Disorder effects on resonant tunneling in double-barrier quantum wells

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We analyze, within the framework of a one-band tight-binding model, the effect of diagonal disorder on the electronic states of a chainlike double-barrier quantum-well structure. Tunneling transmission probabilities together with local densities of states are evaluated in order to study quantum-size effects as a function of disorder in a quantum well.

INTRODUCTION

Resonant tunneling in epitaxially grown semiconductor layered structures, like (Ga,Al)As/GaAs double-barrier quantum wells, is nowadays a well-established phenomenon, which has been under study since the pioneering work by Chang, Esaki, and Tsu.[1] Nevertheless, complete understanding of this problem is far from being achieved. Experimental and theoretical investigations, which have been performed, include magnetotunneling,[2] resonant tunneling of holes,[3] resonant tunneling through multiquantum well structures,[4] through different minima of the conduction bands,[5] and under hydrostatic pressure.[6] The space-charge effects on current-voltage characteristics[7] and the transient time response of resonant tunneling structures[8] are of importance to understand and optimize technological application of the resonant tunneling effect, like new proposals of field effect transistors[9] (FET).

Investigations in this field have followed the improvements in epitaxial growth and device fabrication techniques, leading to observation of resonant tunneling in quantum-well systems other than $GaAs/Ga_{1-x}Al_xAs$, like $In_{1-x}Ga_xAs/InP$ (Ref. 10) and $Hg_xCd_{1-x}Te/CdTe$.[11]

A steady increase in the peak-to-valley ratio in the tunneling current[12] has been observed over the years. Detailed theoretical predictions of this ratio have to take into account the departure from ideal barrier-well interfaces or the presence of defects and impurities in the well and barriers, which lead to a reduction in the ideal peak-to-valley ratio.

In ideal structures the resonant tunneling of electrons is coherent.[13] A carrier which traverses the barriers coherently, but is inelastically scattered in the well, losing phase memory, is said to tunnel sequentially.[14] Inelastic events which destroy phase coherence lead to a broadening and decrease of the resonant transmission peak,[15] equivalently to a broadening of the density of states in the well,[16] and, hence, also to a reduction of the peak-to-valley ratio.

The observation of resonant tunneling in amorphous semiconductor-based heterostructures is rather surprising, when the above considerations are taken into account. The absence of sharp structures in the density of states and an increasing degree of localization of the electronic wave functions as the energy approaches the band edges would suggest the absence of the effect in double-barrier systems fabricated from amorphous semiconductors. However, Miyazaki *et al.*[17] have reported the existence of resonant tunneling through amorphous hydrogenated silicon nitride (barriers) and amorphous hydrogenated silicon (well) double-barrier quantum wells. Similar measurements on amorphous silicon-silicon carbide double barrier diodes, by Pereyra *et al.*[18] confirm the possibility of resonant tunneling through amorphous quantum wells. These experimental results are compared by the authors to transmission probability amplitude calculations based on the effective-mass approximation, where the effective masses are fitted experimental parameters. Recently, Gu Benyuam *et al.*[19] also investigated the effects of scattering centers in order to get an insight on resonant tunneling in amorphous heterostructures.

The aim of this work is to calculate resonant tunneling through a barrier-well-barrier structure, based on a model which takes into account explicitly the existence of disorder and that does not make use of the effective-mass approximation.

MODEL HAMILTONIAN

The present model consists of a one-dimensional chain of s orbitals, treated in the tight-binding approximation. The parameters of the Hamiltonian are chosen to simulate a five-layer structure: semi-infinite contact + barrier + well + barrier + semi-infinite contact. These parameters for well (barrier) materials are the following: atomic energies E_w (E_b) and first-nearest-neighbor hopping element V_{ww} (V_{bb}), which determine the well-known cosine one-band bulk dispersion relation. The parameters for the well and contact segments of the chain are the same. This model was used before to study resonant tunneling

through crystallinelike (ordered) double-barrier quantum-well chains, as reported elsewhere.[20] For the sake of simplicity we consider here only the case $E_w = E_b$, so that the band offset is given by $2 \mid V_{ww} - V_{bb} \mid$. When considering the heterostructure, we write, at the interfaces, $V_{wb} = \mid V_{bb} V_{ww} \mid^{1/2}$.

