Resonant Tunneling with Electron-Phonon Interaction: An Exactly Solvable Model

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The probability for resonant tunneling through a quantum well is calculated for a model including electron-phonon coupling. The interaction of the tunneling electron with optic phonons produces resonant transmission sidebands, which are readily observable in *I-V* characteristics. Our results confirm the recent experimental observation of phonon-assisted resonant tunneling in GaAs.

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The high speeds and novel electronic properties of double-barrier resonant-tunneling structures make them promising candidates for a new generation of electronic devices. Since the seminal work of Tsu and Esaki[1] and the first experimental realization of significant negative differential conductance by Sollner *et al.*,[2] there has been steady progress in both speed[3] and device quality,[4,5] as measured by the peak-to-valley ratio of the current. Qualitatively, the fundamental characteristics of resonant tunneling are well understood (cf. Ricco and Azbel[6]), but quantitative prediction of a complete current-voltage characteristic has remained elusive.

In this Letter, we address one of the most important processes complicating analysis of the tunneling current, namely, electron-phonon scattering. In any real material, an electron tunneling through a double-barrier structure (see Fig. 1) will interact with phonons. The resulting changes in the transmission probability will be manifested in the current—notably, Goldman, Tsui, and Cunningham[7] have recently found evidence for optic-phonon–assisted resonant tunneling in the valley current of a double-barrier resonant-tunneling structure.

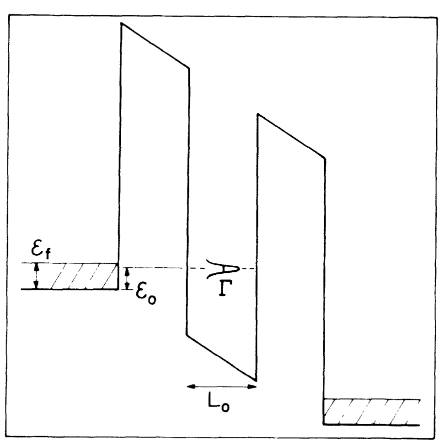

FIG. 1. Schematic band-edge diagram for a semiconductor double-barrier resonant-tunneling structure. The center of the resonant level is an energy ϵ_0 above the band edge in the injecting lead, and the full width of the resonant level is given by Γ. The width of the quantum well is L_0.

In what follows, we present the first solution of a resonant-tunneling model including electron-phonon scattering. We have calculated the probability per unit final energy $T(\epsilon',\epsilon)$ that an electron of energy ϵ, incident from one ideal lead onto a resonant level, where it interacts with phonons, will be transmitted with energy ϵ' into a second ideal lead. Since the dominant electron-phonon interaction in most semiconductor heterostructures involves the polar-optic mode, we explicitly evaluate $T(\epsilon',\epsilon)$ for an Einstein band of optic phonons using a typical polar-optic-phonon coupling strength. The resulting total transmission probability, $T_{\text{tot}}(\epsilon) = \int d\epsilon' T(\epsilon',\epsilon)$, has sidebands spaced at the optic-phonon energy representing phonon-assisted transmission. We compare the current characteristics predicted by our model with those measured for a GaAs/AlGaAs double-barrier resonant-tunneling structure and confirm the experiment observation[7] of phonon-assisted resonant tunneling. From our general expression for the total transmission probability we also obtain a simple analytical expression for the phonon broadening of $T_{\text{tot}}(\epsilon)$ and identify two sum rules satisfied by $T_{\text{tot}}(\epsilon)$ for all temperatures, phonon spectra, and electron-phonon coupling strengths.

The Hamiltonian that we use to model resonant tunneling is the sum of an electron term H_e, a phonon term H_{ph}, and an electron-phonon interaction term H_{int}. The electron Hamiltonian describes a single state of energy ϵ_0 (e.g., the ground state of a quantum well) coupled by hopping matrix elements V_{kL} and V_{kR} to states of energy ϵ_{kL} and ϵ_{kR} in ideal leads on its left and right, respectively. The transmission matrix, $T^0(\epsilon',\epsilon)$, for a noninteracting electron is given by

$$T^0(\epsilon',\epsilon) = \frac{\Gamma_R(\epsilon')\Gamma_L(\epsilon)\delta(\epsilon-\epsilon')}{[\epsilon-\epsilon_0-\Sigma(\epsilon)]^2+[\Gamma(\epsilon)/2]^2},$$

where the resonance width, $\Gamma(\epsilon)=\Gamma_L(\epsilon)+\Gamma_R(\epsilon)$, is determined by the strength of the hopping matrix elements,

$$\Gamma_{L,R}(\epsilon) = 2\pi\sum_k |V_{kL,R}|^2\delta(\epsilon-\epsilon_{kL,R}).$$

