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ELASTIC SCATTERING IN RESONANT TUNNELING DEVICES WITH ONE DEGREE OF FREEDOM

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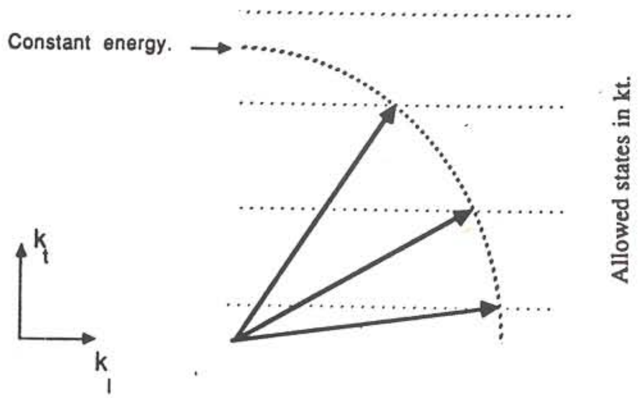
The effect of elastic scattering centers on the current-voltage (I-V) characteristics of double barrier resonant tunneling diodes with transverse confinement is examined. It is shown that elastic scattering centers break the separation of variables condition, and allow transitions between states of different transverse confinement. The changes to the transmission coefficients through the structure due to elastic scattering in the well of a resonant tunneling device are modeled by using perturbation theory. It is shown that additional structure in the I-V characteristics may result.

Resonant tunneling devices (RTD's) have been fabricated by a large number of groups using molecular beam epitaxy and other epitaxial techniques[1,2]. Recent advances in semiconductor processing technology have lead to the possibility of introducing additional quantum confinement perpendicular to the direction of charge transport[3,4]. It has been shown that if the variables can be separated transverse to, and along the direction of transport, that no additional peaks in the current-voltage characteristics of a RTD will result from transverse quantization[5]. In this paper, we show that additional structure in the current-voltage curve can result from breaking the separation of variables condition under transverse confinement. The case of elastic scattering in the well of a transversely confined RTD is studied in detail.

When the variables can be separated perpendicular to, and in the direction of transport in a semiconducting device, the expression for current due to electrons with one degree of freedom tunneling through a barrier system can be written as[5]:

$$I = \sum_{i}^{N} \frac{2q}{h} \int_{0}^{\infty} dE_l \, [f(E)-f(E+qV)] \, |T(E_l,V)|^2 \qquad 1)$$

where q is the magnitude of the electronic charge, E_l is the electron energy in the direction of tunneling, E is the total electron energy, f is the Fermi-Dirac distribution function, V is the applied voltage, h is the Planck constant, $E = E_l + E_t$, in which electronic energy transverse to the tunneling direction, E_t, is quantized, and $|T(E_l,V)|^2$ is the tunneling probability and independent of electron transverse energy. The summation is over the transversely quantized energy levels. Due to the separation of variables condition, transverse energy and momentum are conserved; therefore, only tunneling transitions between states with the same transverse energy contribute to the current.



1. Due to the discrete nature of the transverse states and the conservation of energy condition, only certain states are available for any given incident state. As a result, only well defined energy transitions are available.

Ionized impurities acting as elastic scattering centers break the conservation of transverse energy condition[6,7]. The energy is conserved in the elastic collision, and it becomes possible to scatter elastically between states with different transverse momenta by interchanging longitudinal and transverse energy. As a result, the initial and final longitudinal momenta may be different at the point of scattering as shown in Figure 1. Only certain transitions are allowed due to the discrete nature of the transverse states and the conservation of kinetic energy condition. Unintentional elastic scattering centers within a device can result from impurity diffusion or silicon surface riding. In a structure with a deep quantum well, electrons in the ground state can act as scattering centers for more energetic electrons, though the details of the electron-electron Hamiltonian differ from that of an electron scattering off of a fixed impurity.

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In order to treat the problem of scattering in a system with one degree of freedom, the scattering center is considered as a perturbation to a system with the variables separated in the direction transverse to and along the direction of current flow. The longitudinal potential of the barrier structure is treated as a series of rectangular segments. The wavefunction for each transverse state i is treated as a linear combination of two plane waves:

$$\Psi_i = a_{li}\exp(ikx) + a_{ri}\exp(-ikx) \qquad 2)$$

in each longitudinal rectangular segment. A 2x2 matrix is determined for each interface for a given transverse state and longitudinal energy by wavefunction and flux matching[8,9]. If a system of N transverse states is considered, each interface in the longitudinal direction yields a 2Nx2N matrix which has N 2x2 matrices along the diagonal:

