Differential conductance in three-dimensional resonant tunneling

V. Kalmeyer and R. B. Laughlin
Physics Department, Stanford University, Stanford, California 94305
(Received 6 October 1986)

We report the results of precision numerical calculations of three-dimensional resonant tunneling. Simple fitting formulas are given which parametrize the dependence of the peak differential conductance G_{res} and the resonance broadening Γ on the tunnel barrier parameters. The maximum value attained by G_{res} is universally equal to e^2/h.

Resonant tunneling is an important mechanism of conduction in materials containing localized states. It is responsible for the sharp structure in the differential conductance of metal-insulator-metal junctions,[1] quantum wells,[2] and metal-oxide-semiconductor field-effect transistors (MOSFET's) (Ref. 3) at low temperatures. In these experiments, one tunes the Fermi level of the metallic electrodes by changing the dc bias across the junction and measures the conductance. When the Fermi energy of electrons in the metal matches the energy of an intermediate quantum state localized inside the barrier, tunneling probability increases sharply, producing a peak in the differential conductance $G=dI/dV$ as a function of dc bias. For localized states close to the center of the barrier, the peak value of resonant conductance can exceed the nonresonant contribution due to direct quantum tunneling by many orders of magnitude.

The problem of resonant tunneling via three-dimensional localized states is only partially solved. Accurate calculations of the differential conductance have not been performed up to now, in part because of the complicated structure of eigenstates of the resonant tunnel barrier in three dimensions. The best existing results are those of Knauer, Richter, and Seidel[4] who obtained variational expressions for the resonance width Γ and the tunneling current density for a given incident electron momentum, which were used by Halbritter[5,6] to estimate the resonant conductance. Accurate results exist for one-dimensional models,[7–9] but their applicability to three dimensions is not clear.

We have performed a precision calculation of the resonant differential conductance G and the resonance width Γ in three dimensions (3D). The results are described very well by simple fitting formulas which yield G and Γ directly as functions of tunnel barrier parameters. In particular, we find that the maximum value of the differential conductance on resonance is the same for all tunnel barriers and, for spinless electrons, is equal to e^2/h.

The calculation was carried out for noninteracting electrons at $T=0$, tunneling through a model potential shown in Fig. 1. The barrier has height V_0 and is bounded by two planar interfaces at $z=z_0$ and $z=z_0-d$. The localized state is represented by a bound state of an attractive 3D square well of depth V_1 and radius R, centered at the origin. R and V_1 are chosen to yield the necessary bound-state energy E_0. If the localizing potential is narrow on the scale of its bound-state wave function, the only relevant physical parameter is the binding energy $E_b=E_0-V_0$.

To obtain the differential conductance, we invert the Hamiltonian

$$H=p^2/2m+V(\mathbf{r}) \tag{1}$$

in the manner

$$\mathcal{G}(E)=(E-H+i\eta)^{-1}\,, \tag{2}$$

where $\eta\to 0+$, to form the single-electron Green's function. The matrix element of the Green's function between coordinate basis states satisfies

$$\{E-[-(\hbar^2/2m)\nabla^2+V(\mathbf{r})]+i\eta\}\langle\mathbf{r}\,|\,\mathcal{G}(E)\,|\,\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')\,. \tag{3}$$

For points $\mathbf{r}$ and $\mathbf{r}'$ in (3) on opposite sides of the barrier, i.e., for $z<z_0-d$ and $z'>z_0$, $\langle\mathbf{r}\,|\,\mathcal{G}(E)\,|\,\mathbf{r}'\rangle$ describes an electron at energy E tunneling across the barrier from $\mathbf{r}$ to $\mathbf{r}'$. In terms of the Fourier transform of $\langle\mathbf{r}\,|\,\mathcal{G}(E)\,|\,\mathbf{r}'\rangle$ in

