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Electron Tunneling Through a Quantum Dot Induced by Temperature Gradient: Weak and Strong Coupling Cases

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Abstract

An extended theoretical study for electron transport through a quantum dot embedded between two normal leads is presented; the system under consideration is taken out of equilibrium by induced temperature gradient. We model this quantum dot as single impurity (with two energy levels) to study the electron tunneling process through it. Its occupation numbers and tunneling current are formulated as a function of all important "chemisorption" functions that are 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. The related relations which are spin-dependent are solved self-consistently to calculate the quantum dot energy levels and their occupation numbers and broadenings as well as the correlation energy. The weak and strong coupling regimes will be studied and discussed extendedly.

Keywords: Anderson model, Quantum dot, Thermoelectric effects.

1. Introduction

It is obvious for researchers in the nanotechnology field is that 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 works on thermal transport through a quantum dot attached to external leads have focused on:

1. The linear thermopower in sequential and cotunneling regimes [2,3].
2. The strongly correlated Kondo-type transport regime[4,5].
3. The quantum interference effect in the thermopower in QD ring [6,7].
4. The heat conduction through molecular chains connecting two electrodes at different temperature [8].

Notably, 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 is formulated when the system is in or out equilibrium. The system may be in the case of out equilibrium due to the temperatures gradient or bias voltage (see Fig.(1)). This case is studied to investigate the thermoelectric effects. Our treatment is based on the single impurity Anderson model, this model provides us with good descriptions for the charge and spin on the quantum dot for all cases. Our theoretical treatment is characterized by clear dependence of all the requirements functions and parameters considered in our work to describe the electron transport throughout the quantum dot.

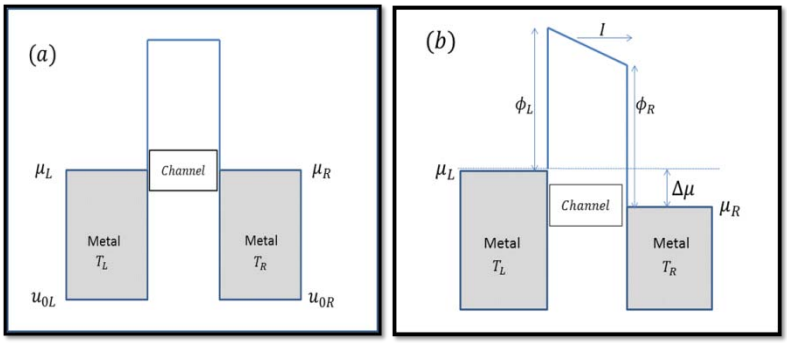


Fig.(1):Simple metal – channel – metal system in the case of (a): equilibrium (b):non-equilibrium.

2. Theoretical treatment

The single "quantum dot" Anderson model [9] 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 enable tunneling process (see Fig.(2)).

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

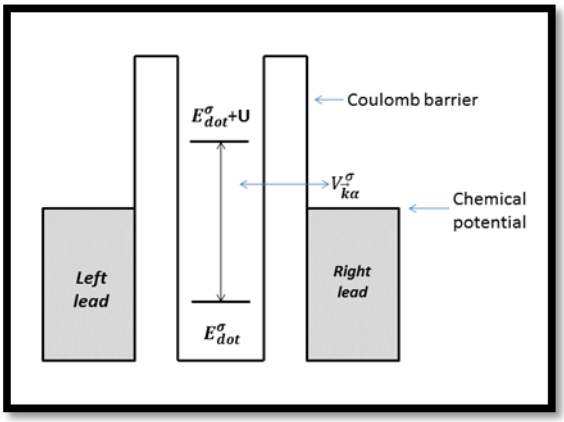


Fig. (2): Single "quantum dot" Anderson Model in the equilibrium case, where $\mu_L = \mu_R$.

The system Hamiltonian can be divided into three parts [9],

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

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 denoted by $n_{dot}^{\sigma} (= d^{\sigma\dagger} d^{\sigma})$ $n_{dot}^{\sigma} (= d^{\sigma\dagger} d^{\sigma})$ where $d^{\sigma\dagger} (d^{\sigma})$ is the creation (annihilation) operator of a localized electron in the level E_{dot}^{σ}.

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,

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

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

$$V_{\vec{k}\alpha} = < \phi_{dot}(r) | H | \psi_{\vec{k}} > \quad (6)$$

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[10],

$$\varphi_{\alpha} = \varphi_0 \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T_{\alpha}}{\varphi_0} \right)^2 - \frac{\pi^4}{80} \left(\frac{k_B T_{\alpha}}{\varphi_0} \right)^4 + ... \right] \quad (7)$$

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 the left one $\Delta T > 0; \Delta\mu > 0$).

The energies of spin-up and spin-down states can take the following form [11],

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

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 [12].

