

Single Quantum Dot as Electronic Rectifier Due to Asymmetric Coupling Interaction

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In this research we present extended theoretical study for electron transport through a quantum dot embedded between two normal leads. We model this quantum dot as single impurity (with two energy levels) to study the electron tunneling process through it, the system under consideration is taken out of equilibrium by induced temperature gradient. Its occupation numbers and tunneling current are formulated as a function of all important "chemisorption" functions that related to the tunneling process. Our treatment allows for the tunneling current through the quantum dot to be calculated depending on the spin-dependent occupation numbers. Our theoretical formulation is applied to study the thermoelectric transport through a quantum dot. The symmetrical and asymmetrical coupling between the quantum dot and leads are studied and investigated to explore the existence of electronic rectification.

Keywords: Anderson model, Quantum dot, Thermoelectric effects

النقطة الكمية كمقوم الكتروني بسبب تفاعل الاقتران اللا متناظر

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المخلص

تم تقديم دراسة نظرية موسعة لنقل الكترون خلال نقطة كمية موصولة بقطبين غير مغناطيسيين. لقد تم نمذجة النقطة كميّة كشائبة مفردة (بمستويي طاقة) لدراسة عملية نفق الإلكترون خلالها، النظام المفترض في حالة انعدام الاتزان بسبب انحدار درجات الحرارة. أعداد الإشغال العائدة لها وتيار النفق تم صيغتهما رياضياً كدالة لكل دوال "الاتصاق الكيميائي" المهمة التي تتعلق بعملية النفق. معالجتنا تتيح لنا حساب تيار النفق خلال النقطة الكمية بالاعتماد على أعداد الإشغال المعتمدة على البرم. صيغتنا الرياضية طبقت لدراسة النقل الكهروحراري خلال النقطة الكمية. حيث تم دراسة وفحص الاقتران المتناظر واللا متناظر بين النقطة الكمية والاقطاب لاستكشاف وجود التقويم الالكتروني.

الكلمات المفتاحية: نموذج اندرسون، النقطة الكمية، التأثيرات الكهروحرارية.

1. Introduction

It is obvious for researchers in the nanotechnology field the required accuracy for studying any subject deals with nanostructures and the importance of the connection of any theoretical treatment with the corresponding experiments. Recently, thermal transport properties of various nanoscale devices have gained considerable attention experimentally and theoretically [1]. Most of the theoretical treatments that deal with the thermal transport do not take into consideration the spin degree of freedom. These cases are experimentally viable due to advances in the

fabrication of nanostructures. The electron transport mechanism throughout a quantum dot embedded between two leads will be formulated when the system is in or out equilibrium.

2. Theoretical Treatment

The single "quantum dot" Anderson model [2] describes a single quantum dot modeled as two energy levels with a local interaction which leads to a hybridization with the left and right leads that enables tunneling process (see Fig.(1)). The local quantum dot energy level with spin up E_{dot}^{σ} is separated from the leads by Coulomb barriers through which electrons can

tunnel. The tunneling strength is determined by the hybridization matrix elements $V_{k\alpha}^\sigma$ with $\alpha = L, R$. The spin down level is separated from the spin up level by the intra-quantum dot Coulomb energy U .

The system Hamiltonian can be divided into three parts [2],

$$H = H_{QD} + H_{leads} + H_{coupling} \quad (2)$$

where, H_{QD} is given by,

$$H_{QD} = \sum_{\sigma} E_{dot}^{\sigma} n_{dot}^{\sigma} + U n_{dot}^{\uparrow} n_{dot}^{\downarrow} \quad (3)$$

This Hamiltonian describes the isolated quantum dot, the first term denotes the energy of electrons on the level E_{dot}^{σ} measured with respect to the chemical potentials (Fermi energies at $T_{\alpha} = 0K$) of the leads. In the presence of temperature gradient that is applied between the leads (by imposing some temperature difference ($\Delta T = T_L - T_R$) the leads chemical potential positions are shifted from each other by $\Delta\mu = \mu_L - \mu_R$ (note that if $\Delta T > 0$ this leads to $\Delta\mu > 0$ and vice versa), where σ indicates the spin of an electron. The second term accounts for the local Coulomb repulsion U on the dot and it is only non-zero if the dot is occupied by both electrons, the occupation number $n_{dot}^{\sigma} (= d^{\sigma\dagger} d^{\sigma})$ $n_{dot}^{\sigma} (= d^{\sigma\dagger} d^{\sigma})$ denoted by where $d^{\sigma\dagger} (d^{\sigma})$ is the creation (annihilation) operator of a localized electron in the level E_{dot}^{σ} .

