$

In the accepted approximation in the rhs of this equation the difference between E and E' has to be neglected.

According to our definition the energy E appearing at the Fourier transform of the transmission amplitude is the total energy of the system while E' is the energy characterizing the electron trajectory. The difference between them is the energy transferred to the phonon system, i.e., the average energy loss of the tunneling electron.

The substitution of $T = L/v$ and calculation of the integral with respect to q_x in Eq. (A8) we obtain for the deformation potential,

$$\Phi_{dyn}(E) = \frac{\Lambda^2 L^2}{8\pi^2 \rho v^3} \int |M_{\mathbf{q}_\perp}|^2 q_\perp^2 d^2\mathbf{q}_\perp . \tag{5.14}$$

For the piezoelectric potential the terms in $|\Xi_{\mathbf{q}\nu}|^2$ containing q_x are small in a/L and the main contribution is

$$\Phi_{dyn}(E) = \frac{L^2}{8\pi^2 \rho v^3} \sum_\nu \int |\Xi_{\mathbf{q}\nu}|^2 |M_{\mathbf{q}_\perp}|^2 d^2\mathbf{q}_\perp . \tag{5.15}$$

For [100] tunneling direction Eq. (5.15) becomes

$$\Phi_{dyn}(E) = \frac{8\beta^2 e^2 L^2}{\rho v^3 \epsilon^2} \int |M_{\mathbf{q}_\perp}|^2 \frac{q_y^2 q_z^2}{q_\perp^4} d^2\mathbf{q}_\perp , \tag{5.16}$$

and for [110] tunneling direction

$$\Phi_{dyn}(E) = \frac{2\beta^2 e^2 L^2}{\rho v^3 \epsilon^2} \int |M_{\mathbf{q}_\perp}|^2 (q_y^4 + 4q_y^2 q_z^2) \frac{d^2\mathbf{q}_\perp}{q_\perp^4}. \tag{5.17}$$

It is worthwhile to note that Φ_{dyn} is positive, i.e., it increases the transmission coefficient as well as Φ_{stat}. One could expect that phonon emission makes the barrier for electrons effectively higher that may lead to a reduction of the transmission probability. However, Φ_{dyn} is calculated for $E = E'$ and this effect can appear only in the next approximation.

The average energy loss resulting from the deformation potential coupling is,

$$E - E' = \frac{3\Lambda^2 L}{8\pi^2 \rho v^2} \int |M_{\mathbf{q}_\perp}|^2 q_\perp^2 d^2\mathbf{q}_\perp . \tag{5.18}$$

Whereas the average energy loss due to the piezoelectric coupling is given by

$$E - E' = \frac{24\beta^2 e^2 L}{\rho v^2 \epsilon^2} \int |M_{\mathbf{q}_\perp}|^2 \frac{q_y^2 q_z^2}{q_\perp^4} d^2\mathbf{q}_\perp , \tag{5.19}$$

for [100] tunneling direction and

$$E - E' = \frac{6\beta^2 e^2 L}{\rho v^2 \epsilon^2} \int |M_{\mathbf{q}_\perp}|^2 (q_y^4 + 4q_y^2 q_z^2) \frac{d^2\mathbf{q}_\perp}{q_\perp^4}. \tag{5.20}$$

for [110] tunneling direction.

The energy loss is proportional to the length of the barrier, which means that it is accumulated along it.

The comparison the static and dynamical phonon corrections to the tunneling probability gives $\Phi_{dyn}/\Phi_{stat} \sim (s/v)(L/a)$ where a is the width of the constriction. Typically the ratio L/a is not very large so the expansion that we used is justified.

VI. DISCUSSION AND SUMMARY

In this paper, we have presented a detailed study of effect of coupling with acoustic phonons on electron tunneling across a rectangular barrier in a realistic situation. We studied piezoelectric and deformation potential coupling at low temperature, which means that $\lambda_T/a \gg 1$, where λ_T is the thermal phonon wavelength (see Appendix). We considered only a one-dimensional problem that can be realized in a quantum wire or a narrow constriction.

