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Resonant Tunneling Devices : Effect of Scattering

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Abstract : The non-equilibrium Green's function (NEGF) formalism provides a general framework for the simulation of quantum devices including electron-phonon and electron-electron interactions. We have used this approach to study the effect of phonon scattering on the dc and ac response of resonant tunneling diodes. In this talk we will discuss the basic results using a simple physical picture.

1. Introduction

Resonant tunneling diode is possibly the most well-known example of a 'quantum device' [1]. Such devices are commonly modeled under the assumption that electrons can traverse the active region coherently without any scattering. The current can then be computed from the expression

$$\hat{I} = \frac{2e}{h} \sum_n \int dE\, T_n(E) \left[f_1(E) - f_2(E) \right] \qquad (1)$$

where $f_1(E)$ and $f_2(E)$ are the Fermi functions for contacts '1' and '2' respectively. The index 'n' labels the different transverse modes and $T_n(E)$ represents the probability that an electron incident in mode 'n' with energy E transmits through the device from one contact to the other. The transmission probability, $T_n(E)$, is calculated by solving the Schrödinger equation for the appropriate device potential. This approach provides a fairly accurate description of the peak current, which is not affected significantly by scattering processes. The valley current, however, is strongly influenced by scattering processes and it is necessary to go beyond the coherent model in order to describe it accurately.

The non-equilibrium Green function (NEGF) formalism provides a general framework for the simulation of quantum devices, comparable to what the Boltzmann formalism provides for classical devices [2]. Recently we have applied this formalism to study the influence of scattering processes on resonant tunneling devices. The details have been described elsewhere [3-5] and will not be repeated here. Instead we will try to convey the main results in simple physical terms. To simplify our discussion we will not worry about different transverse modes and assume the structure to be one-dimensional. We will assume 'zero' temperature so that the Fermi functions appearing in eq.(1) can be replaced by step functions. Also we will assume that the bias is large enough that the injection of carriers

from contact '2' can be neglected (see Figs.1 or 2). With these assumptions, eq.(1) reduces to

$$\hat{I} \approx \frac{2e}{h} \int_0^{\mu_1} dE\, T(E) \qquad (2)$$

2. Peak current

The current through a resonant level is maximum when it lies within the energy range of the incident electrons (Fig.1). Under these conditions, scattering processes have little effect on the current. Let us see why [6-9].

If we neglect scattering then the current can be calculated from eq.(2). The transmission probability can be written approximately in the form of a Lorentzian function

$$T(E) \approx \frac{\Gamma_1 \Gamma_2}{(E - E_r)^2 + (\Gamma/2)^2} \qquad \text{where} \quad \Gamma = \Gamma_1 + \Gamma_2 \qquad (3)$$

The width of the Lorentzian (Γ) is determined by the sum of the escape rates (times $\hbar$) through barriers '1' and '2' respectively. These are obtained by multiplying the attempt frequency (times $\hbar$) by the transmission probabilities T_1 and T_2 through the two barriers : $\Gamma_1 = \hbar\nu\, T_1$ and $\Gamma_2 = \hbar\nu\, T_2$. Substituting eq.(3) into eq.(2) we obtain the peak current in the absence of scattering :

$$\hat{I} = \frac{2e}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2} \qquad (4)$$

Scattering processes can be characterized by a parameter Γ_φ, which is related to the scattering time τ_φ by the relation $\Gamma_\varphi \equiv \hbar / \tau_\varphi$. If this quantity is much larger than the escape rates through the barriers (Γ_1 and Γ_2) then a significant fraction of the electrons will be scattered inside the well and get removed from the coherent stream. One way to model

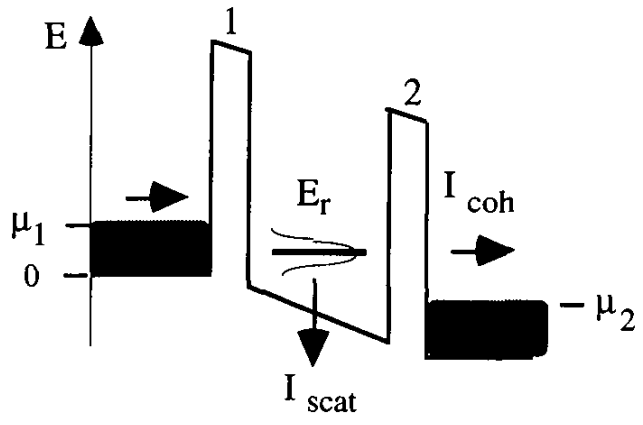


Fig.1. Condition for peak current : the resonant level E_r lies within the energy range of the incident electrons.

this loss of electrons is to introduce an imaginary component of the wavevector 'k' inside the well, causing the electronic wavefunction to decay. The transmission probability can still be written approximately in the form of a Lorentzian function, but the width is larger :

$$T(E) \approx \frac{\Gamma_1 \Gamma_2}{(E - E_r)^2 + (\Gamma/2)^2} \qquad \text{where} \quad \Gamma = \Gamma_1 + \Gamma_2 + \Gamma_\varphi \tag{5}$$

