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The Electron Transport Through Strongly Coupled Double Quantum Dots : Effect of Spin Exchange Interaction

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Abstract
We introduce model calculation for the electron transport through a system consists of two serially coupled quantum dots, embedded between two nonmagnetic leads (source and drain). In our treatment, the time independent Anderson-Newns Hamiltonian model is considered as a basis to study the system dynamics and then to derive spin-dependent analytical formula to calculate the occupation numbers of the quantum dots energy levels, the corresponding quantum dots energy levels and the molecular virtual energy levels, as a function of bias voltage. These relations are solved self-consistently, which are all employed to calculate the tunneling current considering the strong coupling regime. The differential conductance is calculated numerically by using finite differences method. And as the efficiency of electron transport through coupled quantum dots depends on the system parameters, the effective exchange energy is highlighted and studied in details and the role of this parameter in the tunneling current and the differential conductance calculations is presented. Our treatment is utilized to study the following The role of the spin exchange interaction in determining the type of interaction (if it is attractive or repulsive) between the quantum dots. For all values of exchange energy less than $0.2\ \mathrm{eV}$, the bias voltage between the two resonance peaks is equal to $V_{12}+\Gamma_{i\alpha}^{\pm\sigma}+J$. This result is very important to determine the Nano device feature that depends in its operation on two serially coupled quantum dots.

1-Introduction

The electron transport through double quantum dots structure has been the subject of many experimental and theoretical studies during the past few years [1-3]. In particular, a lot of interest and experimental techniques were developed to discover and control double quantum dot systems. A double quantum dots connected in series and coupled to external leads is one of great interest due it possibility of using this kind of systems in quantum computer hard ware, with applications in optical spin manipulation spintronics, spin memories and transistors [4]. The transport properties of the two quantum dots depend on the strength of the inter-dot coupling between the quantum dots, since the weak tunnel coupling between QDs can form ionic like bond, while the strong tunnel coupling can form covalent like bond. In the weak coupling, the electrons are localized in individual quantum dots, while in the strong one, the DQDs can be treated as a molecule. In the weak coupling regime the coupling between the two dots is small as compared with the coupling between the dots and the leads. While in the strong coupling regime the coupling between the two dots is large as compared with the coupling between the dots and the leads. One of the most important interaction is the spin exchange interaction which may called the effective exchange interaction. This interaction is studied and investigated in our study.

2- The Mathematical Model

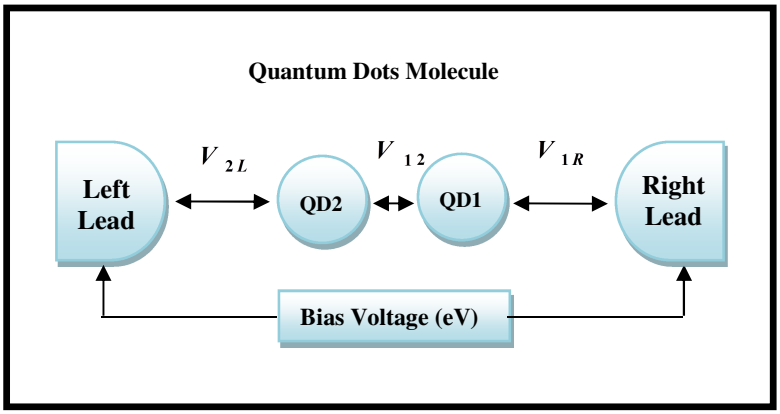
A mathematical model is performed for a system consists of double quantum dots (DQD) serially connected (regarded as an artificial molecule) and placed between two leads, as in Figure (1). V_{1R} in figure (1) represents the coupling interaction between QD1 and right lead, and V_{2L} represents the coupling interaction between QD2 and the left lead . V_{12} represents the direct interaction between QD1 and QD2. The interactions that will be taken into consideration here are the interactions between the right lead and first quantum dot $\Gamma_{1R}^{\pm\sigma}$, the left lead and the second quantum dot $\Gamma_{2L}^{\pm\sigma}$, the interaction between the two quantum dots (V_{12}) in addition to the effective spin exchange interaction between them (J) . The efficiency of electron transport in this system depends on the electronic system properties such as the electrochemical potential of the two leads, the energy band characteristics (such as bandwidth and density of electronic state) as well as energy level of quantum dots. The characteristics of quantum dots are of a great important because of it's role in determining the dynamical properties of electron transfer between the right and left leads, as a function of the bias voltage (eV_{bias}) that applied to the leads which is defined as follow [5]:

$$eV_{bias} = \mu_L - \mu_R \quad (1)$$

The time independent Anderson Hamiltonian [6-8] for (left lead – quantum dots molecule – right lead) system, which is illustrated in Figure (1) , that taking all the coupling and exchange interactions into consideration, is given by:

$$H = H_{DQD} + H_{Leads} + H_{QD-QD} + H_{DQD-Leads} \quad (2)$$

Fig.(1) represents two serially coupled quantum dots placed between two leads.



The first term in equation (2) represents the Hamiltonian of quantum dots molecule (which in fact consists of four terms, two for unperturbed quantum dots before they are coupled with the leads [9,10] :

$$H_{DQD} = \sum_{\sigma}\sum_{i=1}^{2} E_{di}^{\sigma} n_{di}^{\sigma} + \sum_{i=1}^{2} U_i n_{di}^{\sigma} n_{di}^{-\sigma} \quad (3)$$

E_{di}^{σ} represents the energy level i with spin σ while n_{di}^{σ} is the corresponding occupation numbers, where [6]:

$$n_{di}^{\sigma} = C_{di}^{\sigma\dagger} C_{di}^{\sigma} \quad (4)$$

$C_{di}^{\sigma\dagger}$ (C_{di}^{σ}) represent with the creation (annihilation) operator of the quantum dot electronic state i with spin σ . The energy levels of the two dots are defined in the following equations :

$$E_{d1}^{\sigma} = E_1 + U_1 n_{d1}^{-\sigma} - J n_{d2}^{\sigma}$$

$$E_{d2}^{\sigma} = E_2 + U_2 n_{d2}^{-\sigma} - J n_{d1}^{\sigma} \quad (5)$$

E_1, E_2 are the effective energy levels for the two dots. While U_1, U_2 are the Coulomb repulsive energy between electrons with the reverse spin on QD1 and QD2 respectively. The effective exchange energy (J) due to the electron spin exchange between the two dots is given by [11],

$$J = J_{\circ} + 2SV_{12} \quad (6)$$

where $J_{\circ}$ is the non effective spin exchange energy, S is the effect of the electronic wave functions overlapping of the dots when they are close to each other. The second term in equation (2) represents electrons on the right and left leads [12,13].