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 [13],

$$\varepsilon_{nl} = \frac{\hbar^2}{2m^*} \left(\frac{\chi_{nl}}{R_{dot}} \right)^2 \quad , \mathrm{n} = 1,2,3,... \quad , \mathrm{l} = 0,1,2,... \quad (9)$$

where, m^* is the effective mass of the electron at the conduction band minimum, which is $0.067 m_0$ 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 increase 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 $V_{\vec{k}\alpha}$ (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 [14],

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

with R_{dot} represents quantum dot radius, $\gamma_{dot}^{\sigma}=\sqrt{2E_{dot}^{\sigma}}$ (in a.u.) and $N_{F\alpha}$ denotes normalization factor, 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. Here, $N_{F\alpha}$ depends on the quantum dot and leads properties and is given by [14],

$$N_{F\alpha}=\frac{2\gamma_{dot}^{\sigma 3}e^{2R_{dot}\beta_{dot,\alpha}^{\sigma}}}{1+2(R_{dot}\gamma_{dot}^{\sigma})^{-1}+\frac{a}{b}c} \quad (11)$$

and

$$\beta_{dot,\alpha}^{\sigma}=\sqrt{V_{0\alpha}-E_{dot}^{\sigma}} \quad (\text{in a.u.}) \quad (12)$$

$$a=\gamma_{dot}^{\sigma}\left(1+\frac{1}{R_{dot}\gamma_{dot}^{\sigma}}\right)^2$$

$$b=\left(\frac{\sin(R_{dot}\beta_{dot,\alpha}^{\sigma})}{R_{dot}\beta_{dot,\alpha}^{\sigma}}-\cos(R_{dot}\beta_{dot,\alpha}^{\sigma})\right)^2 \quad (13)$$

$$c=\left(R_{dot}+\frac{\sin(2R_{dot}\beta_{dot,\alpha}^{\sigma})}{2\beta_{dot,\alpha}^{\sigma}}-\frac{2\sin^2(R_{dot}\beta_{dot,\alpha}^{\sigma})}{2R_{dot}\beta_{dot,\alpha}^{\sigma}}\right)$$

For certain spin, the level broadening is given by [15],

$$\Delta^\sigma=\Delta_L^\sigma+\Delta_R^\sigma \quad (14)$$

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 [16].In order to point out the importance of Coulomb correlation effect on the electron quantum tunneling through the quantum dot, we use Schrieffer and Mattias [17] formula which is given by,

$$U_{eff}=\frac{U}{1+U\,\Pi(0)} \quad (15)$$

And

$$\Pi(0)=\frac{1}{\pi(E_{dot}^{\sigma}+E_{dot}^{-\sigma})}\left(\tan^{-1}\frac{E_{dot}^{\sigma}}{\Delta^{\sigma}}-\tan^{-1}\frac{E_{dot}^{-\sigma}}{\Delta^{-\sigma}}\right) \quad (16)$$

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.(15) and Δ^σ by using eq.(14) which helps us to characterize two cases of couplings, these are,

1-Weak coupling, where $\Delta^\sigma < U_{eff}$, is also called strong Coulomb interaction.

2-Strong coupling, where $\Delta^\sigma > U_{eff}$, is also called weak Coulomb interaction.

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 $\rho^{\sigma}_{dot}(E)$ (which is obtained from the imaginary part of the retarded Green function $\rho^{\sigma}_{dot}(E) = -\frac{1}{\pi}\mathrm{Im}(G^{r}(E)))$ and the Fermi distribution functions of the leads $f_{\alpha}(E-\mu_{\alpha},T)$. It is well known that the function $\rho^{\sigma}_{dot}(E)$ dependence on energy is related to the range of temperatures, while Fermi distribution function is valid for all temperatures [18-20]. The occupation number n^{σ}_{dot} for the quantum dot levels coupled to the leads can be calculated from this formula [21,22],

$$n^{\sigma}_{dot} = \frac{1}{2}\sum_{\alpha=L,R}\int_{u_{0\alpha}}^{\varphi_{\alpha}} \rho^{\sigma}_{dot}(E)\, f_{\alpha}(E-\mu_{\alpha},T_{\alpha})dE \qquad (17)$$

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

$$\rho^{\sigma}_{d}(E) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{(E-E^{\sigma}_{dot}-\sum_{dot}(E)} \qquad (18)$$

with,

$$\sum_{dot}(E) = -i\Delta^{\sigma}(E) + \Lambda^{\sigma}(E) \qquad (19)$$

and for wide band limit approximation we have,

$$\rho^{\sigma}_{dot}(E) = \frac{1}{\pi}\frac{\Delta^{\sigma}}{(E-E^{\sigma}_{dot})^{2}+\Delta^{\sigma 2}} \qquad (20)$$

and,

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

By using μ_{α} as an energy reference for the lead α we define,

$\varepsilon = E-\mu_{\alpha}$ and $\varepsilon^{\sigma}_{do} = E^{\sigma}_{dot}-\mu_{\alpha}$

The integration in eq.(17) are solved analytically. Then, n^{σ}_{dot} is reduced to the following expression,

$$n^{\sigma}_{dot} = \frac{1}{2\pi}\sum_{\alpha=L,R}\sum_{i=1}^{5} C^{\sigma}_{i,\alpha} I^{\sigma}_{i,\alpha} \qquad (21)$$

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

Table (1) shows $C^{\sigma}_{i,\alpha}$ and $I^{\sigma}_{i,\alpha}$.