In our calculation we assumed that the barrier is high enough to describe tunneling in the semiclassical approximation. Our detailed calculations reveal that the typical phonon interacting with the tunneling electron is chosen through the length of the barrier L and the width of the constriction or quantum wire a. It is thus the geometry of the potential barrier that defines the phonon frequency ω. Under such a condition the electron motion under the barrier is so fast that phonons do not follow it and can be considered nearly static during the time necessary for electron to traverse the barrier. The main effect of phonons in this case is a modulation of the barrier so that its height has to be considered as a quantum-mechanical variable whose probability distribution is controlled by a phonon wave function. In this case, roughly speaking, an electron chooses for tunneling the phonon configurations when the barrier is lower than its average value, that results in an increase of the transmission coefficient compared to that with zero electron-phonon coupling. Thus, the interaction of an electron with the zero point phonon fluctuations increases the tunneling probability.

The correction to the tunneling exponent in the static approximation is proportional to the length of the barrier. That is, the coupling affects the dependence of the transmission coefficient on the height of the barrier only.

The dynamical correction leads to two effects. First, it

describes the reduction of the electron energy due to phonon emission. Second, which is probably more interesting, it gives the dependence of the transmission coefficient on the length of the barrier different from the regular one where the log of the transmission coefficient is linear in the length. We calculated only the first order correction to the exponential dependence. The effect can be stronger and is probably measurable for tunneling near the top of the barrier. One should note that even though the dynamical correction to the transition probability is smaller than the static correction, it is still an exponential correction and it easily can be made larger than unity, i.e., by changing the length of the barrier. In this case it can significantly affect the tunneling probability.

The dependence of transmission coefficient on the height and the length of a barrier can be measured in devices where the barrier is introduced with the help of a gate. In such a device both the height and the length of the barrier are controlled by the gate voltage. Our results point out to a deviation of these dependencies from the standard ones obtained from stationary Schrödinger equation.

The application of our results to a long quantum wire can encounter a difficulty because we did not take into account electron-electron interaction. The effect of this interaction can be reduced for a short wire or a narrow constriction.

We expect nontrivial results through further use of the piezoelectric and deformation potential coupling mechanisms in two- or three-dimensional systems.

We believe that the physical considerations presented here, which greatly simplified the calculations are convenient for extending the calculations to two- and three-dimensional physical situations.

APPENDIX: NONSTATIC CALCULATION OF THE TRANSITION AMPLITUDE AND TRANSITION PROBABILITY

In the Appendix, we carry out the integration with respect to initial and final phonon coordinates and expand the result in two small parameters defined in Sec. III, s/v and $V_{int}/(V-E)$. The calculations presented here are for the finite temperature case.

The explicit form of Eq. (5.10) for $\tilde{T}=T$ is

$$\xi_{ph}(T;T)=g^2(T)\times\int du_{\mathbf{q}i}\int du_{\mathbf{q}f}\int d\tilde{u}_{\mathbf{q}i}\times\exp\left[-\frac{1}{\hbar}\sum_{\mathbf{q}}\alpha_q(T)\,\eta_q(u_{\mathbf{q}f},u_{\mathbf{q}i},\tilde{u}_{\mathbf{q}i};T)\right]\times\frac{1}{Z}\sum_m e^{-\beta E_m}\psi_m(u_{\mathbf{q}i})\psi_m^*(\tilde{u}_{\mathbf{q}i}),\tag{A1}$$

where $Z=\Sigma_m e^{-\beta E_m}$, β is one over the Boltzmann constant times the temperature (we use this notation only in the Appendix and it should not be confused with the piezoelectric module in the body of the paper),

$$\eta_q(u_{\mathbf{q}f},u_{\mathbf{q}i},\tilde{u}_{\mathbf{q}i};T)=\epsilon_q(|u_{\mathbf{q}i}|^2+|u_{\mathbf{q}f}|^2)-(u_{\mathbf{q}i}u_{\mathbf{q}f}^*+u_{\mathbf{q}i}^*u_{\mathbf{q}f})+\epsilon_q(|\tilde{u}_{\mathbf{q}i}|^2+|u_{\mathbf{q}f}|^2)-(\tilde{u}_{\mathbf{q}i}u_{\mathbf{q}f}^*+\tilde{u}_{\mathbf{q}i}^*u_{\mathbf{q}f})+u_{\mathbf{q}i}I_2+u_{\mathbf{q}f}I_1+u_{\mathbf{q}i}^*I_2^*+u_{\mathbf{q}f}^*I_1^*+\tilde{u}_{\mathbf{q}i}^*I_2^*+u_{\mathbf{q}f}^*I_1^*+\tilde{u}_{\mathbf{q}i}I_2+u_{\mathbf{q}f}I_1-I_3,\tag{A2}$$