The real part of the self-energy, $\Sigma(\epsilon)$, is the Hilbert transform of the resonance width $\Gamma(\epsilon)$. The phonon Hamiltonian is just a sum of harmonic oscillators $H_{\rm ph}=\sum_{\bf q}\hbar\omega_{\bf q}a_{\bf q}^\dagger a_{\bf q}$, and the electron-phonon interaction is restricted to the resonant site,

$$H_{\rm int}=c^\dagger c\sum_{\bf q}M_{\bf q}(a_{\bf q}^\dagger+a_{-{\bf q}}),$$

where $c^\dagger$ and c are the fermion operators for the electron on the resonant site.

We will calculate the probability that an electron with energy ϵ incident from the left lead will be transmitted to the right lead with energy ϵ', the "remainder" of the energy being left in the phonon system. Because the electron-phonon interaction is confined to a finite region of space we can apply the S-matrix scattering formalism[8] to evaluate the transmission matrix $T(\epsilon',\epsilon)$. We find that $T(\epsilon',\epsilon)$ is equal to the product of the elastic coupling widths to the two leads and the Fourier transform of a Green's function for the resonant level,[9]

$$T(\epsilon',\epsilon)=\Gamma_L(\epsilon)\Gamma_R(\epsilon')\int\int\int\frac{d\tau\,dt\,ds}{2\pi\hbar^3}e^{i[(\epsilon-\epsilon')\tau+\epsilon' t-\epsilon s]/\hbar}G(\tau,s,t). \tag{1}$$

The three-time Green's function

$$G(\tau,s,t)=\theta(t)\theta(s)\langle c(\tau-s)c^\dagger(\tau)c(t)c^\dagger(0)\rangle \tag{2}$$

is evaluated in an electron vacuum with thermal phonons. The expression for the transmission matrix, Eq. (1), is formally exact and, in the absence of electron-phonon interaction, reproduces the elastic resonant-tunneling result given above.

The problem of evaluating the Green's function of a single site coupled to phonons is well known in the context of core-level x-ray emission.[10-13] The techniques developed to treat the interaction of a stationary core hole with phonons can be adapted directly to evaluate the three-time Green's function that appears in the transport problem. Within the approximation of energy-independent couplings Γ_L and Γ_R, we evaluate $G(\tau,s,t)$ in the same manner as the Green's functions in the core-hole problem. The restriction of energy-independent coupling to the leads corresponds to the condition that the Green's function of the resonant level with no electron-phonon interaction be a simple exponential,[11] $G_R^0(t)=-i\theta(t)\exp[(-i\epsilon_0-\Gamma/2)t]$, where $\Gamma=\Gamma_L+\Gamma_R$. We evaluate $G(\tau,s,t)$, both via a canonical transformation[12] and using a path-integral formulation,[14] and find

$$G(\tau,s,t)=G_R^0(t)[G_R^0(s)]^*\exp\left(i\frac{(t-s)\lambda}{\hbar}-\sum_{\bf q}\left|\frac{M_{\bf q}}{\hbar\omega_{\bf q}}\right|^2[(1+2N_\omega)\,{\rm Re}\{f\}+i\,{\rm Im}\{f\}]\right), \tag{3}$$

$$f=2-e^{-i\omega t}-e^{i\omega s}+e^{-i\omega\tau}(e^{i\omega t}-1)(e^{i\omega s}-1), \tag{4}$$

where $\lambda=\sum_{\bf q}(M_{\bf q}^2/\hbar\omega_{\bf q})$ and N_ω is the Bose-Einstein occupation factor for a phonon mode of energy $\hbar\omega$.

Although direct evaluation of the transmission matrix $T(\epsilon',\epsilon)$ for the general phonon spectrum will require numerical Fourier transforms, certain sum rules and simple analytic results can be derived from the above expressions, for energy-independent Γ_L and Γ_R. First, integrating the total transmission probability over incident energies, we find $\int d\epsilon\,T_{\rm tot}(\epsilon)=2\pi\Gamma_L\Gamma_R/\Gamma$ independent of the electron-phonon interaction. Second, the center of the transmission resonance given by the first moment of $T_{\rm tot}(\epsilon)$ normalized by $\int d\epsilon\,T_{\rm tot}(\epsilon)$ is also unchanged by the electron-phonon interaction.[15] Last, we find that the change in width of the transmission resonance $\delta\langle\epsilon^2\rangle$, given by the difference between the normalized second moment of $T_{\rm tot}(\epsilon)$ and the normalized second moment with no electron-phonon coupling, is always positive and is given by

$$\delta\langle\epsilon^2\rangle=\sum_{\bf q}|M_{\bf q}|^2(1+2N_{\bf q}). \tag{5}$$

