Tunneling in the Presence of Phonons: A Solvable Model

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We obtain the solution for an electron tunneling through a thin potential barrier with local Einstein phonons, by means of a continued-fraction expansion. Our results demonstrate the strong feedback between inelastic and elastic scattering, the associated singularities, an increase in low-energy transmission with a nonmonotonic temperature dependence, and a crossover from quantum to adiabatic behavior with increasing temperature and electron velocity.

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Tunneling is one of the most fundamental quantum processes[1] and tunneling devices are potentially of great technological importance. One of the major issues in this field is the effect of phonons ("dissipation") and its correct theoretical treatment. For example, in a quantum-mechanical problem involving both elastic and inelastic scattering channels, care has to be taken to ensure correct normalization of the particle wave function. If the probability of finding the particle in the initial state is unity then after interaction the sum over all possible final-state probabilities must also be unity. This unitarity condition leads to a feedback mechanism by which inelastic scattering processes change the probability of elastic scattering. Clearly, this feedback mechanism is beyond the scope of simple perturbation theory.[1]

Approximate and exact solutions for quantum-mechanical transmission and reflection of particles in the presence of dissipation have been presented in the past. These studies, e.g., considered two-state systems,[2] WKB approximations,[3] resonant tunneling models,[4] and a unitary one-phonon approximation.[5] In this paper a numerical solution to the problem is outlined for the specific case of an electron tunneling through a thin potential barrier with local Einstein phonons. Using our model, we extract the essential physics of real tunneling structures, in particular the feedback mechanism between elastic and inelastic tunnel current.

Figure 1 represents an electron in the conduction band of a crystal with initial kinetic energy E impinging on a potential barrier of energy V_0 and width δ. Confined within the barrier are Einstein phonons of frequency ω to which the electron couples. The electron may be inelastically scattered inside the barrier, and is either transmitted or reflected emerging with an energy $E'=E+n\omega$, where n is an integer.

We consider the one-dimensional tight-binding Hamiltonian (in the interaction representation) describing the electron subject to the static barrier potential V_{0i} and a deformation potential coupling $V_{1i}(t)$ to the Einstein phonons:

$$H_{ij}(t) = -t_{ij} + \delta_{ij}[V_{0i} + V_{1i}(t)] . \tag{1}$$

t_{ij} is the hopping amplitude and

$$V_{1i}(t) = V_1\delta_{i0}[b\exp(-i\omega t) + b^\dagger\exp(i\omega t)] , \tag{2}$$

where $b^\dagger$ and b are phonon creation and annihilation operators, respectively. The phonons are assumed to be localized at one of the interfaces of V_{0i} which, for convenience, is chosen to be the origin. Experimentally, the localized phonons might correspond to vibrational modes of organic molecules placed in the barrier of a tunneling structure.[6] Note that the solution ψ_i of the time-dependent Schrödinger equation is an amplitude operator, i.e., it is an amplitude for the electron and an operator for the phonons.[5] To calculate observable properties of the electron we will take a thermal average over the phonon states.

After transforming the time-dependent Schrödinger equation into a Lippman-Schwinger equation and dividing ψ_i into an incoming (ψ_i^0) and a scattered (ψ_i^s) wave, we find

$$\psi_i^s(t) = \psi_i^{s0}(t) + \sum_j \int_{-\infty}^{+\infty} dt' G_{ij}^0(t-t') V_{1j}(t')\psi_j(t') , \tag{3a}$$

$$\psi_i^{s0}(t) = \sum_j \int_{-\infty}^{+\infty} dt' G_{ij}^0(t-t') V_{0j}\psi_j^0(t') , \tag{3b}$$

where G_{ij}^0 (ψ_i^{s0}) is the retarded electron propagator

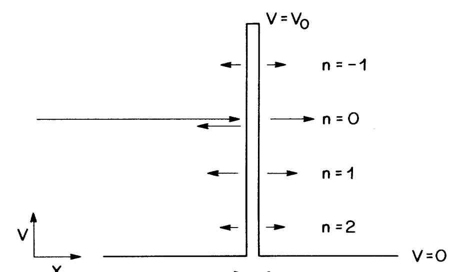

FIG. 1. Schematic diagram of an electron of initial energy E approaching a potential barrier of average energy V_0 and width δ. Inelastically scattered electrons can be transmitted or reflected at the barrier and emerge with energy $E'=E+n\omega$, where n is an integer and ω is the phonon frequency.

