Tunneling in mesoscopic junctions

H. O. Frota  
Departamento de Física-ICE, Universidade Federal do Amazonas,  
69077-000, Manaus-Am, Brazil  
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Abstract

We have applied the Numerical Renormalization Group method to study a mesoscopic system consisting of two samples of metal separated by an insulating barrier, with nanometer dimensions, which allows the tunnelling of a single electron from one to the other side of the junction. The junction is represented by a generalized orthodox model, taking into account the electronic scattering interaction due the hole and the tunnelling electrons, localized in the source and in the drain electrode, respectively. We have calculated the static properties (charge transference, charge average, quadractic charge average and specific heat) and the electric conductivity of the junction, for the model parameters given by the tunneling matrices element $V_T$, the barrier energy $U = e^2/2C$ (where $C$ is the capacitance of the system) and by the electronic scattering potentials $V_L(R)$ acting on the electrons of the left(right) electrode.

1 Introduction

Studies of the tunnelling mesoscopic junctions in the present decade have advanced thanks to the possibilities offered by the new manufacture technologies of these structures, which are increasingly lesser, having reached nanometric dimensions, resulting in capacitance lesser them $10^{-15} F$, which permits to study the effect of the quantization of the charge and electronic energy[1].

The orthodox model for the tunnelling mesoscopic junctions consists of two metal layers intercalated by a fine insulating layer. From the classic point of view there is no tunnelling current through the junction, due to the impediment of electrons to tunnel through the potential barrier represented by the insulator. In this condition the junction behaves as a capacitor with $C$ capacitance. By applying an external potential $V_{ext}$ to the junction, it is loaded with a charge $Q = CV_{ext}$. This charge, which can vary continuously, is originated by the displacement of electrons in the electrodes in relation to the positive ions of metals. Even lowermost, $V_{ext}$ can produce small displacements of electrons, originating a small charge in the electrodes. The interaction between the charges
of these electrodes can be represented by the energy of the capacitor that is given by $E_c = Q^2 / 2C$.

Taking in consideration the quantum effect, when the layer of insulator, intercalated enters the metal layers, will be very fine, it is possible that an electron tunnels from a side to the other side of the junction, through the insulator layer. In this case the process of electronic transport involves discrete charge of only one electron ($e$), in contrast of what occurs with the charges of the electrodes that are continuous. As the electrostatic energy associated with the tunnelling of an electron is $U = e^2 / 2C$, for great values of $C$ this energy is masked by the thermal energy $k_B T$. However, with the advance of the nanostructure manufacture techniques, it is possible to construct junctions with small capacitance, so that the electrostatic energy $U > k_B T$. In these conditions, the effect of the charge transference can be observed. Then, considering that the tunnelling conductance $\Gamma$ also is low, much smaller then the inverse of the quantum resistance of the junction, $\Gamma \ll R_Q^{-1}$, where $R_Q = \pi \Gamma / (2e^2) \simeq 6.5K\Omega$, the tunnelling of a single electron can hinder the tunnelling of the following electrons, giving rise to what is known as Coulomb blockade [1, 2, 3], that has excited great theoretical and experimental interest. Recent works have shown that, even at energies below the energy of capacitor $E_c$, there is tunnelling due to charge fluctuation in the junction [4, 5, 6].

In the present work we have generalized the orthodox model, considering that the charge transference from a side (source) of the junction to the other (drain) creates scattering potentials in the electrodes, originated by the hole left in the source and by the electron that has tunnelled to the drain. The sudden creation of these localized potentials creates electron-hole pairs excitation at the Fermi level, modifying the behavior of the conductivity of the junction. The tunnelling process is in thermal equilibrium when the excess charge in each junction, originated from the tunnelling, is balanced by the phase shift of the conduction electrons, according to the Fridel sum rule. This problem has been treated similarly to the problem related to X-ray threshold singularity [7, 8], where the many particles states, after the tunnelling, are projected on the many particles states before the tunnelling, what can induce X-ray infra-red divergence in the conductivity [8].

Other forms of nanostructures have deserved increasing interest from researchers, as the structure formed by two metal layers intercalated by an insulator layer, inside of which there is a metallic electrode, that usually receives the name of island [9]. The process of charge transport from a metal (source) to the other (drain) occurs by quantum tunnelling through the island, changing its charge by $e$. The effect of the tunnelling of an electron through the island can be enhanced if the dimension of the island is very small, what confers to it a very reduced capacitance and, consequently, a great variation of its potential. This high potential, that produces an electrostatic energy higher then the thermal energy, reduces the probability of tunnelling through the island, as it has been observed in granular metallic materials in the beginning of the studies of the tunnelling junctions [10, 11, 12], where the electronic tunnelling in low voltages is inhibited when the electrostatic energy of an electron of a grain is
greater than the thermal energy. With the development of the manufacture of nanostructure technology it is possible to construct metallic islands with known geometry, separated by tunnelling barriers, that can adequately control the tunnelling of a single electron through the junction, that occurs by the jump of this electron from one to another island [9, 13, 14, 15].

Another geometry of nanostructure that has been studied is constituted by a metal substratum over which a layer of insulator and another one of semiconductor are deposited successively [16], with a pair of electrodes build parallel on the layer of the semiconductor. A positive voltage is applied to the metal substratum, so that the free electrons of the semiconductor are confined to the superior surface of the insulator. This confinement forms a bidimensional free electron gas in the interface semiconductor-insulator. By applying a negative voltage to the pair of electrodes on the layer of the semiconductor, the movement of the electrons is limited throughout a canal in the parallel direction to the electrodes, thus forming a free unidimensional electron gas. Two saliences constructed in the electrodes have the purpose of creating potential barriers that confine electrons between them, producing discrete energy levels in this region, reason why these devices are called quantum points or artificial atoms [17, 18, 19, 20, 21, 22, 23, 24, 25].

In this work, using the Numerical Renormalization Group (NRG) formalism, we have developed an accurate numerical calculation for the generalized orthodox model for mesoscopic junctions, taking into account the electronic scattering [7, 8]. We have initiated by presenting the Hamiltonian of the Model in section I, where the properties that will be studied have been defined; in section II we have developed the formalism adopted for the diagonalization of the Hamiltonian, the calculation of the static properties and the electric conductivity; the section III consists in the central point of this work, where the results obtained for the calculations of the static properties (charge transference, charge average, quadratic charge average and the specific heat) and of the electric conductivity of the model are presented; in section IV we have presented the pertinent conclusions to this work and, finally, in the appendix we have developed a perturbation theory in the tunnelling matrices element \( V_T \) for a particular case of the studied model, whose results are used to verify of the precision of the numerical calculation of the general model.