i	$C^{\sigma}_{i,\alpha}$ *(no units)*	$I^{\sigma}_{i,\alpha}$ *(no units)*
1	*-1*	$tan^{-1}\frac{u_{0\alpha}-E^{\sigma}_{dot}+\mu_{\alpha}}{\Delta^{\sigma}}$
2	$1-\gamma^{\sigma}_{1\alpha}+\Delta^{\sigma 2}\gamma^{\sigma}_{3\alpha}$	$tan^{-1}\frac{-k_{B}T_{\alpha}-E^{\sigma}_{dot}}{\Delta^{\sigma}}$
3	$\gamma^{\sigma}_{1\alpha}-\Delta^{\sigma 2}\gamma^{\sigma}_{3\alpha}$	$tan^{-1}\frac{k_{B}T_{\alpha}-E^{\sigma}_{dot}}{\Delta^{\sigma}}$
4	$\frac{\Delta^{\sigma}}{2}\gamma^{\sigma}_{2\alpha}-\frac{\Delta^{\sigma 3}}{2}\gamma^{\sigma}_{4\alpha}$	$ln\frac{(k_{B}T_{\alpha}-E^{\sigma}_{dot})^{2}+\Delta^{\sigma 2}}{(-k_{B}T_{\alpha}-E^{\sigma}_{dot})^{2}+\Delta^{\sigma 2}}$
5	$2\Delta^{\sigma}k_{B}T_{\alpha}(\gamma^{\sigma}_{3\alpha}-\gamma^{\sigma}_{4\alpha}E^{\sigma}_{dot})$	*1*

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

$$\gamma_{1\alpha} = A_{0\alpha}+A_{1\alpha}(E^{\sigma}_{dot}-\mu_{\alpha})+A_{3\alpha}(E^{\sigma}_{dot}-\mu_{\alpha})^{3}$$

$$\gamma^{\sigma}_{2\alpha} = A_{1\alpha}+3A_{3\alpha}(E^{\sigma}_{dot}-\mu_{\alpha})^{2} \qquad (22)$$

$$\gamma^{\sigma}_{3\alpha} = 3A_{3\alpha}(E^{\sigma}_{dot}-\mu_{\alpha})$$

$$\gamma^{\sigma}_{4\alpha} = A_{3\alpha}$$

Note that, the units of γ^{σ}_{i} function is $1/(eV)^{i-1}$ for $1\le i\le 4$ and $A_{i\alpha}$ are the Taylor expansion coefficients for Fermi distribution function about $\varepsilon = 0$ in the interval $(-k_{B}T_{\alpha}\le\varepsilon\le k_{B}T_{\alpha})$. So, in order to calculate the occupation numbers n^{σ}_{dot} and all the

related functions (i.e. the levels broadening, Coulomb interaction and the quantum dot energy levels positions), eq.(8) and eq.(20) 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 [21],

$$I^{\sigma} = \frac{e}{h}\int_{u_{0\alpha}}^{\varphi_{\alpha}} \pi\Delta^{\sigma}\rho_{dot}^{\sigma}(E)(f_L(E-\mu_L,T_L)-f_R(E-\mu_R,T_R))dE \quad (23)$$

by comparing the integral in eq.(17) with the integral in eq.(23) we can formulate eq.(23) as [23],

$$I^{\sigma} = \frac{e\Delta^{\sigma}}{\hbar}(n_{dot,L}^{\sigma} - n_{dot,R}^{\sigma}) \quad (24)$$

From eq.(24), 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

$$I = \sum_{\sigma} I^{\sigma} \quad (25)$$

2.2 The case of the ultra-low range of temperatures

It has been shown in Ref.[24] 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 is localized on the impurity,

$$\rho_d(E) = \frac{1}{\pi\Delta}\left[1-\left(\frac{E}{\Delta}\right)^2(\tilde{\chi}_{\uparrow\downarrow}^2+\tilde{\chi}_{\uparrow\uparrow}^2)-\frac{1}{2}\frac{\pi^2T^2}{\Delta^2}\tilde{\chi}_{\uparrow\downarrow}^2\right] \quad (26)$$

with, $\frac{E}{\Delta} << 1$

The local susceptibility explains as the two body scattering [25]. 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[25]. For small U_{eff}/Δ^{σ} , it is most usefully expressed in the form of power series

$$\chi_{dot}^{\sigma} = \frac{(g\mu_B)^2}{2\pi\Delta^{\sigma}}\sum_{n=0} C_n\left(\frac{U}{\pi\Delta^{\sigma}}\right)^n \quad (27)$$

Where the coefficients satisfy the recurrence relation,

$$C_n = (2n-1)C_{n-1} - \left(\frac{\pi}{2}\right)^2 C_{n-2} \quad (28)$$

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

$$\chi_{dot}^{\sigma} = \frac{(g\mu_B)^2}{2\pi\Delta^{\sigma}}\tilde{\chi}_{dot}^{\sigma} \quad (29)$$

Where, $\tilde{\chi}_{dot}^{\sigma}$ is the local susceptibility of quantum dot. $\tilde{\chi}_{dot}^{\sigma}$ can be written as the sum of two parts $\tilde{\chi}_{\uparrow\uparrow}^{\sigma}$ and $\tilde{\chi}_{\downarrow\uparrow}^{\sigma}$ which for small U limit can be written as[26],

$$\tilde{\chi}_{\uparrow\uparrow}^{\sigma} = 1+\left(3-\frac{\pi^2}{4}\right)\left(\frac{U_{eff}}{\pi\Delta^{\sigma}}\right)^2 + 0.051\left(\frac{U_{eff}}{\pi\Delta^{\sigma}}\right)^4 \quad (30)$$

$$\tilde{\chi}^{\sigma}_{\uparrow\downarrow} = \frac{U_{eff}}{\pi\Delta^{\sigma}} + \left(15 - \frac{3\pi^2}{2}\right)\left(\frac{U_{eff}}{\pi\Delta^{\sigma}}\right)^2 \qquad (31)$$