(scattered wave) for the static barrier V_{0i}. We consider an incoming plane wave with momentum p and energy E,

$$\psi_j^0(t)=\exp(ipja-iEt)\,, \tag{4}$$

where a is the lattice constant. To solve Eq. (3), we make an *Ansatz* for the scattered wave at the origin, decomposing it into multiphonon components (see Fig. 1),

$$\psi_0^s(t)=\sum_{n=0}^{\infty}(b^\dagger)^n A_n \exp[-i(E-n\omega)t]+\sum_{n=1}^{\infty}(b)^n B_n \exp[-i(E+n\omega)t]\,, \tag{5}$$

where A_n and B_n are diagonal operators. Substituting Eq. (5) into Eq. (3a), we are left with the recurrence relations

$$A_n=V_1G_{00}^0(E-n\omega)[\delta_{n1}+A_{n-1}+(bb^\dagger+n)A_{n+1}],\ \ n\ge 1\,, \tag{6a}$$

$$B_n=V_1G_{00}^0(E+n\omega)[\delta_{n1}+B_{n-1}+(b^\dagger b-n)B_{n+1}],\ \ n\ge 1\,, \tag{6b}$$

$$A_0=B_0=\psi_0^{s0}\exp(iEt)+V_1G_{00}^0(E)[bb^\dagger A_1+b^\dagger bB_1]\,. \tag{6c}$$

Equations of the form (6) have been studied in the past in the context of the dynamical coherent potential approximation for polarons.[7] Given G_{00}^0, (diagonal) matrix elements of A_n and B_n can be easily obtained numerically using a continued-fraction expansion.

In the following, we shall consider tunneling through a thin potential barrier, i.e., $V_{0i}=V_0\delta_{i0}$ and

$$G_{j0}^0(E)=[-\epsilon+\mathrm{sgn}(\epsilon)(\epsilon^2-1)^{1/2}]^{|j|}/[2t\,\mathrm{sgn}(\epsilon)(\epsilon^2-1)^{1/2}-V_0],\ \ |\epsilon|>1 \tag{7a}$$

$$=\exp(ip|j|a)/[2ti(1-\epsilon^2)^{1/2}-V_0],\ \ |\epsilon|<1\,. \tag{7b}$$

Here, nearest-neighbor hopping $[t_{ij}=t\delta_{ij+1},\ E=-2t\cos(pa)]$ has been assumed and $\epsilon=E/2t$. However, our solution can be easily extended to other barrier shapes and dispersion relations by calculating the appropriate Green's function.

The current operator is $j=ita[\psi_{k+1}^*\psi_k-\psi_k^*\psi_{k+1}]$. Using Eqs. (3), (4), (5), and (7), we obtain the thermally averaged transmitted current

$$\langle j_T\rangle=2taZ^{-1}\sum_{l=0}^{\infty}e^{-l\beta\omega}\sum_{n=0}^{\infty}{}'\left[1-\left(\frac{E-n\omega}{2t}\right)^2\right]^{1/2}\left|\delta_{n0}+\left[\frac{(l+n)!}{l!}\right]^{1/2}\langle l|A_n|l\rangle\right|^2$$
$$+2taZ^{-1}\sum_{l=1}^{\infty}e^{-l\beta\omega}\sum_{n=1}^{l}{}'\left[1-\left(\frac{E+n\omega}{2t}\right)^2\right]^{1/2}\frac{l!}{(l-n)!}|\langle l|B_n|l\rangle|^2\,, \tag{8}$$

where $Z=1/[1-\exp(-\beta\omega)]$ is the partition function and the primed sums over n are restricted to current carrying states (positive arguments of the square roots). The expression for the reflected current $\langle j_R\rangle$ is identical to Eq. (8) except for the sign and the absence of the δ_{n0} source term, and

$$\langle j_T\rangle-\langle j_R\rangle=j_0=2ta(1-\epsilon^2)^{1/2}. \tag{9}$$

The static-barrier transmission coefficient $\langle j_T\rangle/j_0$ is given by

$$T_0(\epsilon,V_0)=(1-\epsilon^2)/[1-\epsilon^2+V_0^2/(2t)^2]\,. \tag{10}$$

In addition, we define an adiabatic transmission coefficient

$$T_{\mathrm{ad}}(\epsilon)=\langle T_0(\epsilon,V_0+V_1(b+b^\dagger))\rangle$$
$$=\frac{1}{[2\pi\coth(\beta\omega/2)]^{1/2}}\int_{-\infty}^{+\infty}dQ\exp\left[-\frac{Q^2}{2\coth(\beta\omega/2)}\right]T_0(\epsilon,V_0+V_1Q)\,, \tag{11}$$

which describes current flow in the limit of low phonon frequencies, or high temperatures $T=\beta^{-1}$, in which the phonon potential reduces to Gaussian white noise.

