Theoretical Treatment for Electron Transport throughout Quantum Dots Bridge

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Abstract

In this article we present theoretical treatment for electron transport through one scattering region attached to donor and left lead in the left side, while in the right side attached to acceptor and right lead. Our treatment is based on the time-dependent Anderson – Newns Hamiltonian. The equations of motion are derived for all subsystems then the stationary state is considered to obtain analytical expression for the transmission probability as a function of system energies. The scattering region consists of one, two or three quantum dots. The subsystems eigen values, the coupling interaction between them as well as the leads band width all are taken into consideration and highlighted.

Keyword: Quantum Dot, transport properties.

Introduction

Transport through nano-scale devices based on single molecules has attracted a lot of interest over the last years (Maiti 2010), (Finch *et al*. 2009), (Aradhya *et al*. 2012) and (He *et al*. 2009). The basic idea of such transport devices is that initially two metallic electrodes are separated by a gap, prohibiting any transport of electrons. However, already a single molecule trapped within this gap can serve as bridge and thereby allow for a small current of tunneling electrons. One of the most interesting aspects of such single-molecule devices is their size. The gap can nowadays be fabricated and controlled on the nanometer-scale. The small size of the device makes single-molecule transport devices particularly interesting for information technology, where the demand for device miniaturizing is growing fast. Obviously, at such small scales, quantum mechanical effects become crucial (Reckerman 2010).

In this paper, we study left lead-donor-scattering region-accepter-right lead system (see fig. (1,a)). Where, the scattering region (i.e. the bridge) consists of several nanostructures. These may be one, two or three quantum dots.

In our work, we will present our theoretical treatment to formulate general expression for the electron transport throughout one scattering region to study and calculate the electronic properties for the considered system in our study. So, all the system eigenvalues and coupling interactions are taken into consideration to give obvious view for the system dynamics.

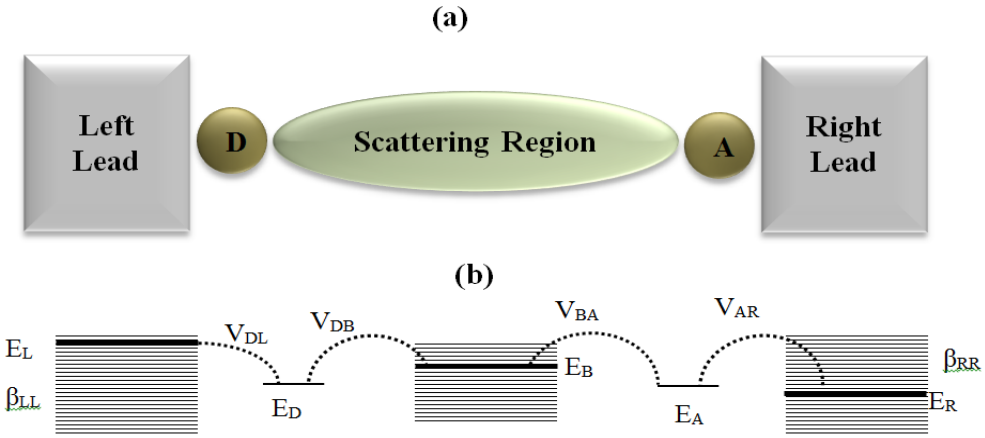


Figure (1):(a) An illustration for left lead-donor-scattering region-accepter-right lead system. (b)The corresponding energy diagram, the energy levels and coupling interactions between the nearest neighbor parts.

1. Theory

In this section, general formula for the transmission probability for one scattering region will be derived for the system shown in fig.(1). The different indices L, D, B, A and R denote left lead, donor, bridge, acceptor and right lead respectively (see fig(1,b)).This energy diagram can be described by using time-dependent and spin less Anderson – Newns Hamiltonian (Newns 1969), which neglects Coulomb interactions. This Hamiltonian is given by

$$\hat{H}(t) = E_D n_D(t) + E_A n_A(t) + \sum_{k_B} E_{k_B} n_{k_B}(t) + \sum_{k_L} E_{k_L} n_{k_L}(t) + \sum_{k_R} E_{k_R} n_{k_R}(t)$$
$$+ \sum_{k_B} (V_{Dk_B} C_D^+(t) C_{k_B}(t) + H.C.) + \sum_{k_B} (V_{Ak_B} C_A^+(t) C_{k_B}(t) + H.C.)$$
$$+ \sum_{k_L} (V_{Dk_L} C_D^+(t) C_{k_L}(t) + H.C.) + \sum_{k_R} (V_{Ak_R} C_A^+(t) C_{k_R}(t) + H.C.) \qquad (1)$$

