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Disorder-Assisted Tunneling through a Double-Barrier Structure

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We consider the effect of disorder on coherent tunneling of electrons through a double-barrier structure. When the disorder potential is treated in leading order we obtain a result with transparent physical consequences. The effect of interface roughness on resonant tunneling is shown to depend qualitatively on the location of the rough interface. Our results may help to explain the often observed asymmetry in the current-voltage characteristics of double-barrier structures.

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The unusual electronic properties of double-barrier resonant-tunneling structures[1] have lead to many proposals for novel devices.[2] While the fundamental characteristics of such systems are well understood,[3] a quantitative understanding of the behavior of a particular device is rarely possible. For example, measured peak-to-valley ratios for the region of negative differential resistance (NDR) are consistently much smaller than those calculated theoretically. It is widely recognized, especially for the case where the barriers are wide resulting in narrow resonances, that the scattering of the tunneling electrons will have to be included in the theoretical description in order to describe experimental results. Recently, studies of the effects of electron-phonon[4-7] and electron-electron[4,8] interactions on resonant-tunneling characteristics have been undertaken.

In this Letter we present a study of the effect of elastic scattering on electrons which are tunneling through a double-barrier structure. This type of scattering process differs from the inelastic ones cited above in that the electron's energy is conserved. The electron, however, is able to exchange its kinetic energy perpendicular to the barrier with its kinetic energy parallel to the barrier and therefore uses tunneling channels that are more conducting. Furthermore, although it suffers a scattering event, the electron's phase coherence is maintained, allowing it to tunnel coherently across the whole structure. To describe elastic scattering, we use a scattering theory formulation in which the double-barrier structure is treated exactly and the disorder potential is treated perturbatively. The formalism is combined with a simple model of interface-roughness scattering which is generally believed to be the dominant source of elastic scattering. When the scattering by the disorder is treated in leading order, a simple result with a clear physical interpretation is obtained.

We start with the Lippman-Schwinger equation:[9]

$$\Psi^+(\mathbf{r}) = \Psi_B^+(\mathbf{r}) + \int d^3\mathbf{r}' G^+(\mathbf{r},\mathbf{r}';E) V_D(\mathbf{r}') \Psi_B^+(\mathbf{r}') , \quad (1)$$

where $\Psi_B^+(\mathbf{r})$ is the wave function for an electron scattered by the barrier alone, $V_D(\mathbf{r})$ is the disorder potential, and $G^+(\mathbf{r},\mathbf{r}';E)$ is the exact advanced Green's function. The barrier potential is dependent on z only, where z is the direction perpendicular to the barrier, and will be taken to be nonzero only for the region $0 \leq z \leq w$, i.e., the barrier region.

So that $G^+(\mathbf{r},\mathbf{r}';E)$ can be found perturbatively, we use Dyson's equation

$$G^+(\mathbf{r},\mathbf{r}';E) = G_B^+(\mathbf{r},\mathbf{r}';E) + \int d^3\mathbf{r}'' G_B^+(\mathbf{r},\mathbf{r}'';E) \times V_D(\mathbf{r}'') G^+(\mathbf{r}'',\mathbf{r}';E) . \quad (2)$$

Here $G_B^+(\mathbf{r},\mathbf{r}';E)$ is the advanced Green's function for the double-barrier structure in the absence of any disorder. Our perturbative treatment of the disorder potential takes advantage of the translational invariance which exists in the planes perpendicular to the double-barrier structure (x-y planes) in the absence of disorder. Expressing the Green's function $G_B^+(\mathbf{r},\mathbf{r}';E)$ in terms of exact eigenstates of the disorder-free problem, it follows that

$$G_B^+(\mathbf{r},\mathbf{r}';E)=\int \frac{d^2\mathbf{k}_\perp}{(2\pi)^2}\exp[i\mathbf{k}_\perp\cdot(\mathbf{r}_\perp-\mathbf{r}'_\perp)] \times G_z^+(z,z';E-\epsilon_0(\mathbf{k}_\perp)), \quad (3)$$

where $\mathbf{k}_\perp$ is the electron's momentum in the x-y plane, $\epsilon_0(\mathbf{k}_\perp)=\hbar^2k_\perp^2/2m^*$, m^* is the effective mass, $\mathbf{r}=(\mathbf{r}_\perp,z)$, and $G_z^+(z,z';E)$ is the Green's function for the one-dimensional (1D) tunneling structure. The 1D Green's function is most easily determined by integrating its differential equation either numerically, or for simple structures analytically, and using the appropriate boundary conditions for the advanced Green's function.[9]

