The I-V Characteristic of Resonant Tunneling Junctions

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Abstract

We calculate the I-V characteristic of a tunnel junction containing resonant centers in the barrier distributed over a finite energy band and having an arbitrary location within the barrier . The on site Coulomb interaction , U, between two electrons of opposite spin causes the I-V characteristic to show some peculiar features when eV $\simeq$ U. The effect of the variation of the energy bandwidth and position of the impurity levels on I-V characteristics is also investigated.

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The presence of localized states in a tunnel junction changes dramatically the I-V characteristic of the junction [1]. At low temperatures two tunneling channels contribute to the current. The first one is the usual direct tunneling between the leads while the second one is a resonant tunneling through impurity states in the barrier. This last mechanism dominates at low temperatures and for thin junctions. This resonant contribution has been observed in several types of semiconductor structures experimentally [2]. Resonant tunneling occurs when the energy of the tunneling electrons is close to the energy of a localized state within the insulating layer. The process of resonant tunneling via localized states is of central importance in many physical systems attracting current attention. In the single electron picture, the total resonant current is simply the sum of the currents passing through each individual resonant channel. In principle, two electrons with opposite spin can occupy each resonant site, and thus each localized site gives rise to two resonant channels. In the presence of a large on-site Coulomb interaction, U, the tunneling becomes strongly correlated [3].

In this paper we restrict ourselves to the case of resonant tunneling and calculate the I-V characteristic of the junction. We calculate the current by taking into account the Coulomb repulsion between two electrons of opposite spin residing simultaneously at the impurity site. In systems such as amorphous silicon (a-Si) junction with short range scattering centers randomly distributed in the barrier [4] each localized site arising from uncoordinated Si-Si bond, is essentially a strongly localized potential well. A simple estimate of the order of magnitude of the on-site Coulomb interaction, $U \simeq e^2/\kappa a$, using the value of the static dielectric constant for crystalline silicon $\kappa \simeq 12$ and localization length $a \simeq 7$Å one finds $U \simeq 0.1$ eV which is very large compared to thermal energy kT, set to be the unit of energy in this work.

We will consider only the resonant tunneling contribution. The hamiltonian describing our system can be written as the sum of the following terms

$$H = H_L + H_I + H_T \tag{1}$$

where H_L is the leads hamiltonian, H_I is the impurity hamiltonian and H_T is the tunneling hamiltonian and are given by

$$H_L = \sum_{k\sigma} \epsilon_{k\sigma} a^+_{k\sigma} a_{k\sigma} + \sum_{p\sigma} \epsilon_{p\sigma} a^+_{p\sigma} a_{p\sigma} \tag{2}$$

$$H_I = \sum_{\sigma}(\epsilon_\sigma a_\sigma^+ a_\sigma + \frac{1}{2}U n_\sigma n_{-\sigma}) \quad (3)$$

$$H_T = \sum_{k\sigma}(T_k a_{k\sigma}^+ a_\sigma + h.c.) + \sum_{p\sigma}(T_p a_{p\sigma}^+ a_\sigma + h.c.) \quad (4)$$

Here $a_{k\sigma}^+$, $a_{p\sigma}^+$ and a_σ^+ are the creation operators for an electron in the spin state σ at the left lead, right lead and the localized state, respectively. T_k is the transition matrix element between wave functions at energy $\epsilon_{k\sigma}$ in the left lead and the localized wave function at ϵ_σ in the barrier, similarly for T_p . U is the on-site Coulomb interaction and $\epsilon_\sigma = \epsilon + \sigma\mu H$ is the energy of an electron with spin $\sigma = \pm$, ϵ is the energy of the localized state reckoned from the Fermi level and μH is the Zeeman magnetic energy. Two types of localized state contribute to tunneling, those with ϵ_σ close to the Fermi level and consequently are able to accept their first electron called A-type and those whose energy ϵ_σ is an amount U below the Fermi level and are able to accept a second electron to such a site near the Fermi level, these are called B-type. In the large U limit the occupation of an A site can be either zero or one while that of B site can be either one of two. However these two energy levels are related by particle-hole symmetry: $n_\sigma \longrightarrow 1 - n_\sigma$ applied to the hamiltonian (3).