We introduce only diagonal disorder in the barrier and well sites, redefining the atomic energy at site n as

$$E_n' = E_n + \delta R_n E_n \ , \tag{1}$$

where E_n is equal to E_w or E_b, R_n is a random function of the site index n, varying between $-1 < R_n < 1$, and δ gives the maximum deviation of E_n' relative to E_n ($\delta = 0$ in the semi-infinite contacts).

For the model Hamiltonian

$$H = \sum_n (E_n' \mid n \rangle \langle n \mid + V_{n,n+1} \mid n \rangle \langle n+1 \mid + V_{n+1,n} \mid n+1 \rangle \langle n \mid) \ , \tag{2}$$

the problem of transmission through the barrier-well-barrier structure can be exactly solved numerically by using a transfer-matrix technique, formally similar to the one used for the effective-mass approximation, described by Price.[21] The transmission probabilities are calculated for relatively short structures (< 30 atomic sites), so averages over several hundred calculations for different random atomic energy sets, with otherwise identical parameters, are necessary. The average of the atomic energies through the chain is $\langle E_n' \rangle = E_n$. Thus, the band offsets are, on the average, the same as in the corresponding ordered case.

We are also interested in investigating electronic densities of states inside the well, so we evaluate Green's functions, from which we obtain the local density of states (LDOS) at a given site n of the chain through the relation

$$g_n(E) = \frac{-1}{\pi} \mathrm{Im}[G_{nn}(E + i\theta^+)] \ , \tag{3}$$

where E is the electron energy and θ an infinitesimal imaginary part added to the energy.

The Green's functions are obtained by solving the following set of equations:

$$\sum_k \left[\left\langle k \left| H - E \right| \sum_m \right| m \right\rangle \langle m \mid G \mid n \rangle - \langle k \mid n \rangle \Bigg] = 0 \ . \tag{4}$$

Here H is the Hamiltonian given by Eq. (2). This set of equations is kept finite by the use of transfer matrices for the ordered semi-infinite chains that act as contacts. The average density of states is calculated over an ensemble of several hundred structures, as mentioned above.

RESULTS AND DISCUSSIONS

In this section we show results for transmission amplitudes and densities of states for very thin structures. For all cases, the barriers are 5 atomic sites wide and the wells are 9, 7, or 5 sites wide. For each site corresponding to a GaAs monolayer, grown in the (100) direction, the well widths would be between, approximately, 25.5 and 15 Å. For epitaxially grown silicon or germanium, on the other hand, these thicknesses would be less. It should be pointed out that we are not able to make direct comparisons with experimental data, but our model is a starting point to study properties of amorphous semiconductor quantum wells. In this case, such thin wells are a reasonable choice, since quantum size effects are only observed in very thin amorphous quantum wells.[22]

For all the results shown here the tight-binding parameters are the same: $E_w = E_b = 1.0$ eV, $V_{ww} = 0.5$ eV, and $V_{bb} = 0.4$ eV. This determines a conduction-band offset of 0.2 eV. The zero on our energy scale coincides with the bottom of the well material conduction band in the ordered case. The disorder amplitude δ is varied from $\delta = 0$ to $\delta = 0.15$, corresponding to variations in atomic energies by an amount smaller than the band offset value.

Figure 1 shows transmission probabilities, as function of incident electron energies, for double-barrier–nine-atom wide well, for different disorder magnitudes. In Fig. 1(a) we show the ordered case, with resonances at the energies of the two quasibound states in the well, $E_0 = 0.034$ eV and $E_1 = 0.124$ eV. The next panels correspond to disordered cases with the following parameters: Fig. 1(b), $\delta = 0.05$; 1(c), $\delta = 0.1$; and 1(d), $\delta = 0.15$. We observe the increasing broadening of the peaks and the decreasing peak-to-valley ratio with increasing disorder, but, on the other hand, there is no shift in the peak maxima positions relative to the ordered case. In the $\delta = 0.15$ case we can only see shoulders related to the now very broad resonances. With further increase of disorder, these shoulders tend to disappear and the transmission probability curve takes the same shape as the corresponding one for a disordered chain, where all atoms are well-like, Fig. 1(e). Notice here, in comparison with Fig. 1(d), the difference in values of the transmission probabilities, of several orders of magnitude, due to the fact that barriers are still present in the $\delta = 0.15$ case. The dashed curve in Fig. 1(c) shows the transmission probability for the same structure, but with disorder $\delta = 0.1$, only in the barriers. This demonstrates that the broadening effects are mostly due to disorder in the well, as expected from the fact that the resonant tunneling state has a larger amplitude inside the well[13] making the influence of disorder in the barriers less important.