By substituting Eq. (2) into Eq. (1) and by realizing that the asymptotic form of the scattered wave function for $z>w$ is

$$\Psi^+(\mathbf{r})=\sum_{\mathbf{k}'_\perp}\exp(i\mathbf{k}'_\perp\cdot\mathbf{r}_\perp)\exp(ik'_z z)t(\mathbf{k}'_\perp,\mathbf{k}_\perp), \quad (4)$$

we are able to identify the interchannel transmission amplitudes as

$$t(\mathbf{k}'_\perp,\mathbf{k}_\perp)=t(E)\delta_{\mathbf{k}'_\perp,\mathbf{k}_\perp}+\frac{-ik'_z}{2AE'_z}\int_0^w dz_1\int_0^w dz_2\,\Psi_R(z_1;E'_z)T_D(z_1,z_2,\mathbf{k}'_\perp,\mathbf{k}_\perp;E)\Psi_L(z_2;E_z). \quad (5)$$

In Eq. (5), A is the cross-sectional area of the system and

$$T_D(z_1,z_2,\mathbf{k}'_\perp,\mathbf{k}_\perp;E)=\delta(z_1-z_2)V_D(z_1:\mathbf{k}'_\perp-\mathbf{k}_\perp) + \int\frac{d^2\mathbf{p}_\perp}{(2\pi)^2}\int_0^w dz'\,G_z^+(z_1,z';E-\epsilon_0(\mathbf{p}_\perp))V_D(z_1:\mathbf{k}'_\perp-\mathbf{p}_\perp)T_D(z',z_2,\mathbf{p}_\perp,\mathbf{k}_\perp;E). \quad (6)$$

$\Psi_L(z;E_z)$ is the solution of the 1D Schrödinger equation describing an electron incident on the barrier from the left-hand side with an energy $E_z=\hbar^2k_z^2/2m^*=E-\hbar^2k_\perp^2/2m^*$, and for $z>w$, $\Psi_L(z;E_z)=t(E_z)e^{ik_z z}$, where $t(E_z)$ is the 1D transmission amplitude. In the derivation of (5) and (6), we have used the relation

$$G_z^+(z,z';E_z)=-e^{ik_z z}ik_z\Psi_R(z';E_z)/2E_z \quad (7)$$

for $z>w$ and $z'<z$, where $\Psi_R(z;E_z)$ is the 1D wave function for an electron incident from the right and normalized to equal $t(E_z)e^{-ik_z z}$ on the left. This relation for $G_z^+(z,z';E_z)$ is derived by noticing that $G_z^-(z',z;E_z)$, the retarded Green's function, has the same form as $\Psi_R(z';E_{z'})$ for $w<z'<z$ and $z>w$. Equation (7) then results by matching the retarded Green's function to either side of z and by using $G^+(z,z')=[G^-(z',z)]^*$. The total transmission coefficient is finally given by $T=\sum_{\mathbf{k}'_\perp}(k'_z/k_z)\,|t(\mathbf{k}'_\perp,\mathbf{k}_\perp)|^2$.

We model a rough interface which is located at z_0 by taking a potential of the form $V_B\Theta(a/4-|z-z_0|)\times\sum_T\theta(\mathbf{r}_\perp-\mathbf{r}_{\perp T})$, where V_B is the band offset between well material and barrier material. The disorder represents scattering from a set of terraces[10] where the barrier material extends one monolayer, $a/2$, of the host material to larger z. Θ is the step function and $\theta(\mathbf{r}_\perp-\mathbf{r}_{\perp T})=1$ on the Tth terrace and is zero otherwise. We have chosen to work with this particular model for the sake of definiteness and it should be noted that our qualitative results are independent of the particular model used. For present purposes it is adequate to take the terraces to be identical and neglect correlations in the planar positions of their centers. Then

$$\langle V_D(z:\mathbf{q}_\perp)\rangle=V_B\Theta(a/4-|z-z_0|)N_T A_T,$$

where N_T is the number of terraces, A_T is their area, and $\langle\cdots\rangle$ denotes an average over the terrace center positions. In principle, $\langle V_D(z:\mathbf{q}_\perp)\rangle$ should be added to $V_B(z)$; however, this is not necessary since a is small compared to envelope-function wavelengths. In either case we may take $\langle V_D(z:\mathbf{q}_\perp)\rangle$ to be zero. The configurational average for a product of two potentials is given by

$$\langle V_D(z:\mathbf{q}_\perp)V_D^*(z';\mathbf{q}'_\perp)\rangle=\tfrac{1}{4}V_B^2N_T a^2\delta(z-z_0) \times\delta(z'-z_0)\,|f_T(\mathbf{q}_\perp)|^2\delta_{\mathbf{q}_\perp,\mathbf{q}'_\perp}, \quad (8)$$

where $f_T(\mathbf{q}_\perp)$ is the Fourier transform of $\theta(\mathbf{r}_\perp-\mathbf{r}_{\perp T})$ and we have used the smallness of a to replace $\Theta(a/4-|z-z_0|)$ by $(a/2)\delta(z-z_0)$. If there are several rough interfaces, their contributions to the right-hand side of Eq. (8) add.