2 The model

The tunnelling junction studied is formed by two metals which are separated by an insulator layer, whose dimensions are nanometrics. The small thickness of the insulator allows the electrons to tunnel from a metal to the other, changing the charge pattern of the junction and giving origin to a tunnelling current. Usually the the Coulomb blockade theory assumes that the conduction electrons, before the tunnelling event, are in an equilibrium state and, after the tunnelling, these electrons enters immediately into a new equilibrium state [1]. This means that the wave functions of the electronic states next to the Fermi
level are not changed with the variation of the charge junction. Only a small displacement in the energy levels of the electrons occurs next to the Fermi level. This theory, therefore, fails to take in consideration the transient effect in the charging patterns between the two states of equilibrium.

To account for the transient effect, some authors [7, 8, 28] have considered that the tunnelling event occurs in two stages, with different time scales. In the first stage of the electron tunnelling through the junction, the charge created in the surface of the metal due to the transference of an electron from one side to the other side of the junction, enter in equilibrium in a time of the order of the inverse of the plasma frequency of the metal, whose corresponding energy is of approximately 1eV. In the second stage, the electrons in the Fermi surface, which are associated to a response time much longer then the correspondent to the first stage, feel the change in the charge states of the junction as if this has occurred quickly and in a localized form. This difference in the time scale, associated with the nature of the localized potential quickly created in the surface of the metal, generates many particles interactions, giving origin to the electron-hole pairs excitations in the Fermi level. This effect is similar to the Mahan-Nozières-Dominicis effect [29, 30] that occurs in the absorption and photoemission of X-rays in metals. In this in case an electron is ejected from a deep atomic level of a metal, changing the charge of an atom. The ion quickly created by the emission of the electron by the ray-X interacts in the final state with conduction electrons, resulting in a divergence in the X-ray absorption and photoemission spectrum.

In this section we have presented the Hamiltonian of the model for a nanostructure metal-insulator-metal, considering the electrostatic screen originated from the tunnelling of the electron through the junction. The model Hamiltonian is written as

\[ H = H_L + H_R + H_T + H_Q + H_V. \]  

The terms \( H_L \) and \( H_R \) represent the left and right electrodes conduction Hamiltonians, respectively, given by

\[ H_L = \sum_k \epsilon_k c_k^\dagger c_k \]  
\[ H_R = \sum_q \epsilon_q d_q^\dagger d_q \]  

where the operators \( c_k^\dagger (c_k) \) and \( d_q^\dagger (d_q) \) create (annihilate) electrons in the respective conduction band and obey the following anticommutation relations:
\[ \{ c_k^\dagger, c_k \} = \delta_{kk}, \]
\[ \{ c_k, c_k \} = \{ c_k^\dagger, c_k^\dagger \} = 0, \]
\[ \{ d_q^\dagger, d_q \} = \delta_{qq}, \]
\[ \{ d_q, d_q \} = \{ d_q^\dagger, d_q^\dagger \} = 0 \]
\[ \{ c_k, d_q \} = 0. \] (4)

The last of the proprieties indicates the independence of the operators of the two conduction bands. The term \( H_T \) describes the tunnelling Hamiltonian

\[ H_T = \sum_{kq} \left( V_T c_k^\dagger d_q + V_T^* d_q^\dagger c_k \right), \] (5)

which allows the electrons be annihilate in the left side conduction band and be create in the right side conduction band, and vice versa, and \( V_T \) is the tunnelling matrices element, which is taken as independent of the moment for energies very close to the Fermi energy. The electrostatic junction energy is represented by the term \( H_Q \),

\[ H_Q = \frac{Q^2}{2C}, \] (6)

where \( C \) is the capacitance, \( Q \) is the junction charge, given by

\[ Q = \frac{e}{2} (N_L - N_R), \] (7)
\[ N_L = \sum_k c_k^\dagger c_k, \] (8)
\[ N_R = \sum_q d_q^\dagger d_q, \] (9)

and \( e \) is the elementary charge.

The last term of the Hamiltonian given by the Eq.(1) corresponds to the free electron scattering by the charges localized in the junctions, written as

\[ H_V = V_L \frac{(N_L - N_R)}{2} \sum_{kk'} c_{k'}^\dagger c_k + V_R \frac{(N_L - N_R)}{2} \sum_{qq'} d_{q'}^\dagger d_q, \] (10)

where \( V_L \) and \( V_R \) represent the changing in the potential of the metals in the left and right side of the junction, respectively, when an electron tunnels through the junction.

3 The Method

The Numerical Renormalization Group formalism used in this paper follows the method proposed originally by K. G. Wilson[31] for the solution of the
static properties of the Kondo model, and applied by Krishna-murthy, Wilkins and Wilson[32, 33] to calculate these properties in the Anderson model, later generalized by Frota and Oliveira[34] to obtain the dynamics properties of these models.

The first study using the Wilson renormalization group method for nanostructures was carried through by Frota and Flensberg [5], having determined the fundamental state and transports properties for these structures, represented by the usual model, which was not taken in consideration that when an electron tunnels through a junction, the conduction electrons quickly readjust its potential, created in the surface of the electrode, producing many particle effects with the creation of electron-hole pairs excitations. In the present work we have introduced this new ingredient and we have analyzed its effect in the fundamental state and transports properties.