In order to analyze the changes of the electronic state at a resonance energy with disorder we calculate the diagonal part of the density matrix defined as

$$\langle \rho(E) \rangle_n = \sum_\alpha P_\alpha \psi_{n\alpha}^*(E) \psi_{n\alpha}(E) \ , \tag{5}$$

where n is the site index. The contribution of each disorder parameters set is weighted by P_α and the summation is over the ensemble of these sets. In the present case all P_α are equal to $1/N$, where N is the number of disorder parameters sets taken in the ensemble average. For the results shown here $N = 500$.

Figure 2 shows $\langle \rho(E) \rangle$ through the symmetric barrier (five atoms)–well (nine atoms)–barrier structure at $E_0 = 0.034$ eV. The curves from top to bottom correspond to increasing disorder, with $\delta = 0.0$, 0.005, 0.01, 0.05, 0.1, 0.15 from (a) to (f), respectively. The ampli-

tudes are normalized to 1.0 at the left contact-barrier interface, since we are assuming electrons incident from the left in our calculations. In (a), the ordered case, we clearly see the resonant quasibound state with the characteristic wave function pick up in the well.[13] This condition is severely perturbed even by very weak disorder, but in (b) and (c) we still see a larger amplitude of the wave function inside the well than at the left contact. Nevertheless the amplitudes at the right contact are orders of magnitude lower than at the left contact, which is characteristic for off-resonance states. These features are more remarkable in the more disordered cases, (d), (e), and (f), where the maxima inside the well, lower than at the left contact, go to the right side of the well, deviating from the *s*-like symmetry of this state (the first quasibound state in the

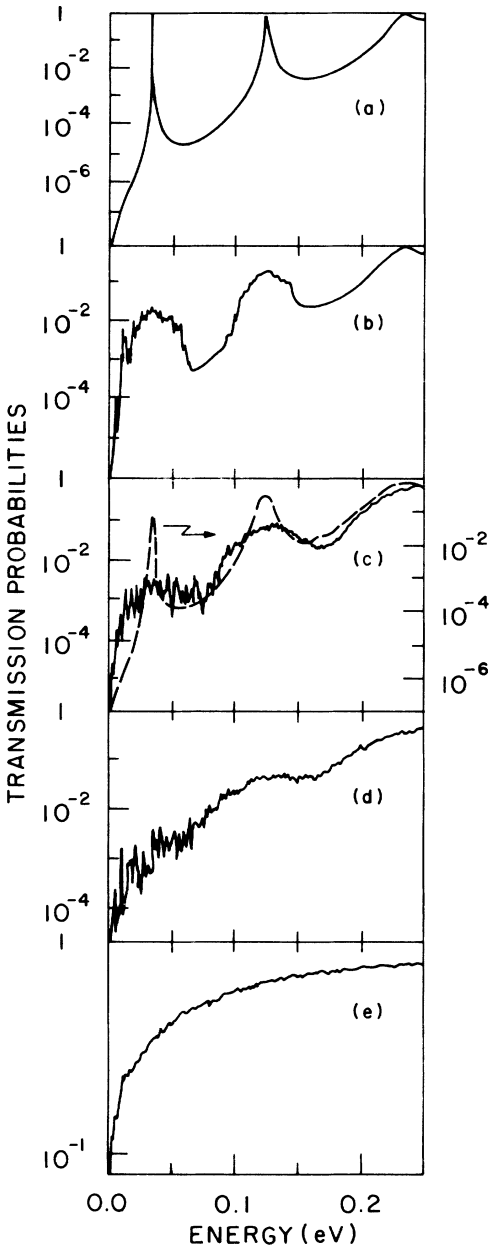

FIG. 1. Transmission probabilities vs incident electron energies, for a symmetric barrier (five atoms)–well (nine atoms)–barrier (five atoms) structure, with increasing disorder (from top to bottom). Disorder is defined by a disorder amplitude parameter, δ: (a) $\delta=0.0$ (ordered structure), (b) $\delta=0.05$, (c) $\delta=0.1$, (d) $\delta=0.15$. The dashed curve in (c) is for a $\delta=0.1$ in the barriers and $\delta=0.0$ in the well. The tight-binding parameters are $E_w=E_b=1.0$ eV, $V_{ww}=0.5$ eV, and $V_{bb}=0.4$ eV. In (e) the transmission probability vs incident electron energy for a chain with $V_w=V_b=0.5$ eV (i.e., there are no barriers) and $\delta=0.15$ is shown.