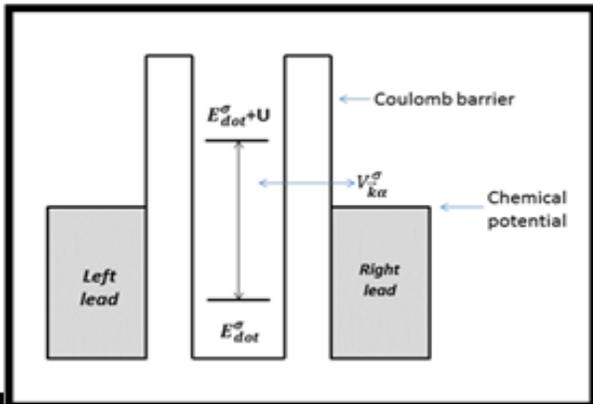


Fig.(1): Single “quantum dot” Anderson Model in the equilibrium case, where $\mu_L = \mu_R$

And, H_{leads} is the Hamiltonian that describes the lead,

$$H_{leads} = \sum_{\alpha=L,R} \sum_{k\sigma} E_{k\sigma}^{\sigma} c_{k\sigma}^{\sigma\dagger} c_{k\sigma}^{\sigma} \quad (4)$$

where, $c_{k\sigma}^{\sigma\dagger} (c_{k\sigma}^{\sigma})$ is the creation(annihilation) operator of the electron, while \vec{k} indicates its wave vector, with spin σ and energy $E_{k\sigma}^{\sigma}$. The coupling part $H_{coupling}$ is given by,

$$H_{coupling} = \sum_{\alpha} \sum_{k\sigma} (V_{k\alpha}^{\sigma} c_{k\alpha}^{\sigma\dagger} d^{\sigma} + V_{k\alpha}^{\sigma*} c_{k\alpha}^{\sigma} d^{\sigma\dagger}) \quad (5)$$

this describes the coupling interaction between the dot and the leads levels which is given by the hybridization matrix element,

$$V_{k\alpha}^{\sigma} = \langle \phi_{dot}(r) | H | \psi_{\vec{k}} \rangle \quad (6)$$

where, ϕ_{dot} is the wave function describing the dot and $\psi_{\vec{k}}$ the wave function of the lead α electron with wave vector \vec{k} . The lead work function φ_{α} as a function of T_{α} , is given by[3],

$$\varphi_{\alpha} = \varphi_0 (1 - 0.0833(\pi k_B T_{\alpha} / \varphi_0)^2 - 0.0125 (\pi k_B T_{\alpha} / \varphi_0)^4 + \dots) \quad (7)$$

So the difference between φ_L and φ_R is $\Delta\varphi = \varphi_L - \varphi_R$, the energy reference $E = 0$ is fixed on μ_L . Notably, in the case where $T_L \neq T_R$, $\Delta\mu$ can be considered as a bias voltage due to cooling the right lead (i.e. lowering its temperature with respect to left one $\Delta T > 0; \Delta\mu > 0$). The energies of spin-up and spin-down states can take the following form [4],

$$E_{dot}^{\sigma} = E_{dot} + U_{eff} n_{dot}^{-\sigma}, \quad (8)$$

where, $n_{dot}^{\pm\sigma}$ are the spin-up and spin-down occupation numbers of QD energy levels. E_{dot} represents the quantum dot energy level in the absence of the leads. U_{eff} is the effective Coulomb correlation on the quantum dot [5]. The similarity between quantum dots and isolated atoms becomes particularly striking in the case of spherical quantum dots, i.e. when the confining potential has spherical symmetry. Then, the quantum dot eigen values are calculated by using the following formula [6],

$$\varepsilon_{nl} = \hbar^2 / 2m^* (\chi_{nl} / R_{dot})^2, \quad n = 1, 2, 3, \dots, \quad l = 0, 1, 2, \dots \quad (9)$$

where, m^* is the effective mass of the electron at the conduction band minimum, which is $0.067m_0$ for GaAs, where m_0 is the free electron mass. The coefficients χ_{nl} are the zeros of spherical Bessel function labeled by integer n in order to increasing energy. The levels can be labeled with usual atomic notation. The quantum dot energy level is broadened by the electron tunneling to and from it due to the presence of the leads. This broadening is determined by calculating the coupling matrix elements $V_{k\alpha}^-$ (eq.(6)). We consider the wide band approximation where the quantum dot energy levels broadening Δ_α^σ does not depend on the system energy. So, according to the wide band approximation Δ_α^σ is given by [7],

$$\Delta_\alpha^\sigma(T_\alpha) = \frac{N_{F\alpha}\gamma_{dot}^{\sigma 2}}{16V_{0\alpha}R_{dot}} \sqrt{2V_{0\alpha} - \gamma_{dot}^{\sigma 2}} \left(1 + \frac{1}{2R_{dot}\gamma_{dot}^\sigma} \right) \quad (10)$$