Figures 2(a)–2(c) show the static-barrier (broken curve) and adiabatic (dotted curve) transmission coefficients for various temperatures T. The adiabatic transmission at low electron velocities is always enhanced [for $\epsilon\to-1$ we have $T_{\mathrm{ad}}(\epsilon)\propto(\epsilon+1)^{1/2}$ and $T_0(\epsilon)\propto\epsilon+1$], proportional to the probability of finding a low potential barrier, i.e., a fluctuation $Q=(-V_0/V_1)$ [see Eq. (11)]. As a function of temperature, this results in a maximum increase for $(V_0/V_1)^2=\coth(\beta\omega/2)$. The behavior at high electron velocities depends on the values of V_0 and V_1, but at high temperatures the transmission is always suppressed [Fig. 2(c)].

The solid curves in Figs. 2(a)–2(c) show the transmission coefficient obtained from the numerical solution of

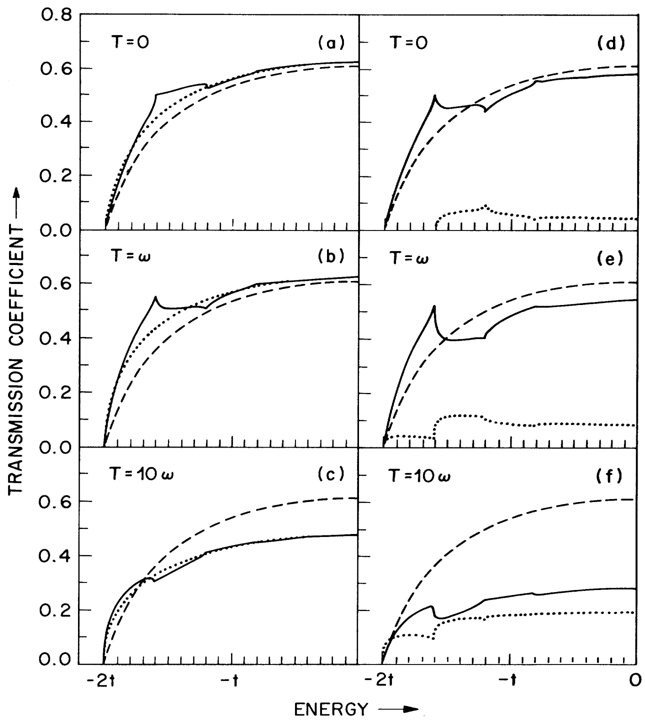

FIG. 2. Transmission coefficient for $V_0=1.6t$, $V_1=0.7t$, and $\omega=0.4t$ for various temperatures T. (a)-(c) show the static-barrier (broken curve), adiabatic (dotted curve), and total (solid curve) transmission; (d)-(f) show the static-barrier (broken curve), elastic (solid curve), and inelastic (dotted curve) transmissions.

Eqs. (6) and (8). The transmission coefficient exhibits singularities (cusps or infinite slopes) at the threshold energies for phonon emission $E=-2t+n\omega$, $n\geq 1$, i.e., whenever a new scattering channel opens up. This interesting threshold behavior is well known from atomic and nuclear reactions[1,8] and is a consequence of unitarity. With increasing electron velocity the lattice has no time to respond and adiabatic behavior is recovered. The same is true at high temperatures [Fig. 2(c)], for which the phonons can be treated classically.