Note that, $\tilde{\chi}^{\sigma}_{\uparrow\uparrow}$ is represented by terms with even power and $\tilde{\chi}^{\sigma}_{\downarrow\uparrow}$ is represented by terms with odd power. Accordingly, the dimensionless values of the spin and charge susceptibilities [27] can be expressed respectively as,

$$\tilde{\chi}^{\sigma}_{c} = \tilde{\chi}^{\sigma}_{\uparrow\uparrow} + \tilde{\chi}^{\sigma}_{\downarrow\downarrow} \qquad (32)$$

$$\tilde{\chi}^{\sigma}_{c} = \tilde{\chi}^{\sigma}_{\uparrow\uparrow} - \tilde{\chi}^{\sigma}_{\downarrow\downarrow} \qquad (33)$$

Note that, we model all the relations in this section to include the spin. Similarly, the occupation numbers can be written as,

$$n^{\sigma}_{dot} = \frac{1}{2}\sum_{\alpha=L,R}\int_{u_{0\alpha}}^{-k_B T_\alpha - \mu_\alpha} \rho^{\sigma}_{dot}\, d\varepsilon + \int_{-k_B T_\alpha - \mu_\alpha}^{k_B T_\alpha - \mu_\alpha} \rho^{\sigma}_{dot,LET}(\varepsilon)\, f_\alpha(\varepsilon, T_\alpha)\, d\varepsilon \qquad (34)$$

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

$$\rho^{\sigma}_{dot,LET}(\varepsilon) = (k^{\sigma}_{1\alpha} - k^{\sigma}_{2}(\varepsilon - \mu_\alpha)^2) \qquad (35)$$

$$k^{\sigma}_{1\alpha} = \frac{1}{\pi\Delta^{\sigma}} - \frac{\pi(k_B T_\alpha)^2}{2\Delta^{\sigma 3}}\chi^{\sigma 2}_{\uparrow\downarrow} \qquad (36)$$

$$k^{\sigma}_{2} = \frac{0.5\chi^{\sigma 2}_{\uparrow\downarrow} + \chi^{\sigma 2}_{\uparrow\uparrow}}{\pi\Delta^{\sigma 3}} \qquad (37)$$

By evaluating the integrals in eq.(34), n^{σ}_{dot} is reduced to the following expression,

$$n^{\sigma}_{dot} = \frac{1}{2\pi}\sum_{\alpha=L,R}\left(\tan^{-1}\frac{-k_B T_\alpha - E^{\sigma}_{dot}}{\Delta^{\sigma}} - \tan^{-1}\frac{u_{0\alpha} - E^{\sigma}_{dot} + \mu_\alpha}{\Delta^{\sigma}}\right) + \frac{1}{2}\sum_{\alpha=L,R}\sum_{j=1}^{6}\frac{1}{j}\beta^{\sigma}_{j\alpha}\left((k_B T_\alpha - \mu_\alpha)^j - (-k_B T_\alpha - \mu_\alpha)^j\right) \qquad (38)$$

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

$$\begin{aligned}
\beta^{\sigma}_{1\alpha} &= (k^{\sigma}_{1\alpha} - k^{\sigma}_{2}\mu^2_\alpha)A_{0\alpha} \\
\beta^{\sigma}_{2\alpha} &= (k^{\sigma}_{1\alpha} - k^{\sigma}_{2}\mu^2_\alpha)A_{1\alpha} - 2k^{\sigma}_{2}A_{0\alpha} \\
\beta^{\sigma}_{3\alpha} &= -2k^{\sigma}_{2}A_{0\alpha} - k^{\sigma}_{2}A_{1\alpha} \\
\beta^{\sigma}_{4\alpha} &= (k^{\sigma}_{1\alpha} - k^{\sigma}_{2}\mu^2_\alpha)A_{3\alpha} - k^{\sigma}_{2}A_{1\alpha} \\
\beta^{\sigma}_{5\alpha} &= -2k^{\sigma}_{2}\mu_\alpha A_{3\alpha} \\
\beta^{\sigma}_{5\alpha} &= -k^{\sigma}_{2}A_{3\alpha}
\end{aligned} \qquad (39)$$

The current through quantum dot at ultralow temperatures can also be calculated from eq.(24) and the occupation numbers must be calculated using eq.(38).

3. Results

It is stated that the conduction depends on the availability of states around $E = \mu$, (see Fig.(1,a)), since the current increases once the energy level comes within the energy window between μ_L and μ_R. So, if we cool the right lead with respect to the left one so that $T_L > T_R$ (with no applied bias voltage and gate voltage), a thermoelectric current will flow in certain direction (see

Fig.(1,b)). Accordingly, Fermi distribution function for the leads can be

$$f_L(E-\mu_L,T_L)=\left[1+\exp(E/k_BT_L)\right]^{-1}$$

$$f_R(E-\Delta\mu,T_R)=\left[1+\exp(E-\Delta\mu/k_BT_R)\right]^{-1}$$

Where, the energy reference $E=0$ is fixed at μ_L. We will call this chemical potential difference $\Delta\mu$ in our treatment as temperature induced bias voltage (see Fig.(2,b)). 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 $5.1eV$ read as,

(40)

(41)

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),.(15) and (21) are solved self consistently. While, equations (8), (10), (15) and (38) are solved self consistently for the ultralow temperature range.

In order to study all the couplings regimes, four values of U are considered in our calculations. It is well known that the Coulomb repulsion U is determined by the size of the quantum dot, the smaller the dot the large is U .

3-1 Weak coupling regime

For this regime, U is chosen to be 0.25eV. 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 are presented in Fig.(3) as a function of the chemical potentials difference. The initial conditions can be read as, $n_{dot}^{\sigma}=1$ and $n_{dot}^{-\sigma}=0$.

