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Study of the Transmission and Reflection of Electron Waves through a Bridge System Consisting of Quan-tum Dots Using the Tight-Binding Approximation

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***Abstract*—In this study, we treat tunneling similarly to the dispersion problem where the wave incident on the barrier is partly transmitted and partly reflected. The transport potential will be related to conduction using the tight-binding model, the steady-state formula, and the Landauer relationship. The tunnel was processed using a bridge model. We studied the effect of changing the size of the quantum dots that make the bridge on the probability of transmission and reflection, the effect of changing the number of quantum dots on them. The transmission and reflection spectrums were compared as functions of the system's energy spectrum. We also noticed the effect of the transmission and reflection spectrum on the conductivity of the system. The results that have been reached, and will contribute significantly to the manufacture of nano-devices in the not-too-distant ture.**

***Keywords*—Transmission, reflection, tight-binding model, conductance.**

I. INTRODUCTION

Louis de Broglie introduced the first crucial concept for understanding quantum tunneling. In 1923, De Broglie proposed that material particles have a wavelength that decreases as momentum increases and vice versa. In 1927 Friedrich Hund was the beginning to postulate the phenomenon of breaking the potential barrier in quantum mechanics [1]. Direct quantum tunneling of electrons is possible by the standards of quantum mechanics. Classical mechanics does not explain the phenomenon of tunneling. Quantum tunneling occurs when particles can cross a barrier that cannot be crossed according to classical mechanics. This barrier is a high-energy area, a vacuum, or an insulator. Tunnel formationis is pivotal in many physical, chemical, and biological features. Electrons can move from the metal surface to the vacuum through a certain barrier. It is possible for an electron to pass through a vacuum if there is a high enough electric field through a barrier that is not thick enough. This emission is called cold emission. Semiconductors are one of the materials in which tunneling is possible. The tunneling of electrons through a dielectric barrier is essential for flash devices. In nanotechnology, quantum tunneling is possible in scanning tunneling microscopes, transistors, and even touch screens. The presence of the assumed particle with energy E inside a well with walls of thickness d. This well is one-dimensional and has a height of V. Classical mechanics holds that if the value of E is less than that of V, then the particle is trapped in the well and never emerges. Unlike quantum mechanics if E is greater than V, the particle can escape from the potential well Even if V is larger than E, the particle can penetrate the barrier and escape, but this is possible depending on The thickness of the sides of the well and the difference between kinetic E and potential energy V.In the electron tunnel in solid materials, the potential well is like a metal region where the electrons are present in the Fermi energy level, and the barrier in it is a material in which electrons cannot spread; that is, there is a Fermi energy gap for the insulating material. Although electrons do not propagate infinitely, vanishing states can extend from the metal to the tunnel barrier. Vanishing states play an essential role in tunnel formation. The fading states consist of the complex bundle structure of the dielectric, which determines how it decays in the dielectric [2,3]. The phenomenon of electron tunneling emerges from the wave nature of electrons, so when the wave encounters an incident, it is partly reflected and partly transmitted. Interface reflection produces interface or junction resistance. In this paper treats tunnel as similar to dispersion, such that the incident wave is partly transmitted over the barrier and partly reflected. The transmission probability is related to conduction based on a model resulting from the Landauer relationship.[4] Brinkmann, Dynes, and Rowell treat the phenomenon of electron tunneling using a simple barrier model, as the model deals with the scattering of electrons based on the

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free electron model. According to this approach, investigating the gap tunnel between the valence band and the conduction band is impossible. We are treated by adopting the tight coupling model to form a barrier whose gap is between the valence band and the conduction band [5]. The models of Bardeen [6] and Slonchevsky [2] consist of two electrodes with a very thick insulator between them, so that electrons cannot form quantum tunneling. Tight-binding approximation takes into account the closest interactions and neglects other farther interactions [7,8]. Nevertheless, this approximation was a great success [9]. To know the basic properties that we obtain through the transfer curve in the system [10], as there are many researchers who use this method [11-13], and the extent to which this approximation agrees with theoretical methods in research. This approximation is considered the cornerstone of special theories in the field of ballistic electron transfer through molecules [14]. The study of the possibility of transferring electrons from one side of the junction to the other side, it takes into account the probability of transport through molecules. The two poles operate as two systems that do not depend on each other, but when one is brought close to the other, their wave functions overlap, and quantum tunneling occurs.