The method consists in the logarithmic discretization of the Hamiltonian of the conduction bands of the two electrodes, and in the determination of a new finite basis in which the Hamiltonian of the model, given by the Eq.(1), is written. After the iterative diagonalization, we obtain its eigenvectors, calculate the charge average and the quadratic charge average of the junction, specific heat and, with the Kubo formula, we obtain the electric conductivity. The conduction bands are divided into logarithmic intervals \( \pm D \Lambda^{-j-z} \) \((j = 1, 2, \ldots; \Lambda > 1; z\) is a continuous parameter), and converted to a “hopping” Hamiltonian [32] given by

\[
H_N^{L} = \frac{(1 + \Lambda^{-1}) D}{2} \sum_{n=0}^{N-1} \varepsilon_{nz} \left( f_{nz}^\dagger f_{(n+1)z} + f_{(n+1)z}^\dagger f_{nz} \right) \\
H_N^{R} = \frac{(1 + \Lambda^{-1}) D}{2} \sum_{n=0}^{N-1} \varepsilon_{nz} \left( g_{nz}^\dagger g_{(n+1)z} + g_{(n+1)z}^\dagger g_{nz} \right),
\]

(11)

(12)

where \( \varepsilon_{nz} \) is obtained numerically. In this basis the electrodes are coupling solely via the first terms of the chains, defined as

\[
f_{nz} = \frac{1}{\sqrt{2}} \sum_k c_k \\
g_{nz} = \frac{1}{\sqrt{2}} \sum_q d_q.
\]

(13)

(14)

In the basis \( \{f_{nz}, g_{nz}\} \), the tunnelling Hamiltonian \( H_T \), the electrostatic junction energy \( H_Q \) and the scattering Hamiltonian \( H_V^S \) are given by
\[ H_T^N = 2 \left( V_T f_{0z}^+ g_{0z} + V_T^* g_{0z}^+ f_{0z} \right) \]  \hspace{1cm} (15) \\
\[ H_Q^N = \frac{U}{4} \left( \sum_{n=0}^{N} f_{nz}^+ f_{nz} - \sum_{n=0}^{N} g_{nz}^+ g_{nz} \right)^2 \]  \hspace{1cm} (16) \\
\[ H_V^N = \left( \sum_{n=0}^{N} f_{nz}^+ f_{nz} - \sum_{n=0}^{N} g_{nz}^+ g_{nz} \right) \left( V_L f_{0z}^+ f_{0z} + V_R g_{0z}^+ g_{0z} \right). \]  \hspace{1cm} (17) 

Rescaling by the factor \( 2\Lambda^{-(N-1)/2}/(1 + \Lambda^{-1})D \) the Hamiltonians given by Eqs.(11,12,15,16 and 17), the diagonalization takes place in the reduced Hamiltonian \( H_N \) that is written as

\[
H_N = \Lambda^{(N-1)/2} \left\{ \sum_{n=0}^{N-1} \varepsilon_{nz} \left( f_{nz}^+ f_{(n+1)z} + f_{(n+1)z}^+ f_{nz} \right) + \sum_{n=0}^{N-1} \varepsilon_{nz} \left( g_{nz}^+ g_{(n+1)z} + g_{(n+1)z}^+ g_{nz} \right) + \bar{V}_T \left( f_{0z}^+ g_{0z} + g_{0z}^+ f_{0z} \right) + \frac{\bar{U}}{4} \left( \sum_{n=0}^{N} f_{nz}^+ f_{nz} - \sum_{n=0}^{N} g_{nz}^+ g_{nz} \right)^2 + \frac{1}{2} \left( \sum_{n=0}^{N} f_{nz}^+ f_{nz} - \sum_{n=0}^{N} g_{nz}^+ g_{nz} \right) \left( \bar{V}_L f_{0z}^+ f_{0z} + \bar{V}_R g_{0z}^+ g_{0z} \right) \right\}, \]

where

\[
\bar{V}_T = \frac{4V_T}{(1 + \Lambda^{-1}) D} \]  \hspace{1cm} (19) \\
\[
\bar{U} = \frac{2U}{(1 + \Lambda^{-1}) D} \]  \hspace{1cm} (20) \\
\[
\bar{V}_L = \frac{4V_L}{(1 + \Lambda^{-1}) D} \]  \hspace{1cm} (21) \\
\[
\bar{V}_R = \frac{4V_R}{(1 + \Lambda^{-1}) D}. \]  \hspace{1cm} (22) 

The scale factor \( \Lambda^{(N-1)/2} \) in the reduced Hamiltonian \( H_N \) is introduced to assure that the smallest eigenvalue is of unity order. The discrete approximation to the Hamiltonian of the model is given as the limit

\[
H = \lim_{N \to \infty} \frac{1}{2} (1 + \Lambda^{-1}) D \Lambda^{-(N-1)/2} H_N \]  \hspace{1cm} (23)
The diagonalization of the Hamiltonian $H_N$, represented by the Eq. (18), is carried out iteratively, using a recurrence relation which allows to calculate the eigenstates of the iteration $(N+1)$ from the eigenstates of the iteration $N$. To obtain this recurrence relation, the charge operator given by Eq. (7) in the basis $\{f_n, g_n\}$ is written as,

$$Q_N \equiv \frac{1}{2} \left( \sum_{n=0}^{N} f_n^\dagger f_n - \sum_{n=0}^{N} g_n^\dagger g_n \right)$$  \hspace{1cm} (24)

which commutes with the operator $H_N$, since $[Q_N, H_N] = 0$. The definition of the charge operator is important to the numerical diagonalization process of the Hamiltonian $H_N$ because, as $Q_N$ and $H_N$ commute, the associated matrices can be written as blocks of matrices that can be diagonalized independently, lowering the computational time. From the definition of $Q_N$, the recurrence relation for the Hamiltonian $H_N$ is written as

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} I_N + 2\Lambda^{N/2} \tilde{U} Q_N q_{N+1} + \Lambda^{N/2} \tilde{U} (q_{N+1})^2 + \Lambda^{N/2} q_{N+1} \left( \tilde{V}_L f_{Nz} f_{0z} + \tilde{V}_R g_{0z} g_{Nz} \right),$$  \hspace{1cm} (25)

where the iterative operator $I_N$, which couples the iteration $(N)$ with the iteration $(N+1)$, is given by

$$I_N = \varepsilon_{Nz} \left[ f_{Nz}^\dagger f_{(N+1)z} + f_{(N+1)z}^\dagger f_{Nz} + g_{Nz}^\dagger g_{(N+1)z} + g_{(N+1)z}^\dagger g_{Nz} \right].$$  \hspace{1cm} (26)

and $q_N$ is defined as

$$q_N = \frac{1}{2} \left( f_{Nz}^\dagger f_{Nz} - g_{Nz}^\dagger g_{Nz} \right)$$  \hspace{1cm} (27)

From Eqs. (24 and 27), the recurrence relation for $Q_N$ and $Q_N^2$ is written as

$$Q_{N+1} = Q_N + q_{N+1}$$  \hspace{1cm} (28)

$$[Q_{N+1}]^2 = [Q_N]^2 + 2 [Q_N] q_{N+1} + [q_{N+1}]^2,$$  \hspace{1cm} (29)

which will be useful for the calculation of the charge average and the quadratic charge average.