$$\begin{vmatrix} B_1 \\ B_2 \\ \cdots \end{vmatrix} = \begin{vmatrix} G_{11} & 0 & \cdots \\ 0 & G_{22} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} A_1 \\ A_2 \\ \cdots \end{vmatrix} \qquad 3a)$$

where the G_{ii}'s are 2x2 matrices which determine the wavefunction amplitudes on either side of the interface. The other elements vanish indicating the lack of interaction between states of different transverse confinement under the separation of variables condition. The vector A has 2N elements, with each of the N transverse states having a set of two elements A_i:

$$A_i = \begin{bmatrix} a_{ri} \\ a_{li} \end{bmatrix} \qquad 3b)$$

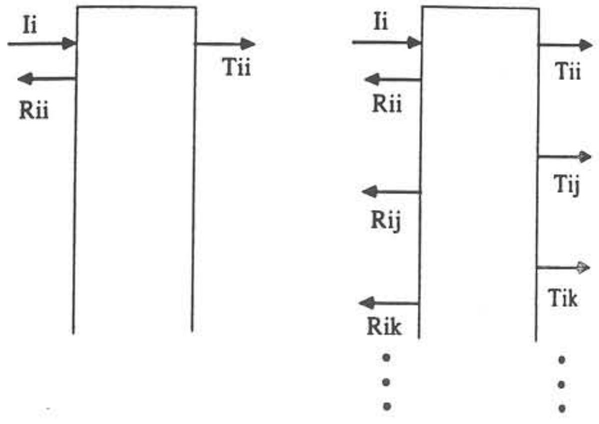
which represent the amplitude of the plane waves one one side of the interface as described in equation 2; the vector B represents the amplitudes the other side. The scattering matrix for the elastic scattering center has off diagonal two by two matrixies with non-zero elements which mix the transverse states:

$$\begin{vmatrix} C_1 \\ C_2 \\ \cdots \end{vmatrix} = \begin{vmatrix} S_{11} S_{21} \cdots \\ S_{12} S_{22} \cdots \\ \cdots\ \cdots\ \cdots \end{vmatrix} \begin{vmatrix} B_1 \\ B_2 \\ \cdots \end{vmatrix} \qquad 3c)$$

where each B_i and C_i are two element vectors, and each S_{ij} is the scattering matrix from transverse states i to j. By assuming a highly localized elastic scattering potential, transmission through a structure with a localized scattering center can now be written as:

$$\begin{vmatrix} D_1 \\ D_2 \\ \cdots \end{vmatrix} = \begin{vmatrix} F_{11} & 0 & \cdots \\ 0 & F_{22} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} S_{11} & S_{21} & \cdots \\ S_{12} & S_{22} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} E_{11} & 0 & \cdots \\ 0 & E_{22} & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix} \begin{vmatrix} A_1 \\ A_2 \\ \cdots \end{vmatrix} \qquad 3d)$$

where the $E_{i\text{-}i}$ matrix elements give the propagation of the wavefunction from the emitter to the scattering center, and the $F_{i\text{-}i}$ matrix elements give the propagation of the wavefunction from the scattering center to the collector.



(a) (b)

2. (a) When the transverse momentum through a barrier system is conserved, only the reflection and transmission coefficients of the incident state need to be considered. (b) When coupling is allowed between different transverse states, multiple transmission and reflection coefficients must be considered.

If an electron is incident upon the structure from the emitter in the transverse state i, and it is energetically possible for the electron to scatter into one of n transverse states (including i), then a total of n transmission and reflection coefficients must be calculated for this event as shown in Figure 2. The n elements of D in Equation 3d) which represent flux away from the barriers will be non-zero, the same is true for A with the exception of state i. By solving n linear equations, it thus becomes possible to obtain the n transmission coefficients, T_{ij}, for the incident state i, which are defined as the ratio of the transmitted flux in state j over the the incident flux in state i.