Consider a junction with a single localized state in it and let P_0,P_σ, and P_2 be the probability for this state to be empty, singly occupied by a spin σ or doubly occupied, respectively, and can be defined as follows

$$P_0 =< (1-n_\uparrow)(1-n_\downarrow) > \ ; P_\sigma =< n_\sigma(1-n_{-\sigma}) > \ ; P_2 =< n_\uparrow n_\downarrow > \quad (5)$$

Where $< \cdots >$ stands for the statistical average. The equantion of motion of n_σ is given by the Heisenberg equation of motion :

$$i\hbar\frac{d}{dt}n_\sigma = [n_\sigma, H] \quad (6)$$

One can then write the exact equations of motion of the occupation probabilities P_X and end up with a higher order correlation functions for which equations of motion should be set up, this process will lead to a hierarchy of equations. A standard procedure enable us to solve these equations by decoupling higher order correlations and expressing them in terms of product of lower order correlations [5]. Another easier way to proceed is to invoke the standard master equation approach [6] which was used in the context

of resonant tunneling in some previous publications [7]. Assuming that the temperature is much larger than the width of the localized state so that one can use the master equation approach to establish the equations of motion. In this formalism the tunneling term is treated as a perturbation so that the Fermi golden rule gives the transition rate of electrons across the junction. In this case the level widths express the degree of hybridization of the resonant center with the extended states at the electrodes. In the limit that the level width of the resonant site is much smaller than all the other relevant energy scales such as the bias voltage and temperature, one can derive the following dynamic equations which can also be derived from the above mentioned equation of motion amended with a decoupling scheme

$$\begin{aligned}\dot{P}_\sigma &= 2\pi \sum_k |T_k|^2 [f_k(\epsilon_\sigma)P_0 - (1 - f_k(\epsilon_\sigma))P_\sigma]\delta(\epsilon_\sigma - \epsilon_{k\sigma}) + 2\pi \sum_k |T_k|^2 \\ &\times [f_k(\epsilon_\sigma)P_{-\sigma} - (1 - f_k(\epsilon_\sigma))P_2]\delta(\epsilon_\sigma + U - \epsilon_{k\sigma}) + (k \longleftrightarrow p) \qquad (7)\end{aligned}$$

$$\begin{aligned}\dot{P}_2 &= 2\pi \sum_{k\sigma} |T_k|^2 [f_k(\epsilon_\sigma)P_{-\sigma} - (1 - f_k(\epsilon_\sigma))P_2]\delta(\epsilon_\sigma + U - \epsilon_{k\sigma}) + \\ &\quad 2\pi \sum_{p\sigma} |T_p|^2 [f_p(\epsilon_\sigma)P_{-\sigma} - (1 - f_p(\epsilon_\sigma))P_2]\delta(\epsilon_\sigma + U - \epsilon_{p\sigma}) \qquad (8)\end{aligned}$$

These equations can simplified to the following compact form

$$\begin{aligned}\dot{P}_\sigma &= 2\Gamma_L[f_L(\epsilon_\sigma)P_0 - (1 - f_L(\epsilon_\sigma))P_\sigma] + 2\Gamma_L[f_L(\epsilon_\sigma + U)P_{-\sigma} \\ &- (1 - f_L(\epsilon_\sigma + U))P_2] + 2\Gamma_R[f_R(\epsilon_\sigma)P_0 - (1 - f_R(\epsilon_\sigma))P_\sigma] \\ &+ 2\Gamma_R[f_R(\epsilon_\sigma + U)P_{-\sigma} - (1 - f_R(\epsilon_\sigma + U))P_2] \qquad (9)\end{aligned}$$

$$\begin{aligned}\dot{P}_2 &= \sum_\sigma 2\Gamma_L[f_L(\epsilon_\sigma + U)P_{-\sigma} - (1 - f_L(\epsilon_\sigma + U))P_2] \\ &+ 2\Gamma_R[f_R(\epsilon_\sigma + U)P_{-\sigma} - (1 - f_R(\epsilon_\sigma + U))P_2] \qquad (10)\end{aligned}$$