with R_{dot} represents quantum dot radius, $\gamma_{dot}^\sigma = \sqrt{2E_{dot}^\sigma}$ (in a.u.) and $N_{F\alpha}$ denotes normalization factor (for more details see[23], which is proportional to $V_{0\alpha} (= |u_{0\alpha}| + \varphi_\alpha)$, where $u_{0\alpha}$ is the band bottom of the leads and φ_α is the work function of the lead α . For certain spin, the level broadening is given by [9],

$$\Delta^\sigma = \Delta_L^\sigma + \Delta_R^\sigma \quad (11)$$

U represents intra-QD Coulomb repulsion for isolated QD. In the presence of the two leads, the effective electron-electron interaction U_{eff} must be taken into account which should be formulated in a manner that includes all the quantum dot and leads properties [10]. In order to point out the importance of Coulomb correlation effect on the electron quantum tunneling through the quantum dot, we use Schrieffer and Mattis [11] formula which is given by,

$$U_{eff} = U / (1 + U \Pi(0)) \quad (12)$$

and

$$\Pi(0) = (\pi(E_{dot}^\sigma + E_{dot}^{-\sigma}))^{-1} \begin{pmatrix} \tan^{-1}(E_{dot}^\sigma / \Delta^\sigma) \\ -\tan^{-1}(E_{dot}^{-\sigma} / \Delta^{-\sigma}) \end{pmatrix} \quad (13)$$

Note that , $\Pi(0)$ depends explicitly on the quantum dot energy levels positions and their broadening and implicitly on their occupation numbers. Calculations of U_{eff} by using eq.(12) and Δ^σ by using eq.(11) help us to characterize the weak and strong cases of couplings. Due to the Fermions behavior at low temperatures, our model calculation can be divided into two ranges of the temperatures, the low range and the ultra-low range of temperatures.

2.1 The case of the low range of temperature

In general, the occupation numbers of the quantum dot depend on the local density of states on the quantum dot $\rho_{dot}^\sigma(E)$ (which is obtained from the imaginary part of the retarded Green function $\rho_{dot}^\sigma(E) = -(1/\pi) \text{Im}(G^r(E))$) and the Fermi distribution functions of the leads $f_\alpha(E - \mu_\alpha, T)$. It is well known that the function $\rho_{dot}^\sigma(E)$ dependence on energy is related to the range of temperatures, while Fermi distribution function is valid for all temperatures [12-14]. The occupation number n_{dot}^σ for the quantum dot levels coupled to the leads can be calculated from this formula [15,16],

$$n_{dot}^\sigma = \frac{1}{2} \sum_{\alpha=L,R} \int_{u_{0\alpha}}^{\varphi_\alpha} \rho_{dot}^\sigma(E) f_\alpha(E - \mu_\alpha, T_\alpha) dE \quad (14)$$

$\rho_{dot}^\sigma(E)$ is the density of states on the quantum dot,

$$\rho_{dot}^\sigma(E) = -\frac{1}{\pi} \text{Im} \frac{1}{(E - E_{dot}^\sigma - \sum_{dot}^\sigma(E))} \quad (15)$$

with,

$$\sum_{dot}^\sigma(E) = -i\Delta^\sigma(E) + \Lambda^\sigma(E) \quad (16)$$

and for wide band limit approximation we have,

$$\rho_{dot}^\sigma(E) = (1/\pi)(\Delta^\sigma / (E - E_{dot}^\sigma)^2 + \Delta^{\sigma 2}) \quad (17)$$

and,

$$f_\alpha(E - \mu_\alpha, T_\alpha) = 1 / (1 + e^{(E - \mu_\alpha) / k_B T_\alpha})$$

By using μ_α as an energy reference for the lead α we define,

$$\varepsilon = E - \mu_\alpha \text{ and } \varepsilon_{do}^\sigma = E_{dot}^\sigma - \mu_\alpha$$

The integration in eq.(14) is solved analytically. Then, n_{dot}^σ is reduced to the following expression,

$$n_{dot}^\sigma = \frac{1}{2\pi} \sum_{\alpha=L,R} \sum_{i=1}^5 C_{i,\alpha}^\sigma I_{i,\alpha}^\sigma \quad (18)$$

Where the functions $C_{i,\alpha}^\sigma$ and $I_{i,\alpha}^\sigma$ are listed in the Table (1).