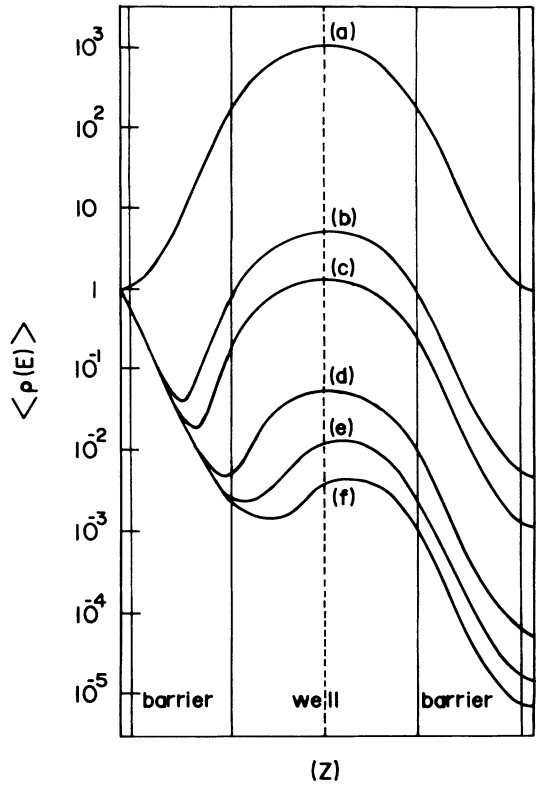

FIG. 2. Diagonal part of the density matrix at $E_0=0.034$ eV for the same structure and tight-binding parameters of Figs. 1(a)–1(d), with increasing disorder parameter: (a) $\delta=0.0$, (b) $\delta=0.005$, (c) $\delta=0.01$, (d) $\delta=0.05$, (e) $\delta=0.1$, and (f) $\delta=0.15$.

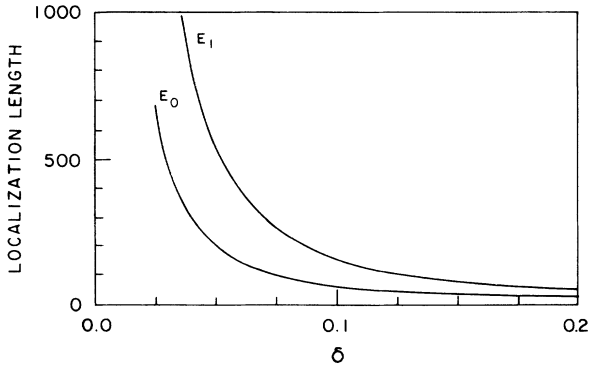

FIG. 3. Localization length as a function of the disorder parameter for a chain 19 contact- (well-) like atoms at $E_0=0.034$ eV and $E_1=0.124$ eV, which correspond to the resonance energies in Fig. 1(a).

quantum well).

It is well known that disorder induces increasing localization of the electronic wave functions, as the energy approaches the bottom of the conduction band. To discuss a relationship between the broadening of the transmission resonance peaks and the degree of localization, we calculate the localization length in disordered chains constituted only by well-like atoms with the same width (19 atoms) of the barrier (five atoms)–well (nine atoms)–barrier (five atoms) structure. The expression used is[23]

$$L(E) = -2L/\ln T(E) , \tag{6}$$

where L is the length of the chain and $T(E)$ the transmission probability. Figure 3 shows average localization length (in number of atomic sites) as a function of the disorder amplitude parameter δ, for energies $E_0 = 0.034$ eV and $E_1 = 0.124$ eV. It is seen that the localization length decreases with increasing disorder. When it is of the same order of magnitude of the length of the chain, the resonance peaks start to be smoothed out.