The terms in $\langle|t(\mathbf{k}'_\perp,\mathbf{k}_\perp)|^2\rangle$ may be placed in one-to-one correspondence with terms in the disorder-averaged perturbation theory for the conductivity and may be represented by the same diagrammatic shorthand. Many interesting qualitative aspects of the influence of disorder in the barrier may be understood by examining the leading order in the perturbation theory. For a single disor-

dered interface the result is

$$T=|t^{(0)}(E)|^2+2\mathrm{Re}[t^{(0)*}(E)t^{(2)}(E)]+\frac{V_B^2\sigma_T a^2}{4\hbar^2}\int\frac{d^2\mathbf{k}'_\perp}{(2\pi)^2}\frac{|\Psi_L(z_0;E_z)|^2|\Psi_R(z_0;E'_z)|^2}{v_z v'_z}|f_T(\mathbf{k}'_\perp-\mathbf{k}_\perp)|^2, \quad (9)$$

where

$$t^{(2)}(E)=\frac{-i}{\hbar v_z}\Psi_R(z_0;E_z)\Psi_L(z_0;E_z)\frac{\sigma_T a^2 V_B^2}{4}\int\frac{d^2\mathbf{p}_\perp}{(2\pi)^2}G_z^+(z_0,z_0;E-\epsilon_0(\mathbf{p}_\perp))|f_T(\mathbf{k}_\perp-\mathbf{p}_\perp)|^2, \quad (10)$$

σ_T is the areal density of terraces, and $v_z=\hbar k_z/m^*$. The second term on the right-hand side of Eq. (9) represents electrons which are virtually scattered into the transverse channel with perpendicular momentum $\mathbf{p}_\perp$ and are then scattered back into the original transverse channel before being transmitted. The last term is the contribution to T in which electrons are scattered between transverse channels before being transmitted and can be thought of as a generalized Fermi "golden rule." This term can be placed in an especially simple form when the terraces are small compared to $|\mathbf{k}_\perp-\mathbf{k}'_+|^{-1}$. In this limit $f_T(\mathbf{k}'_\perp-\mathbf{k}_\perp)=A_T$ and

$$|t^{(1)}(E_z)|^2=\frac{V_B^2\lambda_T A_T g_{2D}}{4}\frac{k_z a|\Psi_L(z_0;E_z)|^2}{2E_z}\times\int_0^E\frac{k'_z a|\Psi_R(z_0;E'_z)|^2}{2E'_z}dE'_z, \quad (11)$$

where $\lambda_T=\sigma_T A_T$ is the fraction of the interface covered by terraces and $g_{2D}=m^*/2\pi\hbar^2$ is the two-dimensional density of states.

We have plotted $|t^{(1)}(E_z)|^2$ using Eq. (11) for scattering at each of the four interfaces of a double-barrier structure. The structure consisted of two 30-Å barriers, 270 meV high separated by a 30-Å well. One bound level exists in the well at 142 meV with a width Γ of $\sim$20 meV. An effective mass of $0.067m_0$ was used where m_0 is the electron rest mass. Realistic numbers for the interface-roughness parameters are $a=5.6$ Å and $A_I\lambda=4\times10^3$ Å^2. Figure 1 displays the results for the electron incident perpendicular to the barriers ($E=E_z$) and Fig. 2 for an incidence of 45° ($E=2E_z$). The distribution of interchannel transmitted electrons will always be strongly peaked around $E'_z\sim E_0$, where E_0 is the resonance energy, independent of E_z. This means that although an incoming electron may not have an E_z that is near resonance, it can scatter into resonance, greatly enhancing its probability of being transmitted.

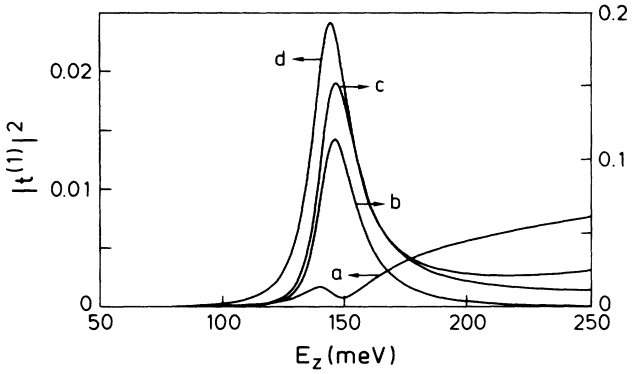

FIG. 1. The leading-order contribution to the transmission coefficient of a double-barrier structure in which electrons are elastically scattered between transverse channels before being transmitted. The electrons are incident with no transverse momentum and so can only scatter to lower-energy E'_z states. The curve representing scattering at the left interface is labeled *a*, at the interface in the well on the left *b*, at the right interface in the well *c*, and for the far-right interface *d*. Notice that curves *b* and *c* are plotted on a different axis from curves *a* and *d* and they give a contribution that is nearly an order of magnitude greater. The resonance energy E_0 is 142 meV and has a width Γ of 20 meV.

