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RESEARCH ARTICLE

Characteristics of Single Electron Transport in a Quantum Dots System

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In this paper, we investigated the time-dependent single electron transport process in a quantum dots system. This system is consisted from three quantum dots linked with donor and acceptor electron as tight-bending model. The calculations of this system are done using time dependent Schrödinger equations, which is utilized theoretically to calculate the occupation probability for the all quantum dots and study the characteristics of this system. we observed that the occupation probabilities are oscillatory behavior with time, and the number of oscillations in the occupation probabilities is increased by increasing the coupling interaction strength. We also calculated the transmission probability density using a scattering theory, we observed that its peaks decreased at $E = 0$ with increasing the coupling interaction strength.

Keywords: Electron Transport, Quantum Dots, Donor-Bridge-Acceptor System.

1. INTRODUCTION

The electron transport (ET) process in quantum dots (QDs) systems has a significant physical, chemical and biological fields.[1–4] The electron tunnelling between the donor (D) and the acceptor (A) through a quantum dot is the important mechanical transmission of both electron and electronic energy in quantum dots systems.[5,6] The main role of the quantum dot in these cases is the M. C. Connells-model (super-exchange process), which controls the transmission of the electron when the energy gap is positive between the levels of the donor/acceptor and the quantum dots, especially when it is much higher than thermal energy $k_B T$.[7–9] Because the resonance tunnelling, there is a great benefit for theoretical analysis due to the difference of the electronic tunnelling path and dependence on the distance in the tunnelling rate.[10] According to the mechanics of super-exchange, there is also an important factor affecting on the electron transfer rate, which is the association with the electronic motion of the nuclei, which controls the transmission rate of the electron.[11] The electronic coupling between the donor and the QDs controls the decay of the charge build-up at the donor level and its accumulation on the QDs, while the electronic coupling between the QDs and the acceptor reduces the accumulation of charge on the QDs and its growth at the acceptor level depending on the donor and acceptor dimension.[12]

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2. THEORETICAL METHOD

We consider the isolated coupled system, which under study is consisted from three QDs, with energy level ε_d, and linked with D and A, with effective energy level ε_{DA}. The electronic states in such a coupled system can be writing by the Hamiltonian (Eq. (1)):

$$H = \varepsilon_{DA} n_D(t) + \varepsilon_{DA} n_A(t) + E_d \sum_i^3 n_i(t) + V(C_D^\dagger(t)C_1(t) + C_A^\dagger(t)C_3(t) + C_1^\dagger(t)C_2(t) + C_2^\dagger(t)C_3(t)) + h.c. \quad (1)$$

In which, $C_i^\dagger(t) - C_i(t)$ are the creation-annihilation operators of an electron on i-th quantum dot, V is the D, A and the i-th QD electronic coupling-interaction between all them. The wave function of the system under consideration is a linear combination of the D, A, and QDs wave functions. The system of equations of motion can be obtained according to the time dependent Schrödinger equations, $dC_i(t)/dt = -i(dH(t)/dC_i^\dagger(t))$,[13,14] are (with $\hbar = e = 1$):

$$\frac{dC_D(t)}{dt} = -i\varepsilon_{DA} C_D(t) - iVC_1(t) \quad (2)$$

$$\frac{dC_1(t)}{dt} = -i\varepsilon_d C_1(t) - iVC_D(t) - iV_d C_2(t) \quad (3)$$

$$\frac{dC_2(t)}{dt} = -i\varepsilon_d C_2(t) - iV_d C_1(t) - iV_d C_3(t) \quad (4)$$

$$\frac{dC_3(t)}{dt} = -i\varepsilon_d C_3(t) - iVC_A(t) - iV_d C_2(t) \quad (5)$$

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$$\frac{dC_A(t)}{dt} = -i\varepsilon_{DA}C_A(t) - iVC_3(t) \tag{6}$$