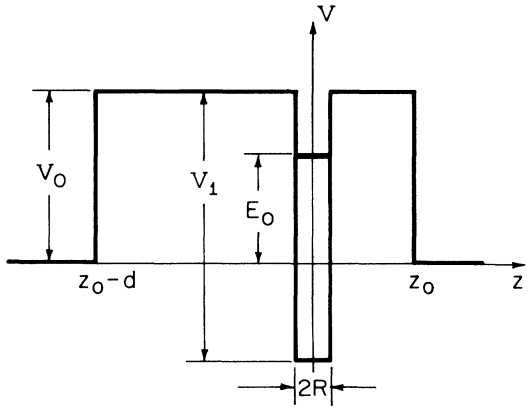

FIG. 1. Potential energy diagram of the resonant tunnel barrier. The origin of coordinates is at the center of the 3D spherical well of radius R.

the xy plane

$$\langle \mathbf{k}_{||},z \mid \mathcal{G}(E) \mid \mathbf{k}'_{||},z' \rangle = \int\int\int\int dx\,dy\,dx'dy' e^{-i(\mathbf{k}_{||}\cdot\mathbf{r}+\mathbf{k}'_{||}\cdot\mathbf{r}')} \times \langle \mathbf{r} \mid \mathcal{G}(E) \mid \mathbf{r}' \rangle , \quad (4)$$

where $\mathbf{k}_{||}=(k_x,k_y,0)$ and $\mathbf{k}'_{||}=(k'_x,k'_y,0)$ are the components of the incident and transmitted electron momenta parallel to the barrier interface, the differential conductance is given by

$$G(E)=(2\pi)^{-5}\int\int d\mathbf{k}_{||}d\mathbf{k}'_{||}k_{\perp}k'_{\perp} \times |\langle \mathbf{k}_{||},z \mid \mathcal{G}(E) \mid \mathbf{k}'_{||},z' \rangle|^2 , \quad (5)$$

where $k_{\perp}=[E-(2m/\hbar^2)k_{||}^2]^{1/2}$ and $k'_{\perp}=[E-(2m/\hbar^2)k'^2_{||}]^{1/2}$. G does not depend on z or z' as long as $\mathbf{r}$ and $\mathbf{r}'$ in (3) are on the opposite sides of the barrier.

The differential conductance given by (5) is defined by aligning the chemical potentials on both sides of the tunnel junction at a common level μ, and then raising the potential of one electrode by a small amount $d\mu$. Then $G=dI/d\mu$, where dI is the current carried by electronic states in the energy range $(\mu,\mu+d\mu)$. Such a definition is relevant to experimental situations where electron densities in the two electrodes are nearly equal and the Fermi level shift across the junction is small compared to the resonance width, as is the case in some recent experiments on short MOSFET's.[3]

The resonant part of the required Green's function $\langle \mathbf{k}_{||},z \mid \mathcal{G}(E) \mid \mathbf{k}'_{||},z' \rangle$ was computed numerically using the following algorithm. We define the bare Green's function $\mathcal{G}_0(E)$ by an equation similar to (2) with H replaced by H_0, the Hamiltonian for a barrier without the attractive spherical well. The bare Green's-function matrix elements $\langle \mathbf{r} \mid \mathcal{G}_0(E) \mid \mathbf{r}' \rangle$ are easily computed[4] because translational symmetry in the xy plane renders the problem one-dimensional. We then calculate from this the full Green's function at the trapping site using the Koster-Slater method.[10] We make the size of the well sufficiently small compared with the spread of its bound-state wave function, $(\langle r^2 \rangle)^{1/2}$, that the zero-angular-momentum (s-wave) channel dominates the scattering of electrons by the trapping potential well. Having chosen R to be small, one need calculate only the bare on-site Green's-function matrix element

$$\mathcal{G}_0^{\text{on site}}(E)=(4\pi)^{-1}\int_{r=r'=R}\int d\Omega\,d\Omega' \langle \mathbf{r} \mid \mathcal{G}_0(E) \mid \mathbf{r}' \rangle , \quad (6)$$