$$H_{Leads} = \sum_{\sigma}\sum_{\alpha}\sum_{k_\alpha} E_{k_\alpha}^{\sigma} n_{k_\alpha}^{\sigma} \quad (7)$$

where $E_{k_\alpha}^{\sigma}$ is the single electron energy level in the lead α with quantum numbers k and spin σ , and

$n_{k_\alpha}^{\sigma}$ is the corresponding occupation number. Note that the spin on the electrodes are not taken into account in our study. The third term in equation (2) represents the Hamiltonian concerned to the interaction between the two dots, which is written with the help of the reference [11] :

$$H_{QD-QD} = \sum_{\sigma} (V_{12} C_1^{\sigma\dagger} C_2^{\sigma} + V_{21} C_2^{\sigma\dagger} C_1^{\sigma})$$

$$+ \frac{1}{2} J_{\circ} (C_1^{\sigma\dagger} C_2^{\sigma} C_1^{\sigma} C_2^{\sigma} + H.C.) \qquad (8)$$

The tunneling process between the DQD molecule and the two leads are described by the fourth part of the Hamiltonian of equation (2),

$$H_{DQD-Leads} = \sum_{\sigma} \sum_{\alpha} \sum_{i=1}^{2} \sum_{k_\alpha} (V_{ik_\alpha} C_i^{\sigma\dagger} C_{k_\alpha}^{\sigma} + H.C.) \qquad (9)$$

$C_{k_\alpha}^{\dagger\sigma}$, $C_{k_\alpha}^{\sigma}$ are the creation (annihilation) operators of the electronic states of the left and right leads. And V_{ik_α} is the coupling matrix elements between the quantum dot i and lead α . The occupation numbers of the quantum dots energy levels n_{di}^{σ} ($i = 1, 2$) can be calculated according to Anderson model, at zero temperature, by using the following relation [14] :

$$n_{di}^{\sigma} = \int_{u_{0\alpha}}^{\mu_\alpha} \rho_{i\alpha}^{\sigma}(E) dE \qquad i = 1,2 \quad , \quad \alpha = L, R \qquad (10)$$

$u_{0\alpha}$ represents the bottom of the conduction band of lead α and $\rho_{i\alpha}^{\pm\sigma}(E)$ is the electronic density of states for quantum dot i that connected to the lead α . The density of states can be formed by using the following relation [15,16] :

$$\rho_{i\alpha}^{\sigma}(E) = -\frac{1}{\pi} \mathrm{Im} G_{i\alpha}^{\sigma}(E) \qquad (11)$$

$G_{i\alpha}^{\pm\sigma}(E)$ are the Green functions on the quantum dot i of spin σ according to the coupling with the lead α [16] :

$$G_{1R}^{\sigma}(E) = \frac{1}{2} \left\{ \frac{(1 + W_1^{\sigma} / V_1^{\sigma})}{(E - E_{1+}^{\sigma}) + i\Gamma_{1R}^{\sigma}} + \frac{(1 - W_1^{\sigma} / V_1^{\sigma})}{(E - E_{1-}^{\sigma}) + i\Gamma_{1R}^{\sigma}} \right\} \qquad (12a)$$

$$G_{2L}^{\sigma}(E) = \frac{1}{2} \left\{ \frac{(1 - W_2^{\sigma} / V_2^{\sigma})}{(E - E_{2+}^{\sigma}) + i\Gamma_{2L}^{\sigma}} + \frac{(1 + W_2^{\sigma} / V_2^{\sigma})}{(E - E_{2-}^{\sigma}) + i\Gamma_{2L}^{\sigma}} \right\} \qquad (12b)$$

$\Gamma_{i\alpha}^{\sigma}$ represents the broadening in quantum dot i energy levels due to the coupling with lead (α), and it is function of the distance between the quantum dot and lead. By using the Wide Band approximation, the broadening functions $\Gamma_{i\alpha}^{\sigma}$ are independent on energy [17,18].

The energies $E_{i\pm}^{\sigma}$ are defined by the following relation [19],

$$E_{i\pm}^{\sigma} = E_i + U_i n^{-\sigma} - J n^{\sigma} \pm V_i^{\sigma} \qquad (13)$$

The functions in equation (13) are defined as [19] :

$$V_i^{\sigma} = \sqrt{V_{12}^2 + (W_i^{\sigma})^2} \quad ; \quad W_i^{\sigma} = U_i M^{\sigma} + J M^{\sigma} \qquad (14)$$

$$n^{\sigma} = \frac{n_{d1}^{\sigma} + n_{d2}^{\sigma}}{2} \quad ; \quad M^{\sigma} = \frac{n_{d1}^{\sigma} - n_{d2}^{\sigma}}{2} \qquad (15)$$

Getting use of equ. (11) and substituting equ. (12) into equ. (10) then by solving these equations analytically, we

get the occupation numbers for the quantum dots QD1 and QD2 energy levels as follows :

$$n_{d1}^{\sigma}=\frac{(1+W_1^{\sigma}/V_1^{\sigma})}{2\pi}\left\{\tan^{-1}\left(\frac{\mu_R-E_{1+}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)+\tan^{-1}\left(\frac{u_{0R}-E_{1+}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)\right\}$$
$$+\frac{(1-W_1^{\sigma}/V_1^{\sigma})}{2\pi}\left\{\tan^{-1}\left(\frac{\mu_R-E_{1-}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)+\tan^{-1}\left(\frac{u_{0R}-E_{1-}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)\right\} \quad (16a)$$

$$n_{d2}^{\sigma}=\frac{(1-W_2^{\sigma}/V_2^{\sigma})}{2\pi}\left\{\tan^{-1}\left(\frac{\mu_L-E_{2+}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)+\tan^{-1}\left(\frac{u_{0L}-E_{2+}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)\right\}$$
$$+\frac{(1+W_2^{\sigma}/V_2^{\sigma})}{2\pi}\left\{\tan^{-1}\left(\frac{\mu_L-E_{2-}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)+\tan^{-1}\left(\frac{u_{0L}-E_{2-}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)\right\} \quad (16b)$$