Although the second moment of $T_{\rm tot}(\epsilon)$ itself cannot be defined because the line shape dies as $1/\epsilon^2$ in the tails, a useful estimate of the phonon-induced broadening can still be obtained from (5) if the important contributions to $\delta\langle\epsilon^2\rangle$ are from the region near the resonance. This condition is satisfied in the case of optic phonons (discussed below) where $\delta\langle\epsilon^2\rangle$ approaches its asymptotic value within a few phonon energies of the resonance center.

Because of the strong polarization interaction in III-V and II-VI semiconductors, the largest electron-phonon matrix elements are those involving longitudinal optic phonons. To determine the effect of optic-phonon interaction on resonant tunneling, we have evaluated the transmission matrix $T(\epsilon',\epsilon)$ at zero temperature for an Einstein band of phonons with energy $\hbar\omega_0$,

$$T(\epsilon',\epsilon)=\Gamma_L\Gamma_R e^{-2g}\sum_{m=0}^{\infty}\frac{g^m}{m!}\delta(\epsilon-\epsilon'-m\hbar\omega_0)\left|\sum_{j=0}^{m}(-1)^j\binom{m}{j}\sum_{l=0}^{\infty}\frac{g^l}{l!}\left(\frac{1}{[\epsilon-(\epsilon_0-\lambda)-\hbar\omega_0(j+l)]+i\Gamma/2}\right)\right|^2, \tag{6}$$

where the coupling constant $g=\sum_{\mathbf{q}}(|M_{\mathbf{q}}|/\hbar\omega_0)^2$. For a quantum well of width L_0 we estimate g by

$$g=\frac{e^2}{L_0\hbar\omega_0}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]. \qquad (7)$$

In Fig. 2, we have plotted $T_{\rm tot}(\epsilon)$ for the Einstein model with no electron-phonon coupling and with a coupling constant[16] $g=0.1$, which is appropriate for a state of width $L_0=100$ Å in CdTe. The sum rules imply that the integrals under both curves are equal and that their centers are at the same energy. At zero temperature no optic phonons are present, and the phonon-assisted resonances appear only at energies above the elastic resonance. The center of the transmission curve remains fixed, however, because there is an overall shift down in energy by $\lambda=g\hbar\omega_0$ associated with the deformation of the lattice about the tunneling electron.

To make comparison with the experiment[7] on a GaAs/AlGaAs structure, it is necessary to calculate the current from $T(\epsilon',\epsilon)$. The current from the left[17] in a given transverse momentum channel is the sum over incoming momenta of the product of the incoming velocity, the Fermi function of incoming states ϵ, and the probability of transmission $T(\epsilon',\epsilon)$ integrated over final energies ϵ'. Provided that $T(\epsilon',\epsilon)$ does not depend strongly on transverse momentum, the transverse integral for low temperatures gives a factor $m^*(\epsilon_F-\epsilon)/\hbar^2$, the momentum sum combines with the factor of velocity into an integral over incident energies, and the definition of $T_{\rm tot}(\epsilon)$ can be employed to write

$$J=\frac{Aem^*}{2\pi^2\hbar^3}\int_0^{\epsilon_F}d\epsilon(\epsilon_F-\epsilon)T_{\rm tot}(\epsilon), \qquad (8)$$

where A is the cross-sectional area and m^* is the effective mass. Under the assumption that the elastic couplings Γ_L and Γ_R can be taken as constant, the current depends on the total bias across the device only through the position of the resonant level. Accordingly, in Fig. 3 we have plotted the current J versus the position of the resonant level. The elastic width used in Fig. 3 is chosen to be $\Gamma=0.2\hbar\omega_0$ and the electron-phonon coupling is estimated to be $g=0.03$. The shoulder in the current is a replica of the main current peak produced by phonon-assisted resonant tunneling. To obtain the current-voltage characteristic from Fig. 3 one must relate the resonant-level energy to the total applied bias[18];

