Model of Phonon-Associated Electron Tunneling through a Semiconductor Double Barrier

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We propose an approach to study one-dimensional electron tunneling in an arbitrarily shaped barrier in the presense of electron-optical-phonon scattering. An independent-boson model is used for the electron-phonon scattering. Our result for a double-barrier structure shows the occurrence of phonon-assisted resonant tunneling.

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Since the pioneering work of Esaki and Tsu,[1] there has been great interest in double-barrier resonant tunneling devices. One of the important problems in the study of these devices is the effect of electron-phonon scattering on the tunneling current. Recently Goldman, Tsui, and Cunningham[2] have found the existence of optical-phonon-assisted resonant tunneling in the valley current region in a double-barrier structure. This effect was theoretically confirmed by Wingreen, Jacobsen, and Wilkins[3] and others.[4] In Ref. 3 the problem of phonon-associated electron tunneling through a barrier has been converted to that of scattering of electron in a single resonant state with phonons.

The quantum tunneling with dissipation and its correct theoretical treatment is an interesting issue. As pointed out by Gelfand, Schmitt-Rink, and Levi,[5] the unitarity condition (or the current conservation) leads to a feedback mechanism by which inelastic scattering processes change the probability of elastic scattering. This feedback mechanism is beyond the scope of simple perturbation theory. Several works[3-10] have been presented on different methods of solving this problem.

In this Letter we present the first calculation of an optical-phonon-associated electron tunneling through an actual double barrier. Using a solvable model for the electron-phonon interaction we propose an approach to calculate the 1D electron tunneling with dissipation in an arbitrary barrier, and indicate how the boundary conditions uniquely determine the transmitted current and the reflected current of an electron. Our approach also clearly shows why phonon-assisted resonant tunneling appears when the electron injects at sideband $E \pm n\omega$ (E is the energy level of elastic resonant tunneling, ω is the energy of optical phonon) in a double-barrier structure.

An incident electron from the left lead (in region I, $x<0$) enters the barrier region II and is scattered by phonons (between $x=0$ and d), and arrives at the right lead (in region III, $x>d$). The Hamiltonian of the electron-optical-phonon interaction has the form

$$H_{\text{int}} = \left[\sum_{\mathbf{q}} M(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}} e^{-i\omega t} a_{\mathbf{q}} + \text{H.c.}\right] \Theta(x)\Theta(d-x),$$

with $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^{\dagger}$, respectively, the phonon annihilation and creation operators, $M(\mathbf{q})$ the electron-phonon scattering matrix, and $\mathbf{R}$ the electron position. $\Theta(x)$ is the Heaviside step function. In the following we use a model that replaces $e^{i\mathbf{q}\cdot\mathbf{R}}$ by 1 in H_{int}. This model is similar to the independent-boson model[3,11] used to describe electron-phonon scattering. Using this model, the Schrödinger equation for a one-dimensional electron in a barrier with arbitrary shape, $V_0(x)$, in region II is given by ($\hbar=1$)

$$i\frac{\partial \psi^{\text{II}}}{\partial t} = -\frac{1}{2}\frac{\partial}{\partial x}\left(\frac{1}{m(x)}\frac{\partial \psi^{\text{II}}}{\partial x}\right) + [V_0(x) + Ve^{-i\omega t} + V^{\dagger}e^{i\omega t}]\psi^{\text{II}}, \qquad (1)$$

where $V = \sum_{\mathbf{q}} M(\mathbf{q}) a_{\mathbf{q}}$ and $V^{\dagger} = \sum_{\mathbf{q}} M^*(\mathbf{q}) a_{\mathbf{q}}^{\dagger}$. Here $m(x)$ is the effective mass of the electron. In regions I and III the electron is in free motion. By neglecting the effect of the electron-phonon interaction on the phonon system, we assume phonon variables are in free motion and in equilibrium with a heat bath. Equation (1) is separable in space and time. The general solution of Eq. (1) can be written as

$$\psi^{\text{II}}(x,t) = \exp\left(\frac{V}{\omega}e^{-i\omega t} - \frac{V^{\dagger}}{\omega}e^{i\omega t}\right)\int dE' [A_{E'}\phi_{E'}^{a}(x) + B_{E'}\phi_{E'}^{b}(x)] e^{-iE't}, \qquad (2)$$