II. THEORETICAL FORMULATION OF THE MODEL

The bridge system was proposed to study the relationship between transmission and reflectivity and the extent to which they are affected by changes in the energy and number of quantum dots. This system consists of two poles, the right pole , and the left pole, and between them, the quantum dots are located or placed, as shown in Figure (1).

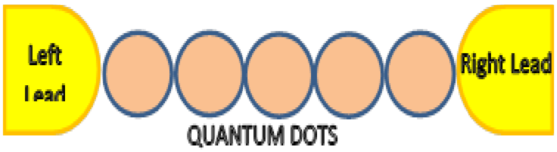

Fig.1. represents the bridge system consisting of two electrodes in yellow, and the pink circles represent quantum dots.

In tight binding therapy, the system is converted to a potential series model, in which the energy levels of each molecule and the coupling interaction between each two molecules are considered calculating the eigenvalues of the system is done based on the tight coupling model, such as [15],

$$E_j = E_Q - 2V_{mn}\cos\left(\frac{\pi j}{N+1}\right), \tag{1}$$

E_Q represents the energy level of the molecule. V_{mn} is the coupling interaction between the nearst neighboring molecules. N refers to the total number of molecules. The tight connection process of the bridge system is prepared as a one-dimensional chain. Any bonding between sites is a coupling interaction. Depicting the system as a single scattering region simplifies the model with wires. The system under study (as in Figure 1) is represented by a time-independent Hamiltonian (using Dirac- symbols). The Hamiltonian includes all the interactions of the subsystems, as shown below:

$$H = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + \sum_{k_{L1}} E_{k_{L1}}|k_{L1}\rangle\langle k_{L1}| + \sum_{k_{L2}} E_{k_{L2}}|k_{L2}\rangle\langle k_{L2}| + \sum_{k_b} E_{k_b}|k_b\rangle\langle k_b| + \sum_{k_b}[(V_{Ak_b}\,|A\rangle\langle k_b| + h.c) + (V_{Dk_b}|D\rangle\langle k_b| + h.c) + h.c)] + \sum_{k_L}(V_{Dk_{L1}}\,|D\rangle\langle k_{L1}| + h.c) + \sum_{k_R}(V_{Ak_{L2}}\,|A\rangle\langle k_{L2}| + h.c) \tag{2}$$

The following symbols D, A, $L1$, $L2$, and b indicate the donor, acceptor, first strand, and second strand, while N represents the total number of molecules. The symbol k_i is the wave vector with i representing the symbols indexes D, A, $L1$, $L2$, and b. E_i represents the location of the energy level and $|i\rangle$ and $\langle i|$ represents ket and bra states, respectively. While V_{ij} is the coupling interaction between subsystems i and j. The wave function of the system is written as follows:

$$\psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_{k_b} C_{k_b}(t)|k_b\rangle + \sum_{k_{L1}} C_{k_{L1}}(t)|k_{L1}\rangle + \sum_{k_{L2}} C_{k_{L2}}(t)|k_{L2}\rangle, \tag{3}$$