Where $\dot{X}$ stands for the time derivative of the variable X and the level widths due to tunneling to the right and left leads are defined as usual by

$$\Gamma_L = \pi \sum_k |T_k|^2 \delta(\epsilon_k - \epsilon) \;\; ; \;\; \Gamma_R = \pi \sum_p |T_p|^2 \delta(\epsilon_p - \epsilon) \qquad (11)$$

The Fermi functions in the left ($f_L(x)$) and right ($f_R(x)$) leads are defined by

$$f_{L/R}(x) = (\exp[\beta(x - \mu_{L/R})] + 1)^{-1} \tag{12}$$

The quantity β is the inverse temperature , and μ_L and μ_R are the left and right chemical potentials, respectively. We have choosen the chemical potential at the right lead as our origin for the energies (i.e. $\mu_R = 0$ and $\mu_L = eV$, V is the applied voltage). Probability conservation allows P_0 to be expressed in terms of P_σ and P_2 while the current through the junction is defined in terms of the total electronic charge in one of the leads, say the right lead, $Q = e\sum_{p\sigma} < n_{p\sigma} >$ and is given by

$$\begin{aligned} I &= e\sum_{p\sigma} < \dot{n}_{p\sigma} > \\ &= 2e\Gamma_L \sum_{\sigma}[f_L(\epsilon_\sigma)P_0 - (1 - f_L(\epsilon_\sigma))P_\sigma + f_L(\epsilon_\sigma + U)P_{-\sigma} \\ &- (1 - f_L(\epsilon_\sigma + U))P_2] \end{aligned} \tag{13}$$

Since we are interested in studying the I-V characteristic in the absence of applied magnetic field, the spins do not play any role in our present problem. The density of states in the leads will be constant if the bands are broad (wide band model). If the hopping matrix elements also vary slowly with energy, then the width of the resonant level, Γ, will be independent of energy and will be treated as a constant in this paper. Under steady state conditions we can solve our equations (9-10) for P_σ and P_2 which, in their turn, are plugged into equation (13) to give the following expression for the current due to a single resonant level at ϵ

$$I(\epsilon) = 2e\Gamma_R \times \frac{f_L(\epsilon)(1 - f_R(\epsilon + U)) - f_R(\epsilon)(1 - f_L(\epsilon + U))}{[A_L(\epsilon) + A_R(\epsilon)/\alpha]} \tag{14}$$

The quantities $A_L(\epsilon)$ and $A_R(\epsilon)$ are defined by

$$A_L(\epsilon) = 1 + f_L(\epsilon) - f_L(\epsilon + U)\ ;\ A_R(\epsilon) = 1 + f_R(\epsilon) - f_R(\epsilon + U) \tag{15}$$

Where $\alpha = \Gamma_L/\Gamma_R$ defines the asymmetry parameter between the impurity couplings to left and right leads. We have chosen the chemical potential at the right lead as our origin for the energies, $\mu_R = 0.$, since the results are independent of the value of the right chemical potential. The current will

depend only on the applied voltage , V, between the leads. While doing the numerics we have chosen our energy unit to be the thermal energy kT . In figure 1 we show $I(V)$ due to a single impurity level in the symmetric Anderson model where $\epsilon = -U/2$ in our case we chose U = 20, $\epsilon = -10$ and different values of the asymmetry parameter α. The curve show two sharp peaks around ϵ and $\epsilon + U$ which are basically the resonant centers contributing to tunneling and called A-type and B-type, previously. The strength of these peaks decreases as the asymmetry parameter α decreases. The area under these curves basically represents the current averaged over a uniform distribution of impurity centers. Thus we can conclude that the major contribution to the current comes from impurities located at the center of the junction ($\alpha = 1$) in accord with previous work[3, 8].