Where, $n_j(t) = C_j^+(t) C_j(t)$ and the $C_j(t)$ ($C_j^+(t)$) denotes annihilation (creation) operators. The index k_j being a set of quantum numbers, with j=*L, B, R*. The equation of motion for $C_j(t)$ can be obtained by using (Ballentine 2000),

$$\dot{C}_j(t) = -i \frac{d\hat{H}(t)}{dC_j^+(t)} \qquad (2)$$

to get,

$$\dot{C}_D(t) = -iE_D C_D(t) - i\sum_{k_B} V_{Dk_B} C_{k_B}(t) - i\sum_{k_L} V_{Dk_L} C_{k_L}(t) \quad (3)$$

$$\dot{C}_A(t) = -iE_A C_A(t) - i\sum_{k_B} V_{Ak_B} C_{k_B}(t) - i\sum_{k_R} V_{Ak_R} C_{k_R}(t) \quad (4)$$

$$\dot{C}_{k_B}(t) = -iE_{k_B} C_{k_B}(t) - iV_{k_B D} C_D(t) - iV_{k_B A} C_A(t) \quad (5)$$

$$\dot{C}_{k_L}(t) = -iE_{k_L} C_{k_L}(t) - iV_{k_L D} C_D(t) \quad (6)$$

$$\dot{C}_{k_R}(t) = -iE_{k_R} C_{k_R}(t) - iV_{k_R A} C_A(t) \quad (7)$$

For stationary state we define $C_j(t)$ by the following:

$$C_j(t) = \overline{C}_j(E) e^{-iEt} \quad (8)$$

where E denotes the system eigenvalues, then accordingly, $\dot{\overline{C}}_j(E) = 0$.

In order to get logic and simple formula for the transmission probability amplitude, we assume the following energy separation procedure (Stamfi 1994):

$$V_{k_B\alpha} = \nu_{k_B} V^{B\alpha}; V_{k_L D} = \nu_{k_L} V^{LD} \;;\; V_{k_R A} = \nu_{k_R} V^{RA} \;;\; \overline{C}_{k_\beta}(E) = \nu_{k_\beta} \overline{\overline{C}}_\beta \quad (9)$$

where α=D,A and β=D,A,B ,then we get,

$$\overline{C}_A = \frac{1}{E - E_A}\left\{ V^{AB}\Gamma_B(E)[V^{BD}\overline{C}_D + V^{BA}\overline{C}_A] + \left|V^{AR}\right|^2 \Gamma_R(E)\overline{C}_A \right\} \quad (10)$$

Then the transmission probability amplitude and transmission probability (Ihn 2010) can be calculated respectively as:

$$t(E) = \frac{\overline{C}_A(E)}{\overline{C}_D(E)} \quad (11)$$

$$T(E) = \left|t(E)\right|^2 \quad (12)$$

Where

$$\Gamma_\ell(E) = \sum_{k_\ell}\left\{ \frac{\left|V_{k_\ell}\right|^2}{E - E_{k_\ell}} \right\} \qquad \ell = B, R \quad (13)$$

By using the following operator equation,

$$\lim_{\gamma\to 0} \frac{1}{E - E_n + i\gamma} = -i\pi\delta(E - E_n) + P\frac{1}{E - E_n} \quad (14)$$

Where P(…) denotes the principal part of (…).

Accordingly, the functions $\Gamma_B(E)$ and $\Gamma_R(E)$ will take the following formulas,

$$\Gamma_\ell(E) = -i\pi\rho_\ell(E) + P\int \frac{\rho_\ell(E')}{E-E'}dE' \qquad \ell = B,R \qquad (15)$$

Where $\rho_\ell(E)$ represents the density of electronic states for the nanostructure which is given by (Amos 1989)

$$\rho_\ell(E) = \sum_{k_\ell} \left|V_{k_\ell}\right|^2 \delta(E-E_\ell) \qquad (16)$$

Then we can write the level self-energy (Galperin 2004),

$$\begin{aligned}\sum_{A\ell}(E) &= \left|V^{A\ell}\right|^2 \Gamma_\ell(E) \\ &= -i\Delta_{A\ell}(E) + \Lambda_{A\ell}(E) \qquad \ell = B,R\end{aligned} \qquad (17)$$