The current flowing, in the active region (quantum dots molecule) in the case of nonequilibrium under applying bias voltage, is given by the following equation [20-22]:

$$I=\frac{e}{\hbar}\sum_{\sigma}\int_{\mu_R}^{\mu_L}dE\ \Gamma^{\sigma}\rho^{\sigma}(E)(f_L(E)-f_R(E)) \quad (17)$$

Where $f_{\alpha}(E)$ is the Fermi distribution function of the lead α , μ_{α} is the chemical potential of the lead α , with [21],

$$\rho^{\sigma}(E)=\rho_{1R}^{\sigma}(E)+\rho_{2L}^{\sigma}(E)\quad,\quad \Gamma^{\sigma}=\frac{\Gamma_{1R}^{\sigma}\Gamma_{2L}^{\sigma}}{\Gamma_{1R}^{\sigma}+\Gamma_{2L}^{\sigma}} \quad (18)$$

In order to obtain an analytic formula for the tunneling current as a function of bias voltage we will discuss two cases :

Firstly if ($\mu_R < \mu_L$), then the Fermi functions values, at the electrodes temperature $T=0$ for the values of energy ($\mu_R \le E \le \mu_L$), are equal to,

$$f_L(E)=1$$
$$f_R(E)=0$$

Thus, we get,

$$I=\frac{e}{\hbar}\sum_{\sigma}\sum_{j=+,-}[\Gamma^{\sigma}K_{1j}^{\sigma}\ \tan^{-1}\left(\frac{\mu_L-E_{1j}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)-\Gamma^{\sigma}K_{1j}^{\sigma}\ \tan^{-1}\left(\frac{\mu_R-E_{1j}^{\sigma}}{\Gamma_{1R}^{\sigma}}\right)$$
$$+\Gamma^{\sigma}K_{2j}^{\sigma}\ \tan^{-1}\left(\frac{\mu_L-E_{2j}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)-\Gamma^{\sigma}K_{2j}^{\sigma}\ \tan^{-1}\left(\frac{\mu_R-E_{2j}^{\sigma}}{\Gamma_{2L}^{\sigma}}\right)] \quad (19)$$

Secondly, if ($\mu_R > \mu_L$) , then the Fermi functions values, at electrodes temperature $T=0$ for the values of energy ($\mu_L \le E \le \mu_R$), are equal to,

$$f_R(E)=1$$
$$f_L(E)=0$$

And, we get,

$$I = \frac{-e}{\hbar}\sum_{\sigma}\sum_{j=+,-}[\Gamma^{\sigma}K_{1j}^{\sigma}\ \tan^{-1}(\frac{\mu_R - E_{1j}^{\sigma}}{\Gamma_{1R}^{\sigma}}) - \Gamma^{\sigma}K_{1j}^{\sigma}\ \tan^{-1}(\frac{\mu_L - E_{1j}^{\sigma}}{\Gamma_{1R}^{\sigma}})$$
$$+\Gamma^{\sigma}K_{2j}^{\sigma}\ \tan^{-1}(\frac{\mu_R - E_{2j}^{\sigma}}{\Gamma_{2L}^{\sigma}}) - \Gamma^{\sigma}K_{2j}^{\sigma}\ \tan^{-1}(\frac{\mu_L - E_{2j}^{\sigma}}{\Gamma_{2L}^{\sigma}})] \quad (20)$$

The functions K_j^{σ} are defined as :

$$K_{1j}^{\sigma} = \frac{1}{2\pi}(1 + j\frac{W_1^{\sigma}}{V_1^{\sigma}}) \quad , \quad K_{2j}^{\sigma} = \frac{1}{2\pi}(1 - j\frac{W_2^{\sigma}}{V_2^{\sigma}}) \quad (21)$$

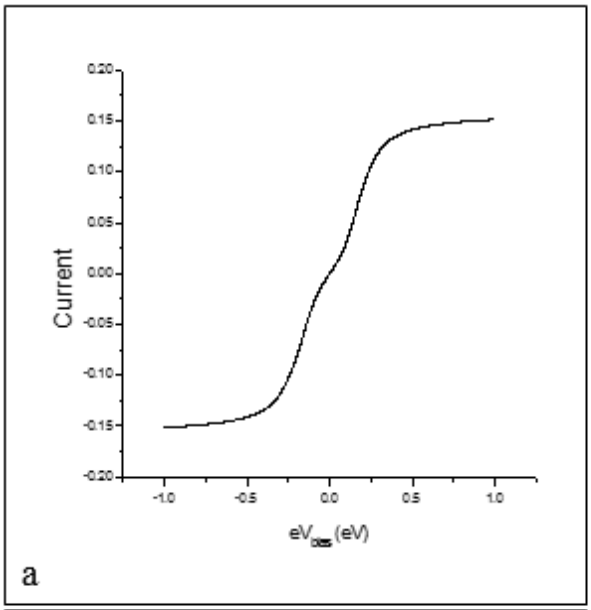
For the purpose of checking the functional characteristics of the system we calculate the differential conductivity by using the following relation [24-26] :

$$G_{diff} = \frac{\partial I}{\partial(eV_{bias})} \quad (22)$$

Where G_{diff} is calculated numerically by using finite differences method.