Table (1) shows $C_{i,\alpha}^\sigma$ and $I_{i,\alpha}^\sigma$

i	$C_{i,\alpha}^\sigma$ (no units)	$I_{i,\alpha}^\sigma$ (no units)
1	-1	$\tan^{-1} \frac{u_{0\alpha} - E_{dot}^\sigma + \mu_\alpha}{\Delta^\sigma}$
2	$1 - \gamma_{1\alpha}^\sigma + \Delta^{\sigma^2} \gamma_{3\alpha}^\sigma$	$\tan^{-1} \frac{-k_B T_\alpha - E_{dot}^\sigma}{\Delta^\sigma}$
3	$\gamma_{1\alpha}^\sigma - \Delta^{\sigma^2} \gamma_{3\alpha}^\sigma$	$\tan^{-1} \frac{k_B T_\alpha - E_{dot}^\sigma}{\Delta^\sigma}$
4	$\frac{\Delta^\sigma}{2} \gamma_{2\alpha}^\sigma - \frac{\Delta^{\sigma^3}}{2} \gamma_{4\alpha}^\sigma$	$\ln \frac{(k_B T_\alpha - E_{dot}^\sigma)^2 + \Delta^{\sigma^2}}{(-k_B T_\alpha - E_{dot}^\sigma)^2 + \Delta^{\sigma^2}}$
5	$2\Delta^\sigma k_B T_\alpha (\gamma_{3\alpha}^\sigma - \gamma_{4\alpha}^\sigma E_{dot}^\sigma)$	1

Where, the functions $\gamma_{i\alpha}^\sigma$ are given by,

$$\begin{aligned} \gamma_{1\alpha}^\sigma &= A_{0\alpha} + A_{1\alpha} (E_{dot}^\sigma - \mu_\alpha) + A_{3\alpha} (E_{dot}^\sigma - \mu_\alpha)^3 \\ \gamma_{2\alpha}^\sigma &= A_{1\alpha} + 3A_{3\alpha} (E_{dot}^\sigma - \mu_\alpha)^2 \\ \gamma_{3\alpha}^\sigma &= 3A_{3\alpha} (E_{dot}^\sigma - \mu_\alpha) \\ \gamma_{4\alpha}^\sigma &= A_{3\alpha} \end{aligned} \quad (19)$$

Note that, the units of γ_i^σ function is $1/(eV)^{i-1}$ for $1 \leq i \leq 4$ and $A_{i\alpha}$ are the Taylor expansion coefficients for Fermi distribution function about $\varepsilon = 0$ in the interval $(-k_B T_\alpha \leq \varepsilon \leq k_B T_\alpha)$. So, in order to calculate the occupation numbers n_{dot}^σ and all the related functions (i.e. the levels broadening, Coulomb interaction and the quantum dot energy levels positions), eq.(8) and eq.(18) must be solved self consistently for all values of the required parameters.

The thermoelectric current I^σ flowing through the QD is given by the following formula [15],

$$I^\sigma = \frac{e}{h} \int_{u_{0\alpha}}^{\varphi_\alpha} \pi \Delta^\sigma \rho_{dot}^\sigma(E) (f_L(E - \mu_L, T_L) - f_R(E - \mu_R, T_R)) dE \quad (20)$$

by comparing the integral in eq.(14) with the integral in eq.(20) we can formulate eq.(20) as [8],

$$I^\sigma = (e\Delta^\sigma / \hbar) (n_{dot,L}^\sigma - n_{dot,R}^\sigma) \quad (21)$$

From eq.(21), it is obvious that the current is related to the occupation numbers of the quantum dot energy levels as well as their broadening. So, the total current is given by

$$I = \sum_\sigma I^\sigma \quad (22)$$

2.2 The case of the ultra-low range of temperatures

It has been shown in Ref.[17] that for the single impurity Anderson Hamiltonian the susceptibility and the electric resistivity at low temperature can be written in terms of two physical quantities $\tilde{\chi}_{\uparrow\uparrow}^\sigma$ and $\tilde{\chi}_{\uparrow\downarrow}^\sigma$. This fact holds also for other physical quantities such as the density of states that localized on the impurity,

$$\rho_d(E) = \frac{1}{\pi \Delta} \left[1 - \left(\frac{E}{\Delta} \right)^2 (\tilde{\chi}_{\uparrow\downarrow}^2 + \tilde{\chi}_{\uparrow\uparrow}^2) - \frac{1}{2} \frac{\pi^2 T^2}{\Delta^2} \tilde{\chi}_{\uparrow\downarrow}^2 \right] \quad (23)$$

with, $(E/\Delta) \ll 1$

The local susceptibility explain as the two body scattering [18]. The above $k_i \uparrow$ and $k_i \downarrow$ represent the system energy states. As we know, the full expression for the local susceptibility can be expressed in various forms [18]. For small U_{eff}/Δ^σ , it is most usefully expressed in the form of power series

$$\chi_{dot}^\sigma = \frac{(g\mu_B)^2}{2\pi\Delta^\sigma} \sum_{n=0} C_n \left(\frac{U}{\pi\Delta^\sigma} \right)^n \quad (24)$$

Where the coefficients satisfy the recurrence relation,

$$C_n = (2n-1)C_{n-1} - (0.5\pi)^2 C_{n-2} \quad (25)$$

With, $C_0 = C_1 = 1$. Notably, the coefficients up to C_4 correspond to the fourth order perturbation[5],

$$\chi_{dot}^\sigma = (g\mu_B)^2 \tilde{\chi}_{dot}^\sigma / 2\pi\Delta^\sigma \quad (26)$$

Where, $\tilde{\chi}_{dot}^\sigma$ is the local susceptibility of quantum dot.