The broadening of the resonance peaks with disorder is accompanied by a broadening of the density of states in the well. Figure 4 shows the LDOS at the central site of the well in the barrier (five atoms)–well (nine atoms)–barrier (five atoms) structure. In Fig. 4(a) we see the peak in the LDOS due to the s-like state at $E_0 = 0.034$ eV, which has its maximum amplitude at the center. The arrow indicates the position in energy of the second state, $E_1 = 0.124$ eV, which gives no contribution to the LDOS at the central site. Figures 4(b), 4(c), and 4(d) show the

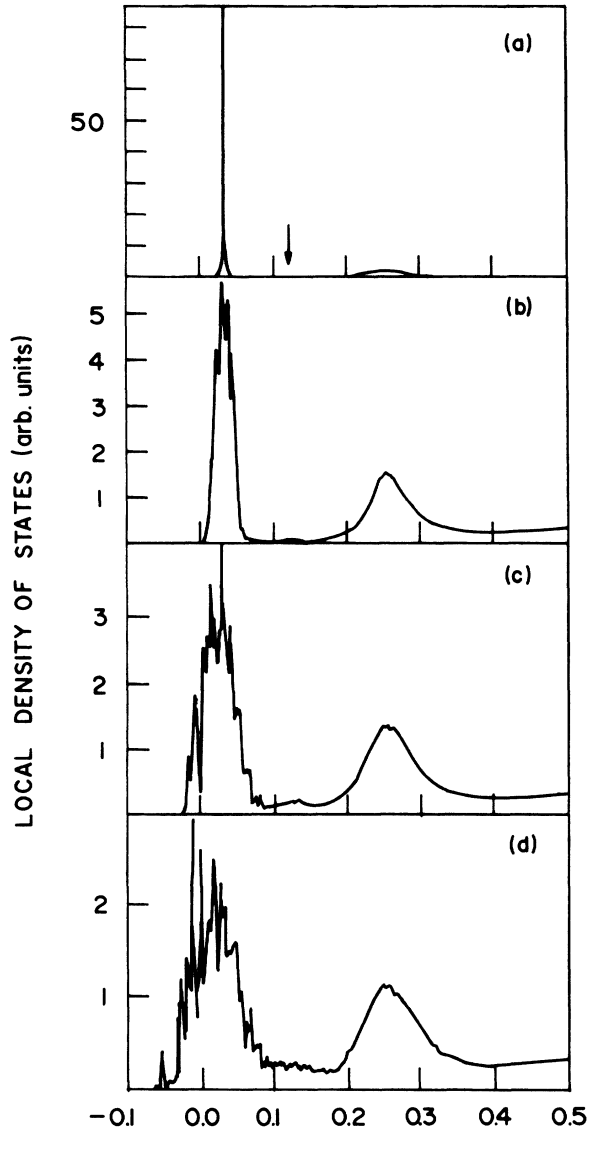

FIG. 4. Local density of states at the central site of the barrier (five atoms)–well (nine atoms)–barrier (five atoms) structure. In (a) we have the ordered case, $\delta = 0.0$, with the arrow indicating the position in energy of the second quasibound state, $E_1 = 0.124$ eV. The subsequent figures are for increasing disorder: (b) $\delta = 0.05$, (c) $\delta = 0.1$, and (d) $\delta = 0.15$. The tight-binding parameters are the same as Figs. 1(a)–1(d).