The Eq.(25) consists in the core of the renormalization group method used in the present work. It permits that, once the eigenvalues and eigenvectors of the Hamiltonian $H_N$ are known, the eigenvalues and the eigenvectors of the Hamiltonian $H_{N+1}$ can be determined.

For a given iteration $N$, the eigenstates consist in the following Fermi operators: $f_{0z}, f_{1z}, ..., f_{Nz}$ and $g_{0z}, g_{1z}, ..., g_{Nz}$. Each one of these operators can assume two states, occupied and empty, so that for the iteration $N$ the number of states is given by $2^{2(N+1)}$ and the matrices associate to the Hamiltonian $H_N$
in the basis \( \{ f_{nz}, g_{nz} \} \) is of the order \( 2^{2(N+1)} \times 2^{2(N+1)} \). For typical values of \( N \) used in the present work (\( N = 20 \)), the matrices that will be diagonalized are of the order \( 2^{42} \times 2^{42} \), which makes the numerical diagonalization impossible. To by-pass these difficulties were carried out, two procedures which are reported as follows: 1) As the operator \( Q_N \) commutes with the Hamiltonian \( H_N \), then the eigenstates of \( H_N \) also are eigenstates of \( Q_N \), which means that we can diagonalize \( H_N \) in independent subspaces of \( Q_N \). Thus, the matrices associated with the Hamiltonian \( H_N \) can be written in diagonal blocks that are diagonalized separately, which reduces the dimensions of the matrices to be diagonalized. 2) Even if diagonalizing in subspaces of same charge, the matrices continue with dimensions that makes the numerical diagonalization process inadequate. However, as in the calculation of the static and dynamic proprieties the energies are close to the Fermi energy, the procedure consists in generating the basis for the diagonalization of the iteration (\( N + 1 \)) taking into account only the lower energy eigenstates of the iteration (\( N \)), according with the references [31] and [32].

The iterative process begins with the diagonalization of the Hamiltonian \( H_0 \), written as

\[
H_0 = \frac{1}{\sqrt{\Lambda}} \left\{ \tilde{V}_T \left( f_{0z}^\dagger g_{0z} + g_{0z}^\dagger f_{0z} \right) + \tilde{U} \left[ \frac{1}{2} \left( f_{0z}^\dagger f_{0z} - g_{0z}^\dagger g_{0z} \right) \right]^2 \right\} + \frac{1}{2} \left( f_{0z}^\dagger f_{0z} - g_{0z}^\dagger g_{0z} \right) \left( \tilde{V}_L f_{0z}^\dagger f_{0z} + \tilde{V}_R g_{0z}^\dagger g_{0z} \right),
\]

where only the operators \( f_{0z} \) and \( g_{0z} \) appear. In the second step, the operators \( f_{1z} \) and \( g_{1z} \) are added and the Hamiltonian

\[
H_1 = \sqrt{\Lambda} H_0 + I_0 + 2 \tilde{U} Q_q q_1 + \tilde{U} q_1^2 + q_1 \left( \tilde{V}_L f_{0z}^\dagger f_{0z} + \tilde{V}_R g_{0z}^\dagger g_{0z} \right),
\]

is diagonalized in relation to a basis formed by the eigenstates of the Hamiltonian in the first step \( H_0 \) and the states that are constructed by the operators \( f_{1z}^\dagger, g_{1z}^\dagger \) and \( f_{1z}^\dagger g_{1z}^\dagger \) applied to the eigenstates of \( H_0 \). Following this procedure, the Hamiltonian \( H_{N+1} \) is diagonalized in relation to a basis formed by the eigenstates of \( H_N \) and the states given by the operator \( f_{(N+1)z}^\dagger, g_{(N+1)z}^\dagger \) and \( f_{(N+1)z}^\dagger g_{(N+1)z}^\dagger \) applied to the eigenstates of \( H_N \).

For each iteration the charge average \( \langle Q_N \rangle \), the quadratic charge average \( \langle Q_N^2 \rangle \), the specific heat \( C_V \), the charge transference \( \tau \) and the electrical current \( \sigma(\omega) \) are calculated, in relation to the basis \( \{ f_{0z}, g_{0z}, f_{1z}, g_{1z}, ..., f_{Nz}, g_{Nz} \} \), as follows,
\[
\langle Q_N \rangle = \frac{\text{Tr} Q_N \exp(-\bar{\beta} H_N)}{\text{Tr} \exp(-\beta H_N)}
\]
(32)

\[
\langle Q_N^2 \rangle = \frac{\text{Tr} Q_N^2 \exp(-\bar{\beta} H_N)}{\text{Tr} \exp(-\beta H_N)}
\]
(33)

\[
\frac{C_V}{k_B} = \beta^2 \left[ \frac{\text{Tr} (H_N)^2 \exp(-\bar{\beta} H_N)}{\text{Tr} \exp(-\beta H_N)} - \left( \frac{\text{Tr} H_N \exp(-\bar{\beta} H_N)}{\text{Tr} \exp(-\beta H_N)} \right)^2 \right]
\]
(34)

where the Boltzmann factor is written in terms of the reduced Hamiltonian \( H_N \) as

\[
\exp(-\beta H) = \exp \left[ -\bar{\beta} H_N \right]
\]
(35)

where \( \beta = 1/k_B T \), \( k_B \) is the Boltzmann constant, \( T \) is the temperature and \( \bar{\beta} \) a constant that is defined according with reference [32],

\[
\bar{\beta} = -\beta \left[ \frac{1}{2} \left( 1 + \Lambda^{-1} \right) \Lambda^{-(N-1)/2} \right]
\]
(36)

Then, taking a fixed \( \bar{\beta} < 1 \) [32], the temperature \( T_N \), corresponding to the iteration \( N \), is given by

\[
T_N = \frac{D}{k_B \beta} \left[ \frac{1}{2} \left( 1 + \Lambda^{-1} \right) \Lambda^{-(N-1)/2} \right].
\]
(37)