$\Delta_{AB}(E)$ is the acceptor level broadening due to acceptor level-bridge level coupling interaction, while $\Delta_{AR}(E)$ is the acceptor level broadening due to acceptor level-right lead's levels coupling interaction. $\Lambda_{AB}(E)$ and $\Lambda_{AR}(E)$ are the quantum shift that happen in the acceptor level due to the over mentioned coupling interactions. With (Newns 1983),

$$\Delta_{A\ell}(E) = \pi\left|V^{A\ell}\right|^2 \rho_\ell(E) \qquad \ell = B,R \qquad (18)$$

and

$$\Lambda_{A\ell}(E) = P\frac{1}{\pi}\int \frac{\Delta_{A\ell}(E')}{E-E'}dE' \qquad (19)$$

Also, we can define the self-energy $V^{AB}V^{BD}\Gamma_B(E)$,which refers to the indirect coupling interaction between the donor and the acceptor levels throughout the bridge, as

$$\begin{aligned}\sum_{ABD}(E) &= V^{AB}V^{BD}\Gamma_B(E) \\ &= -i\Delta_{ABD}(E) + \Lambda_{ABD}(E)\end{aligned} \qquad (20)$$

With,

$$\Delta_{ABD}(E) = \pi V^{AB}V^{BD}\rho_B(E) \qquad (21)$$

$$\Lambda_{ABD}(E) = P\frac{1}{\pi}\int \frac{\Delta_{ABD}(E')}{E-E'}dE' \qquad (22)$$

Notably, $\Delta_{ABD}(E)$ determines the interference energy and $\Lambda_{AB}(E)$ is its corresponding quantum shift.

Now we can write the transmission probability amplitude as

$$t(E)=\frac{\sum_{ABD}(E)}{E-E_A-\sum_{AB}(E)-\sum_{AR}(E)} \quad (23)$$

Note that, the acceptor and donor levels are broadened and thus they will have local density of states which take the following Gaussian forms respectively (Kjollerstrom 1966), (Anderson 1961) and (Al-Muhk 1997),

$$\rho_A(E)=\frac{1}{\pi}\frac{\Delta_{AR}(E)}{(E-E_A-\Lambda_{AR}(E))^2+\Delta_{AR}^2(E)} \quad (24a)$$

$$\rho_D(E)=\frac{1}{\pi}\frac{\Delta_{DL}(E)}{(E-E_D-\Lambda_{DL}(E))^2+\Delta_{DL}^2(E)} \quad (24b)$$

where Δ_{DL} (E) is the donor level broadening due to donor level-left lead's levels coupling interaction and Λ_{DL}(E) is the corresponding quantum shift.

2. Model Parameterization

(3-1) One Quantum Dot

The first case is the case when the bridge's system is considered as one quantum dot with effective energy level E_B, with local density of states given by (Havison 2005),

$$\rho_B(E_{k_B})=\delta(E_{k_B}-E_B) \quad (25)$$

Accordingly, the third term in eq. (1) will be $E_B n_B(t)$ while the sixth and seventh terms are written respectively as,

$V_{DB}C_D^+(t)C_B(t)+h.c$

$V_{AB}C_A^+(t)C_B(t)+h.c$

Then by using the definitions in eqs.(13-15) with,

$$\sum_{AB}(E)=\frac{\left|V^{AB}\right|^2}{E-E_B} \quad (26a)$$

and,

$$\sum_{DBA}(E)=\frac{V^{DB}V^{AB}}{E-E_B} \quad (26b)$$

The self-energy $\sum_{AR}(E)$ is calculated by using eq.(17), for this purpose the density of states formula used for the right lead is given by (Sulston 1988),

$$\rho_R(E)=\frac{1}{\pi|\beta_R|}\sqrt{1-\left(\frac{E-E_{FR}}{2\beta_R}\right)^2} \quad (27)$$

E_{FR} is the position of Fermi energy level on the right lead. β_R is related to the occupied band width of the right leads which is equal to 2 β_R.