The current through the device based on the transition i-j can now be written:

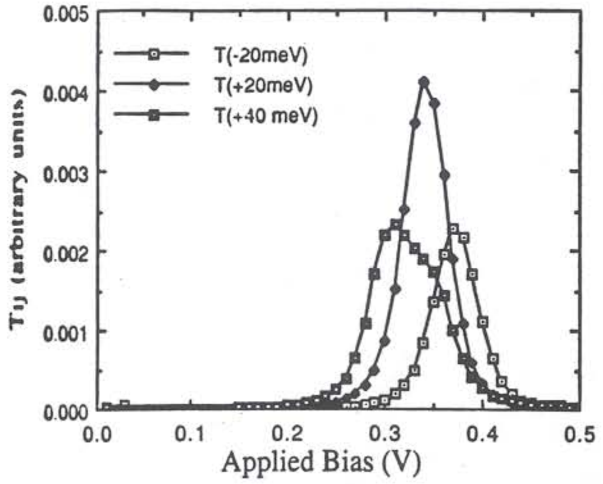
$$J_{i\text{-}j} = \frac{2q}{h}\int_0^{\infty} |T(E_l,V)_{ij}|^2\,[f(E)-f(E+qV)]\,dE_l \qquad 4)$$

where $|T(E_l,V)_{ij}|^2$ is derived in the manner outlined above Several transverse states are available for incident electrons, and each transverse state may be coupled to several other transverse states due to the scattering matrix Thus we can write the total tunneling current, J, as:

$$J = \sum_{i}^{N} \sum_{j}^{n(i)} J_{ij} \qquad 5)$$

where the outer summation is over initial transverse states i, and the inner summation is over the final states f, which are allowed by conservation of energy. In the absence of scattering between transverse states, the above expression reduces to Equation 1.

Consider the case of only two transverse states denoted i and j. For $|X|=|E||S||F|$, the ratio of the



The transmission coefficient T_{ij} is plotted for several different energy transitions.

transmitted flux in the transverse channel j to the incident flux in the transverse channel i is:

$$T_{ij} = \frac{\dot{x}_{13} \qquad \sqrt{k_f}}{[\dot{x}_{11}\dot{x}_{33}-\dot{x}_{31}\dot{x}_{13}]\sqrt{k_i}} \tag{6}$$

where k_i and k_f are the initial and final longitudinal wavevectors of state i and j repectively, and T_{ij} is the ratio of the transmitted flux in state j over the incident flux in state i. The unitary properties of the scattering matrix, $|X|$, have been used, in particular, $U^{-1} = U^*$.

To first order in the scattering potential, the scattering matrix elements are given by:

$$S_{if} = 2m_{eff} < \Psi_i | V | \Psi_j > (2\pi)^2 h^{-2} k^{-1/2} k'^{-1/2} \tag{7}$$

This expression can be derived through a time independent formulation. The wavefunctions Ψ_i and Ψ_j consist of a normalized transverse wavefunction multiplied by longitudinal plane wave states, V is the scattering potential, and k is the longitudinal wavevector of the incident state at the point of scattering. The longitudinal final state wavevector, k', is chosen on the side of the device where the final density of states is determined.

For the sake of tractability, we approximate the potential of the elastic scattering center by a Dirac delta function[7]. As a result, the transmission coefficient is weighted by a factor $|\Psi_{ti}(r_o)|^2\ |\Psi_{tj}(r_o)|^2$, where $\Psi_{ti}(r_o)$ and $\Psi_{tj}(r_o)$ are the transverse wavefunctions for states i and j evaluated at the position of the scattering center $\mathbf{r_o}$. Within this approximation, it is possible that a given transition would be very weak by the coincident location of a transverse wave node and the scattering center.

The transmission coefficients calculated in the above manner are plotted in Figure 3 as a function of applied bias. A structure with 50 Å $Al_xGa_{1-x}As$ (x=0.3) barriers, and a 50 Å $In_yGa_{1-y}As$ (y=0.1) well was assumed and resonant tunneling through the excited state was used. Transverse energy levels spaced 20 meV apart and an incident electron energy of 25 meV were assumed for this calculation. Three different values of energy transitions were used to calculate the transmission coefficient as a function of applied bias, each showing distinct peak positions. A constant weighting of the scattering was assumed for the three transitions. Less bias is needed to achieve a resonance condition for electrons which gain longitudinal energy in the well, and more bias is needed to obtain resonance for electrons which lose longitudinal energy in the well. The magnitude of the transmission coefficient decreases with larger changes in longitudinal energy.

Due to the shift in the transmission coefficient, there will be a different rensonant peak in the current-voltage characteristics of the device for each different transverse energy transition, $S_{i\text{-}j}$. The resulting additional currents which occur due to electrons scattering to different transverse energy states in the well may account for the additional peaks that have been observed in the current voltage characteristics of these structures.

We have shown that it is possible to elastically scatter between states with different transverse momenta in a RTD with transverse confinement. The effect on the transmission coefficient through the device was derived using a perturbation approach. By computing the transmission coefficients for several different energy transitions, we showed that additional structure in the current-voltage characteristics of such devices could result.

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