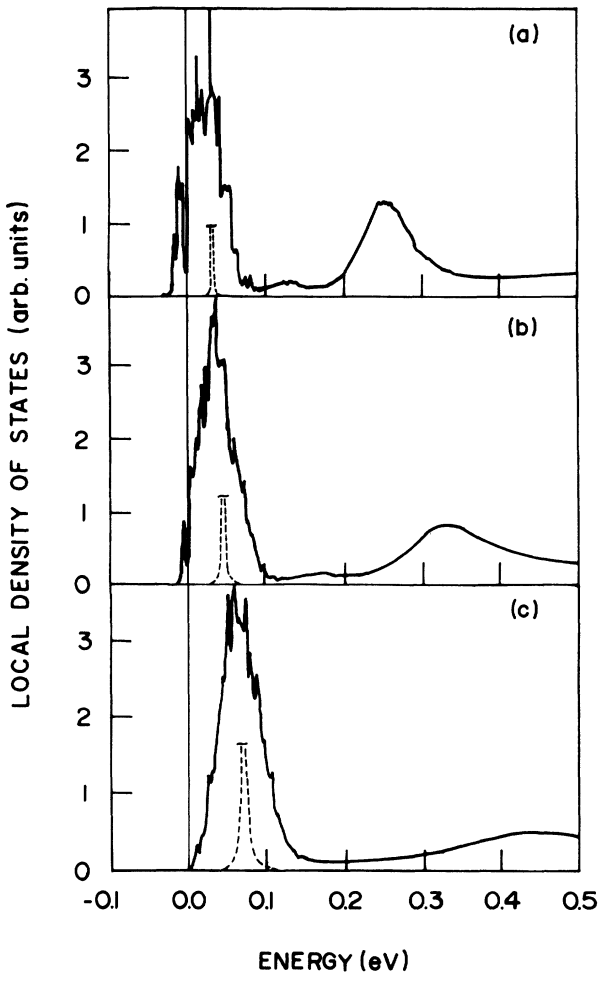

FIG. 5. Local density of states at the central site of symmetric barrier-well-barrier structures. The barrier thicknesses are kept fixed in all the cases (five atoms), but the well width is varied: (a) nine atoms, (b) seven atoms, and (c) five atoms. The solid curves are for the disordered cases with $\delta = 0.1$ and the dashed ones show the contribution of the first resonance state in the respective ordered structures. The vertical line at $E = 0.0$ eV visualizes the position in energy of the bottom of the well.

LDOS at the same central site for increasing disorder, with $\delta=0.05$, 0.1, and 0.15, respectively. The increasing broadening in the density of states with disorder is clearly seen. The appearance of a small peak at the position in energy of the second quasibound state indicates a mixing of states induced by disorder. With enough disorder, like in Figs. 4(c) and 4(d), there are states below the conduction-band edge, resulting in a "red-shift" instead of a blue-shift in the effective band gap. In a system like the one shown in Fig. 4(d) one would not expect experimental observation of quantum size effects, because of the strong localization of the states.

By comparing Figs. 1 and 4, we can see that the disappearance of sharp resonance structures in the transmission probability with increasing disorder correlates well with the smoothing out of the density of states under the same conditions.

The red- versus blue-shift competition, mentioned above, in disordered quantum-well systems is illustrated in Fig. 5. Here we show LDOS at the well center of structures with nine sites [Fig. 5(a)], seven sites [Fig. 5(b)], and five sites [Fig. 5(c)] in the well and the same disorder amplitude parameter, $\delta=0.1$. The dashed curves show the corresponding peaks in the LDOS for the respective ordered structures. We see the state mixing in Figs. 5(a) and 5(b) and no structure is seen in the last case, for no second state is quasibound in this well. The vertical solid line at the zero of energy indicates the bottom of the conduction band. This result points out that, whereas in the ordered case, space quantization effects are already seen in large quantum wells with a well-defined quasibound state above the conduction-band edge; in the disordered case one should go to thinner quantum wells to see clearly this kind of effect.

CONCLUSIONS

The disorder-induced broadening of transmission probabilities and LDOS discussed above is produced by elastic scattering, unlike that discussed by Buttiker,[16] which is due to inelastic effects. In our case, we are dealing with heterogeneous broadening, since for each member of the statistical ensemble of disordered chains, the resonance energy is different. In a realistic calculation both contributions must be taken into account. The relative contributions of broadening in transmission amplitude due to elastic scattering and due to inelastic scattering should be studied in greater detail to understand the experimental results and the threshold in well width to observe quantum size effects in this kind of amorphous systems. In the present calculation, moreover, the true three-dimensional situation in a disordered heterostructure is modeled through an ensemble average over one-dimensional elastic scattering channels. An important effect, lateral scattering, which would couple these one-dimensional channels is neglected. Hence, our model is not adequate for a calculation of the current density in these systems. However, it indicates that, in agreement with the experimental data, quantum size effects should really exist in amorphous semiconductor heterostructures in a similar way as in the crystalline ones.

Finally, a central question concerns the dynamics of the tunneling electron, which involves the concept of a tunneling time. The definition of this time is still a controversial question[24] although the recent suggestion by Luryi[25] indicates that this quantity may soon be actually measured. By carefully designing the experiments, we may then be able to begin to separate the effects of elastic and inelastic scatterings in the resonant tunneling phenomenon. Until now the only attempt to measure tunneling times was done by Tsuchiya *et al.*[26]

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