To solve the above equations, we can using Laplace transform method,[15] $F(s) = L\{f(t)\} = \int_0^\infty e^{-st} f(t)\,dt$ with initial condition $C_D(0) = 1$ and $C_A(0) = C_1(0) = C_2(0) = C_3(0) = 0$, and then applying the inverse Laplace transform on the results one gets,

$$\begin{aligned} C_D(t) = -i\Bigg[& \frac{(\alpha_1^4 + \gamma_{1d}\alpha_1^3 + \gamma_{2d}\alpha_1^2 + \gamma_{3d}\alpha_1 + \gamma_{4d})e^{\alpha_1 t}}{(\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_1-\alpha_4)(\alpha_1-\alpha_5)} \\ & - \frac{(\alpha_2^4 + \gamma_{1d}\alpha_2^3 + \gamma_{2d}\alpha_2^2 + \gamma_{3d}\alpha_2 + \gamma_{4d})e^{\alpha_2 t}}{(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_2-\alpha_4)(\alpha_2-\alpha_5)} \\ & + \frac{(\alpha_3^4 + \gamma_{1d}\alpha_3^3 + \gamma_{2d}\alpha_3^2 + \gamma_{3d}\alpha_3 + \gamma_{4d})e^{\alpha_3 t}}{(\alpha_1-\alpha_3)(\alpha_2-\alpha_3)(\alpha_3-\alpha_4)(\alpha_3-\alpha_5)} \\ & - \frac{(\alpha_4^4 + \gamma_{1d}\alpha_4^3 + \gamma_{2d}\alpha_4^2 + \gamma_{3d}\alpha_4 + \gamma_{4d})e^{\alpha_4 t}}{(\alpha_1-\alpha_4)(\alpha_2-\alpha_4)(\alpha_3-\alpha_4)(\alpha_4-\alpha_5)} \\ & + \frac{(\alpha_5^4 + \gamma_{1d}\alpha_5^3 + \gamma_{2d}\alpha_5^2 + \gamma_{3d}\alpha_5 + \gamma_{4d})e^{\alpha_5 t}}{(\alpha_1-\alpha_5)(\alpha_2-\alpha_5)(\alpha_3-\alpha_5)(\alpha_4-\alpha_5)} \Bigg] \end{aligned} \tag{7}$$