Accordingly, the broadening and the quantum shift functions read as,

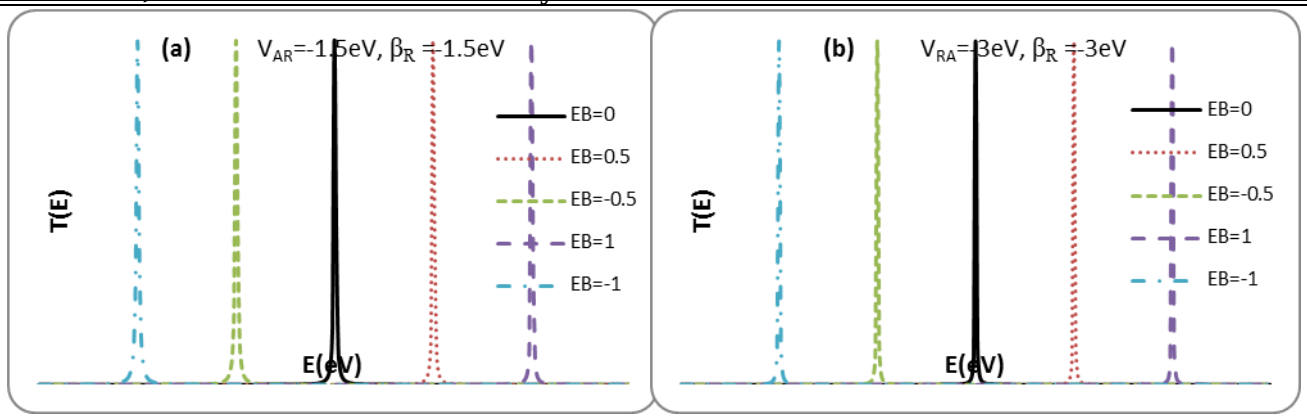
$$\Delta_{AR}(E) = \frac{|V_{AR}|^2}{|\beta_R|}\sqrt{1-\left(\frac{E-E_{FR}}{2|\beta_R|}\right)^2} \qquad (28a)$$

$$\Lambda_{AR}(E) = \frac{|V_{AR}|^2}{2\pi|\beta_R|^2}(E-E_{FR}) \qquad (28b)$$

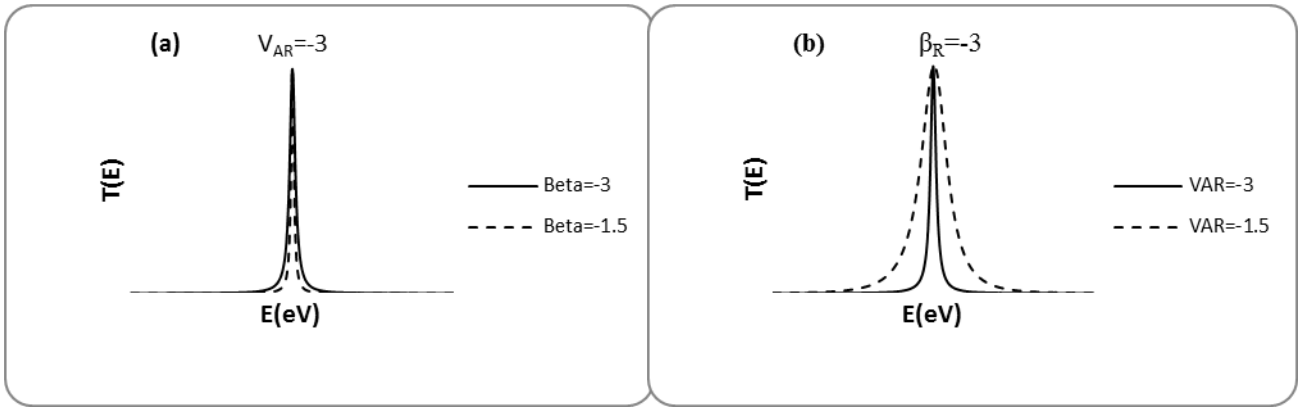
As a model parameterization, the transmission probability is calculated as a function of energy for different values of the coupling interactions as well as the leads band width. These calculations are shown in the figures (2-4). Fig.(2) shows our results for the cases V^{AR}=-1.5eV and β_R =-1.5eV in (a) and V^{AR}=-3eV and β_R =-3 eV in (b) for different quantum dot's energy level positions (relative to leads Fermi levels E_{FR}=0 and E_{FL}=0). It is obvious that T(E)=1 at E=E_B. It is also obvious that there is a pronounced broadening in T(E) curve as E_B lies more below the leads Fermi levels. In Fig. (3), T(E) is calculated for different values of β_R with V^{AR}=-3.0eV in (a), while in (b) T(E) is calculated for different values of V^{AR} with β_R =-3.0eV. Fig. (3) shows that the broadening of T(E) increases as the band width increases and as coupling interaction between the acceptor and the right lead decreases. fig. (4) shows that the broadening of T(E) increases as the coupling interactions of the bridge with the donor and acceptor increase. It is obvious that the effect of these coupling interactions is dominant.

The solid lines In Fig. 4 represent the results in the limit of weak-coupling, while, the dash lines denote the results in the strong-coupling limit. In the weak coupling limit, the transmission shows very sharp resonant peak for bridge energy E_B=-1. At this resonance the transmission probability T(E) achieves the value 1.