$C_i(t)$ represents the linear expansion coefficients. We obtain the equations of motion for $C_i(t)$ using the time-dependent Schrödinger equation,

$$\frac{\partial\psi(t)}{\partial t} = -iH\psi(t). \tag{4}$$

By substituting equations (2) and (3) into (4), we get the following:

$$\frac{\bar{C}_A(E)}{\bar{C}_D(E)} = \frac{X(E)}{Y(E)}, \tag{5}$$

where,

$$X(E) = V^{Ab}\,\Gamma_b(E)V^{bD}\ , \tag{6}$$

$$Y(E) = E - E_A - \sum\nolimits_{AL1}(E) - \sum\nolimits_{Ab}(\mathrm{E}), \tag{7}$$

here $\sum_{Ai}(E) = -i\Delta_{Ai}(E) + \Lambda_{Ai}(E)$, where $\Delta_{Ai}(E)$ is the broadening function, while $\Lambda_{Ai}(E)$ is the quantum shift function, where $i = L1, b$. The transmission amplitude, the transmission probability , and the reflection probability are respectively defined by [16],

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)}, \tag{8}$$

$$T(E) = |t(E)|^2. \tag{9}$$

$$Ref(E) = 1 - T(E) \tag{10}$$

Calculations of the current passing through the scattering region are based on the Landauer transfer formula[17],

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_{L1}(E) - f_{L2}(E)]dE, \qquad (11)$$

Conductivity calculations are made based on calculations of the probability of access for the bridge system of the model under study using the following formula [18],

$$G = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\, T(E)\frac{\partial f_\alpha(E)}{\partial E}\ , \qquad (12)$$

where $f_\alpha(E) = \{1 + \exp[E - \mu_\alpha/k_B Te_\alpha]\}^{-1}$ is the firmi disribution function of electrons in the lead $\alpha = L1, L2$. The chemical potential of the lead α is μ_α with $\mu_{L1} = -V/2$ and $\mu_{L2} = +V/2$ where V is the bias voltage. The temperature Te_α of the lead α. Here we use Te_{L1}=Te_{L2}=Te is fixed at 300 K, meaning the leads are in thermal equilibrium.

III. Results and Discussion

The values of the factors used in our numerical calculations are indicated. The bonding strength of the nearest neighbors V_{nm} is set at 0.01 eV, while the coupling interaction between the bridge with the donor and the bridge with the acceptor is 0.1 eV. Also, the coupling interaction between the donor with the left wire and the acceptor with the right wire is 1 eV. The Fermi energy level, E_F, is set at zero in equilibrium. The most important of all is the energy level of quantum dots, which is equal to 10 eV. We note in Fig.2. that the probability of penetration will be high in locations close to the energies of the eigenvalues of the quantum dots, and this is logical due to the coupling interactions in the active region with the donor and acceptor, which cause a state of resonance between the eigenvalues of the quantum dots and the energy spectrum of the system. It can be These resonances are called Fano resonances that arise due to the interference of coupling interactions, that is, due to interference effects. The number of states of the peak transmission potential is N-1 due to the decay state that occurs for the levels of eigenvalues of quantum dots with the energy spectrum of the system. Also, in Fig. 2, we notice that the resonant peaks start from the left side, meaning the lower negative values of energy are very sharp, and as we move to the right towards the peaks of larger negative values, we find that the intensity of the resonance peaks decreases and exposure occurs until we finally reach a drop. It is so sharp that the system is almost continuously open. Fig.3 shows that the reflection probability of the electron's wave function works the opposite way to the penetration probability function. This is because when the eigenvalues of the quantum dots match the energy spectrum of the system, the resonant peaks of the reflection probability spectrum are the smallest possible, while the other values are the largest possible , the farther away from the values. Resonance of eigenvalues with the energy spectrum of the system. In Fig.3. we notice that the resonant peaks start from the left side; that is, the lower negative values of energy are blunt and appear as if they are continuous. As we move to the right towards the peaks of larger negative values, we find that the sharpness of the resonant peaks increases and the exposure decreases until we reach the end. Ultimately, the decline is so wide that the system is almost constantly reversing.