The term \( H_T \) of the Hamiltonian \( H \) allows the tunnelling through the junction, given by the charge transference operator \( \tau = \sum_k c_k^\dagger d_k \) in the basis \( \{ f_{nz}, g_{nz} \} \) as

\[
\tau = 2 f_{0z}^\dagger g_{0z}.
\]
(38)

The charge transference through the junction is given by the thermal average of the operator \( \tau \),

\[
\langle \tau \rangle = \frac{\text{Tr} \left( 2 f_{0z}^\dagger g_{0z} \right) \exp(-\bar{\beta} H_N)}{\text{Tr} \exp(-\beta H_N)}.
\]
(39)

The electrical current operator through the junction, \( I \), is written as a function of the time rate of the charge \( Q \) as

\[
I = \frac{dQ}{dt} = \frac{e}{2} \frac{d(N_L - N_R)}{dt}.
\]
(40)

The above time derivative is obtained from the commutation of the operator \( N_L - N_R \) with the Hamiltonian \( H \) given by Eq.(1). As \( N_L - N_R \) commutes with \( H_L, H_R, H_Q \) and \( H_V \), then
\[
\frac{d(N_L - N_R)}{dt} = \frac{i}{\hbar} [H_L, (N_L - N_R)],
\]

and the electrical current operator is written in terms of the operators \(c_k\) and \(d_q\) as

\[
I = \frac{e i}{2\hbar} \sum_{k,q} \left( V_T c_k d_q - V_T^* d_q^* c_k \right).
\]

(41)

The electrical conductivity through the junction is obtained from the Kubo formula\[29\]:

\[
\sigma(\omega) = \frac{\pi}{\omega} \sum_F |\langle F | I | \Omega \rangle|^2 \delta \left( E^F - E^\Omega - \omega \right),
\]

(42)

where \(\omega\) is the frequency, \(|\Omega\rangle\) and \(|F\rangle\) are the fundamental and the final many particles states of the Hamiltonian \(H\), with eigenvalues \(E^\Omega\) and \(E^F\), respectively.

For NRG purpose, the operator \(I\), given by Eq.(41), is written in terms of the operators \(f_0^z\) and \(g_0^z\) (Eq. (13 and 14), respectively),

\[
I(z) = \frac{e i}{\hbar} \left( V_T f_0^z g_0^z - V_T^* g_0^z f_0^z \right),
\]

(43)

and \(\sigma(\omega)\) (Eq.(42)) is written in terms of the eigenstates of the reduced Hamiltonian \(H_N\) (Eq.(18)), as

\[
\sigma(\omega_N, z) = \frac{\pi}{\omega_N} \sum_F \frac{|\langle F(z) | I(z) | \Omega(z) \rangle|^2}{\left( \frac{1 + \Lambda^{-1}}{2} \Lambda^{-(N-1)/2} \right)^2} \delta \left( E^F_N(z) - E^\Omega_N(z) - \omega_N \right),
\]

(44)

where the reduced energy \(E^F_N(z)\), \(E^\Omega_N(z)\) and \(\omega_N\) are given by

\[
E^F_N(z) = \frac{2}{1 + \Lambda^{-1}} \Lambda^{(N-1)/2} E^F(z)
\]

(45)

\[
E^\Omega_N(z) = \frac{2}{1 + \Lambda^{-1}} \Lambda^{(N-1)/2} E^\Omega(z)
\]

(46)

\[
\omega_N = \frac{2}{1 + \Lambda^{-1}} \Lambda^{(N-1)/2} \omega.
\]

(47)

In Eq.(43) an electron is destroyed in the orbital \(f_0^z\) of the left conduction band and another electron is created in the orbital \(g_0^z\) of the right conduction band, and vice versa, so that the application of the operator \(I(z)\) conserves the charge. In the matrices elements \(|\langle F(z) | I(z) | \Omega(z) \rangle|\) of the Eq.(44) we take as initial state the fundamental state \(|\Omega(z)\rangle\), and as final states \(|F(z)\rangle\) all the excited states whose charges are equal to the charge of the initial state. As the energy levels of the conduction bands (left and right) are discretized, the lines
\(|\langle F(z) | I(z) | \Omega(z) \rangle|\) that appear in Eq.(44) are discontinuous in \(\omega_N\), so that rarely the final energy is equal to the initial energy plus \(\omega_N\) \((E_{FN}^k(z) = E_{\Omega N}^k(z) + \omega_N)\). If the numerical approach for \(\Lambda = 1\) were possible, there would be the continuous limit, where the energy levels of the conduction bands would originate a dense spectrum for those lines. However, in this limit \((\Lambda \to 1)\) the computational costs would be infinite. To recover the continuous limit the continuous parameter \(z\) in the discretization process of the conduction bands was introduced. The continuous limit is obtained averaging in \(z\) the conductivity \(\sigma(\omega_N, z)\) given by Eq.(44). The function \(\delta(\Phi(z)) = \delta(E_{FN}^k(z) - E_{\Omega N}^k(z) - \omega_N)\) can be written in terms of the roots \(z_i\) of \(\Phi(z)\):

\[
\delta[\Phi(z)] = \sum_i \delta(z - z_i) \frac{d\Phi}{dz} \bigg|_{z=z_i}.
\]

The average \(\bar{\sigma}(\omega_N)\) in \(z\) of the function \(\sigma(\omega_N, z)\), given by \(\bar{\sigma}(\omega_N) = \int_{z_a}^{z_b} \sigma(\omega_N, z) dz / \Delta z\), with \(\Delta z = z_a - z_b\), represents the continuous spectrum of the electric conductivity, that is written as

\[
\bar{\sigma}(\omega_N) = \frac{\pi}{\omega_N} \sum_i \frac{|\langle F(z_i) | I(z_i) | \Omega(z_i) \rangle|^2}{\left[1 + \frac{\Lambda - 1}{2} \Lambda^{-(N-1)/2}\right]^2} \frac{1}{\left| \frac{d\Phi}{dz} \right|_{z=z_i}}.
\]

4 Results and discussion

In this section the results of the charge transference \(\tau\) as a function of \(U\), the charge average \(\langle Q_N \rangle\) as a function of \(V_{ext}\), the quadratic charge average \(\langle Q_N^2 \rangle\) and the specific heat \(C_V\) as a function of the temperature \(T\), and the electrical current \(\sigma(\omega)\) are shown.