For scattering at the left interface, labeled *a*, $|\Psi_L(z_0;E_z)|^2\sim1$, while $|\Psi_R(z_0;E'_z)|^2$ is very small unless E'_z is near the resonance, in which case $|\Psi_R(z_0;E'_z)|^2\sim1$ for the symmetric barrier considered here. Once $E\sim E_0$ or $E>E_0$, $|t^{(1)}(E_z)|^2$ tends to rise gradually as the upper limits of the integral include more exit channels. The feature which occurs for $E_z\sim E_0$ is caused by $|\Psi_L(z_0;E_z)|^2$ being exactly 1 when the reflection coefficient vanishes. For scattering at the right interface, labeled *d*, $|\Psi_L(z_0;E_z)|^2\ll1$, except for $|E_z-E_0|\sim\Gamma$. In this case it goes to 1. On the other hand, $|\Psi_R(z_0;E'_z)|^2$ has no strong energy dependence at resonance. Therefore, $|t^{(1)}(E_z)|^2$ will have a strong peak for $E_z\sim E_0$ in both Figs. 1 and 2. The most

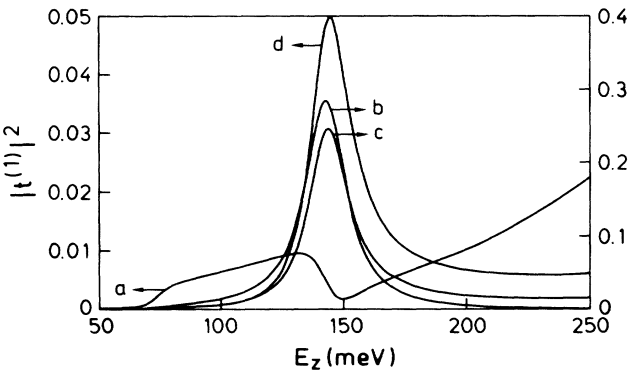

FIG. 2. As Fig. 1 but now the electrons are incident with the same amount of kinetic energy both perpendicular and parallel to the barriers. Consequently, the electrons are now able to scatter to higher-energy E'_z states.

effective disorder for interchannel scattering occurs at the interfaces surrounding the well, labeled b for the left interface and labeled c for the right one, since both $|\Psi_L(z_0;E_z)|^2$ and $|\Psi_R(z_0;E_z')|^2$ are large when E_z and E_z' are near E_0. For normal incidence we see that $|t^{(1)}(E_z)|^2$ rises extremely rapidly as $E_z=E_0$ is approached since resonant exit channels are becoming available just as the resonance develops for the incident channel. For 45° incidence, $|t^{(1)}(E_z)|^2$ switches on when $E_z\sim E_0/2$ as it is now possible for the electron to exit resonantly by increasing E_z.

In conclusion, it is clear from Figs. 1 and 2 that this type of elastic scattering will lead to an asymmetry in the voltage-current characteristics of resonant-tunneling diodes since interfaces in which GaAs is grown on $Al_xGa_{1-x}As$ are much rougher than interfaces in which $Al_xGa_{1-x}As$ is grown on GaAs. Thus in Figs. 1 and 2 curves a and c correspond to electrons incident towards the substrate and curves b and d to electrons incident in the opposite direction.[11] Furthermore, for electrons incident with energies above the resonance, scattering off the a interface increases in relative importance. This effect will be even more pronounced in structures with wider barriers, i.e., narrower resonances. Indeed, scattering off this interface may control the peak-to-valley ratio in the NDR region.

The current could also be calculated by integrating the product of T and the supply function up to the Fermi energy. The supply function takes account of the density of states in the contact regions and allows current to flow against the electric field. This will be undertaken in a future publication, but it is expected that the asymmetries which are seen here in T will also be observable in the current. Moreover, introducing structure in the transverse density of states by applying a magnetic field parallel to the current will allow the rate of elastic scattering to be studied experimentally in some detail.[12,13] For narrower resonances with longer tunneling times or rougher interfaces, interchannel scattering will be more dominant. To study this regime it will be necessary to carry out the perturbation expansion to higher order. Work in this direction is proceeding.

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Note added.—A recent paper by Fertig and Das Sarma[14] that appeared after this Letter was submitted for publication also treats elastic scattering in a double-barrier structure. However, these authors use a tight-binding formalism to calculate T and consider scattering in the well region.

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