3- Results and discussion

In order to calculate the tunneling current and the differential conductance, equations (5) and (16) are solved self-consistently. The strong coupling regime ($V_{12} > \Gamma_{i\alpha}^{\pm\sigma}$) is considered in this work. Our calculations are performed for symmetrical system, i.e. for two identical quantum dots with equal coupling to the leads. All the transport properties are calculated as a function of bias voltage that applied to the leads. The quantum dots energy levels are $E_1 = E_2 = 0.05\ \text{eV}$, the tunneling coupling between the dots and the leads are $\Gamma_{1R}^{\pm\sigma} = \Gamma_{2L}^{\pm\sigma} = 0.08\ \text{eV}$, the hopping energy between the dots is equal to $0.2\ \text{eV}$ and the coulomb repulsive interaction energy on the dots are $U_1 = U_2 = 0.04\ \text{eV}$. Various values of effective spin exchange interaction are considered in our calculation, $J = (\pm 0.04,\ \pm 0.1,\ \pm 0.2,\ \pm 0.3,\ \pm 0.4)$ eV . All our calculation for the tunneling current and G_{diff} are presented in figs ((2)-(6)) for positive values of J and in figs. ((7)-(11)) for negative values. According to our results the tunneling current in all figures is inversely symmetric with respect to the bias voltage polarity, with $I = 0$ at $eV_{bias} = 0$. The differential conductance shows symmetric peaks with the bias voltage for all values of $J < 0.2\ \text{eV}$, while there are additional peaks when $J \geq 0.2\ \text{eV}$, which means that the interaction between the quantum dots is attractive, and the two dots can be treated as a molecule weakly coupled the leads. According to figures (9,10,11) with lower values of negative J, the resonant peak presented in the G_{diff} reemphasizes that the interaction between the two dots is repulsive even at strong coupling regime. In the limits of strong coupling with $J < 0.2\ \text{eV}$, the bias voltage between the two resonance peaks is equal to $V_{12} + \Gamma_{i\alpha}^{\pm\sigma} + J$. This notification is very important to determine the Nano device feature that depends in its operation on two coupled quantum dots. Finally figs. (12) illustrate the relation between the tunneling current and the exchange interaction at finite values of $eV_{bias} = (0,\ \pm 0.25)\ \text{eV}$. For $eV_{bias} = 0.25\ \text{eV}$, the current decreases as J increasing, while it increases as the polarity is reversed. This figure makes sure that for positive values of J the interaction between the two dots is attractive and it is repulsive for negative values of J .



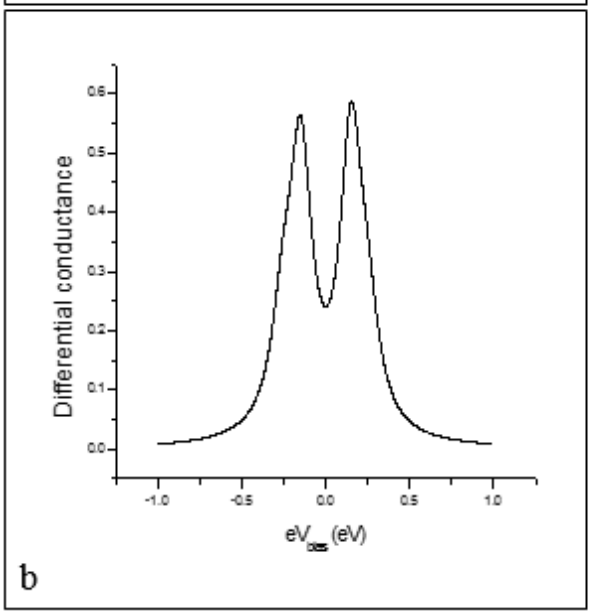
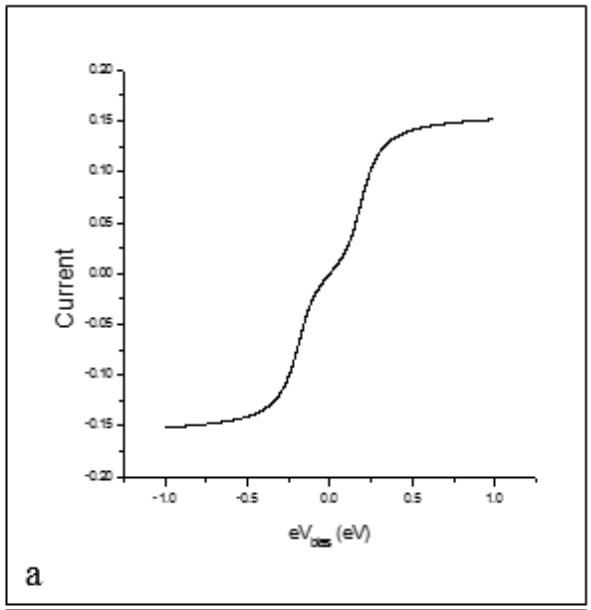


Fig. (2) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = 0.04$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



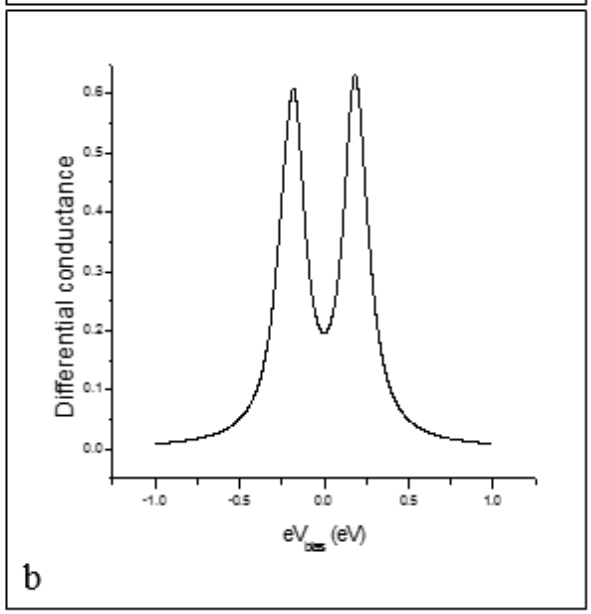


Fig. (3) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = 0.1$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .

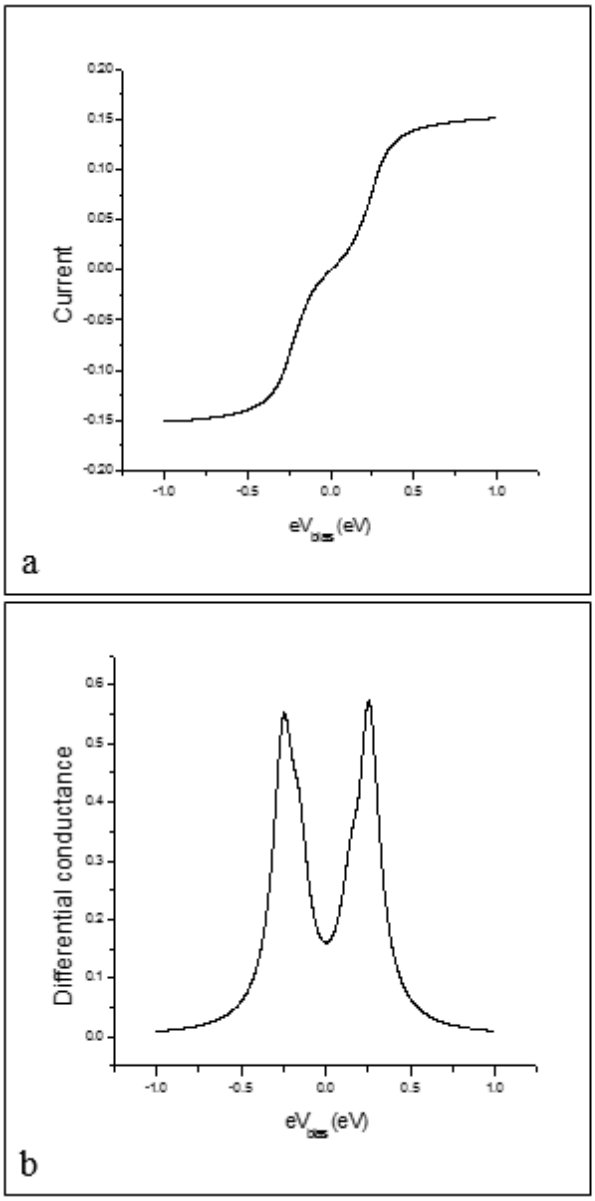


Fig. (4) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = 0.2$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .

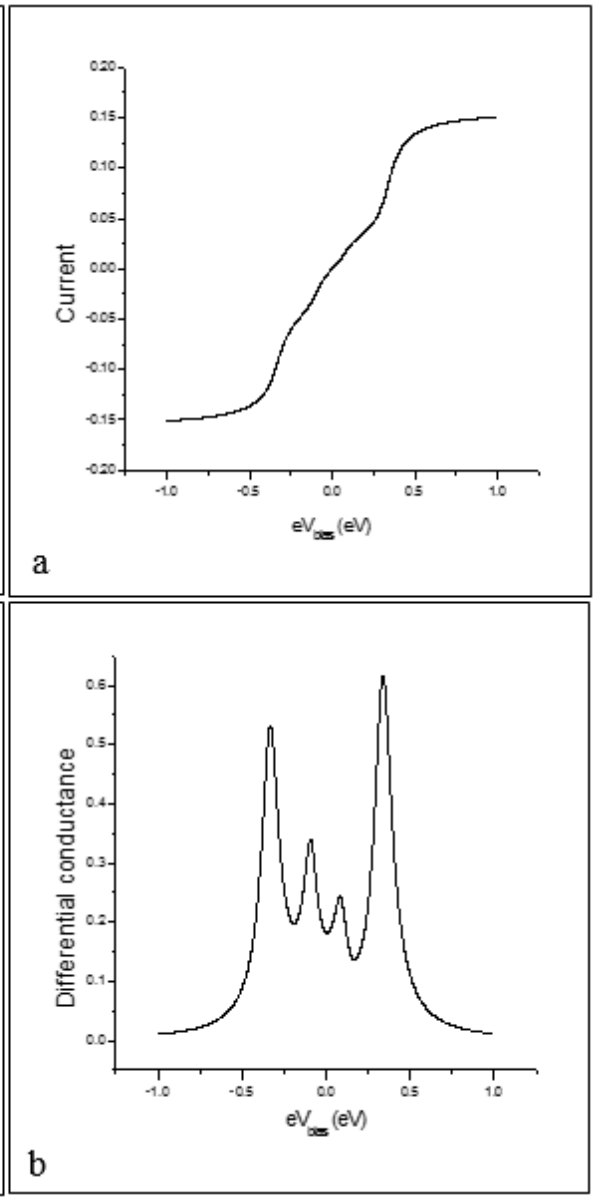
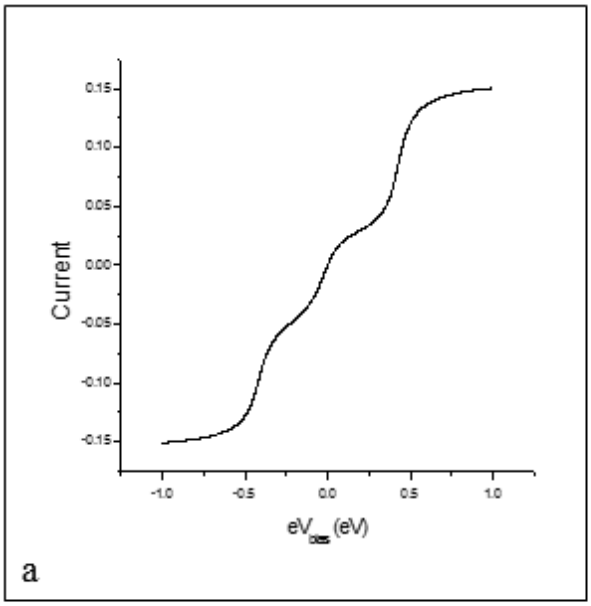


Fig. (5) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = 0.3$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