To verify the precision of the calculation, we present in Fig.(1) the results of the charge transference \(\langle \tau \rangle = 2 \langle \hat{f}_{0z}^\dagger \hat{g}_0^z \rangle\) as a function of \(V_T\) (the tunnelling matrices element), in the fundamental state, calculated by the NRG (black circles) and the exact result obtained from the Green’s function equation of motion (full line). In the limit of \(V_T \to 0\), \(\tau\) is null, since in this limit the two conduction bands are decoupled. For large \(V_T\), the orbitals \(f_{0z}\) and \(g_{0z}\) are strongly coupled, disconnected from the remain of the conduction bands. In this case the Hamiltonian \(H_N\) is reduced to two decoupled conduction bands with two energy levels, one below the base and the other above the top of the conduction bands, forming ligating and antiligating states, \((f_{0z}^\dagger - g_{0z}^\dagger) | 0 \rangle / \sqrt{2}\) and \((f_{0z}^\dagger + g_{0z}^\dagger) | 0 \rangle / \sqrt{2}\), respectively, with \(2 \langle \hat{f}_{0z}^\dagger \hat{g}_0^z \rangle \to 1\). From Fig.(1) it can be noticed that the analytical and NRG results are in very good agreement, with an error less than 2%.
The results of $\langle \tau \rangle$ as a function of $U/D$ calculated by NRG (black circles) and by second order perturbation theory in $V_T$ (full line), for three cases: $V_T = 0.01D$, $V_T = 0.1D$ and $V_T = 0.3D$ are shown in Fig.(2). For small $V_T$, the second order perturbation theory developed in Appendices A, given by

$$\langle \tau \rangle = -2V_T \ln \frac{U^U(2+U)^{(2+U)}}{(1+U)^{2(1+U)}},$$

is in good agreement with NRG calculation. However, for large $V_T$, the perturbation theory results are precarious, mainly for small $U$.

The parameters $V_L$ and $V_R$, corresponding to the scattering potentials of the localized charges in the mesoscopic junction, are introduced in Fig.(3), taking $V_T = 0.3D$ and $V_L = -V_R = 0, 0.1D$ and $0.2D$. The NRG shows that the scattering potentials reduce the charge transference, with more prominent effect for small $U$.

The NRG results for $\langle Q \rangle$ as a function of $eV_{ext}/U$, taking $V_L = V_R = 0$, $U = 0.1D$ and $V_T = 0.01D$ are shown in Fig.(4). For zero temperature, the stairs, with steps spaced by $U/e$, is associated with the quantization of the charge transference in the mesoscopic junction. As $Q = e(N_L - N_R)/2$, the difference between the number of particles in the two metals assumes integer values due to the effect of the charge quantization in the tunnelling process. The thermal excitation smooths the stairs as is shown in the results for $k_B T = 0.02D$ (traced-point line) and $k_B T = 0.005D$ (traced line). At high temperatures the thermal excitations mask the Coulomb blockade effect, reducing the spectrum of the charge as a function of the external potential to a straight line. The introduction of the scattering potential $V_L = -V_R = 0.2D$ reduces the width of the steps, due the electron-hole excitations that are created when an electron pass from one side to the other of the mesoscopic junction. This result suggests that the electron-hole excitations can reduce the Coulomb blockade, by the renormalization of the parameter $U$ that, for these values of $V_L$ and $V_R$, assumes the reduced value $U^* = 0.881U$. For $V_L \neq V_R$, as is shown in Fig.(6), the results present an asymmetry in the charge of the junction as a function of the applied external potential.

In Fig.(7) is shown the quadratic charge average $\langle Q^2 \rangle$ as a function of $T$ for $V_T = 0.1D$, $V_L = V_R = 0$ and different values of $U$. For fixed $U$, $\langle Q^2 \rangle$ increases with the temperature due the thermal fluctuation. Even for temperature zero, there is $\langle Q^2 \rangle \neq 0$ originated from the quantum fluctuations in consequence of the tunnelling from one side to the other side of the junction. The introduction of the scattering potentials $V_L$ and $V_R$ modify the quantum fluctuation, reflecting in the quadratic charge average, as it is shown in Fig.(8).

In the analysis of the charge of the junction as a function of the external potential we have observed that the Coulomb potential $U$ is reduced by the effect of the electron-hole pairs excitation, originated from the scattering potentials $V_L$ and $V_R$, decreasing the effect of the Coulomb blockade. From the calculation of the specific heat it is found out that the tunnelling matrices $V_T$ also renormalize the potential $U$. The specific heat is shown in Figs.(9 and 10). As now we wish
to analysis only the effect of the tunnelling matrices $V_T$ on the renormalization of $U$, we will consider the scattering potential $V_L = V_R = 0$. In Fig.(9) is shown the specific heat $C_V/k_B$ as a function of $T$ for $V_T = 0.01D$ and different values of $U$, $U = 0.1D, 0.3D$ and $0.5D$. The results can be analyzed in terms of a simple two-level system. According to the Eqs. (6 and 7), the electrostatic energy of the junction is $U(N_L - N_R)^2/4$, so that when there is an excess electron, the energy of the junction is $\Delta = U/4$. In the limit of $V_T = 0$, the model reduces to two decoupled conduction bands, separated by an energy barrier $\Delta$. On the other hand, at the other extreme, when $V_T$ is very large, the two conduction bands are strongly coupled by the term $V_T(f^\dagger_0 g_{0z} + g^\dagger_{0z} f_0)$, as is represented in Eq.(18). In this limit, the orbitals $f_{0z}$ and $g_{0z}$ are disconnected from the two conduction bands and the system reduces to two decoupled conduction bands, with two located states below the base and above the top of the conduction bands, identified as $(f^\dagger_{0z} \pm g^\dagger_{0z})/\sqrt{2}$, where the signals $-$ and $+$ represent the ligant and anti-ligant states, respectively. Again the system is reduced to two bands separated by an energy barrier $\Delta$. In those two extremes, free bands and strongly coupled bands, the specific heat is given by the specific heat of two energy levels separated by $\Delta$. In Fig.(9) the full line represent $C_V/k_B$ of a two level system separated by an energy $U/4$, which is in very good agreement with the NRG results for small $V_T = 0.01D$.