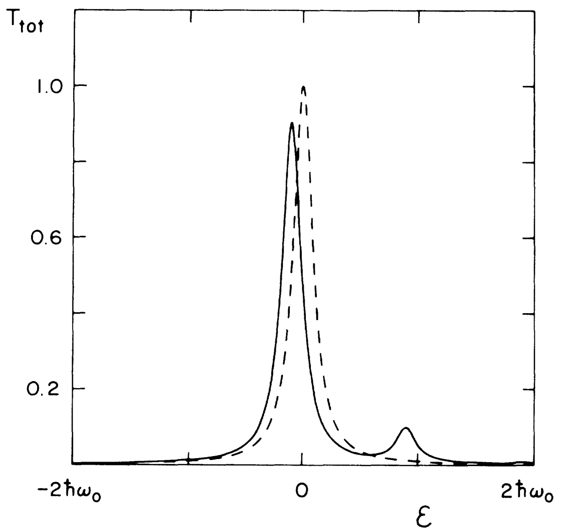

FIG. 2. Total transmission probability $T_{\rm tot}(\epsilon)$ vs incoming energy for an electron incident on a double-barrier resonant-tunneling structure with an elastic width $\Gamma=0.2\hbar\omega_0$ at $T=0$ K. The dashed curve is calculated in the absence of electron-phonon coupling, while the solid curve is for a coupling $g=0.1$ to optic phonons in CdTe (see text). If the couplings to the contacts, Γ_L and Γ_R, are not equal, as is typically the case under bias, then the transmission probability is reduced by a factor $4\Gamma_L\Gamma_R/\Gamma^2$. The effect of phonon coupling is to shift the elastic resonance down in energy by $\lambda=g\hbar\omega_0$ and to produce inelastic transmission sidebands. At $T=0$ K, only the phonon emission sidebands appear because there are no thermal phonons to absorb. Both the integrated total transmission probability and the center of the resonance in energy are independent of the electron-phonon interaction.

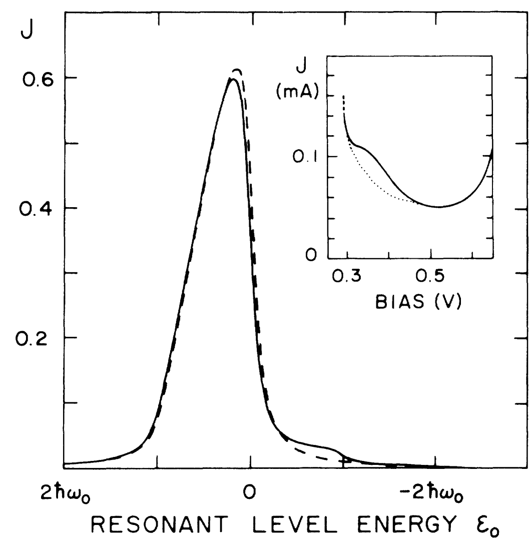

FIG. 3. Current vs resonant-level energy for the resonant-tunneling structure shown in Fig. 1, calculated from Eq. (8). The dashed curve is for no electron-phonon coupling while the solid curve is for a coupling $g=0.03$. The Fermi energy is taken to be $\hbar\omega_0$ and the current is in units of $Aem^*\Gamma_L\Gamma_R\epsilon_F/2\pi^2\hbar^3\Gamma$. The shoulder in the current when $g=0.03$ is due to transmission through the first inelastic transmission sideband. For comparison, the inset is an experimental I-V characteristic for a GaAs/AlGaAs resonant-tunneling structure (Ref. 7). The similarity between the experimental and theoretical curves for the realistic value of the electron-phonon coupling $g=0.03$ confirms the presence of phonon-assisted resonant tunneling in the experimental structure.

since this relation is expected to be linear in the valley region of the current, the phonon-induced shoulder in Fig. 3 will be roughly unchanged in the *I-V* characteristic. For a stronger polar-optic coupling as in CdTe or other II-VI compounds, the phonon replica in the current-voltage characteristic should be more pronounced.

In conclusion, we have found an expression for the probability of resonant tunneling in a model including electron-phonon interactions. The inelastic character of phonon scattering broadens the transmission resonance but does not change the integrated transmission through the barrier nor does it shift the average energy of the resonance. In the important case of optic phonons, we have explicitly derived the phonon-mediated transmission probability. Finally, by calculating the current characteristic for a double-barrier resonant-tunneling structure including a realistic optic-phonon coupling we have provided a theoretical confirmation of the experimentally observed magnitude[7] of phonon-assisted resonant tunneling.

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$$R(\epsilon',\epsilon)=\Gamma_L(\epsilon')T(\epsilon',\epsilon)/\Gamma_R(\epsilon'),$$

which is valid except at $\epsilon=\epsilon'$.

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