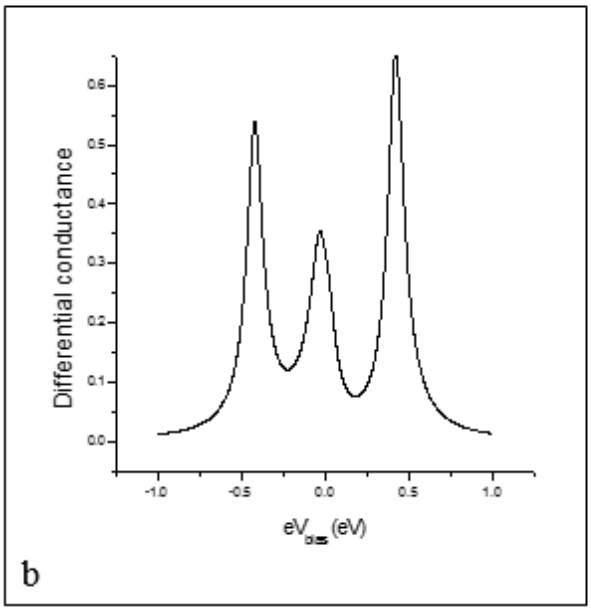
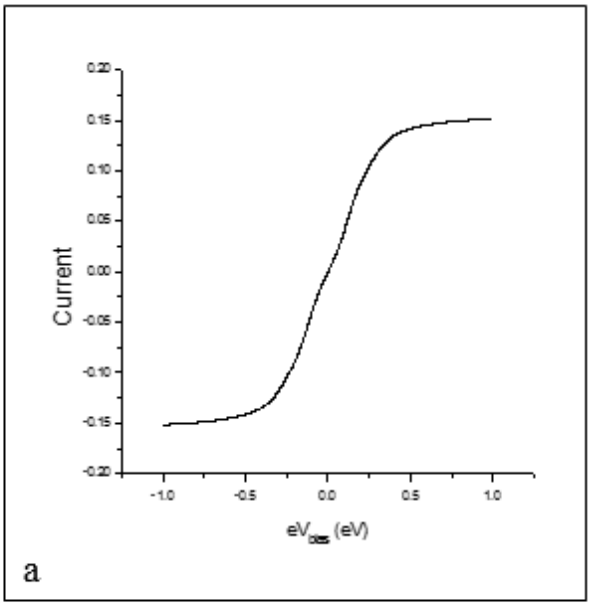


Fig. (6) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = 0.4$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



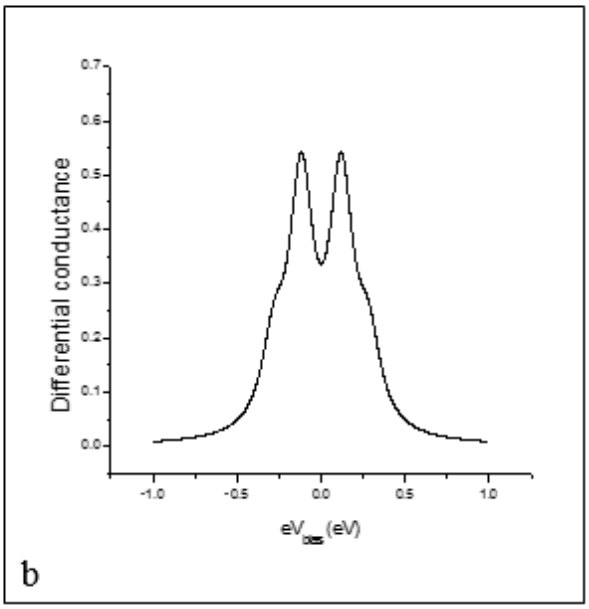
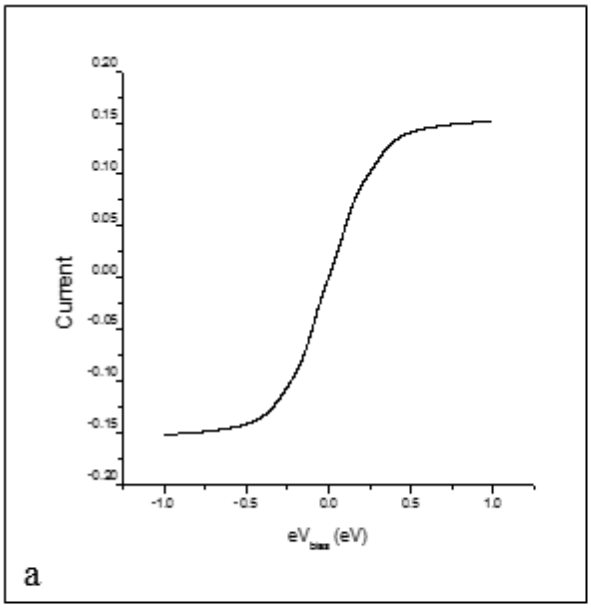


Fig. (7) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = -0.04$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



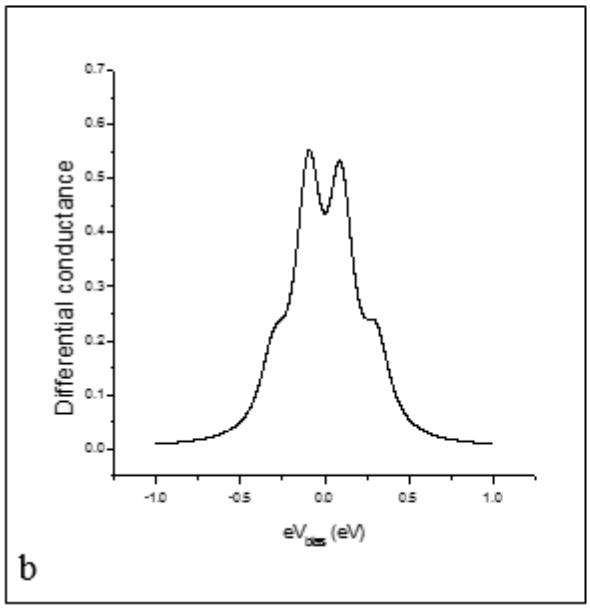
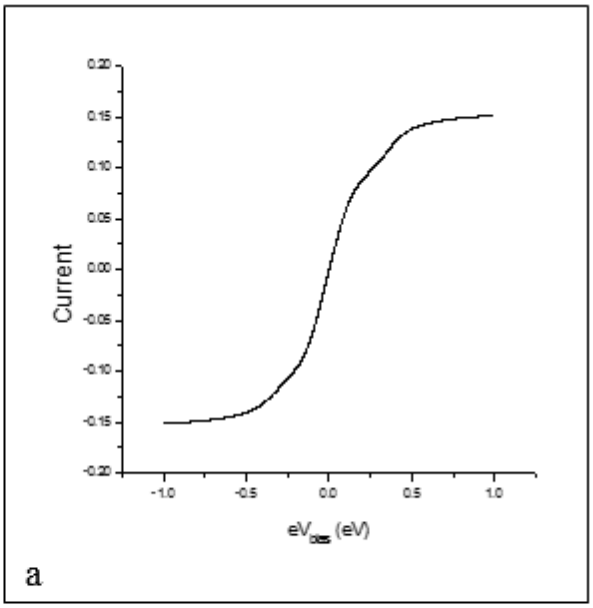