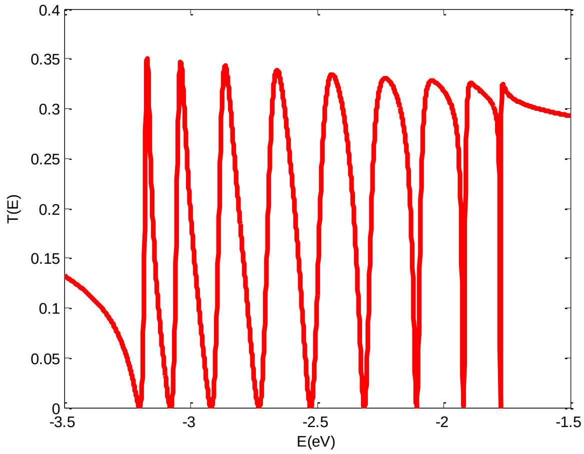

Fig.2. represents the relationship between the transmission probability as a function of the system energy spectrum.

By comparing the transmittance spectrum and the reflection spectrum as functions of the system's energy spectrum, it was found that there is a region in which there is neither the probability of reflection nor the probability of penetration of the wave function of the electron, and because in our quantitative treatment of the case studied we focused on the probability of transmission and the probability of reflection and did not give much importance to the case of capture. Alternatively, the loss of the electron within the system, which became clear to us through this comparison that there is a specific region or values in which there is no possibility of penetration and no possibility of reflection of the electron wave due to capture or loss within the system or due to the case of destructive interference of the electron wave within the system. Thus the possibility of the existence of The electrons in this region are almost zero, or the probability of implosion and the probability of running out are equal, or what is called the superposition state.

Fig.5. Represents the relationship between conductivity and the probability of permeation, as this relationship appears as a direct linear relationship. The greater permeability leads to the greater conductivity. This is intuitive because when the probability of an electron transferring through the system increases, the conductivity increases accordingly.

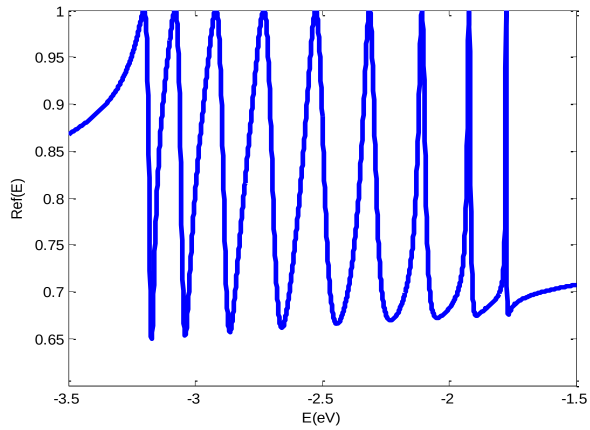

Fig.3. represents the relationship between the reflection probability as a function of the system energy spectrum.

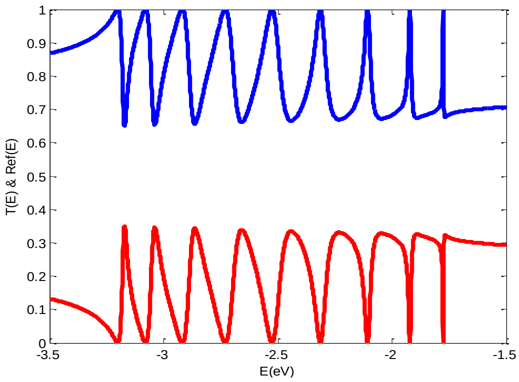

Fig.4. shows a comparison of the transmission probability spectrum (red line) with the reflection probability spectrum (blue line) as a function of the system energy spectrum.

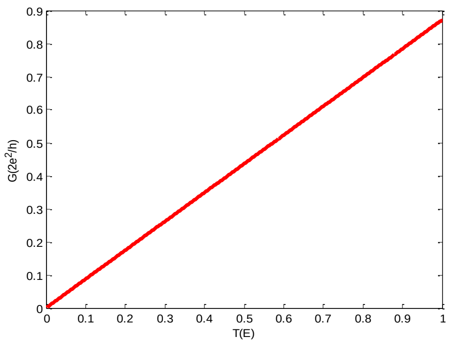

Fig. 5. The Conductivity as a function of transmission probability.

