Behavior of Current in a Semiconductor Nanostructure under Influence of Embedded Quantum Dots

H. Paredes Gutiérrez, S. T. Pérez-Merchancano

Abstract—Motivated by recent experimental and theoretical developments, we investigate the influence of embedded quantum dot (EQD) of different geometries (lens, ring and pyramidal) in a double barrier heterostructure (DBH). We work with a general theory of quantum transport that accounts the tight-binding model for the spin dependent resonant tunneling in a semiconductor nanostructure, and Rashba spin orbital to study the spin orbit coupling. In this context, we use the second quantization theory for Rashba effect and the standard Green functions method. We calculate the current density as a function of the voltage without and in the presence of quantum dots. In the second case, we considered the size and shape of the quantum dot, and in the two cases, we worked considering the spin polarization affected by external electric fields. We found that the EQD generates significant changes in current when we consider different morphologies of EQD, as those described above. The first thing shown is that the current decreases significantly, such as the geometry of EQD is changed, prevailing the geometrical confinement. Likewise, we see that the current density decreases when the voltage is increased, showing that the quantum system studied here is more efficient when the morphology of the quantum dot changes.

Keywords—Quantum semiconductors, nanostructures, quantum dots, spin polarization.

I. INTRODUCTION

SPINTRONICS is a developing branch of modern sciences that currently raises a huge scientific and technological interest in different theoretical and experimental fields [1]-[10]. One of the main reasons is that in the future, this branch of sciences will become a very important technological line in the study of the electron spin. This compendium of physics has different advantages, among which we highlight: The increased speed of information processing will generate a lower power consumption, better overlap and of course, a more accurate reading of the electronic states information, and increased devices density on a chip [5]-[10]. This shows that the spintronics is of great practical interest for nano electronics when the spin effects are present in nanostructures of condensed matter. In this context, currently the spin orbit coupling (SO) in semiconductors has attracted great attention due to the crucial role it plays in the freedom spin degrees and

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the electron orbital dynamics when affected by the presence of impurities, electric and magnetic external fields [7]-[12].

Recently, the Rashba effect has gained great attention in different quantum low dimensional structures such as multiple wells [4], quantum dots [5], [15] and nanotubes [16] due to the changes that occur in the energy of these systems. In particular, Rashba effect is relevant in quantum dots and semiconductor nanostructures when the spin reversal modifies the tunneling information processing. Currently, the study of the Rashba effect in nanostructures involving self-assembled quantum dots is of great experimental and theoretical interest because of the potential spin filter manufacturing that analyzes the resonant tunneling in presence of electric and magnetic fields.

In the last decade, theoretical works such as Sun et al. [2] analyzed the metal semiconductor nanostructures behavior that included quantum dots. They showed that both spin orbital effects and conductance behavior are important in such systems when spin inversion is influenced by Rashba interaction in the presence of EQD and magnetic field flux. Likewise, they studied the spin polarization influenced by external fields, showing the appearance of a phase in the spin analysis and spin investment generated by the Rashba [6] effect.

In the same decade, other theoretical works such as Murakami et al. [7] and Sinova et al. [8] showed substantial changes in the current behavior when it took into account the spin dissipation, and electric fields, and interaction S.O. Such theoretical predictions are consistent with different analysis of experimental resonant quantum tunneling structures InGaAs/ GaAsSb studies in the presence parallel to the planes of the layers and temperature dependence [17], where the behavior of spin filters based on Rashba effect using nonmagnetic tunneling diodes resonant was investigated. In particular, symmetrical structures that consider the presence of the emitter and collector and a system of two separated quantum wells separated by a thin potential barrier were analyzed. These studies show a detailed analysis of the current and the spin polarization between the emitter and the collector in presence of the Rashba effect.

In this work, we focus on a theoretical investigation of a semiconductor nanostructure that analyzes the behavior of a quantum mechanical system of double potential barrier that considers quantum dots of different geometries, which are embedded. In order to determine the spin orbit coupling and the Rashba effect in this model, we use a Hamiltonian of close

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neighbors or tight binding model, which also takes into account the hopping between, sites i and j, the Rashba effect and spin orbit coupling. This analysis is performed following a treatment in second quantized under the Keldysh formalism, which considers Green's functions out of balance in the presence of electric fields [13].