Due to coupling with the leads, the occupations on the quantum dot levels as a function of $\Delta\mu$ are as in Fig.(3a), where $n_{dot}^{\sigma}<1$, and $n_{dot}^{-\sigma}>0$ and $n_{dot}^{\sigma}>n_{dot}^{-\sigma}$ for all values of $\Delta\mu$. This determines the type of solution, which is a magnetic one. By magnetic solution, we mean that there is a net spin on the quantum dot. The occupation numbers with spin $\sigma(-\sigma)$ are decreasing (increasing) slowly with $\Delta\mu$, where the positive value of $\Delta\mu$ corresponds to the case $T_L>T_R$ while, the negative value corresponds to the case $T_L<T_R$. The positions of the quantum dot levels with respect to $\mu_L(=0)$ are presented in Fig.(3b). The physical features in Fig.(3a) are in agreement with that in Fig.(3b). 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.(3c). 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.(3d) 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.(24) 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.(3e) 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.(3f)). $I^{-\sigma} > I^{\sigma}$ 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.

We also check another value for $U = 0.16eV$ in this regime. For this value, the solution is nonmagnetic where $n_{dot}^{\sigma} = n_{dot}^{-\sigma} = 0.5$ (see Fig.((4a)-(4b))). The values of $U_{eff} > \Delta^{\pm\sigma}$ for all values of $\Delta\mu$, but they are increasing with cooling (see Figs.(4c) and (4d). The total current and its components are shown in Figs.(4e) and (4f) respectively, where $I^{\sigma} = I^{-\sigma}$. This means that the thermoelectric current is spin independently.

3.2 Strong Coupling Regime

Similarly, we choose U to be equal to 0.0016eV and our results are presented in a similar manner. Fig.(5a) and Fig.(5b) 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 nonmagnetic where $n_{dot}^{\sigma} = n_{dot}^{-\sigma}$ for all values of $\Delta\mu$. Fig.(5c) and Fig.(5d) 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 conditions that make the system in the strong coupling regime are:

1-The type of solution is nonmagnetic.

2- $\Delta^{\pm\sigma} > U_{eff}$

The behavior of the thermoelectric current and its contributions as a function of the chemical potentials difference are represented in Figs.(5e) and (5f). The current I increases as $\Delta\mu$ increases. The increasing of the total current can be explained as increasing of the electronic tunneling through both the spin up and spin down levels.