With the increase of the dot-donor V_{DB} and dot-acceptor V_{AB} coupling strengths, the width of this resonance get enhanced substantially, as illustrated by the dash curves in Fig. 4. This is due to the substantial broadening of the quantized energy levels in the limit of strong-coupling.



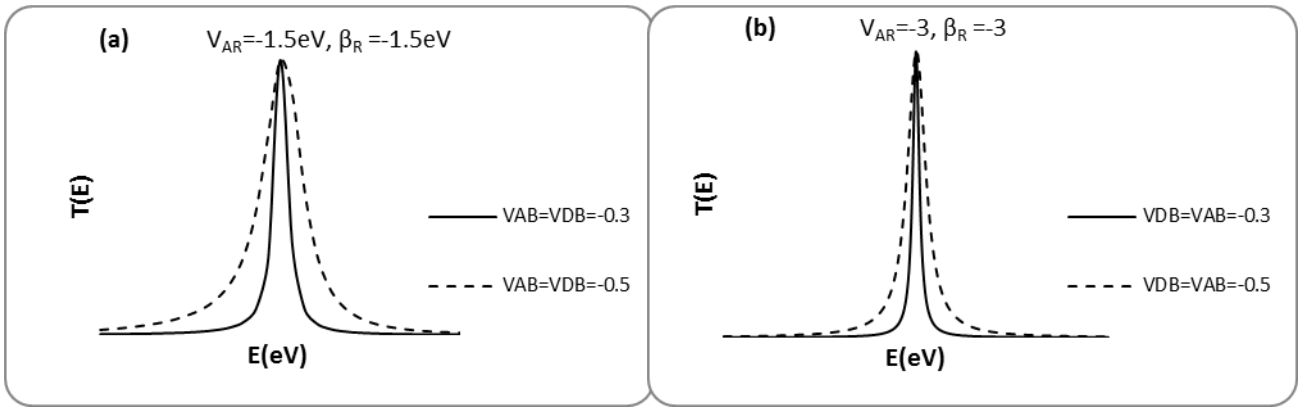
Figure(2): the transmission probability as function of the system energy with $V^{DB}=V^{AB}$=-0.1eV.



Figure(3): the transmission probability as function of the system energy with E_B=-1eV, $V^{DB}=V^{AB}$=-0.3eV.

Thus for the strong-coupling limit, the electron conducts through the dots for the wide range of energies, while, a fine tuning in the energy scale is necessary to get the electron conduction through these systems in the limit of weak coupling.

Therefore, it can be predicted that the dot-donor and dot-acceptor coupling strength has a significant role in the determination of the electron conduction through the bridge systems. This feature provides a key information in the study of molecular transport phenomena.



Figure(4): the transmission probability as function of the system energy with E_B=-1eV.

(3-2) Two Quantum Dots

The second case is the case when the bridge's system is considered as two quantum dots with two effective energy levels E_{B1} and E_{B2}.The local density of states on each quantum dot is calculated by using the following formula,

$$\rho_B(E_j)=\left|\frac{N}{4V^{BB}\pi\sin(\frac{j\pi}{N+1})}\right| \qquad (29)$$

So $\rho_B(E_1)=\rho_B(E_2)=\frac{1}{\sqrt{3}\pi V^{BB}}$, where V^{BB} is the coupling interaction between the two quantum dots. The two quantum dots are connected serially and E_{B1} = E_{B2}=E_B.

If the interaction between the two quantum dots is switched on, then the interaction will lifted the degeneracy and the two quantum dot levels will be

$$E_{B1}=E_B-V^{BB} \qquad (30a)$$

$$E_{B2}=E_B+V^{BB} \qquad (30b)$$

which corresponds to the case of two levels interaction.

Notably, the two quantum dots are connected serially, so V_{DB2}=0 and V_{AB1}=0. This case is also parameterized. The calculations are performed for V_{DB1}=V_{AB2}=-0.1eV, V^{BB}=-0.1,-0.2 and -0.3eV with V_{AR}=-3eV, β_R=-3eV and E_B=-1, 0, 1eV (see figs.(5- 7)).