which propagates an electron in the state with zero angular momentum on the surface $r=R$ to the same state. The exact on-site Green's-function matrix element in the presence of the well is then given by

$$\mathcal{G}^{\text{on site}}(E)=\left[\mathcal{G}_0^{\text{on site}}(E)^{-1} - \frac{\hbar^2 R}{2m}[x\cot(x)-x_0\coth(x_0)]\right]^{-1} , \quad (7)$$

where $x_0=R[2m(V_0-E)/\hbar^2]^{1/2}$, $x=R[2m(E-V_0+V_1)/\hbar^2]^{1/2}$, for $0<E<V_0$. The tunneling Green's function in coordinate space is

$$\langle \mathbf{r} \mid \mathcal{G}(E) \mid \mathbf{r}' \rangle = \frac{R^2\hbar^4}{16\pi m^2}\int_{r_1=r_2=R}\int d\Omega_1 d\Omega_2 \langle \mathbf{r} \mid \mathcal{G}_0(E) \mid \mathbf{r}_1 \rangle \langle \mathbf{r}_2 \mid \mathcal{G}_0(E) \mid \mathbf{r}' \rangle \times [x_0\coth(x_0)-x\cot(x)]\mathcal{G}^{\text{on site}}(E)[x_0\coth(x_0)-1-\varphi_0] , \quad (8)$$

where x_0 and x are defined above and

$$\varphi_0=[\mathcal{G}_0^{\text{on site}}(E)]^{-1} \times \left[(a/4\pi)\frac{\partial}{\partial a}\int_{r=r'=a}\int d\Omega\,d\Omega' \langle \mathbf{r} \mid \mathcal{G}_0(E) \mid \mathbf{r}' \rangle\right]_{a=R} . \quad (9)$$

The Fourier transform of (8) with respect to (x,y) and (x',y') is the resonant part of the tunneling Green's function which appears in (5). The momentum integrals in (5) are then evaluated numerically. This procedure is arbitrarily accurate in the limit $R\to 0$, and the conductance converges to a well-defined value in this limit.

The differential conductance (5) exhibits a Lorentzian resonance peak centered at $E_r \simeq E_0$:

$$G(E)=G_{\text{res}}\Gamma^2/[(E-E_r)^2+\Gamma^2] . \quad (10)$$

In Fig. 2 we have plotted the differential conductance on resonance G_{res} versus the reduced distance from the center of the wall to an interface, z_0/d. Note that the quantity G_{res} has been computed by two completely different methods: one based on Eqs. (5)—(9) (solid curves), the other numerically integrating the variational solution of Ref. 4 (dashed curves). We observe that G_{res} grows roughly exponentially as the well gets farther away from an interface. The increase in G_{res} is faster for more deeply bound states and for wider barriers. As the well approaches the midplane of the barrier ($z_0=d/2$), the conductance flattens out and reaches a maximum value of $\simeq 0.998$ in units of e^2/h. Qualitative arguments by Ricco, Azbel, and Brodsky[11] predict a maximum value of $(h/e^2)G_{\text{res}}$ of order unity. Our calculations suggest strongly that this maximum value is equal to 1 *exactly and universally* for all tunnel barriers.