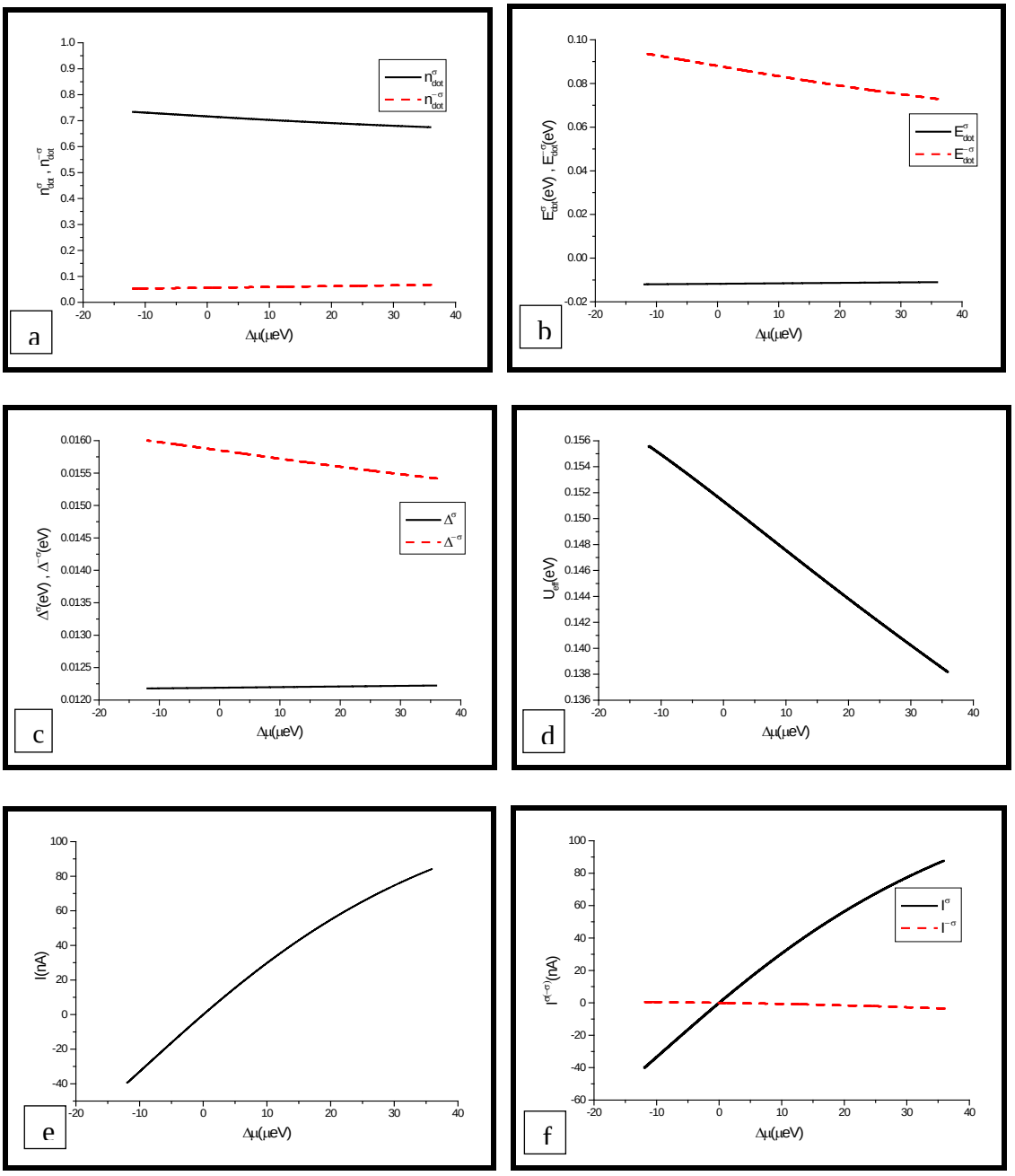
3-3 Intermediate Regime

For this regime, we choose U to be 0.016eV. From these calculations, we can report the following notes:

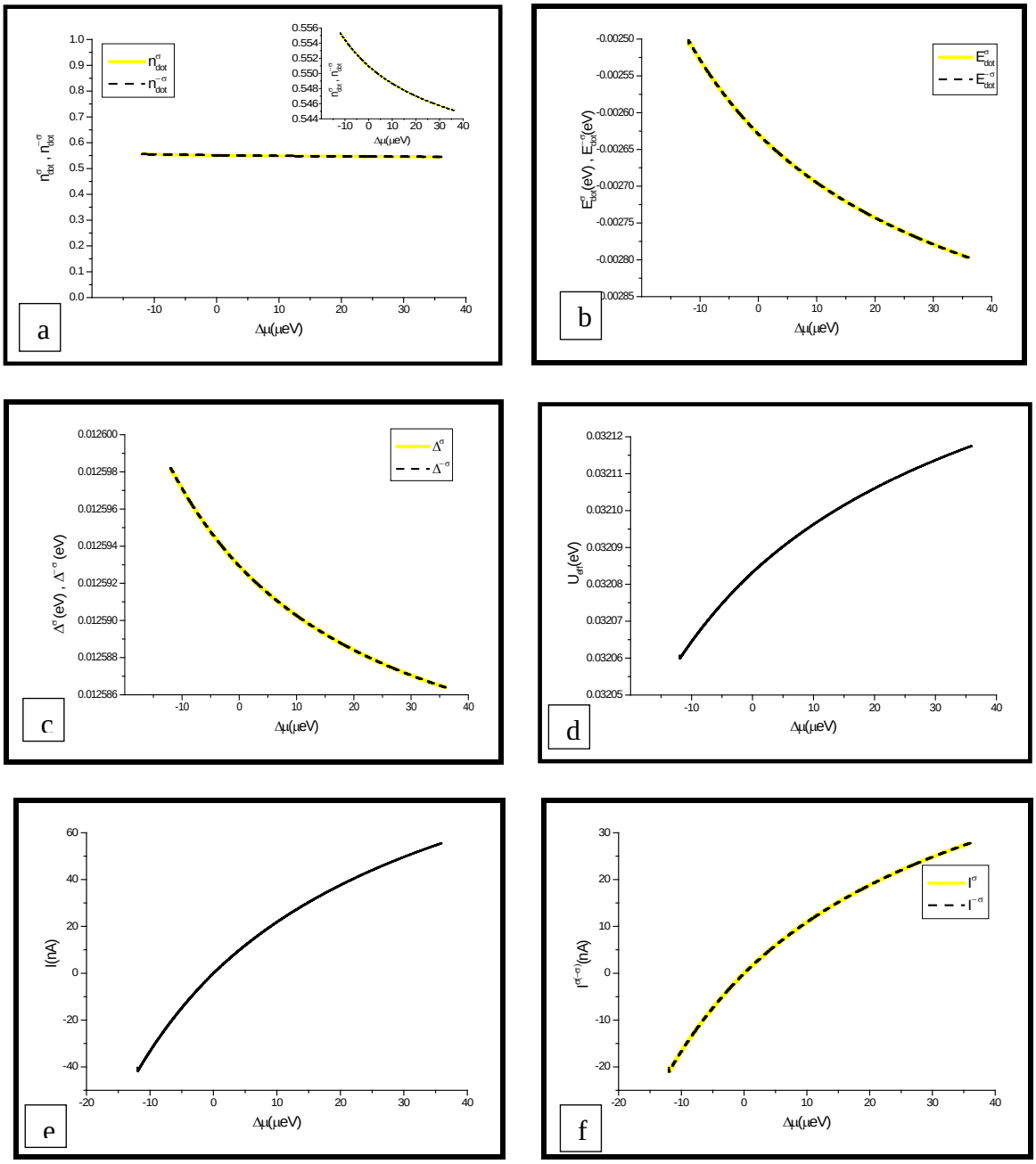
1- $n_{dot}^{\sigma} = n_{dot}^{-\sigma}$ for all values of $\Delta\mu$, this solution is nonmagnetic, i.e. there is no net spin on the quantum dot (see Fig.(6a)).
2- Both E_{dot}^{σ} and E_{dot}^{σ} are lying below the energy reference. Their positions are agreed with the high values of their occupations(see Fig.(6b)).
3- Figs.(6c) and (6d) show that U_{eff} is greater than $\Delta^{\pm\sigma}$ nearly for all values of $\Delta\mu$.
4- For the thermoelectric current calculation, we get the same behavior as in the case of strong coupling regime (see Figs.(6e) and (6f)).