Figures 2(d)-2(f) show the elastic (solid curves) and inelastic (dotted curves) transmission coefficients for the same parameters as in Figs. 2(a)-2(c) and in Fig. 3 the decomposition of the inelastic transmission into its multiphonon components is shown for $T=0$. Figures 2(d)-2(f) illustrate the complementary behavior of elastic and inelastic transmissions, i.e., the former decreases when the latter increases, and vice versa. This is again a manifestation of unitarity. At $T=0$, the inelastic transmission sets in at the threshold for one-phonon emission, $E=-2t+\omega$. The elastic (zero phonon) transmission decreases drastically at that point, because states with lower velocity are mixed in [Fig. 2(d)]. At $E=-2t+2\omega$, two-phonon emission becomes possible and now

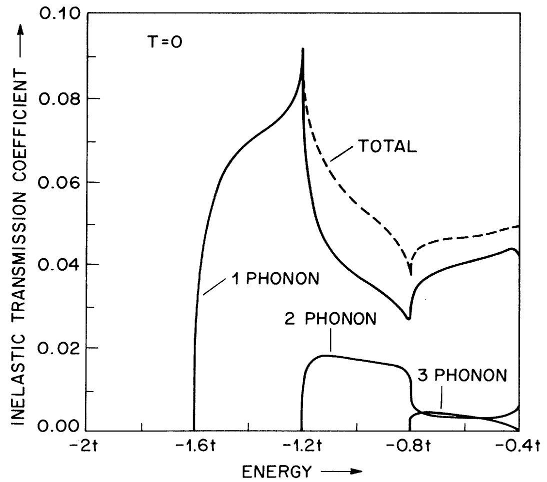

FIG. 3. Inelastic transmission coefficient for $V_0=1.6t$, $V_1=0.7t$, and $\omega=0.4t$, for $T=0$.

the one-phonon transmission decreases, again because of the admixture of lower velocity states (Fig. 3). For the particularly large value of the coupling used in the calculation, the total inelastic transmission actually decreases (Fig. 3) and hence the elastic transmission is enhanced [Fig. 2(d)]. Similar arguments explain the behavior above the three-phonon threshold.

For temperatures $T>0$, one-phonon absorption initially enhances the low-energy elastic transmission by admixing higher velocity states [Fig. 2(e)], but ultimately it leads to its reduction because of unitarity [Fig. 2(f)]. This results in a nonmonotonic temperature dependence of the low-energy elastic and total transmis-

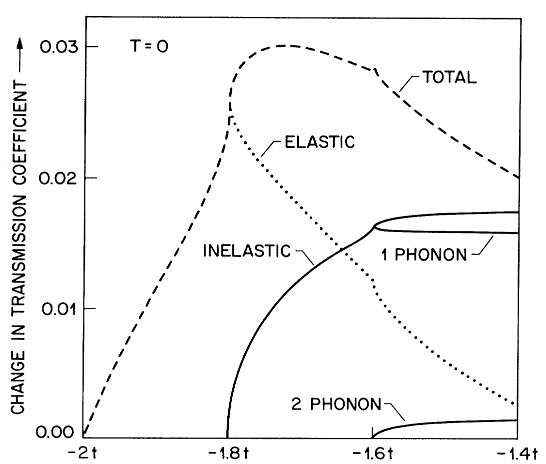

FIG. 4. Change in transmission coefficient (relative to the static-barrier case) for $V_0=1.6t$, $V_1=0.4t$, and $\omega=0.2t$, for $T=0$.

sion similar to that in the adiabatic case [Figs. 2(a)-2(c)].

Realistic tunneling structures usually have couplings and phonon frequencies smaller than in Figs. 2 and 3, so that the changes in transmission due to phonons can only be seen on a differential scale. Typically, for $T=0$ we find a change in total transmission with infinite slope at the one-phonon threshold and a small cusp at the two-phonon threshold (Fig. 4). This translates, respectively, into a peak and a dispersive signal in the second derivative of a typical tunnel junction's current-voltage characteristic. Experimentally, one-phonon peaks are observed and the measured two-phonon structure appears to have just such a dispersive signature.[9]

In summary, we have developed a nonperturbative formalism to describe electron transport across abrupt changes in potential in the presence of inelastic scattering with local Einstein phonons. We have applied our technique to the case of electron tunneling through a thin potential barrier. Our numerical results demonstrate (i) the existence of a feedback mechanism in which inelastic scattering processes substantially influence elastic tunnel current, (ii) associated singularities, (iii) an increase in low-energy elastic and total transmission with a nonmonotonic temperature dependence, and (iv) a crossover from quantum to adiabatic behavior with increasing temperature and electron velocity. The total transmitted current in a tunnel device depends in a subtle, but understandable, way on the initial electron energy, barrier energy, phonon frequency, interaction strength, and device temperature. It remains to be seen whether experiments can be devised that directly measure the feedback mechanism between elastic and inelastic channels, as well as the associated singularities.

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