Fig.6. represents the relationship between conductivity and the probability of reflection. This relationship appears as an inverse linear relationship. The greater reflectivity leads to the lower the conductivity. This is logical because when the probability of reflection of the electron through the system increases, the probability of the electron being transmitted through the system decreases, and therefore, the conductivity decreases accordingly.

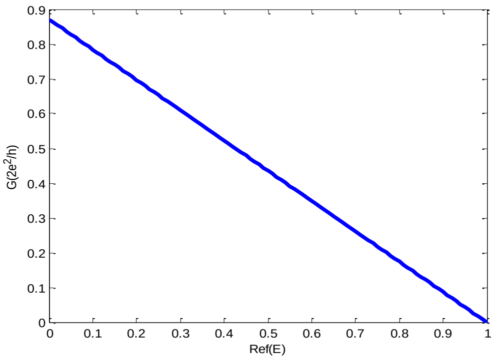

Fig. 6. The Conductivity as a function of reflection probability.

Fig.6. represents the probability of transmission as a function of the energy spectrum of the system. We notice that the probability of penetration decreases with the increase in the number of quantum dots, because the probability of tunneling decreases as the number of quantum dots increases. In other words, the resistance of the system to the transfer of electrons through it increases, and therefore , the probability of penetration decreases accordingly.

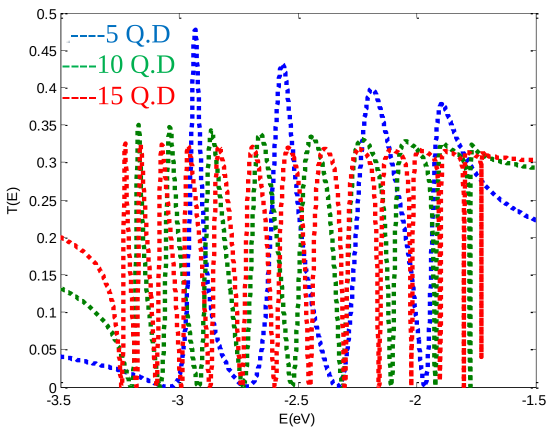

Fig.6. The probability of transmission as a function of the system energy spectrum for different numbers of quantum dots (the blue dotted line represents 5 quantum dots, the green dotted line represents 10 quantum dots, and the red dotted line represents 15 quantum dots).

Fig.7. represents the probability of reflection as a function of the energy spectrum of the system. We notice that the probability of reflection increases with the increase in the number of quantum dots, because the probability of tunneling decreases as the number of quantum dots increases. In other words, the system becomes more closed for the passage and transfer of an electron, and accordingly, the probability increases.

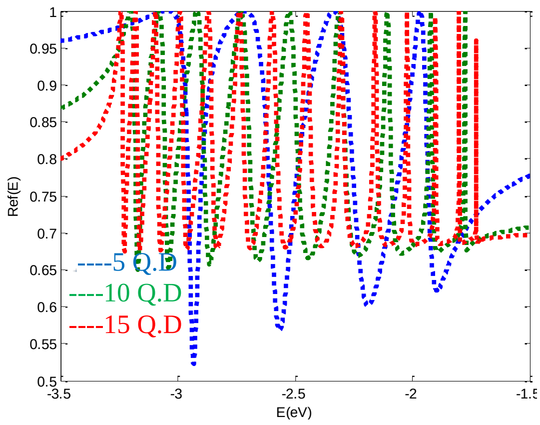

Fig.7. The probability of reflection as a function of the system energy spectrum for different numbers of quantum dots (the blue dotted line represents 5 quantum dots, the green dotted line represents 10 quantum dots, and the red dotted line represents 15 quantum dots).