It is concluded that in this regime, the solution is nonmagnetic and $\left|\Delta^{\pm\sigma} - U_{eff}\right|$ is small.

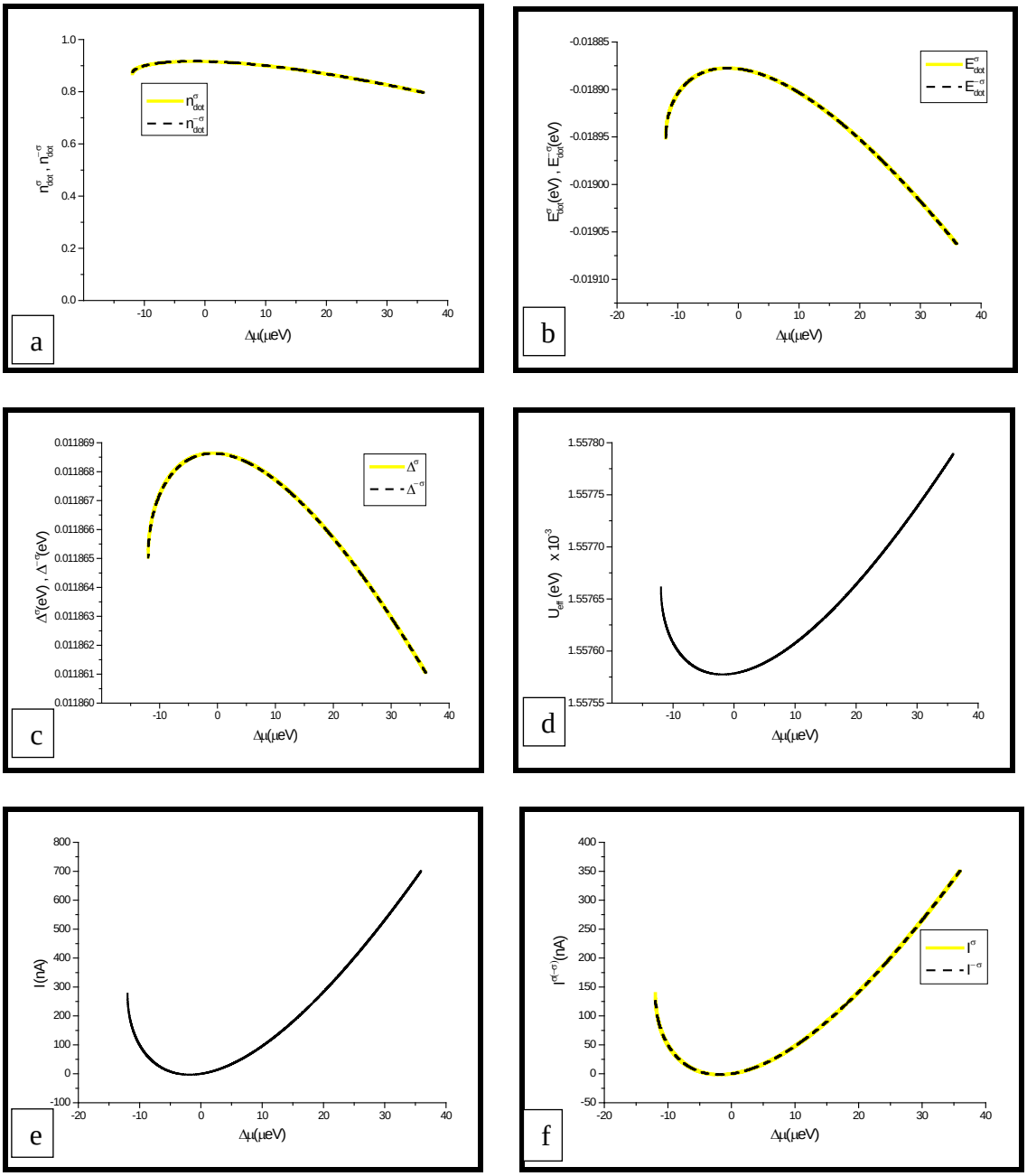
Accordingly, we conclude that the system considered in our model can be used as a spin filter in the weak coupling regime. And the results for $U = 0.16eV$ can also considered as intermediate regime. In general, our results are in agreement with many results be performed for the nanostructures and nanodevices. So, we can use our treatment to calculate the tunneling current throughout any devices whenever, the parameters chosen are coinciding with the electronic structure and phenomenological properties of the system.