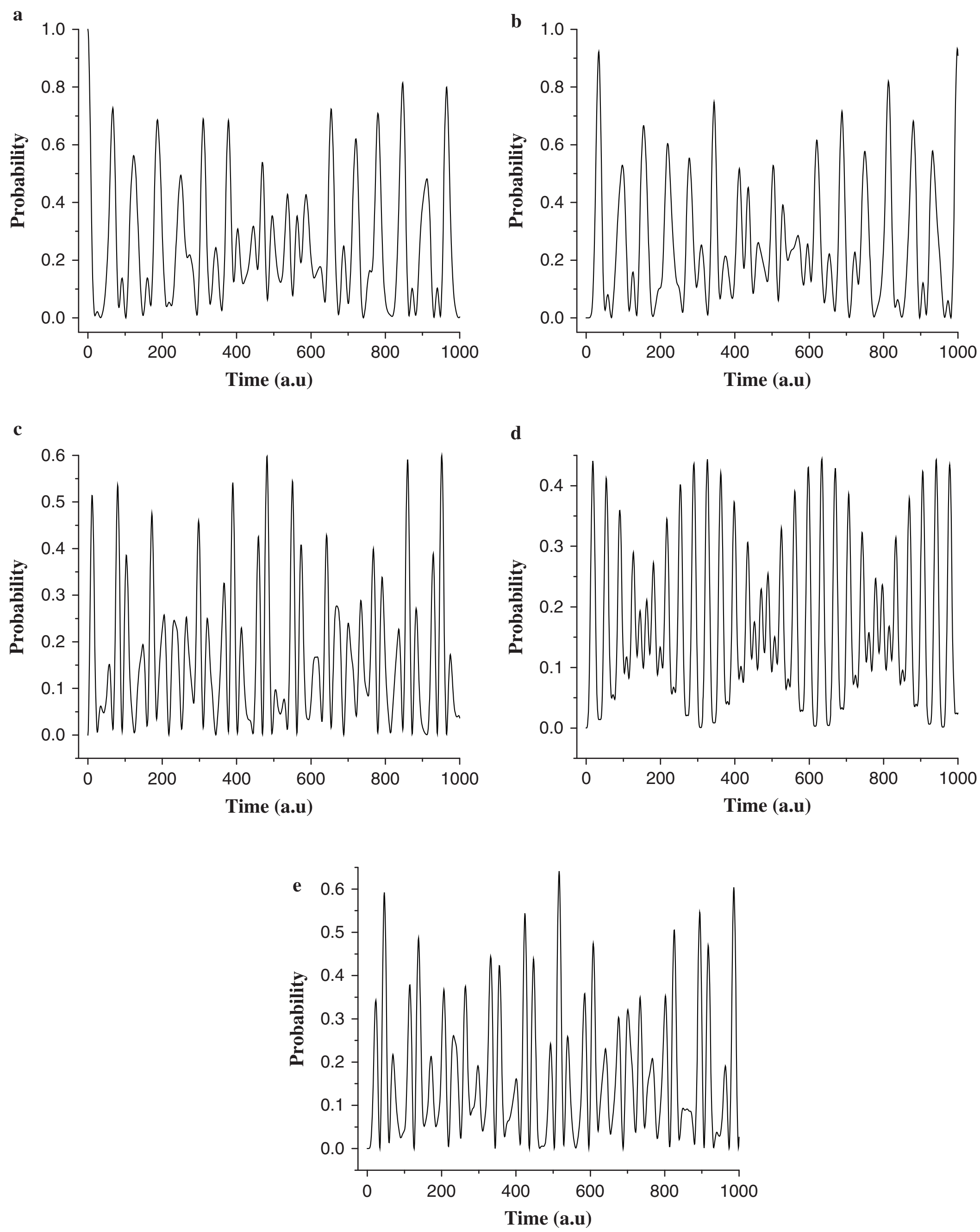

Fig. 1. Occupation probabilities versus the time of a donor (a), acceptor (b), Q.D1 (c), Q.D2 (d) and Q.D3 (e) with $\varepsilon_{DA} = -0.12$ eV, $\varepsilon_d = -0.14$ eV, $V = 0.1$ eV.

$$C_A(t) = -i|V|^2|V|^2 \times \left[\frac{e^{\alpha_1 t}}{(\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_1-\alpha_4)(\alpha_1-\alpha_5)} - \frac{e^{\alpha_2 t}}{(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_2-\alpha_4)(\alpha_2-\alpha_5)} + \frac{e^{\alpha_3 t}}{(\alpha_1-\alpha_3)(\alpha_2-\alpha_3)(\alpha_3-\alpha_4)(\alpha_3-\alpha_5)} - \frac{e^{\alpha_4 t}}{(\alpha_1-\alpha_4)(\alpha_2-\alpha_4)(\alpha_3-\alpha_4)(\alpha_4-\alpha_5)} + \frac{e^{\alpha_5 t}}{(\alpha_1-\alpha_5)(\alpha_2-\alpha_5)(\alpha_3-\alpha_5)(\alpha_4-\alpha_5)}\right] \quad (8)$$

$$C_1(t) = iV\left[\frac{(\alpha_1^3+\gamma_1\alpha_1^2+\gamma_2\alpha_1+\gamma_3)e^{\alpha_1 t}}{(\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_1-\alpha_4)(\alpha_1-\alpha_5)} - \frac{(\alpha_2^3+\gamma_1\alpha_2^2+\gamma_2\alpha_2+\gamma_3)e^{\alpha_2 t}}{(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_2-\alpha_4)(\alpha_2-\alpha_5)}\right.$$