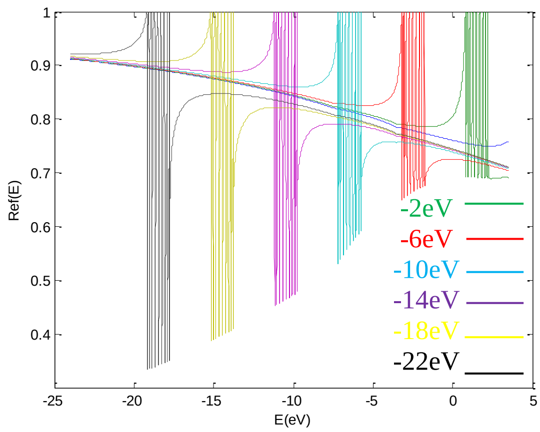

Fig.9. Reflection probability as a function of the system energy spectrum for different values of quantum dot energy(-2 ,-6,-10, -14, -18, -22 eV).

Fig. 8 indicates the transmittance spectrum as a function of the energy spectrum. We notice that the resonant peaks of the transmittance spectrum decrease with the increase in the ionization energy of the quantum dots, and this can be interpreted as the potential barrier represented by the quantum dots; as the value of the ionization energy increases, this means that the barrier has become more Thicker, and therefore the probability of the electron wave penetrating through this barrier decreases, and in return, the reflectivity spectrum increases with the increase in the ionization energy of the quantum dots, which is intuitive, meaning that if the probability of penetration decreases, this necessarily means an increase in the probability of electron wave reflection, as shown in Fig.9.

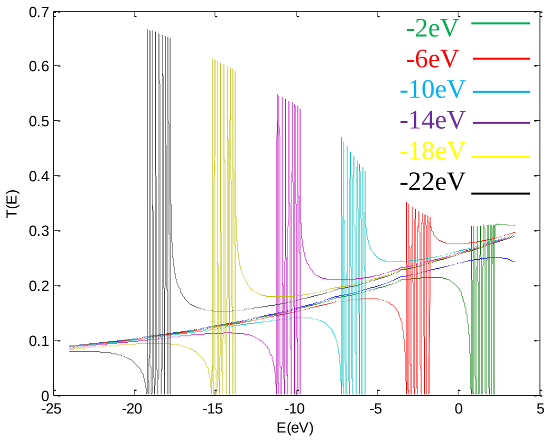

Figure (8) Transmittance probability as a function of the system energy spectrum for different values of quantum dot energy(-2,-6,-10, -14, -18, -22 eV).

IV. CONCLUSION

Through the results obtained for the proposed model, we conclude that the transmission and energy spctrums are significantly affected by the number of quantum dots placed between the electrodes as a quantum bridge. We notice that the system opens or a resonant state occurs during which the electron can form a quantum tunnel through the bridge and cross between the poles, taking advantage of the state of convergence between the levels due to the resonant states that are generated as a result of the equality that occurs between the intrinsic values of the energies and the energy spectrum of the system. It has been observed that the reflectivity spectrum is also affected in one way or another by the number of quantum dots, so that it increases with the increase in the number of quantum dots. This is very logical because the voltage barrier becomes thicker with the increase in the number of quantum dots between the electrodes, and therefore, the probability of the electron wave being reflected increases with the increase in quantum dots. We also note that the transmittance spectrum is affected by the increase and decrease of the ionization energy of the quantum dots, as it was observed that as the ionization energy increases, the resonant peaks of the transmittance spectrum decrease in contrast in the case of the reflection spectrum, the relationship is opposite to the transmittance spectrum, so that the probability of reflection increases with the increase in the ionization energy of the quantum dots. Results that have been reached to that consistent with our results in terms of behavior [19]. Other researchers have studied electronic properties at then nano scale level by studying the possibility of transmission through some molecules.[20] The results as mentioned earlier give us a clear idea about the factors that can increase the probability of electron wave reflection and decrease the probability of transmission, and vice versa, and how to deal with similar bridge systems to design electronic devices at the nanoscale**.**

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CONFLICT OF INTEREST

Authors declare that they have no conflict of interest.

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