Substituting into eq.(2) we obtain the coherent current :

$$I_{coh} = \frac{2e}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2 + \Gamma_\varphi} \tag{6}$$

But this is not the total current. The electrons that are scattered out of the coherent stream give rise to a scattered current which is given by an expression that looks just like that for the coherent current (see Eq.(6)) with Γ_2 replaced by Γ_φ :

$$I_{scat} = \frac{2e}{\hbar} \frac{\Gamma_1 \Gamma_\varphi}{\Gamma_1 + \Gamma_2 + \Gamma_\varphi} \tag{7}$$

This result (known as the Breit-Wigner result) seems quite reasonable if we view the scattered current as a current that escapes into a fictitious third terminal having a coupling of Γ_φ [9]. The scattered current eventually exits from the device partially through barrier '1' and partially through barrier '2' in the ratio $\Gamma_1 : \Gamma_2$. The fraction coming out through '2' contributes to the net current and is referred to as the sequential current :

$$I_{seq} = \frac{\Gamma_2}{\Gamma_1 + \Gamma_2} I_{scat} = \frac{\Gamma_\varphi}{\Gamma_1 + \Gamma_2} I_{coh} \tag{8}$$

The total current (coherent + sequential) is given by

$$I_{tot} = I_{coh} + I_{seq} = \frac{2e}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2} \tag{9}$$

This is *exactly the same* as the result obtained earlier (eq.(4)), neglecting scattering processes altogether ! Thus scattering has no effect on the peak current within this approximate model. More accurate calculations, however, do show small effects [10].

3. Valley current

The current through a resonant level is very small when it lies outside the energy range of the incident electrons (Fig.2). A number of authors have studied the influence of scattering processes on the valley current that flows under these conditions (see [11] and references therein]. In our simple model, we can calculate the coherent component simply by substituting eq.(5) into eq.(2), just as we did for the peak current (cf. eq.(6))

$$I_{coh} = \frac{2e}{\hbar} \Gamma_1 K \qquad \text{where} \qquad K \approx \int_0^{\mu_1} \frac{\Gamma_2 \, dE}{(E - E_r)^2} \tag{10}$$

assuming that the linewidth is much smaller than the energy difference, E - E_r, between the incident electrons and the resonant energy. Actually we should not be using the Lorentzian approximation far from resonance, but that only changes the precise value of K and does not affect the following arguments. The scattered current is obtained by replacing Γ_2 with Γ_φ, just as we did before :

$$I_{scat} = \frac{2e}{\hbar}\,\Gamma_1 g \qquad \text{where} \qquad g \approx \int_0^{\mu_1} \frac{\Gamma_\varphi\, dE}{(E - E_r)^2} \tag{11}$$

Earlier we had argued that the scattered current exits through the two barriers in the ratio Γ_1 : Γ_2 and the fraction coming out through '2' contributes to the sequential current. However, in the present case the scattered current must come entirely out of '2' since there are no states in '1' corresponding to E_r. We are assuming that the electrons scatter down in energy into the resonance by phonon emission and the temperature is low enough that they cannot climb out by absorbing phonons. Under these conditions the sequential current is simply equal to the scattered current so that the total valley current is given by

$$I_{tot} = I_{coh} + I_{scat} = \frac{2e}{\hbar}\left[K\Gamma_1 + g\Gamma_1\right] \tag{12}$$

But this cannot be right. Suppose we make barrier 2 so thick that Γ_2 (and hence 'K') is essentially zero. Eq.(12) still predicts a non-zero valley current equal to (2e / $\hbar$) $g\Gamma_1$! How can any current flow if electrons cannot transmit across barrier 2 ? What happens for very thick barriers is that the resonant level fills up, since it cannot empty anywhere. To include this effect we should modify Eq.(12) to write the valley current as

$$I_{tot} = \frac{2e}{\hbar}\left[\, K\Gamma_1 + g\Gamma_1\,(1 - f_r)\right] \tag{13}$$

To complete the story we need to calculate the occupation factor f_r for the resonant level. This can be done quite simply using a sequential model as described below.

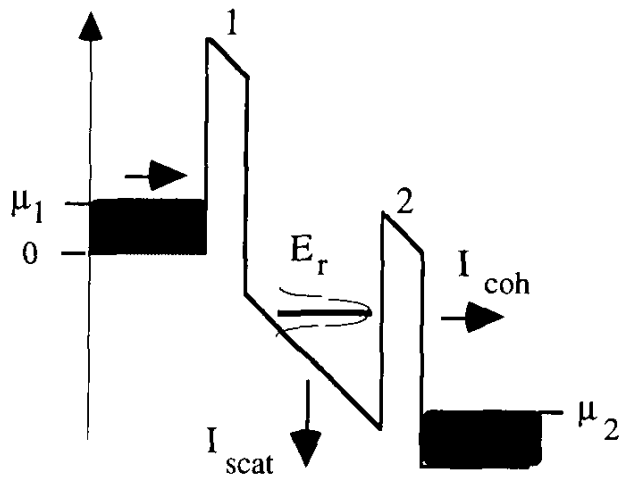


Fig.2. Condition for valley current : the resonant level E_r lies outside the energy range of the incident electrons.