In Fig.(10) $C_V/k_B$ as a function of $T$ for a fixed $U = 0.2D$ and different values of $V_T = 0.2D, 0.3D, 0.4D, 0.5D$ and $0.6D$ are shown. The results obtained from the NRG calculation are perfectly fitted by the specific heat of a two level system separated by an effective Coulomb potential $U^*/4$. The renormalized $U^*$ as a function of $V_T$ is presented in Fig.(11), which shows that $U^* \rightarrow U$ in the limit of small and high $V_T$, corresponding to the regimes of decoupled and strongly coupled conduction bands, respectively.

The electrical conductivity is determined by the Kubo formula and is shown in Fig.(12) as a function of the frequency $\omega$, for the Coulomb energy $U = 0.01D$, the scattering potential $V_L = V_R = 0$, and three values of the tunnelling matrices element $V_T = 0.05D, 0.10D$ and $0.15D$, with the energy scaled by $U$ and the conductivity scaled by the conductivity $G_0$ for the limit of $\omega \rightarrow \infty [5]$, given by

$$G_0 = \frac{e^2}{h} \frac{\pi^2 (V_T/D)^2}{(1 + (\pi V_T/2D)^2)^2}. \quad (51)$$

The rate $G/G_0$ tends to the unit limit as $\omega/U \gg 1$ and drops to zero when $\omega/U \rightarrow 0$, as is pointed out in the inset of Fig.(12). In contrast with the classical behavior, where there is conductivity only for $\omega/U > 1$, here there is conductivity through the junction also for energy lower than the Coulomb gap ($\omega/U < 1$), due to the quantum fluctuations that introduces uncertainty in the charge of the junction, as is shown in the inset of Fig.(12). We also verify that the conductivity is an universal function of $\omega/U$ (not shown in the figure), depending only on $V_T$. The effect of the scattering potential $V_L$ and $V_R$ is to reduce the conductivity, as it is shown in Fig.(13) for $V_T = 0.1D, U = 0.01D$ and three different values of $V_L$ and $V_R$. 

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5 Conclusion

In this work we have studied the static and dynamic properties of a mesoscopic junction, by using NRG to calculate the charge transference in the fundamental state, the charge average and the quadratic charge average, the specific heat and the electric conductivity of the junction.

For $V_T/D \gg 1$ the orbitals $f_{0z}$ and $g_{0z}$ are decoupled from their conduction bands, forming the states $(f_{0z}^{\dagger} - g_{0z}^{\dagger}) |0\rangle / \sqrt{2}$ and $(f_{0z}^{\dagger} + g_{0z}^{\dagger}) |0\rangle / \sqrt{2}$, and the charge transference $2 \langle f_{0z}^{\dagger} g_{0z} \rangle \rightarrow 1$. For any value of $V_T/D$, the charge transference is reduced by the scattering potential $V_L$ and $V_R$. The charge average $\langle Q \rangle$ as a function of the external potential $V_{ext}$ presents a stairs spectrum, suggesting the charge quantization. The width of the steps is equal to $U$ for $V_L = V_R = 0$, and is reduced by the effect of the electron-hole pairs excitations for $V_L = V_R \neq 0$. For different values of $U$, the results have shown that, even for zero temperature, quadratic charge average $\langle Q^2 \rangle \neq 0$, as a consequence of the quantum fluctuations in the junction. The calculation of the specific heat discloses that the junction can be represented by a system of two energy levels separated $U^*$, that depends on the tunnelling matrices element $T$. In the limit of $V_T = 0$ or $V_T \rightarrow \infty$, $U^* = U$, since in these limits the two conduction bands are decoupled. For intermediate values of $V_T$, $U^*$ varies between zero and $U$. The electrical conductivity as a function of the frequency was obtained from the Kubo formula. The quantum fluctuations originate electrical conductivity different of zero, even for energies less then $U$, in contrast with the classical behavior, where the electrical conductivity is zero for energies less then $U$. The scattering potentials $V_L$ and $V_R$ introduce electron-hole pairs excitations near the Fermi level, reducing the conductivity of the junction for all frequency scales. The formalism developed in the present work can be extended for Hamiltonians that represent other models of mesoscopic junction, as for instance metallic islands or quantum dot, with several tunnelling canals.
A Second order perturbation theory in $V_T$

In this Appendices we have used the second order perturbation theory in $V_T$ to calculate analytically the quadratic charge average and the charge transference in the fundamental state for the Hamiltonian $H_N$ given by Eq.(18), considering $V_L = V_R = 0$. In this case the Hamiltonian $H_N$ is written as

$$H_N = H_N^0 + H_N^T,$$

where

$$H_N^0 = \Lambda^{(N-1)/2} \left\{ \sum_{n=0}^{N-1} \varepsilon_{nz} \left( f_{nz}^\dagger f_{(n+1)z} + f_{(n+1)z}^\dagger f_{nz} \right) + \sum_{n=0}^{N-1} \varepsilon_{nz} \left( g_{nz}^\dagger g_{(n+1)z} + g_{(n+1)z}^\dagger g_{nz} \right) + U Q_N^2 \right\}$$

$$H_N^T = \Lambda^{(N-1)/2} V_T \left( f_{0z}^\dagger g_{0z} + g_{0z}^\dagger f_{0z} \right),$$

where $H_N^T$ is treated as a perturbation. The charge transference $\langle \tau \rangle$ and the quadratic charge average $\langle Q^2 \rangle$ in the fundamental state are given by

$$\langle Q^2 \rangle = \frac{\partial}{\partial U} \langle \Omega | H | \Omega \rangle$$

$$\langle \tau \rangle = \frac{1}{2} \frac{\partial}{\partial V_T} \langle \Omega | H | \Omega \rangle,$$

where $H$ is given by Eq.(23).