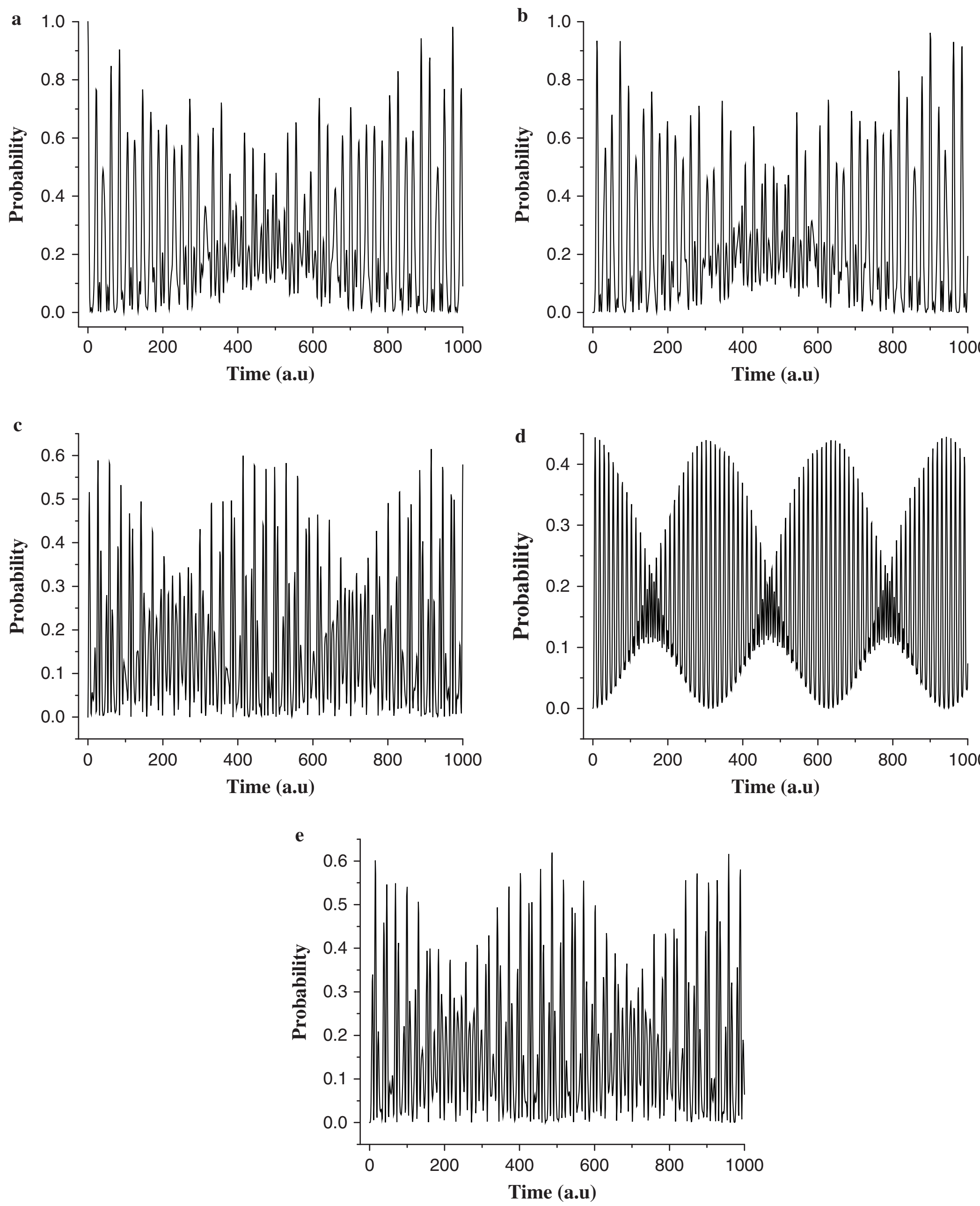

Fig. 2. Occupation probabilities versus the time of a donor (a), acceptor (b), Q.D1 (c), Q.D 2 (d) and Q.D3 (e) with $\varepsilon_{DA} = -0.12$ eV, $\varepsilon_d = -0.14$ eV, $V = 0.3$ eV.