$\alpha_q=\rho\omega_q/2\sinh(\omega_qT)$, $\epsilon_q=\cosh(\omega_qT)$,

$$I_1=\frac{1}{\rho\omega_q v}\int_0^L dx f_{\mathbf{q}}(x)\sinh\left(\frac{\omega_q x}{v}\right),\tag{A3a}$$

$$I_2=\frac{1}{\rho\omega_q v}\int_0^L dx f_{\mathbf{q}}(x)\sinh\left[\frac{\omega_q(L-x)}{v}\right],\tag{A3b}$$

$$I_3=\frac{2}{\rho^2\omega_q^2v^2}\int_0^L dx\int_0^x dy[f_{\mathbf{q}}(x)f_{\mathbf{q}}^*(y)+f_{\mathbf{q}}^*(x)f_{\mathbf{q}}(y)]\sinh\left(\frac{\omega_q y}{v}\right)\sinh\left[\frac{\omega_q(L-x)}{v}\right].\tag{A3c}$$

Using the well known result for the density matrix[21]

$$\frac{1}{Z}\sum_m e^{-\beta E_m}\psi_m(u_{\mathbf{q}i})\psi_m^*(\tilde{u}_{\mathbf{q}i})=g(\beta)\exp\left[-\frac{2}{\hbar}\sum_{\mathbf{q}}\rho\omega_q\left|u_{\tilde{\mathbf{q}}i}\right|^2\tanh\left(\frac{\hbar\omega_q\beta}{2}\right)\right],\tag{A4}$$

where $g(\beta)$ is given by

$$g(\beta)=\prod_{\mathbf{q}}\sqrt{\frac{\rho\omega_q}{2\pi\hbar\sinh\hbar\omega_q\beta}}.\tag{A5}$$

The result of the integration with respect to initial and final phonon coordinates gives $\xi_{ph}(T;T)=A\exp[2\Phi_{ph}(T)/\hbar]$ where

$$\Phi_{ph}(T)=\sum_q\frac{\alpha_q}{\epsilon_q}\left[\frac{|\epsilon_q\cdot I_2+I_1|^2}{\epsilon_q^2+\rho s q\gamma_q/2-1}+|I_1|^2+\frac{\epsilon_q\cdot I_3}{2}\right],\tag{A6}$$

$\gamma_q=\epsilon_q\tanh(\hbar\omega_q\beta/2)/\alpha_q$

Finite temperature effects in Eq. (A6) can be neglected if $\tanh(\hbar\omega_q\beta/2)\approx 1$. The physical meaning of this approximation is that the phonon thermal wavelength is much larger than the quantum wires width, i.e., $\lambda_T/a\gg 1$. For the width of the constriction of 100 Å or larger this condition is satisfied up to room temperature. From this estimate it is also follows that the matrix element for high-energy phonons that could activate a tunneling electron to energy comparable with the height of the barrier is small and we neglect it. Thus, the rest of the calculations will be performed for the zero-temperature case.

One should note that the phonon part of the transition probability, $\xi_{ph}(T;T)$, is larger than 1, causing an enhancement of the electron tunneling probability.

It is convenient to separate in $\Phi_{ph}(T)$ a static part that is obtained by putting $s/v=0$ and a dynamical correction,

$$\Phi_{ph}(T)=\Phi_{stat}(T)+\Phi_{dyn}(T). \tag{A7}$$

The static part

$$\Phi_{stat}=\sum_{q}\frac{1}{\rho q s v^2}\left|\int_0^L dx f_{\mathbf{q}}(x)\right|^2, \tag{A8}$$

is equal to the expression appearing in Eq. (4.7). The dynamical correction is necessary for the calculation of phonon emission and it is calculated in the leading order in $s/v \ll 1$. For the deformation potential the dynamical correction is given by

$$\Phi_{dyn}(E)=\frac{4\Lambda^2 T}{\rho v^2 V_{vol}}\sum_{\mathbf{q}}\left[\frac{\sin(q_x L)}{q_x^3 L}-\frac{\cos(q_x L)}{q_x^2}\right]q_\perp^2|M_{\mathbf{q}_\perp}|^2. \tag{A9}$$

For the piezoelectric coupling, one gets

$$\Phi_{dyn}(E)=\frac{4T}{\rho v^2 V_{vol}}\sum_{\mathbf{q}\nu}\left[\frac{\sin(q_x L)}{q_x^3 L}-\frac{\cos(q_x L)}{q_x^2}\right]|\Xi_{\mathbf{q}\nu}|^2|M_{\mathbf{q}_\perp}|^2. \tag{A10}$$

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