$\tilde{\chi}_{dot}^\sigma$ can be written as sum of two parts $\tilde{\chi}_{\uparrow\uparrow}^\sigma$ and $\tilde{\chi}_{\uparrow\downarrow}^\sigma$ which for small U limit can be written as[19],

$$\tilde{\chi}_{\uparrow\uparrow}^\sigma = 1 + \left(3 - \frac{\pi^2}{4} \right) \left(\frac{U_{eff}}{\pi\Delta^\sigma} \right)^2 + 0.051 \left(\frac{U_{eff}}{\pi\Delta^\sigma} \right)^4 \quad (27)$$

$$\tilde{\chi}_{\uparrow\downarrow}^\sigma = \frac{U_{eff}}{\pi\Delta^\sigma} + \left(15 - \frac{3\pi^2}{2} \right) \left(\frac{U_{eff}}{\pi\Delta^\sigma} \right)^2 \quad (28)$$

Note that, $\tilde{\chi}_{\uparrow}^{\sigma}$ is represented by terms with even power and $\tilde{\chi}_{\downarrow}^{\sigma}$ is represented by terms with odd power. Accordingly, the dimensionless values of the spin and charge susceptibilities [20] can be expressed respectively as,

$$\tilde{\chi}_s^{\sigma} = \tilde{\chi}_{\uparrow}^{\sigma} + \tilde{\chi}_{\downarrow}^{\sigma} \quad (29)$$

$$\tilde{\chi}_c^{\sigma} = \tilde{\chi}_{\uparrow}^{\sigma} - \tilde{\chi}_{\downarrow}^{\sigma} \quad (30)$$

Similarly, the occupation numbers can be written as,

$$n_{dot}^{\sigma} = \frac{1}{2} \sum_{\alpha=L,R} \int_{u_{0\alpha}}^{-k_B T_{\alpha} - \mu_{\alpha}} \rho_{dot}^{\sigma} d\varepsilon + \int_{-k_B T_{\alpha} - \mu_{\alpha}}^{k_B T_{\alpha} - \mu_{\alpha}} \rho_{dot,LET}^{\sigma}(\varepsilon) f_{\alpha}(\varepsilon, T_{\alpha}) d\varepsilon \quad (31)$$

Where, $\rho_{dot,LET}^{\sigma}(\varepsilon)$, is the density of states of the quantum dot at low energy and low temperature, can be written as,

$$\rho_{dot,LET}^{\sigma}(\varepsilon) = (k_{1\alpha}^{\sigma} - k_2^{\sigma}(\varepsilon - \mu_{\alpha})^2) \quad (32)$$

$$k_{1\alpha}^{\sigma} = \frac{1}{\pi \Delta^{\sigma}} - \frac{\pi(k_B T_{\alpha})^2}{2\Delta^{\sigma^3}} \chi_{\uparrow\downarrow}^{\sigma^2} \quad (33)$$

$$k_2^{\sigma} = (0.5\chi_{\uparrow\downarrow}^{\sigma^2} + \chi_{\uparrow\uparrow}^{\sigma^2}) / \pi \Delta^{\sigma^3} \quad (34)$$

By evaluating the integrals in eq.(31), n_{dot}^{σ} is reduced to the following expression,

$$n_{dot}^{\sigma} = \frac{1}{2\pi} \sum_{\alpha=L,R} \left(\tan^{-1} \frac{-k_B T_{\alpha} - E_{dot}^{\sigma}}{\Delta^{\sigma}} - \tan^{-1} \frac{u_{0\alpha} - E_{dot}^{\sigma} + \mu_{\alpha}}{\Delta^{\sigma}} \right) + \frac{1}{2} \sum_{\alpha=L,R} \sum_{j=1}^6 \frac{1}{j} \beta_{j\alpha}^{\sigma} \left((k_B T_{\alpha} - \mu_{\alpha})^j - (-k_B T_{\alpha} - \mu_{\alpha})^j \right) \quad (35)$$