The reduced energy of the fundamental state is

$$\langle \Omega | H_N | \Omega \rangle = E_{\Omega,N}^0 + \sum_F \frac{|\langle F | H_N^T | \Omega \rangle|^2}{E_{F,N}^0 - E_{\Omega,N}^0},$$

where $|\Omega \rangle (|F \rangle)$ is the many particles fundamental (excited) satate of $H_N^0$, before (after) the tunnelling event, with reduced energy $E_{\Omega,N}^0 (E_{F,N}^0)$. Following Wilson [31], the many particles states are constructed from many one body states, whose energy levels are given by

$$\eta_{\ell} = \pm \Lambda^{\ell-1} \quad \text{for } N \text{ odd}$$

$$\tilde{\eta}_{\ell} = \pm \Lambda^{\ell-1/2} \quad \text{for } N \text{ even}$$

In the fundamental sate $|\Omega \rangle$ all the energy levels of the two conduct bands below (above) the Fermi level are occupied (empty). In the final state $|F \rangle$, after the tunnelling, an electron is transfered from the level $m$ of the left conduction
band, below the Fermi level, to level $\ell$ of the right conduction band, above the Fermi level, with energy given by
\[ E_{F,N}^0 = E_{\Omega,N}^0 + \eta_\ell + |\eta_m| + \Lambda^{(N-1)/2} \tilde{U}. \] (60)

The operators $f_{0z}$ and $g_{0z}$ are written in terms of the operators $a_k$ and $b_k$, which diagonalize the left and right conduction bands, respectively, as follows
\[ f_{0z} = \Lambda^{(N-1)/4} \sum_{k=-J}^{J} \alpha_{0k} a_k \] (61)
\[ g_{0z} = \Lambda^{(N-1)/4} \sum_{k=-J}^{J} \alpha_{0k} b_k \] (62)
where
\[ \alpha_{0k} = \alpha_0 \Lambda^{(k-1)/2} \] (63)
\[ \alpha_0 = \left( \frac{1 - \Lambda^{-1}}{2} \right)^{1/2} \] (64)
and $J = (N+1)/2$. Substituting the Eqs. (61 e 62) into the Eq. (54), and the result inserted into the Eq. (57), with $E_{F,N}^0$ given by Eq. (60), we obtain
\[ \langle \Omega | H_N | \Omega \rangle = E_{\Omega,N}^0 - 2 V_T^2 \Lambda^{(N-1)/2} \tilde{V}_T \sum_{m=1}^{J} \sum_{\ell=1}^{J} \frac{\Lambda^{-(N-1)/2} \alpha_{0m} \alpha_{0\ell}}{\eta_\ell + \eta_m + \Lambda^{(N-1)/2} \tilde{U}^2}, \] (65)

To obtain $\langle \Omega | H | \Omega \rangle$, we multiply both the members of the Eq. (65) by the factor $\frac{\Lambda^{1/2} - \Lambda^{-(N-1)/2}}{2}$, with $\eta$ and $\alpha_0$ given by the Eqs. (58 and 63), respectively. In the limit of $\Lambda \rightarrow 1$, $\langle \Omega | H | \Omega \rangle$ is written as
\[ \langle \Omega | H | \Omega \rangle = E_{\Omega}^0 - 2 V_T^2 \ln \left[ \frac{U^2 + (2+U)^2}{(1+U)^2(1+U)} \right]. \] (66)

From the Eqs. (55, 56 and 66) we finally have
\[ \langle Q^2 \rangle = -2 V_T^2 \ln \left[ \frac{U^2 + (2+U)^2}{(1+U)^2} \right] \] (67)
\[ \langle \tau \rangle = -2 V_T \ln \left[ \frac{U^2 + (2+U)^2}{(1+U)^2(1+U)} \right]. \] (68)
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FIGURE CAPTIONS

Figure 1. Charge transference as a function of $V_T/D$, for $U = V_L = V_R = 0$. The full line represents the exact solution using the Green's function equation of motion; the black circles are the results of NRG calculation, considering the discretization parameter $\Lambda = 3$.

Figure 2. Charge transference as a function of $U/D$, taking $V_L = V_R = 0$. The full lines represent the results of the second order perturbation theory in $V_T$ and the black circles are the results obtained from the NRG for $\Lambda = 3$.

Figure 3. Charge transference as a function of $U/D$, for $V_T = 0$. The full lines represent the results of the second order perturbation theory in $V_T$ and the black circles are the results obtained from the NRG for $\Lambda = 3$.

Figure 4. The stairs bahavior of the charge of the junction as a function of $V_{ext}$, for $V_T = 0$, $U = 0$, $V_L = V_R = 0$, and three different temperatures. The quantization of the charge and the width of the stairs equal to $U$, which is smoothed by the temperature, are shown.

Figure 5. Charge of the junction as a function of $V_{ext}$, for a symetric junction with $V_T = 0$, $U = 0$, $V_L = V_R = 0$, and three different temperatures. The width of the steps is $U^* = 0.881U$, which is reduced by the effect of the electron-hole pairs excitation due to the scaterring potential.

Figure 6. Charge transference as a function of $V_{ext}$ fo an assymetric junction with $V_L = 0.2D$, $V_R = -0.1D$, $V_T = 0.01D$, $U = 0.1D$ and three values of the temperature.

Figure 7. The square charge average $\langle Q^2 \rangle$ as a function of the temperature, for $V_T = 0.1D$, $U = 0.1D$, $V_L = V_R = 0$, and several values of $U$. The values $\langle Q^2 \rangle$ tend for a finite values in the limit of $T = 0$, due to the quantum fluctuations in the fundamental state.

Figure 8. The square charge average $\langle Q^2 \rangle$ as a function of the temperature $T$, for $V_T = 0.1D$, $U = 0.2D$ and several values of $V_L$ and $V_R$.

Figure 9. The specific heat as a function of $T$ without Coulomb scattering, for small $V_T$ and several values of $U$. The full line represents the specific heat for a two level system separated by $U/4$.

Figure 10. The specific heat as a function of $T$ for $U = 0.2D$ and several values of $V_T$. The full line represents the specific heat for a two level system, separated by $U/4$ renormalized by the $V_T$ tunnelling matrice.

Figure 11. From the fitting of the NRG results for specific heat by the results of a two-level system we have verified that the capacitor energy $U$ is renormalized by the tunnelling matrice $V_T$ as is shwon in this figure. $U^* \rightarrow U$ in the limits of $V_T = 0$ and $V_T \rightarrow \infty$, since the two bands are decoupled in these two limits.
Figure 12. Electrical conductivity $G$ scaled by $G_0$ (conductivity for large frequency) as a function of the frequency $\omega$ scaled by $U$, without Coulomb scattering, with $U = 0.01$ and several values of $V_T$.

Figure 13. Electrical conductivity $G$ scaled by $G_0$ (conductivity for large frequency) as a function of the frequency $\omega$ scaled by $U$, with Coulomb scattering, with $V_T = 0.1D$, $U = 0.01$ and several values of $V_L$ and $V_R$. 
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