$$
- \frac{(\alpha_3^3+\gamma_1\alpha_3^2+\gamma_2\alpha_3+\gamma_3)e^{\alpha_3 t}}{(\alpha_1-\alpha_3)(\alpha_3-\alpha_2)(\alpha_3-\alpha_4)(\alpha_3-\alpha_5)}
- \frac{(\alpha_4^3+\gamma_1\alpha_4^2+\gamma_2\alpha_4+\gamma_3)e^{\alpha_4 t}}{(\alpha_1-\alpha_4)(\alpha_4-\alpha_2)(\alpha_4-\alpha_3)(\alpha_4-\alpha_5)}
- \frac{(\alpha_5^3+\gamma_1\alpha_5^2+\gamma_2\alpha_5+\gamma_3)e^{\alpha_5 t}}{(\alpha_1-\alpha_5)(\alpha_5-\alpha_2)(\alpha_5-\alpha_3)(\alpha_5-\alpha_4)}\Bigg] \tag{9}
$$

$$
C_2(t) = |V|^2\Bigg[\frac{(\alpha_1^2+i(\varepsilon_{DA}+\varepsilon_d)\alpha_1+|V|^2-\varepsilon_{DA}\varepsilon_d)e^{\alpha_1 t}}{(\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_1-\alpha_4)(\alpha_1-\alpha_5)}
- \frac{(\alpha_2^2+i(\varepsilon_{DA}+\varepsilon_d)\alpha_2+|V|^2-\varepsilon_{DA}\varepsilon_d)e^{\alpha_2 t}}{(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_2-\alpha_4)(\alpha_2-\alpha_5)}
- \frac{(\alpha_3^2+i(\varepsilon_{DA}+\varepsilon_d)\alpha_3+|V|^2-\varepsilon_{DA}\varepsilon_d)e^{\alpha_3 t}}{(\alpha_1-\alpha_3)(\alpha_3-\alpha_2)(\alpha_3-\alpha_4)(\alpha_3-\alpha_5)}
- \frac{(\alpha_4^2+i(\varepsilon_{DA}+\varepsilon_d)\alpha_4+|V|^2-\varepsilon_{DA}\varepsilon_d)e^{\alpha_4 t}}{(\alpha_1-\alpha_4)(\alpha_4-\alpha_2)(\alpha_4-\alpha_3)(\alpha_4-\alpha_5)}
- \frac{(\alpha_5^2+i(\varepsilon_{DA}+\varepsilon_d)\alpha_5+|V|^2-\varepsilon_{DA}\varepsilon_d)e^{\alpha_5 t}}{(\alpha_1-\alpha_5)(\alpha_5-\alpha_2)(\alpha_5-\alpha_3)(\alpha_5-\alpha_4)}\Bigg] \tag{10}
$$

$$
C_3(t) = iV|V|^2\Bigg[\frac{(\alpha_1+i\varepsilon_{DA})e^{\alpha_1 t}}{(\alpha_1-\alpha_2)(\alpha_1-\alpha_3)(\alpha_1-\alpha_4)(\alpha_1-\alpha_5)}
- \frac{(\alpha_2+i\varepsilon_{DA})e^{\alpha_2 t}}{(\alpha_1-\alpha_2)(\alpha_2-\alpha_3)(\alpha_2-\alpha_4)(\alpha_2-\alpha_5)}
- \frac{(\alpha_3+i\varepsilon_{DA})e^{\alpha_3 t}}{(\alpha_1-\alpha_3)(\alpha_3-\alpha_2)(\alpha_3-\alpha_4)(\alpha_3-\alpha_5)}
- \frac{(\alpha_4+i\varepsilon_{DA})e^{\alpha_4 t}}{(\alpha_1-\alpha_4)(\alpha_4-\alpha_2)(\alpha_4-\alpha_3)(\alpha_4-\alpha_5)}
- \frac{(\alpha_5+i\varepsilon_{DA})e^{\alpha_5 t}}{(\alpha_1-\alpha_5)(\alpha_5-\alpha_2)(\alpha_5-\alpha_3)(\alpha_5-\alpha_4)}\Bigg] \tag{11}
$$