Where, the functions $\beta_{j\alpha}^{\sigma}$ are given by,

$$\begin{aligned} \beta_{1\alpha}^{\sigma} &= (k_{1\alpha}^{\sigma} - k_2^{\sigma} \mu_{\alpha}^2) A_{0\alpha} \\ \beta_{2\alpha}^{\sigma} &= (k_{1\alpha}^{\sigma} - k_2^{\sigma} \mu_{\alpha}^2) A_{1\alpha} - 2k_2^{\sigma} A_{0\alpha} \\ \beta_{3\alpha}^{\sigma} &= -2k_2^{\sigma} A_{0\alpha} - k_2^{\sigma} A_{1\alpha} \\ \beta_{4\alpha}^{\sigma} &= (k_{1\alpha}^{\sigma} - k_2^{\sigma} \mu_{\alpha}^2) A_{3\alpha} - k_2^{\sigma} A_{1\alpha} \\ \beta_{5\alpha}^{\sigma} &= -2k_2^{\sigma} \mu_{\alpha} A_{3\alpha} \\ \beta_{5\alpha}^{\sigma} &= -k_2^{\sigma} A_{3\alpha} \end{aligned} \quad (36)$$

The current through quantum dot at ultralow temperatures can also be calculated from eq.(21) and

the occupation numbers must be calculated using eq.(35).

3. Results and Conclusions

In this paper, we will apply our theoretical formulation to study the quantum electron tunneling due to temperature gradient in the asymmetrical coupling between the quantum dot and leads, i.e. $\Delta_R^{\sigma} = 0$ while $\Delta_R^{-\sigma}$ and $\Delta_R^{\pm\sigma}$ are calculated according to eq.(10). The temperature T_L is firstly fixed at 100K while T_R is varied from 200K to 0K, i.e. cooling the right lead with respect to the left one (see Fig.(1)). ϕ_L and ϕ_R are calculated using eq.(6), so μ_L is constant and equals to 0.0eV. This means that we use the temperature difference $T_L - T_R$ to control the difference in the chemical potentials. E_{dot} is calculated by using eq.(9) and it is equal to $(-5.1203eV)$ (measured with respect to vacuum level), since its radius $R_{dot} = 4.8nm$ and μ_0 is equal to 5.1eV for golden lead. The bottom of energy band $u_{0\alpha} = u_{0R} = u_{0L} = 15.1eV$, this value corresponds to a flat band. In order to get the occupation numbers $n_{dot}^{\pm\sigma}$ of the quantum dot energy levels $E_{dot}^{\pm\sigma}$ in the low temperature range, eqs.(8), (10), (12) and (18) are solved self consistently. While, equations (8), (10), (12) and (35) are solved self consistently for the ultralow temperature range. As the charge transport is accomplished through the quantum dot by cooling right lead with respect to the left one, all the functions calculated in our treatment will be presented as a function of $\Delta\mu$. The occupation numbers of the quantum dot energy levels and all the "chemisorption functions" as well as the tunneling current are presented in Fig.(2) and Fig.(3) for the cases of coupling $U = 0.16eV$ and $U = 0.0016eV$ respectively. From Fig.(2a), it is visible that n_{dot}^{σ} increases as T_L decreases while $n_{dot}^{-\sigma}$ increases as T_L increases (i.e. T_R decreases). Therefore, in the region of $(\Delta\mu = -)$ for $(T_R > T_L)$, this difference in temperature implies a higher occupation possibility for electrons in the right lead to enter the E_{dot}^{σ} level of the QD, i.e. resulting in a higher n_{dot}^{σ} and lesser $n_{dot}^{-\sigma}$ due to the strong Coulomb correlation. In contrast, in the region of