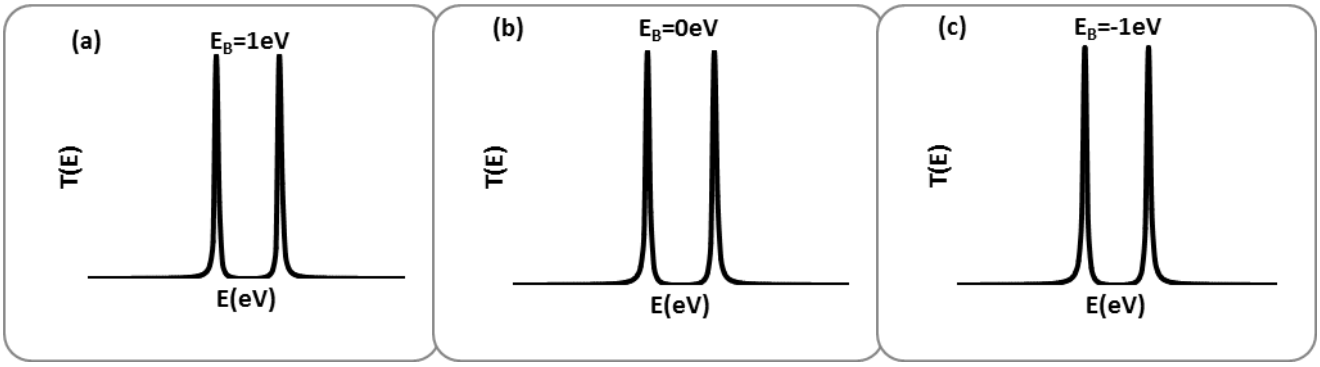


Figure (5): the transmission probability as function of the system energy with $V^{DB}=V^{AB}=V^{BB}$=-0.1eV, V^{AR}=-3eV, β_R=-3eV.

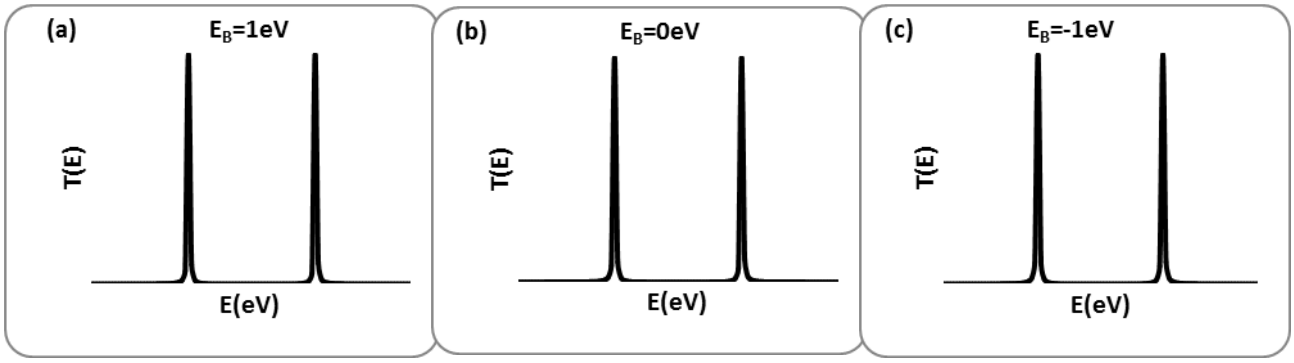


Figure (6): the transmission probability as function of the system energy with $V^{DB}=V^{AB}$=-0.1eV, V^{BB}=-0.2eV, V^{AR}=-3eV,β_R=-3eV.

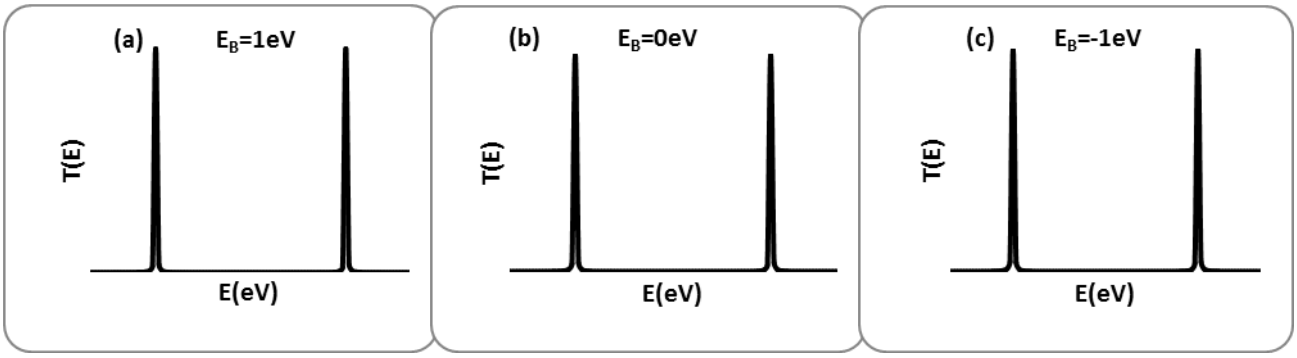


Figure (7): the transmission probability as function of the system energy with $V^{DB}=V^{AB}$=-0.1eV, V^{BB}=-0.3eV,V^{AR}=-3eV, β_R=-3eV.