where $\phi_{E'}^{a}(x)$ and $\phi_{E'}^{b}(x)$ are two independent eigenfunctions at eigenvalue E' for the equation without phonons. The coefficients $A_{E'}$ and $B_{E'}$ are constants, which will be determined by the boundary conditions. We assume the electron injects at energy E, with time-independent amplitude, A^{in} (the steady-state case). In this case only components of $\psi(x,t)$

with energy $E+n\omega$ ($n=0,\pm 1,\ldots$) exist. In region II,

$$\psi^{\rm II}(x,t)=\sum_n \psi^{II}_{E+n\omega}(x)\exp[-i(E+n\omega)t]\,,$$

with

$$\psi^{\rm II}_{E+n\omega}(x)=\sum_j\sum_k \frac{(V/\omega)^k}{k!}\frac{(-V^\dagger/\omega)^{j-n+k}}{(j-n+k)!}[A_j^{\rm II}\phi_j^a(x)+B_j^{\rm II}\phi_j^b(x)]\,, \tag{3}$$

where the subscript index j corresponds to the energy $E+j\omega$ ($j=0,\pm 1,\ldots$), $k\geq 0$, $j-n+k\geq 0$. To obtain Eq. (3) we have used $e^{A+B}=e^Ae^Be^{-(1/2)[A,B]}$ for phonon operators. It is easy to see that the magnitudes of $A_n^{\rm II}$ and $B_n^{\rm II}$ have the order of $|V|^{|n|}$. Assuming the electron-phonon interaction is weak, a cutoff of $|n|$ and $|m|$ up to N will ensure the results for the transmitted and the reflected current with an accuracy up to $|V|^{2N}$. In Eq. (3) terms for the nth branch should be maintained to the order of $|V|^{2N-|n|}$. For example, for computing the current with an accuracy up to $|V|^2$, we should keep the following terms:

$$\psi^{\rm II}_{E+\omega}(x)\simeq\frac{V}{\omega}[A_0^{\rm II}\phi_0^a(x)+B_0^{\rm II}\phi_0^b(x)]+[A_{+1}^{\rm II}\phi_{+1}^a(x)+B_{+1}^{\rm II}\phi_{+1}^b(x)]\,, \tag{4a}$$

$$\psi^{\rm II}_{E}(x)\simeq\left(1-\frac{VV^\dagger}{\omega^2}\right)[A_0^{\rm II}\phi_0^a(x)+B_0^{\rm II}\phi_0^b(x)]+\frac{V}{\omega}[A_{-1}^{\rm II}\phi_{-1}^a(x)+B_{-1}^{\rm II}\phi_{-1}^b(x)]-\frac{V^\dagger}{\omega}[A_{+1}^{\rm II}\phi_{+1}^a(x)+B_{+1}^{\rm II}\phi_{+1}^b(x)]\,, \tag{4b}$$

$$\psi^{\rm II}_{E-\omega}(x)\simeq\frac{-V^\dagger}{\omega}[A_0^{\rm II}\phi_0^a(x)+B_0^{\rm II}\phi_0^b(x)]+[A_{-1}^{\rm II}\phi_{-1}^a(x)+B_{-1}^{\rm II}\phi_{-1}^b(x)]\,. \tag{4c}$$

In the incident channel it is necessary to deep the terms $\psi_E^{(2)}\sim|V|^2$, which are related to the coherent double phonons process, since the cross term of $|\psi_E^{(0)}+\psi_E^{(2)}|^2$ contributes the lowest order of phonon effect to the current in the incident channel. The physical requirement is that only the reflected wave exists at region I except for the incident wave,

$$\psi^{\rm I}(x,t)=A^{\rm in}\exp(ik_0^{\rm I}x-iEt)+\sum_n B_n^{\rm I}\exp[-ik_n^{\rm I}x-i(E+n\omega)t]\,,$$

with $B_n^{\rm I}$ the amplitude of the reflected wave. Also, only the transmitted wave exists in region III, $\psi^{\rm III}(x,t)=A_n^{\rm III}\times\exp[ik_n^{\rm III}x-i(E+n\omega)t]$, with $A_n^{\rm III}$ the amplitude of the transmitted wave. Here $k_n^L=[2m_L(E+n\omega-V_0^L)]^{1/2}$, with m_L the effective mass of electron in L region and V_0^L the flat potential level in L region. Using the continuity condition of the wave function and its derivative, we obtain the following equations:

$$\begin{aligned}
&\sum_j f(j-n)[A_j^{\rm II}\phi_j^a(0)+B_j^{\rm II}\phi_j^b(0)]=A^{\rm in}\delta_{n,0}+B_n^{\rm I}\,,\\
&\frac{1}{m_{\rm II}(0)}\sum_j f(j-n)[A_j^{\rm II}\phi_j'^a(0)+B_j^{\rm II}\phi_j'^b(0)]=\frac{1}{m_{\rm I}}ik_n^{\rm I}(A^{\rm in}\delta_{n,0}-B_n^{\rm I})\,,\\
&\sum_j f(j-n)[A_j^{\rm II}\phi_j^a(d)+B_j^{\rm II}\phi_j^b(d)]=A_n^{\rm III}\exp(ik_n^{\rm III}d)\,,\\
&\frac{1}{m_{\rm II}(d)}\sum_j f(j-n)[A_j^{\rm II}\phi_j'^a(d)+B_j^{\rm II}\phi_j'^b(d)]=\frac{1}{m_{\rm III}}ik_n^{\rm III}A_n^{\rm III}\exp(ik_n^{\rm III}d)\,,
\end{aligned} \tag{5}$$

with

$$f(j-n)=\sum_k\frac{(V/\omega)^k}{k!}\frac{(-V^\dagger/\omega)^{j-n+k}}{(j-n+k)!}$$

and $\phi_j'^a$ the derivative of ϕ_j^a. Equation (5) consists of a group of coupled equations through which components of the wave function in different energy channels couple with each other through phonon emission and absorption. We can solve Eq. (5) to determine $A_n^{\rm II}$ and $B_n^{\rm II}$, and then obtain $B_n^{\rm I}$ and $A_n^{\rm III}$. By use of a serial substitution method to solve these equations, i.e., step by step to obtain $\psi_E^{(0)}$, $\psi_{E\pm\omega}^{(1)}$, $\psi_E^{(2)}$, $\psi_{E\pm 2\omega}^{(2)}$, $\psi_{E\pm\omega}^{(3)}$, $\psi_E^{(4)},\ldots$, where the superscript index (n) corresponds to the term $\sim|V|^n$, the order of phonon operators in each term is determined. The transmitted current at energy $E+n\omega$ is $J_n^{\rm trans}=(k_n^{\rm III}/m_{\rm III})\langle A_n^{\rm III\dagger}A_n^{\rm III}\rangle$, and the reflected current at energy $E+n\omega$ is $J_n^{\rm ref}=(k_n^{\rm I}/m_{\rm I})\langle B_n^{\rm I\dagger}B_n^{\rm I}\rangle$, where $\langle\cdots\rangle$ means the average over the phonon assemble (below the bottom of the barrier k_n^L becomes imaginary, and $J_n^{\rm trans\,(ref)}$ is zero). Assuming phonons are in equilibrium at temperature T_L, we have $\langle V^\dagger V\rangle=\sum_{\bf q}|M({\bf q})|^2n_{\bf q}$ and $\langle VV^\dagger\rangle=\sum_{\bf q}|M({\bf q})|^2(1+n_{\bf q})$, with the phonon occupation number $n_{\bf q}=[\exp(\omega/k_BT_L)-1]^{-1}$. Also, we can calculate the average value for the assemble of a product of V's and $V^\dagger$'s. The transmission coefficient is given by $T_{\rm trans}=(\sum_n J_n^{\rm trans})/J^{\rm in}$, with $J^{\rm in}=(k_0^{\rm I}/m_{\rm I})|A^{\rm in}|^2$. Current conservation is ensured, namely, $J^{\rm in}=\sum_n(J_n^{\rm trans}+J_n^{\rm ref})$.