Where: $\gamma_{1d} = i(\varepsilon_{DA} + 3\varepsilon_d)$, $\gamma_{2d} = 3|V|^2 - 3\varepsilon_d(\varepsilon_{DA} + \varepsilon_d)$, $\gamma_{3d} = i[2|V|^2\varepsilon_{DA} + 4\varepsilon_d|V|^2 - \varepsilon_d^2(\varepsilon_d + 3\varepsilon_{DA})]$, $\gamma_{4d} = \varepsilon_{DA}\varepsilon_d(\varepsilon_d^2 - 2|V|^2) + |V|^2(|V|^2 - \varepsilon_d^2)$, $\gamma_1 = \gamma_{1d} - 2i\varepsilon_d$, $\gamma_2 = |V|^2 + |V_d|^2 - \varepsilon_d(2\varepsilon_{DA} + \varepsilon_d)$, $\gamma_3 = i[\varepsilon_{DA}(|V_d|^2 - \varepsilon_d^2) + |V|^2\varepsilon_d]$, $\alpha_{1,2} = -(1/2)i(\varepsilon_{DA} + \varepsilon_d \pm \sqrt{(\varepsilon_{DA} - \varepsilon_d)^2 + 4|V|^2})$, $\alpha_3 = (1/6)(a_1 + 12\sqrt{a_2})^{1/3} - 6a_3/(a_1 + 12\sqrt{a_2})^{1/3} - (1/3)i(\varepsilon_{DA} + 2\varepsilon_d)$, $\alpha_{4,5} = -(1/12)(a_1 + 12\sqrt{a_2})^{1/3}(1 - i\sqrt{3}) + 3a_3/(a_1 + 12\sqrt{a_2})^{1/3}(1 \pm i\sqrt{3}) - (1/3)i(\varepsilon_{DA} + 2\varepsilon_d)$, $a_1 = 8i(\varepsilon_{DA} - \varepsilon_d)(\varepsilon_{DA}^2 - 2\varepsilon_{DA}\varepsilon_d + \varepsilon_d^2 - (27/2)|V|^2)$, $a_2 = 3|V|^2[8(\varepsilon_{DA}^4 + \varepsilon_d^4) + (9|V|^2 - 32\varepsilon_{DA}\varepsilon_d)(\varepsilon_{DA}^2 + \varepsilon_d^2) + 6\varepsilon_{DA}\varepsilon_d(8\varepsilon_{DA}\varepsilon_d - 3|V|^2) + 108|V|^2|V|^2]$, and $a_3 = (1/9)[\varepsilon_{DA}^2 + \varepsilon_d^2 - 2\varepsilon_{DA}\varepsilon_d + 9|V|^2]$.

3. RESULTS AND DISCUSSION

There are numerous parameters characterize of the (donor-bridge-acceptor) system, which are affected on the ET process. Also, they are affected on the occupation possibilities, such as time variation (t), energy deference $(\varepsilon_{DA} - \varepsilon_d)$ and the coupling interaction (V) between donor, acceptor and quantum dots, which are dependent on a spatial variation of a corresponding wave functions. Results of the ET are performed by using the above theoretical method. So, we are arranged the QDs in a tight-bending model between the D and the A, which displayed in the following figures. When the coupling interaction is effective, the charge is decay on the donor site and growing on the acceptor site as well as observing the oscillatory behavior of the occupation probabilities with time, as shown in Figure 1. By increasing the coupling interaction strength, the number of oscillations in the occupation probabilities is increased, as displayed in Figure 2.

Figure 3 shows the occupation probabilities of charge for both donor and acceptor as a function of the energy gap at $t = 2000$ a.u. It's clearly to show that probabilities are symmetric on the energy difference due to the dependence on the absolute value of the energy difference. So, by increasing the interaction, the existence of the electron on the acceptor is increased and decreases on the donor at $\varepsilon_{DA} - \varepsilon_d = 0$.