As a check on the accuracy of our calculations, we have

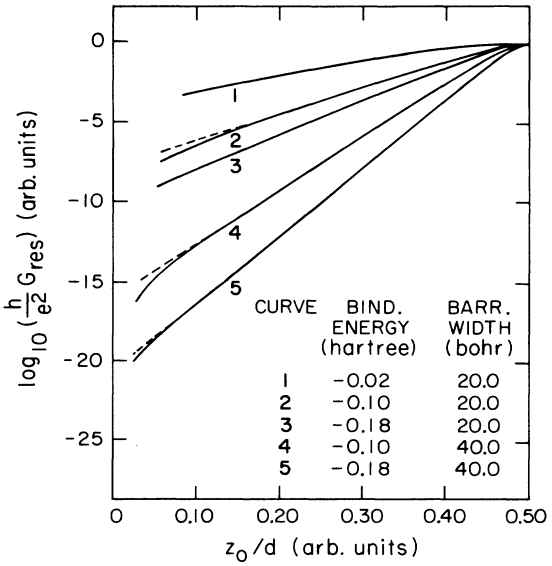

FIG. 2. Peak differential conductance at resonance, G_{res}, as a function of reduced distance of the well from an interface, z_0/d, for several binding energies and barrier widths. Energies are in hartrees, 1 hartree=27.2 eV; lengths are in bohrs, 1 bohr=0.529 Å. Barrier height is $V_0=0.2$ and binding energies are measured from the top of the barrier. Solid lines, numerical results (this work); dashed lines, variational results (Ref. 4); fit to G_{res} by Eqs. (12), (15), and (16) is within line thickness from numerical curves.

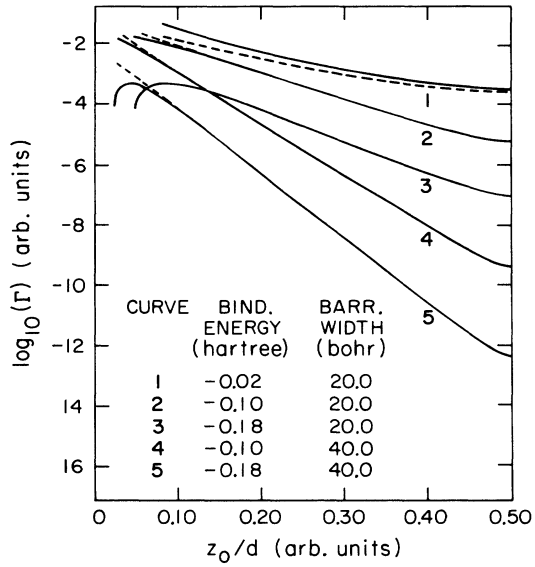

FIG. 3. Resonance width Γ as a function of reduced location of the well, z_0/d. Parameters used are the same as in Fig. 2.

plotted in Fig. 3 the resonance width Γ, defined by (10), versus the same reduced distance z_0/d as in Fig. 2. Γ is proportional to the rate for an electron trapped in the well to tunnel out of the barrier. Therefore, we expect Γ to reach a minimum at $z_0=d/2$, i.e., when the trap is maximally distant from either interface. The close agreement of the numerical (solid curves) and variational (dashed curves) results over a broad range of barrier parameters[12] justifies our neglecting the $l>0$ contributions to G_{res} and Γ and demonstrates the accuracy of the numerical algorithm.

This behavior of resonant conductance can be understood in the following way. Consider a set of energy levels E_j connected to an intermediate level E_0 by tunneling matrix elements T_j, but not connected to each other. The states with $j<0$ form the continuum on the left-hand side of the barrier; those with $j>0$ form the one on the right-hand side. The on-site Green's-function matrix element is

$$\mathcal{G}_{00}(E)=\left[E-E_0-\sum_{j\,(\neq 0)}|T_j|^2/(E-E_j+i\eta)\right]^{-1}. \quad (11)$$

The real part of the sum in (11) shifts the resonant energy E_0 slightly to its renormalized value E_r while the imaginary part gives the resonance width

$$\Gamma=\Gamma^L+\Gamma^R, \quad (12)$$

where

$$\Gamma^{L,R}=-\mathrm{Im}\left[\sum_{L,R}|T_j|^2/(E_r-E_j+i\eta)\right]. \quad (13)$$