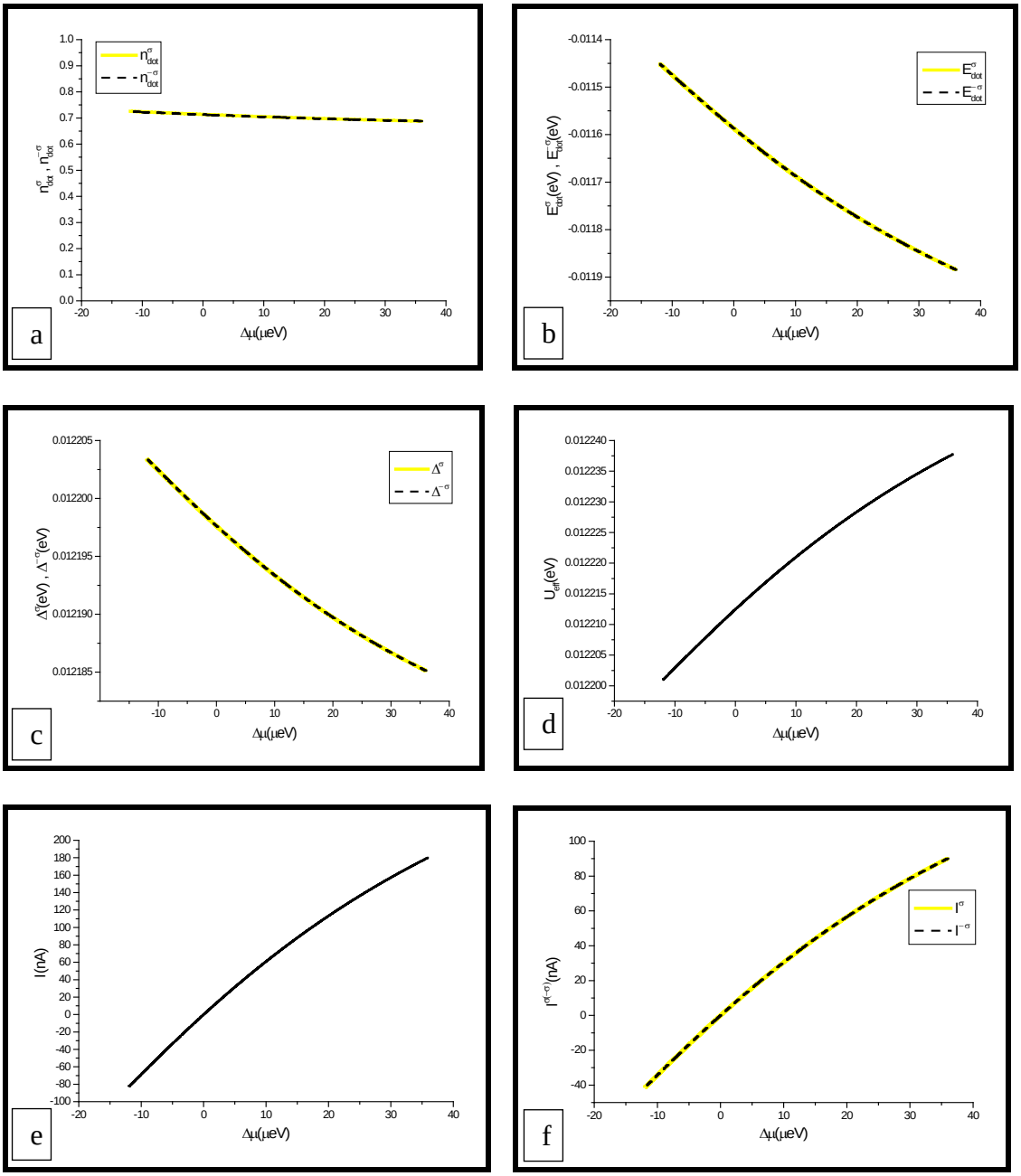
Figure(3):(a)The occupation numbers of quantum dot energy levels, (b) The quantum dot energy levels, (c) The broadening of the quantum dot energy levels, (d) The effective electron-electron interaction of quantum dot energy levels, (e) The current through a quantum dot and (f) The components of current $I^{\pm\sigma}$ through a quantum dot as a function of chemical potentials difference ,when U=0.25eV.



Figure(4):(a)The occupation numbers of quantum dot energy levels, (b) The quantum dot energy levels, (c) The broadening of the quantum dot energy levels, (d) The effective electron-electron interaction of quantum dot energy levels, (e) The current through a quantum dot and (f) The components of current $I^{\pm\sigma}$ through a quantum dot as a function of chemical potentials difference ,when U=0.16eV.



Figure(5):(a)The occupation numbers of quantum dot energy levels, (b) The quantum dot energy levels, (c) The broadening of the quantum dot energy levels, (d) The effective electron-electron interaction of quantum dot energy levels, (e) The current through a quantum dot and (f) The components of current $I^{\pm\sigma}$ through a quantum dot as a function of chemical potentials difference ,when U=0.0016eV.



Figure(6):(a)The occupation numbers of quantum dot energy levels, (b) The quantum dot energy levels, (c) The broadening of the quantum dot energy levels, (d) The effective electron-electron interaction of quantum dot energy levels, (e) The current through a quantum dot and (f) The components of current $I^{\pm\sigma}$ through a quantum dot as a function of chemical potentials difference ,when U=0.016eV.

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نفق الإلكترون خلال النقطة الكمية يحث بواسطة انحدار درجات الحرارة: حالات الاقتران الضعيف والقوي

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الملخص

تم تقديم دراسة نظرية موسعة لنقل الكترون خلال نقطة كمية موصولة بقطبين غير مغناطيسين للنظام المفترض في حالة انعدام الاتزان بسبب انحدار درجات الحرارة. لقد تم نمذجة النقطة الكمية كشائبة مفردة (بمستويا طاقة) لدراسة عملية نفق الإلكترون خلالها. اعداد الإشغال العائدة لها وتيار النفق تم صيغتهما رياضياً كدالة لكل دوال " الالتصاق الكيميائي" المهمة التي تتعلق بعملية النفق.معالجتنا تتيح لنا حساب تيار النفق خلال النقطة الكمية بالاعتماد على إعداد الإشغال المعتمدة على البرم. حيث تم حل العلاقات المتعلقة المعتمدة على البرم حلاً ذاتياً لحساب طاقة مستويات النقطة الكمية واعداد الإشغال ودوال التعريض و طاقة التبادل العائدة لها. لقد تمت دراسة نهج الاقتران الضعيف والقوي ومناقشته بصورة موسعة.

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