We emphasize that the above boundary conditions uniquely determine the solution of an electron tunneling wave function in the case with dissipation as well as in the case without dissipation. This key point was not properly considered in some previous works. In Ref. 8, for example, the wave function is described by $\psi = e^{i(s_0+s_1)}$, where s_0 is the action without phonons and s_1 is the correction due to the phonon effect. In the equation for s_1 the authors neglect the terms $\partial^2 s_1/\partial x^2$ (WKB) and $(\partial s_1/\partial x)^2$ $(\sim |V|^2)$, and reduce the equation for s_1 to a first-order differential equation to x. They then arbitrarily impose the left-hand boundary condition $s_1(x=0,t)=0$. This forces s_1 to be zero for $x<0$, so that one finds the incorrect result that there is no phonon correction to the reflected current. This correction is needed to obtain the proper physical results on the right-hand side. By use of the WKB method with the neglect of the $(\partial s_1/\partial x)^2$ term they have lost one of the two solutions, and hence cannot impose the correct boundary conditions at both sides.[12] Moreover, $(\partial s_1/\partial x)^2$ is of order $|V|^2$ and must be kept to retain this accuracy in the transmission, as discussed before.

It is obvious from our approach that a process with emission (or absorption) of n phonons must involve the electron eigenfunctions up to the $E \pm n\omega$ sidebands. Therefore, if a resonant state in a double-barrier structure appears at energy level $\bar{E}$ in the case of elastic tunneling, a phonon-assisted resonant tunneling can appear when electron injects at energy $\bar{E}+n\omega$, since the resonant eigenfunctions $\phi^a_{\bar{E}}(x)$ and $\phi^b_{\bar{E}}(x)$ are included in the expression of the wave function of electron injected at $\bar{E}+n\omega$ through electron-phonon coupling. We have calculated the transmission of electrons in a double-barrier structure. Since we are interested in the phonon effect inside the double-barrier region (as in Ref. 3), electron-phonon scattering is considered only inside the double-barrier region (although our approach allows the region II beyond the double-barrier region). The calculation is made with accuracy up to $|V|^2$ (one phonon process). By neglecting V and $V^\dagger$ into Eq. (4b), we can obtain the elastic solution $\psi^{(0)}_E$ at E channel. Substituting $\psi^{(0)}_E$ into Eqs. (4a) and (4c), and solving Eq. (5) at $E \pm \omega$ channels, we obtain the $J^{\text{trans (ref)}}_{\pm 1}$, which represents the phonon effect at inelastic channels. We then go back to Eq. (4b) to calculate $\psi^{(2)}_E$ $(\sim |V|^2)$, which represents the feedback effect of inelastic scattering on the elastic channel. Therefore, the transmitted current and the reflected current at each energy channel are obtained and our numerical results indicate that current conservation is exactly satisfied. In Fig. 1, we plot the total transmission coefficient of electron T_{trans} in a square double-barrier structure as a function of the energy E of the incident electron. The structure parameters are for a GaAs well sandwiched between two $Al_{0.3}Ga_{0.7}As$ barriers.[13] The optical-phonon energy ω is 36.2 meV. For comparison with Ref. 3, the electron-phonon coupling constant is taken as $g \equiv \sum_{\mathbf{q}} (|M(\mathbf{q})|/\omega)^2 = 0.1$. At zero temperature, only a phonon-assisted resonant peak appears at $\bar{E}+\omega$, since only emission of phonons is allowed. At $T_L = 300$ K peaks at both $\bar{E} \pm \omega$ appear. The amplitude of the resonant peak at incident energy $\bar{E}$ decreases when electron-phonon scattering is included. The effects of inelastic scattering alone at $T_L = 0$ K are displayed in curve C of Fig. 1, where peaks occur at incident energy $\bar{E}+\omega$ and $\bar{E}$. From Eq. (4c), it is clear that the inelastic peak can occur when either $\phi_0(x)$ or $\phi_{-1}(x)$ is an elastic resonant eigenfunction. In Fig. 2, we plot the transmission coefficient T_{trans} as a function of the potential drop of the applied electric field, V_a, in the same structure as that for Fig. 1, when incident electron is at energy $E_0 = 70$ meV. We see the phonon-assisted resonant peak appears at the potential drop $V_a = 108$ meV, at which an elastic resonance occurs at energy $E_0 - \omega$. The coupling constant $g = 0.03$ is more realistic for a GaAs-AlGaAs structure;[3] Fig. 2 shows that the peak position at $g = 0.03$ and 0.1 are the same, but the amplitude of the phonon-assisted resonant peak decreases with decrease of g.