4. Sequential model

In the sequential model the *peak current* is calculated by writing a rate equation for the currents I_1 and I_2 from the two terminals :

$$I_1 = \frac{2e}{\hbar}\Gamma_1 (f_1 - f_r) \qquad \text{and} \qquad I_2 = \frac{2e}{\hbar}\Gamma_2 (f_r - f_2) \tag{14}$$

Setting $f_1 = 1$, $f_2 = 0$ and $I_1 = I_2 \equiv I_P$, we obtain

$$f_r = \frac{\Gamma_1}{\Gamma_1 + \Gamma_2} \qquad \text{and} \qquad I_P = \frac{2e}{\hbar}\frac{\Gamma_1\Gamma_2}{\Gamma_1 + \Gamma_2} \tag{15}$$

in agreement with our earlier results (see eqs.(4), (9)). We can use the same approach to describe the *valley current* , simply by modifying the rate equation as follows (cf. eq.(14)) :

$$I_1 = \frac{2e}{\hbar} g\Gamma_1 (f_1 - f_r) \qquad \text{and} \qquad I_2 = \frac{2e}{\hbar}\Gamma_2 (f_r - f_2) \tag{16}$$

All that we have done is to reduce the rate constant for barrier 1 from Γ_1 to $g\Gamma_1$, where the factor 'g' (<< 1) is determined by the electron-phonon coupling constant. This seems reasonable since an electron in order to get into the resonant level from terminal 1 must tunnel through barrier 1 *and* emit a phonon simultaneously. Setting $I_1 = I_2 \equiv I_V$ and $f_1 = 1$, $f_2 = 0$ we obtain (cf. eq.(15))

$$f_r = \frac{g\Gamma_1}{g\Gamma_1 + \Gamma_2} \qquad \text{and} \qquad I_V = \frac{2e}{\hbar}\frac{g\Gamma_1\Gamma_2}{g\Gamma_1 + \Gamma_2} \tag{17}$$

Eq.(17) has also been derived from the NEGF formalism with suitable approximations and is found to describe the exact results obtained from a full numerical simulation fairly well [3].

Generally we assume that the valley current will be a small fraction of the peak current, independent of Γ_1 and Γ_2 . But it is easy to see from Eqs.(15) and (17) that this is not true in general :

$$I_P \sim \frac{1}{\Gamma_1} + \frac{1}{\Gamma_2} \qquad \text{and} \qquad I_V \sim \frac{1}{g\Gamma_1} + \frac{1}{\Gamma_2}$$

For very asymmetric devices having $\Gamma_2 << g\ \Gamma_1$, the peak and valley currents can even become equal! This has been observed experimentally [12].

5. High frequency response

We have also used the NEGF formalism to study the ac response of resonant tunneling devices in the presence of inelastic scattering processes. The results can be understood fairly simply in terms of the sequential model. Under time-varying conditions we cannot assume that I_1 is equal to I_2. Instead, $I_1 - I_2 = 2e\ (df_r / dt)$, so that for the *peak* current we can use eq.(14) to write

$$\frac{df_r}{dt} + \frac{\Gamma_1+\Gamma_2}{\hbar} f_r = \frac{1}{\hbar}(\Gamma_1 f_1 + \Gamma_2 f_2) \qquad \textit{peak} \qquad (19)$$

while for the *valley* current we can use eq.(16) to write

$$\frac{df_r}{dt} + \frac{g\Gamma_1+\Gamma_2}{\hbar} f_r = \frac{1}{\hbar}(\Gamma_1 f_1 + \Gamma_2 f_2) \qquad \textit{valley} \qquad (20)$$

From eqs.(19) and (20) we would expect that if we modulate f_1 and/or f_2 through an ac signal applied across the contacts, the peak current should respond with a time constant of $(\Gamma_1 + \Gamma_2)$ while the valley current should respond with a time constant of $(g\Gamma_1 + \Gamma_2)$. This is exactly what we find from the NEGF formalism [5].

5. Concluding remarks

In this talk we have shown how the effect of scattering processes on the valley current can be understood in simple intuitive terms using rate equations based on a sequential model. In general for quantitative calculations one needs to go beyond simple models and include multiple levels, level broadening, non-zero temperature, transverse modes, details of scattering processes, band-structure etc. The NEGF formalism provides a rigorous approach suitable for this purpose (see [2,3] and references therein). Since it incorporates the physics of the interactions correctly from first principles, a device simulator based on this formalism should have significant predictive value. It should be mentioned, however, that in resonant tunneling devices with small cross-section, the electron-electron interactions can be very strong leading to Coulomb blockade and related effects [13]. The utility of the NEGF formalism in this transport regime is still unclear.

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