Fig. (8) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = -0.1$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



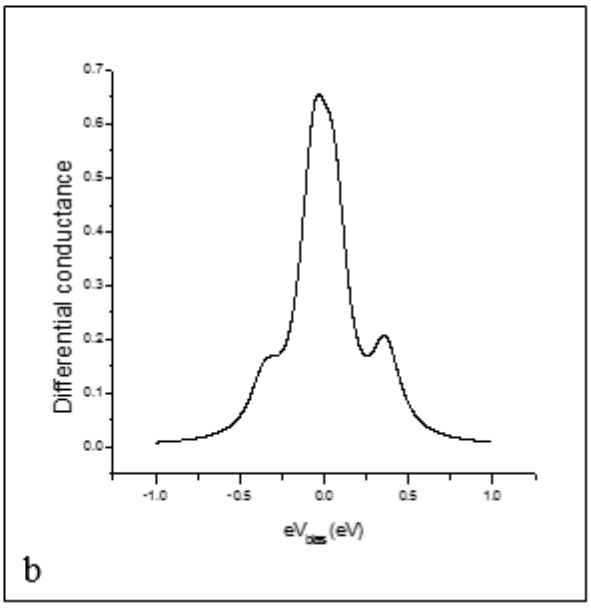
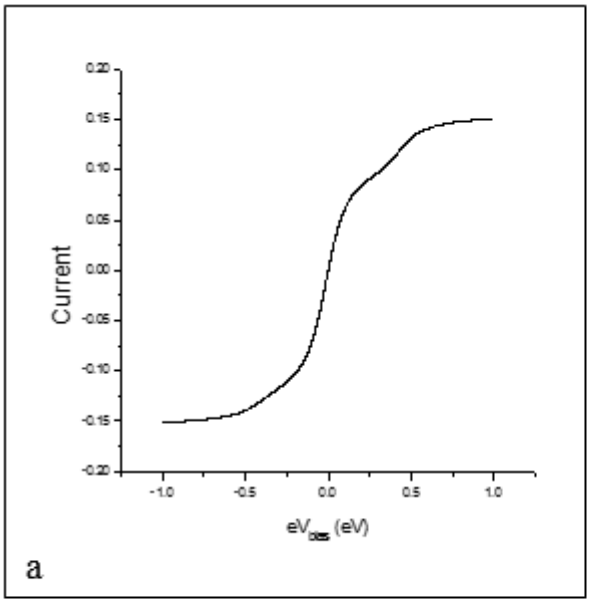


Fig. (9) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J = -0.2$ eV $U_1 = U_2 = 0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV $E_1 = E_2 = 0.05$ eV , $V_{12} = 0.2$ eV .



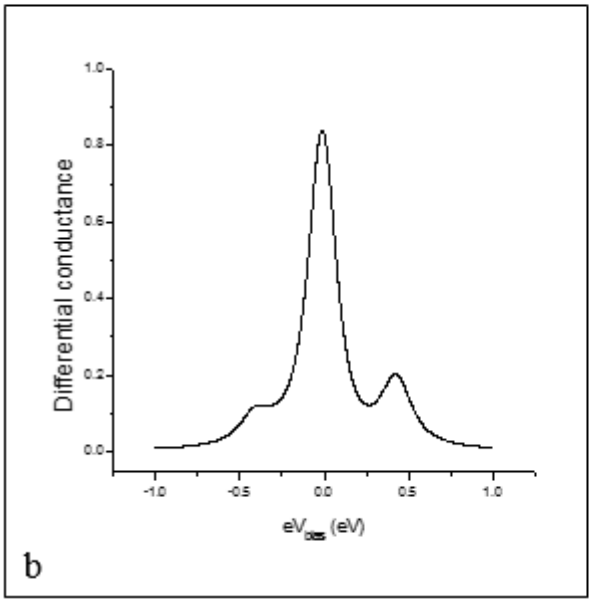
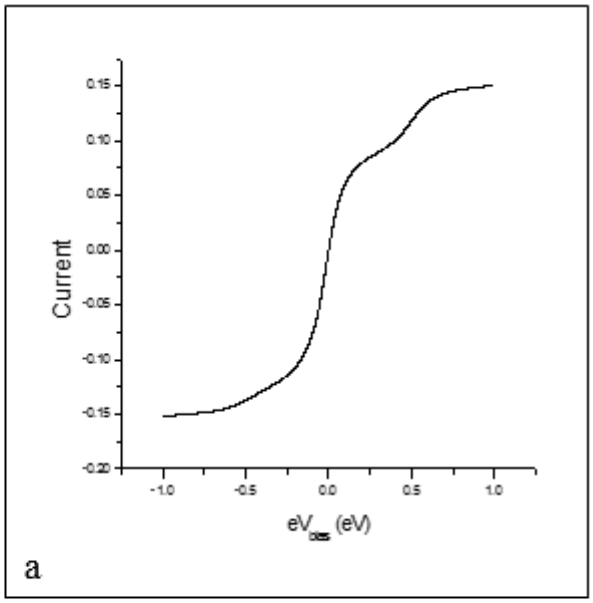


Fig. (10) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J=-0.3$ eV $U_1=U_2=0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma}=0.08$ eV $E_1=E_2=0.05$ eV , $V_{12}=0.2$ eV .