The sum in (13) is over $j<0$ for Γ^L and over $j>0$ for Γ^R. The tunneling rate from level E_j on the left to level E_k on the right is governed by the transition matrix element

$$\mathcal{T}_{jk}=T_jT_k/(E_j-E_r+i\Gamma). \quad (14)$$

The differential conductance on resonance is given in terms of $\mathcal{T}$ by

$$G_{res}=(4e^2/h)\sum_{j\,(<0)}\sum_{k\,(>0)}\mathrm{Im}\left[\frac{1}{E_r-E_j+i\eta}\right]|\mathcal{T}_{jk}|^2\mathrm{Im}\left[\frac{1}{E_r-E_k+i\eta}\right]$$
$$=(4e^2/h)\Gamma^L\Gamma^R(\Gamma^L+\Gamma^R)^{-2}, \quad (15)$$

for spinless electrons. When the resonant state is in the midplane of the barrier, $\Gamma^L=\Gamma^R$, and G_{res} reaches its universal maximum value of e^2/h. This argument does not depend on the shape of the trapping potential which creates the intermediate state or on the details of the tunneling process. The only critical assumption is the existence of two sets of electronic states on either side of the tunnel barrier and a localized state in the middle. Therefore, even in three dimensions, the resonant behavior of the tunneling current can be understood in terms of a nar-

row quasi-one-dimensional channel of conduction.

The quantitative differences between one- and three-dimensional resonant tunneling systems arise from different dependences of the widths $\Gamma^{L,R}$ on the tunnel-barrier parameters. Using a stripped-down version of the variational expression[4] for Γ, we identify $\Gamma^{L,R}$ in 3D as follows:

$$\Gamma^{L,R} \simeq \frac{k\kappa^2}{V_0 z_{L,R}} f\left[\frac{k^2}{\kappa} z_{L,R}\right] e^{-\kappa z_{L,R}} . \tag{16}$$

Here $z_R = z_0$, $z_L = d - z_0$, $k = (2E_r)^{1/2}$, $\kappa = [2(V_0 - E_r)]^{1/2}$, $f(x) = 1 - \exp(-3x/2)$, and we have set $\hbar = m_e = 1$. The difference between the solid (dashed) lines in Fig. 2 (3) and the fits to Γ and $G_{\rm res}$ defined by Eqs. (12), (15), and (16) is less than the line thickness. The quality of the fit is limited only by extreme broadening of the resonance and deviations of its shape from Lorentzian at very small z_0 and E_b, and is better than 6% for $d > 40$, $0.1d < z_0 < 0.9d$. In fact, Figs. 2 and 3 show that, for most values of tunnel-barrier parameters, $G_{\rm res}$ and Γ as given by (12), (15), and (16), are indistinguishable from their "exact" values.

Any real tunnel barrier will probably contain many localized states, so even at zero temperature tunneling via several intermediate states is not excluded. However, if the density of localized states is low compared with $1/\Gamma d^3$, where d is the barrier width, then interference between tunneling channels involving different intermediate states can be ignored. The result is a simple (incoherent) superposition of conductance peaks, one for each resonant energy.

Our results put a fundamental upper limit on the single-channel resonant tunneling conductance, which, for real electrons with spin, is $2e^2/h$. This limit should be observable as the maximum height of conductance peaks in MOSFET's and narrow metal-insulator-metal junctions provided the temperature is below the crossover from the Mott hopping conductivity to resonant tunneling.[9] Temperatures reached in the recent experiments on short MOSFET's (Ref. 3) are already within the resonant tunneling regime, as indicated by the temperature-independent behavior of conductance. So far, the maximum peak conductance reported[3] is $0.1e^2/h$. This is consistent with our upper bound, the rather small value being related to the exponential dependence of $G_{\rm res}$ on the position of the localized state which, in most cases, is off the center of the barrier.

This work was supported by the National Science Foundation—Materials Research Laboratory program through the Center for Materials Research at Stanford University and by the National Science Foundation under Grant No. DMR-8510062. We thank M. R. Beasley for helpful discussions of his experimental results.

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