In order to calculate the I-V characteristic of the junction we must proceed through some averaging because from the experimental point of view the total current measured is due to a large number of impurities. We assume that the localized states have a finite band with a constant density of states g, while the spacial distribution of the localized state obey the so called δ-distribution where the localized states are uniformly distributed over a plane parallel to the junction interface having a specific coordinate z from the left interface inside the insulating layer. In recent years molecular beam epitaxy techniques have been developed in semiconductor technology in which dopant atoms are confined in a single plane of the host material, the so called δ- doping [10]. The measured thickness of the doping layer is limited by the resolution of the technique. However, in general we can say that dopants can be confined to within $15\mathring{A}$, which correspond roughly to three atomic layers. Hence to compare our results with experiment we need to perform averaging energies of the impurities. Note that the expression of the current we obtained (14) strongly depends on the position of impurity which is reflected in the parameters Γ_L and Γ_R. Assuming a wide band approximation in which the bandwidth in the leads is much larger than the resonance width so that the density of states can be taken as constant. The hopping matrix elements are assumed to be energy independent and decay exponentially

$$|T_{k,p}| = T_0 \exp(-z_{L,R}/a) \tag{16}$$

where $z_{L,R}$ denotes the distance from the localized state to the left and right lead, respectively, while a is the localization length and T_0 is a constant.

Under these assumptions the decay widths to the left and leads (Eq.7) will reduce to the following forms [9]

$$\Gamma_L = E\exp(-2z/a) \;\; ; \;\; \Gamma_R = E\exp(-2(d-z)/a) \tag{17}$$

Here z denotes the distance from the impurity to the left lead, d is the width of the junction, a is the impurity localization length which is known to be around $7\mathring{A}$ in Mo/a-Si/Mo tunnel junction [8]. To the first order approximation the pre-exponential factor, E, may be considered as independent of the coordinates and is a measure of the effective depth of the localized state. The formula of the single impurity current (14) depends on the coordinates only through Γ_L and Γ_R in its denominator.

Using the above mentioned averaging technique we can evaluate the averaged current $< I >$ assuming a uniform distribution of impurities over the barrier

$$< I >= S\int d\epsilon g(\epsilon) I(\epsilon) \tag{18}$$

where $I(\epsilon)$ stands for equation (14) which gives the current due to a single impurity at a given position z and with a given energy ϵ, S is the lateral area of the junction. The quantity $g(\epsilon)$ is the density of impurity states , assuming it to be constant within a finite band of width D so that

$$g(\epsilon) = \begin{cases} 1/D & if \;\; |\epsilon| < D \\ 0 & if \;\; |\epsilon| > D \end{cases} \tag{19}$$

the averaged current reads

$$< I(U) >= I_0 \int_{-D}^{D} d\epsilon \frac{f_L(\epsilon)[1-f_R(\epsilon+U)] - f_R(\epsilon)[1-f_L(\epsilon+U)]}{[A_R(\epsilon) + A_L(\epsilon)/\alpha]} \tag{20}$$

where I_0 is a constant that depend on the characteristics of the junction and the width of the energy distribution

$$I_0 = 2eS\Gamma_R/2D \tag{21}$$

Formula (20) is symmetric under left/right transformation , that is when ($\Gamma_R, \alpha) \rightarrow (\Gamma_L, 1/\alpha)$. That is why we restrict ourselves to values of α in the range [0,1] in our numerical computations. Evaluating the current (20), for a fixed value of the potential U, we found that it shows a kink (Fig.2) at a value of the applied voltage equal to the Coulomb energy, U. The slope of

the I-V characteristic (the differential conductance) changes abruptly from applied voltages less than U to voltages greater than U (see Fig.2). Hence it is more instructive to plot the conductance as a function of the applied voltage (Fig.3). One important feature to notice is that there is a step in the differential conductance as the applied voltage V becomes comparable to U. The magnitude of this step gets reduced when α decreases from 1 to 0. At finite temperature the step itself get smoothed out due to thermal fluctuations. In Fig.3 we have considered only positive values of the applied voltages, the region $V < 0$ can be obtained by reflection symmetry about the V = 0 axis.