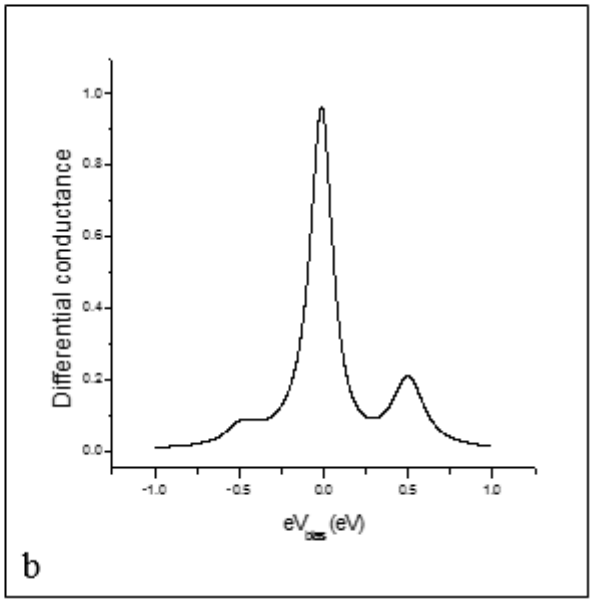


Fig. (11) showing (a) tunneling current as a function of bias voltage, (b) differential conductance as a function of bias voltage, when $J=-0.4$ eV $U_1=U_2=0.04$ eV , $\Gamma_{i\alpha}^{\pm\sigma}=0.08$ eV $E_1=E_2=0.05$ eV , $V_{12}=0.2$ eV .

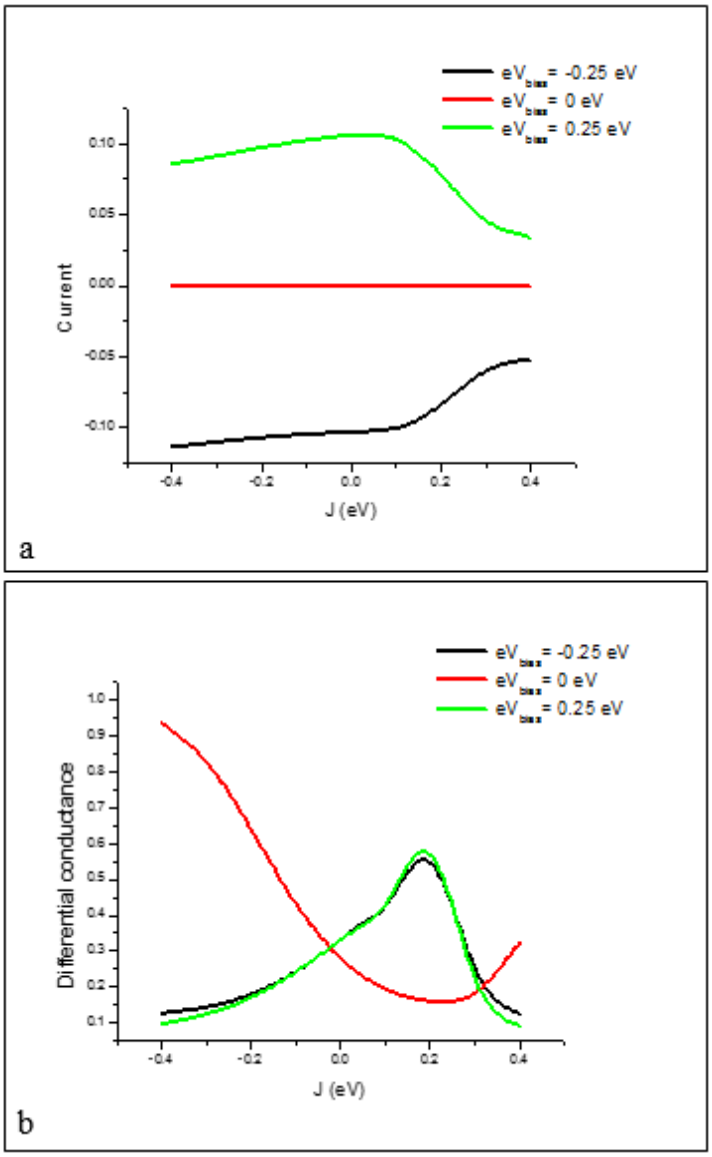


Fig (12) showing (a) tunneling current as a function of the exchange effective, (b) differential conductance as a function of the exchange effective, when $\Gamma_{i\alpha}^{\pm\sigma} = 0.08$ eV

$E_1 = E_2 = 0.05$ eV , $U_1 = U_2 = 0.04$ eV , $V_{12} = 0.2$ eV .

4- Conclusion

Effect of Spin Exchange Interaction (J) on electron transport across double quantum dots connected in series and coupled to external electrode have been investigated. Our results clearly show that the spin exchange interaction strongly affected the tunneling current and the differential conductance G_{diff} values . According to our results the tunneling current is inversely symmetric with respect to the bias voltage polarity, with $I = 0$ at $eV_{bias} = 0$. The differential conductance shows symmetric peaks with the bias voltage for all values of $J < 0.2$ eV , while there are additional peaks when $J \geq 0.2$ eV , which means that the interaction between the quantum dots is attractive, and the two dots can be treated as a molecule weakly coupled the leads. While at lower values of negative J , the resonant peak presented in the G_{diff} reemphasizes that the interaction between the two dots is repulsive even at strong coupling regime. Moreover the bias voltage between the two

resonance peaks is equal to $V_{12}+\Gamma_{i\alpha}^{\pm\sigma}+J$, this notification is very important in determine the Nano device feature that depends in its operation on a double coupled quantum dots.

5- References

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