The transmission probability density of electron $T(E)$ can obtained using the scattering theory

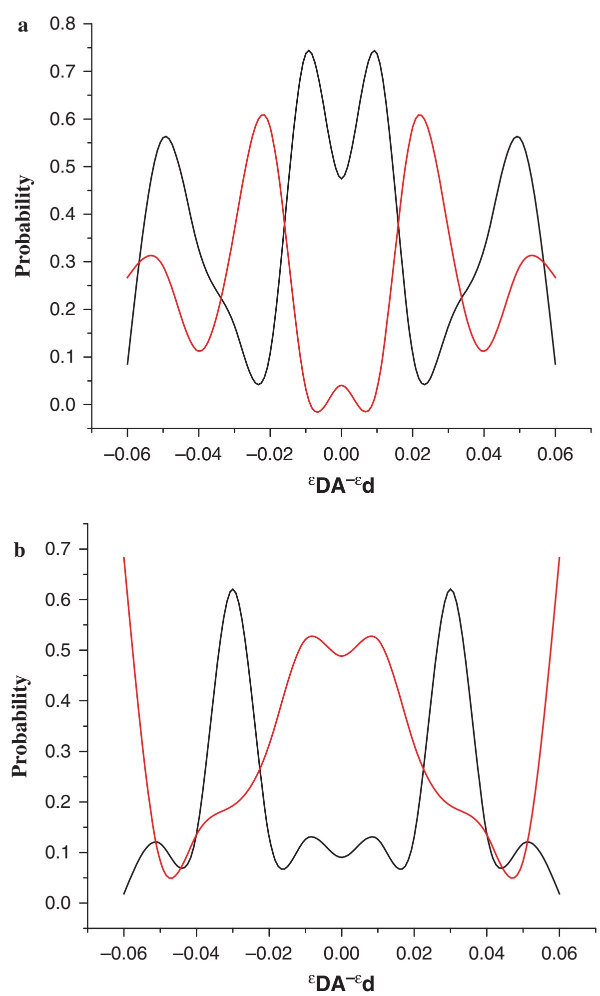

Fig. 3. Occupation probabilities versus the energy gap of a donor (black line) and acceptor (read line), with $V = 0.1$ eV (a) and $V = 0.3$ eV (b).

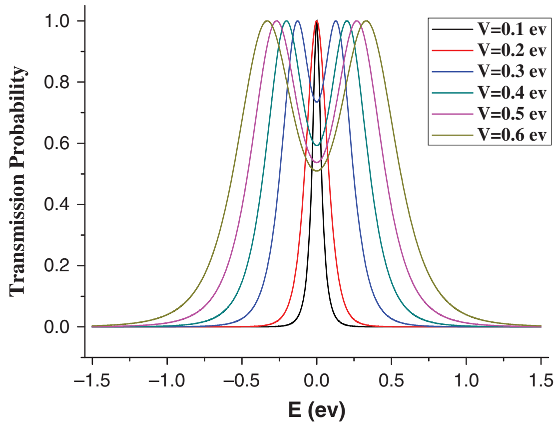

Fig. 4. Transmission probability density versus the scattering energy, with $\varepsilon_{DA} = \varepsilon_d = 0$.

(Fourier-Transform), which is expressed in this approach as $T(E) = |\psi^{\text{out}}(E)|^2/|\psi^{\text{in}}(E)|^2$.[16] Figure 4 demonstrations the transmission probability density as a function of the scattering energy (E). The location of the peaks in the transmission probability are determined by the quantum dots characteristics, coupling interaction. For coupling interaction, we observed that the transmission probability peak is decrease at $E = 0$.

4. CONCLUSION

We investigated electron transport process of a system of three QDs coupled to the D and A. The occupation probabilities of QDs, D, and A are oscillatory behavior with time, and the number of oscillations is increased by increasing the coupling interaction strength. Also, the probabilities of D and A are symmetric on the energy difference due to the dependence on the absolute value of the energy difference. The peaks of transmission probability density decreased at $E = 0$ with increasing the coupling interaction strength.

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