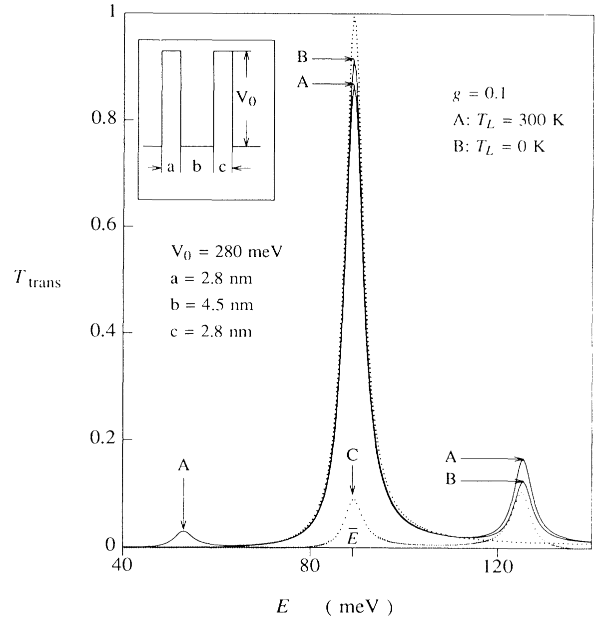

FIG. 1. The transmission coefficient, T_{trans}, as function of energy of incident electron E in a GaAs-AlGaAs double barrier including electron-optical-phonon scattering. We use the electron effective-mass parameters: $m_{\text{GaAs}} = 0.067m_0$, $m_{\text{AlGaAs}} = 0.092m_0$, with m_0 the free-electron mass. The mass of electron in the lead regions is assumed as m_{GaAs}. The energy of the phonon is $\omega = 36.2$ meV. The solid curves include the phonon effect. The dotted curve omits the phonon effect. Curve labeled A applies at room temperature, that labeled B applies at 0 K. Curve C (+) represents the contribution to T_{trans} of the transmitted current in the $E-\omega$ channel at $T_L = 0$ K.

In conclusion, based on an independent-boson model

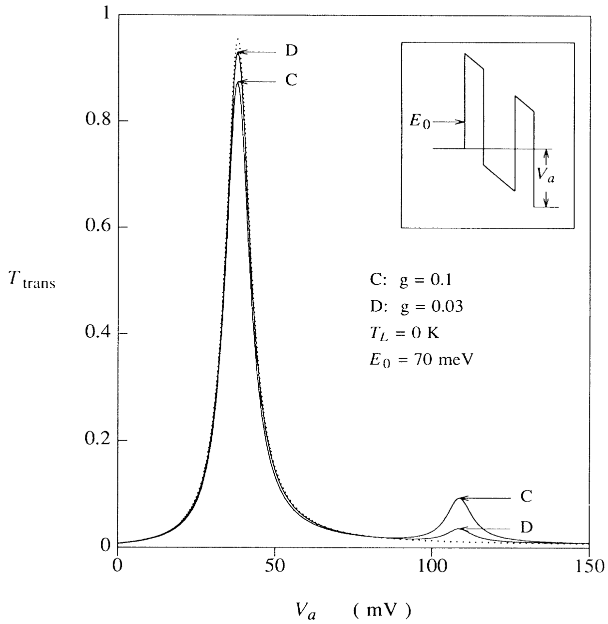

FIG. 2. The transmission coefficient of electron, T_{trans}, in a GaAs-AlGaAs double barrier as function of potential drop of an applied electric field, V_a, when the electron-phonon scattering is included. The incident electron is at the energy level $E_0 = 70$ meV. The double-barrier structure is the same as that of Fig. 1. The solid curves include the phonon effect. The dotted curve omits the phonon effect. Here curve C refers to calculations with coupling constant $g = 0.1$ and curve D refers to $g = 0.03$.

for electron-phonon interaction, we have proposed an approach for the study of phonon-assisted electron tunneling through an arbitrary barrier. The algebra in this approach is simple and straightforward. The correct boundary conditions and current conservation are ensured. Our results for double-barrier tunneling show the presence at the sidebands of phonon-assisted resonant tunneling, which has been shown in experiments.[2] Our model is good for phonons with long wavelength, but can only qualitatively describe the properties of a realistic device, where the three-dimensional electron-phonon interaction, statistics, and screening effect of electrons should be taken into account.

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