In Fig.4 we show the I-V characteristic for small values of the Coulomb interaction compared to the energy bandwidth (U = 5 and D = 20). In this case the current shows a negative differential resistance (NDR) contrary to Fig.2 where such an important feature of electronic devices is missing. It is well known in the literature [11] that the ability of a resonant tunneling diode to show NDR is not exhibited in the infinite band model. Our point here is that NDR are exhibited not solely by the finiteness of the energy bands in the leads but it can also result from the finiteness of the impurity band as it is the case in our situation.

In Fig.5 we show the I-V characteristic for a Coulomb interaction larger than the impurity bandwidth, here the current shows some extra structures due to the competition of the applied voltage with the other energy scales in the problem: U and D. Basically the current reaches its maximum value when impurity levels: ϵ and $\epsilon + U$ are within the transport window of the junction (between μ_R and μ_L). In Fig.6 we show the current through the localized state as a function of the energy of the localized state for different values of the applied voltage while U was fixed to 20. At small voltages the main contributions to the current originate from the two resonant peaks (dotted curve). Thus for $eV < U$ the I (ϵ) presents two peaks, the lower comes from tunneling through the upper level for impurities deep below μ_R (thus the current flows through the upper level only) while the upper peak is due to impurities whose resonant level is above μ_R and the upper level is above μ_L (thus the current flows predominantly through the resonant level). As we increase the Voltage this resonant structure is suppressed (dashed) and shoulders appear at -U, 0, U and 2U for extremely high voltages (continuous curves).

The calculations presented in this work shows that the width of the

localized states energy distribution within the barrier plays an important role in the I-V characteristic. In the case of wide energy bands ($D > eV_{max}$, V_{max} is the maximum value of the applied voltage) and in the absence of applied magnetic field the Coulomb blockade effect is reflected in the existence of a current step in the differential conductance, G. This step gets reduced with a decrease of the asymmetry parameter α. The I-V characteristic has a non-Ohmic behavior since it has a kink at eV = U, whose magnitude depend on α. The current is linear in the applied voltage only in the wide band limit ($D > eV_{max}$) and change slope at V = U. Of course for extreme values of the asymmetry $\alpha \simeq 0$ and $\alpha \simeq \infty$,our present approach should be modified so as to take into account the strong Coulomb interaction between the lead and the localized state which became very close to it in this limit. In the case of narrow impurity band ($D < eV_{max}$) the current displays a nonlinear behavior. The most important feature of resonant tunneling diodes i.e. their ability to show negative differential resistance is also restored in the case of narrow impurity bands. Generally speaking, due to the presence of strong Coulomb on-site interaction the current is maximum only when the two impurity levels ϵ and $\epsilon + U$ are within the transport window (between μ_R and μ_L). In fact the current is almost zero when both impurity levels are well below the right chemical potential or well above the left chemical potential.

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Figure Captions

Fig.1 The I-V characteristic (in arbitrary units) for a single localized state at $\epsilon = -U/2$ with U = 20.

Fig.2 The I-V characteristic of the tunnel junction averaged over a wide energy band (D = 100) of localized states for different values of the asymmetry parameter α. The parameter U is fixed to be 20 in units of kT.

Fig.3 The conductance (in arbitrary units) as a function of the applied voltage for different values of the asymmetry parameter α, the parameter U is fixed to 20.

Fig.4 The I-V characteristic of the tunnel junction for U = 5 , D = 20 (units of kT) and different values of the asymmetry parameter (α).

Fig.5 The I-V characteristic of the tunnel junction for U = 20 , D = 5 (units of kT) and different values of the asymmetry parameter (α).

Fig.6 The current through the localized state (in arbitrary units) as a function of the localized state energy for different values of the applied voltage and U = 20.