Interesting features are noticed:-

1- The energy difference between the energy levels positions is equal to $2|V^{BB}|$ for all cases.
2- As the coupling interactions V_{DB1} *and* V_{AB2} increase the transmission probability curves are broadened more.

(3-3) Three Quantum Dots

The third case is the case when the bridge's system is considered as three quantum dots with three effective energy levels E_{B1}, E_{B2} and E_{B3} .The local density of states on each quantum dot is calculated by using eq.(29), so $\rho_B(E_1) = \rho_B(E_3) = \frac{3\sqrt{2}}{4\pi V^{BB}}$ and $\rho_B(E_2) = \frac{3}{4\pi V^{BB}}$.

The bridge energy levels positions must be obtained following the tight binding model formula (Patterson 2007),

$$E_{B_j} = E_B + 2V^{BB}\cos\left(\frac{j\pi}{N+1}\right) \qquad j=1,2,3 \qquad (31)$$

Here V^{BB} is the coupling interaction between any two nearest neighbors quantum dots and N=3. In this case the interaction will partially lifted the degeneracy and the three quantum dots levels will be,

$$E_{B1} = E_B - \sqrt{2}V^{BB} \qquad (32a)$$

$$E_{B2} = E_B \qquad (32b)$$

$$E_{B3} = E_B + \sqrt{2}V^{BB} \qquad (32c)$$

This case is also parameterized. The calculations are performed for V^{DB1}=V^{AB3}=-0.1eV, V^{BB}=-0.1, -0.2 and -0.3eV with V^{AR}=-3eV, β_R=-3eV and E_B=-1, 0, 1eV (see figs.(8-10)). Interesting features are noticed:-

1- The energy difference between any two adjacent energy levels positions is equal to $\sqrt{2}|V^{BB}|$ for all cases.
2- As the coupling interaction V^{DB1}, V^{AB3} increases the transmission probability curves are broadened more.

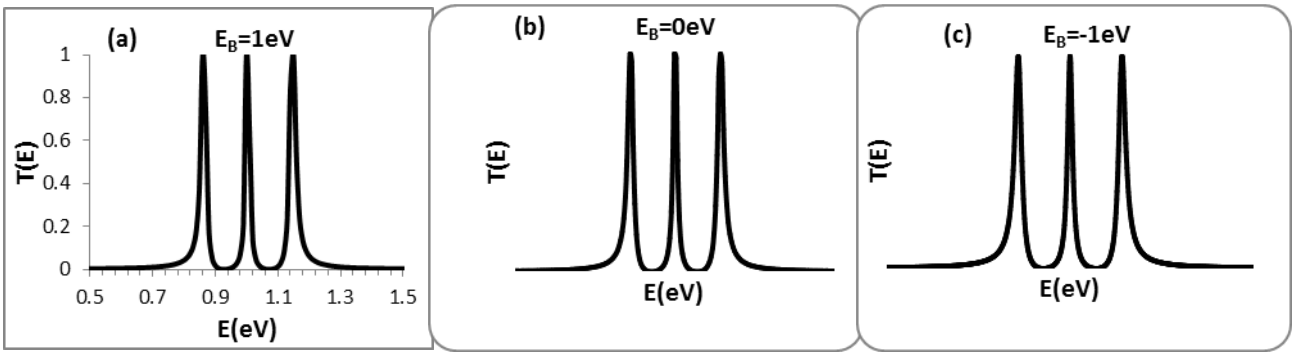


Figure (8): the transmission probability as function of the system energy with $V_{DB}=V_{AB}=V^{BB}$=-0.1eV, V_{AR}=-3eV,β_R=-3eV.