($\Delta\mu = +$) for ($T_L > T_R$), the difference implies a lesser occupation possibility for electrons in the left lead to enter the E_{dot}^{σ} level of the QD due to the asymmetric coupling ($\Delta_R^{\sigma} = 0$, while $\Delta_R^{-\sigma} \neq 0$), i.e. resulting in a lower n_{dot}^{σ} and higher $n_{dot}^{-\sigma}$ for the same reason. The positions of the quantum dot levels with respect to $\mu_L (= 0)$ are presented in Fig.(2b). The physical features in Fig.(2a) are in agreement with that in Fig.(2b). As E_{dot}^{σ} lies below the energy reference $\mu_L = 0$, it is nearly constant as compared with $E_{dot}^{-\sigma}$ which lies above the energy reference. So $E_{dot}^{-\sigma}$ decreases with cooling. The spin up and spin down broadening functions are shown in Fig.(2c). It is clear that $\Delta^{-\sigma} > \Delta^{\sigma}$, since the energy level of spin up coincides with occupied energy levels in the left and the right leads while the energy level of spin down coincides with empty energy levels in the left and right leads. Writing final conclusion about the broadening functions is not easy because the calculation of Δ^{σ} depends implicitly on $\Delta^{-\sigma}$ calculation and vice versa. Fig.(2d) represents the Coulomb correlation variation with $\Delta\mu$ where $U_{eff} > \Delta^{\pm\sigma}$ for all values of $\Delta\mu$. This determines the weak coupling regime, in which the energy level E_{dot}^{σ} is nearly occupied and $E_{dot}^{-\sigma}$ is nearly empty. One can conclude that in this regime U_{eff} decreases with cooling. It is obvious from eq.(21) that the current can be easily calculated, where its direction can be determined by its sign. As we cool the right lead with respect to the left one, then the tunneled electron will transport from the left lead to the right one. This tunneling is due to temperature gradient, accordingly one can call this current as thermoelectric tunneling current. The calculated current is presented in Fig.(2e) where I is increasing with cooling. The negative sign of the current indicates that the direction of tunneling is from the right to the left one. However, $I = 0$, in the case of equilibrium where there is no temperature gradient. The components of the current I^{σ} and $I^{-\sigma}$ give us good idea about the spin polarization due to cooling (see Fig.(2f)). $I^{-\sigma} > I^{\sigma}$ for $T_L < T_R$ while $I^{\sigma} > I^{-\sigma}$ for $T_L > T_R$, while $I^{\sigma} = I^{-\sigma} = 0$ at

$\Delta\mu = 0$. The current $I^{-\sigma}$ vanishes because the occupation numbers for this spin are nearly zero. Hence, the total current I takes the same values of I^{σ} . From this figure, one can conclude that the variation of the right lead temperature T_R from heating to cooling changes the direction of the spin up contribution of the current. The direction of the spin down contribution is also changed but in the opposite to that of the spin up one.

Similarly, we also choose U to be equal to 0.0016eV and our results are presented in a similar manner. Fig.(3a) and Fig.(3b) show the occupation numbers of the quantum dot energy levels and the position of the energy level with respect to $\mu_L (= 0)$ respectively, both have the same behavior with $\Delta\mu$. The type of solution is magnetic where $n_{dot}^{\sigma} \neq n_{dot}^{-\sigma}$ for all values of $\Delta\mu$. Fig.(3c) and Fig.(3d) represent the broadening functions and Coulomb correlation as a function of $\Delta\mu$, where $\Delta^{\pm\sigma} > U_{eff}$ for all values of $\Delta\mu$. The behavior of the thermoelectric current and its contributions as a function of the chemical potentials difference are represented in Figs.(3e) and (3f). It seems in Fig.(3e) that the charge current increases with the temperature difference induced bias voltage only in the positive direction ($\Delta\mu > 0$) and it is blocked in the opposite direction. Note that this strong asymmetric behavior is found for small U , i.e. $U = 0.0016eV$. This indicates the occurrence of certain rectification in charge current, it may considered as electronic rectification due to temperature gradient. The results motivate us to formulate, the thermal rectification which is also formulated and investigated, this will be our future paper.