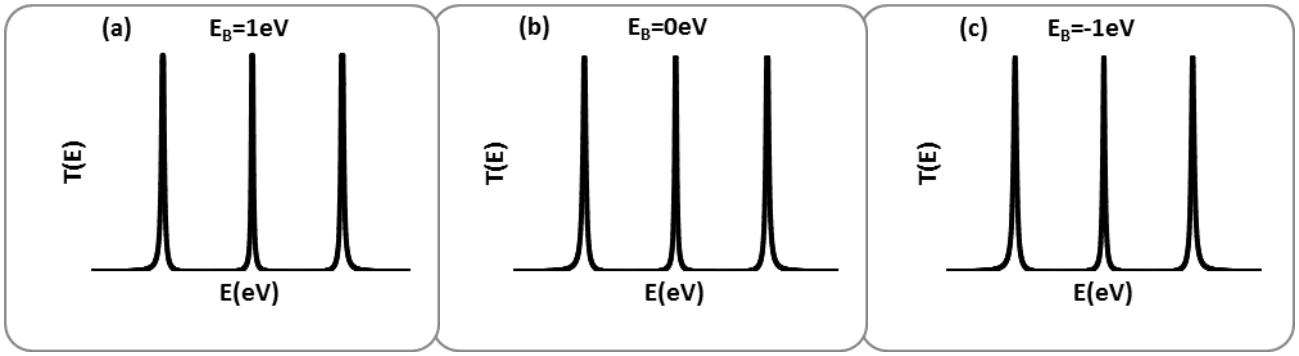


Figure (9): the transmission probability as function of the system energy with $V_{DB}=V_{AB}$=-0.1eV, V^{BB}=-0.2eV, V_{AR}=-3eV, β_R=-3eV.

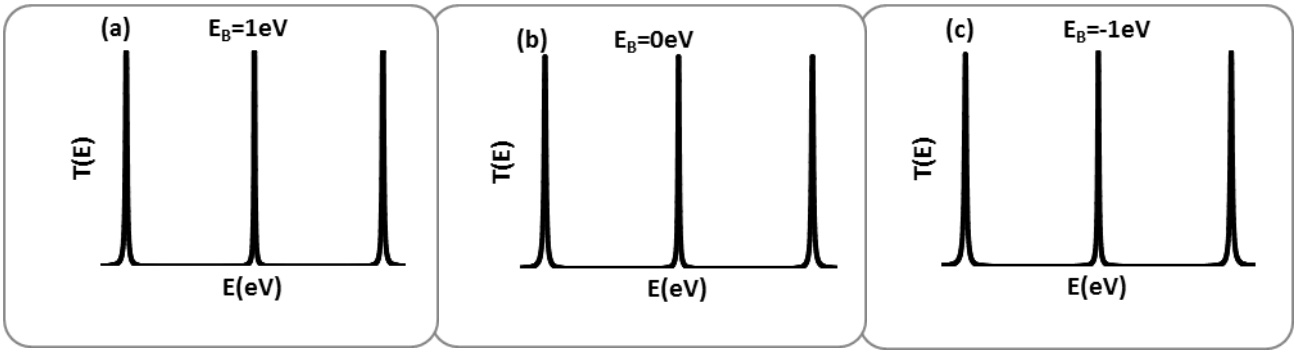


Figure (10): the transmission probability as function of the system energy with $V_{DB}=V_{AB}$=-0.1eV,V^{BB}=-0.3eV, V_{AR}=-3eV, β_R=-3eV.

4. Conclusions

From our results we can predict that the electron transport is significantly influenced by (a) the bridge-donor and bridge-acceptor coupling strength, (b) the acceptor-right lead

coupling strength and (c) the band width of leads.

The transmission probability shows sharp resonant peak for the weak-coupling limit (solid curves in Fig. (4)), while, they get broadened in the limit of strong-coupling (dash curves of Fig. (4)). Such increment of the resonant width is due to the broadening of the quantized energy levels of the donor and the acceptor. All these resonant peaks are associated with the energy eigenvalues of the bridge, and hence, we can predict that the transmission probability spectrum manifests itself the electronic structure of the bridge.

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معالجة نظرية لنقل الألكترون خلال جسر من النقاط الكمية

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الملخص

في هذا البحث تم تقديم معالجة لنظرية لنقل الألكترون خلال منطقة أستطارة واحدة رُبطت بواهب وقطب أيسر في الجانب الأيسر بينما في الجانب الأيمن ربطت بمستقبل وقطب أيمن. بنيت معالجتنا على هاملتونين أندرسون-نيونز المعتمد على الزمن. أُشتقت معادلات الحركة لكل أجزاء النظام ثم تم إعتبار الحالة المستقرة لإيجاد صيغة تحليلية لأحتمالية النفاذية كدالة لطاقات النظام. تتكون منطقة الأستطارة من واحد أو أثنان أو ثلاثة نقاط كمية. القيم الذاتية لأجزاء النظام وتفاعل الأقتران بينهما بالإضافة إلى عرض حزمة الأقطاب ثم أخذها جميعاً بنظر الأعتبار.