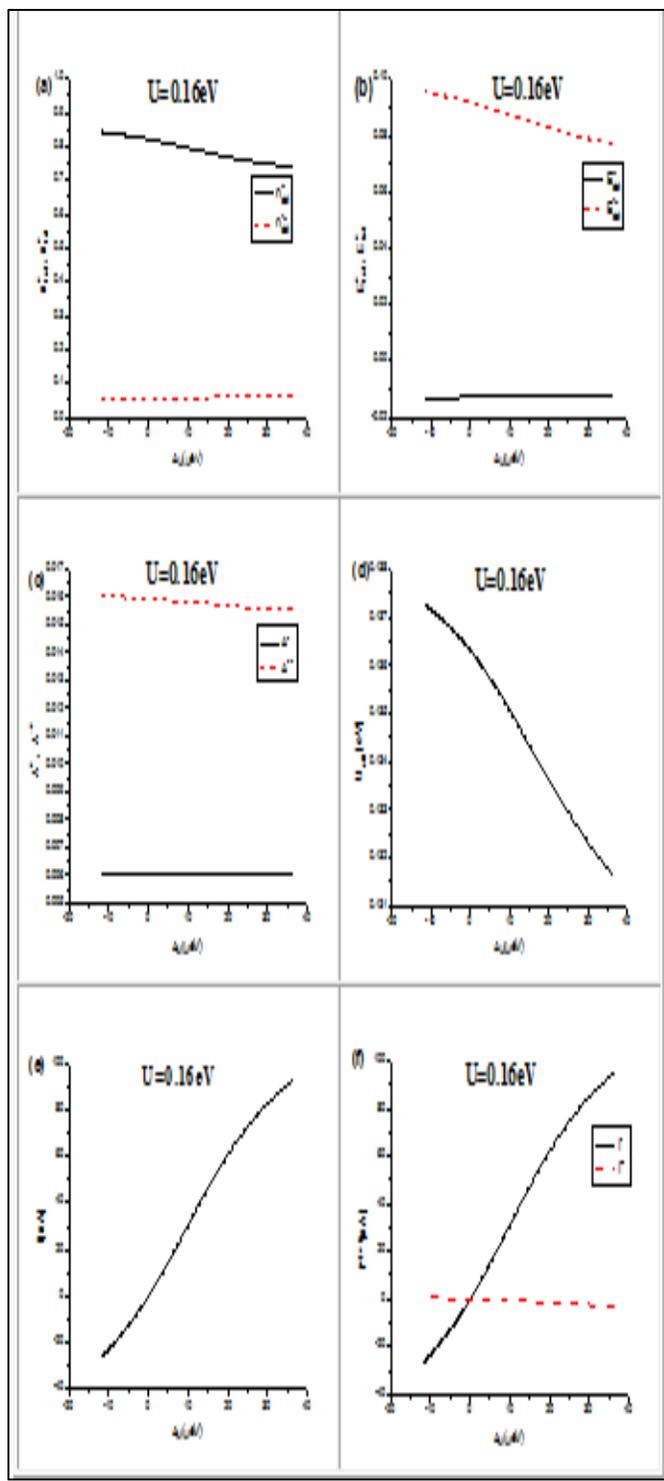


Fig.(2)

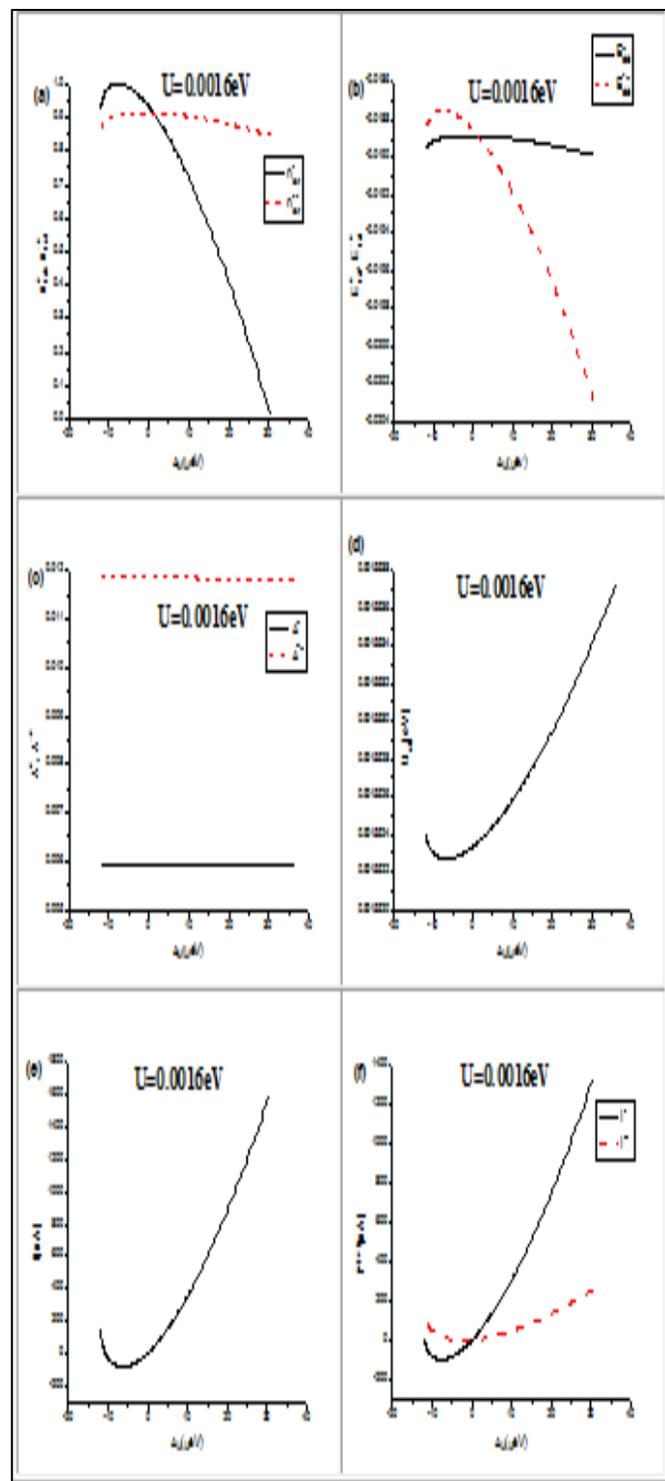


Fig.(3)

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