The article was organized as follows: in Section II we present and discuss the many body Hamiltonian that analyzes the behavior of the double barrier system that takes into account the different geometries EQDs that allow us to involve quantum states. In Section III, the results obtained and their respective analysis are shown.
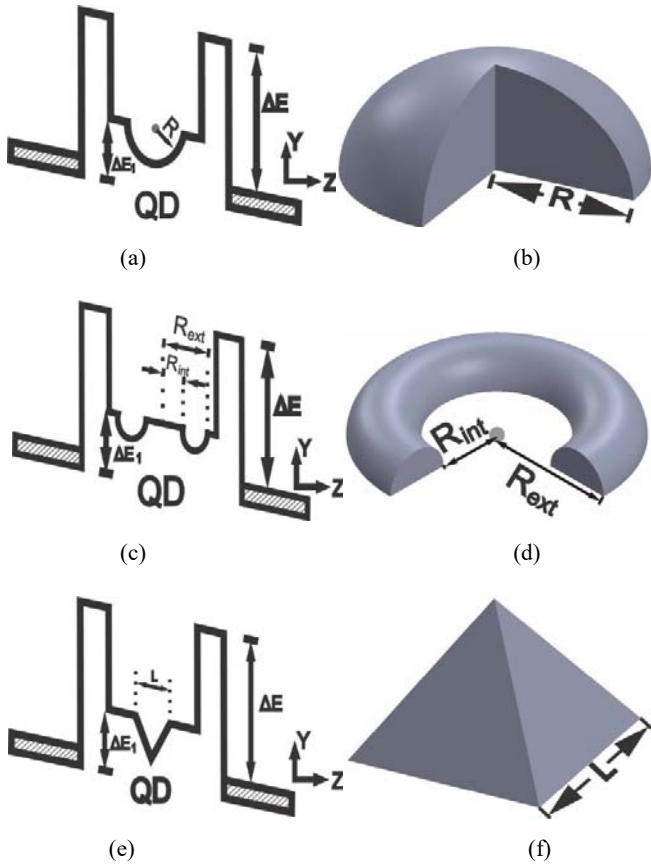
II. THEORETICAL MODEL

(a) (b)

(c) (d)

(e) (f)

Fig. 1 The effective potential in the growing z-direction of our DBH system with different *QDs* embedded: (a) *QDs* in lens form of radio R = 50 Å (b) ring of internal radio R_{int} = 30 Å and external radio R_{ext} = 50 Å and (c) Pyramid, whose base is an equilateral triangle of side L = 100 Å. 80 Å wide barriers, $\Delta E = 300 meV$ height, the 100 Å wide QW and $\Delta E_1 = 262 meV$

In this work, we study the electrons resonant tunneling through a quantum dot (QD) of (InGa)As of different form (lens, ring and pyramid) embedded in a DBH of *GaAS-(Ga,Al)As*, that was grown in the z-direction and connected to two semiconductor leads, as shown in Fig. 1. Our system is subjected to an external electric field applied in the z direction and an asymmetric confinement potential, this brings a consequence to the presence of the Rashba (SO) spin orbital

interaction.

The Hamiltonian H(r) associated to the electron transport through a quantic mechanical system is QD-DBH given by:

$$H(r) = \frac{p^2}{2m^*} + V(r) + H_{SO}(r), \qquad (1)$$

$$H_{SO} = \frac{\hat{z}}{2\hbar} \bullet \left[\alpha \left(\hat{\sigma} \times \vec{p} \right) + \left(\vec{p} \times \hat{\sigma} \right) \alpha \right], \qquad (2)$$

The vector $\hat{\sigma} = \left(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z \right)$ represents the Pauli matrices and the vector *p* of the momentum operator. The Rashba interaction that expresses (2) can be divided in two terms, H_{R1} and H_{R2} [2]:

$$H_{SO} = H_{R1} - H_{R2}, \qquad (3)$$

where

$$H_{R1} = \frac{1}{2\hbar} \left[\alpha \hat{\sigma}_x p_y + \hat{\sigma}_x p_y \alpha \right], \qquad (4)$$

H_{R1} results in a spin precession and the H_{R2} term can cause spin flips between different energy levels.

$$H_{R2} = \frac{1}{\hbar} \alpha \hat{\sigma}_y, \qquad (5)$$

The Hamiltonian in (1) of the *DBH* device connected to two leads $\left(\beta = L, R \right)$, and considering the Rashba spin orbit interaction (H_{SO} with $\alpha \neq 0$), can be approximately written in the standard Anderson model:

$$H = H_{QD-DBH} + \sum_{\beta=L,R} H_\beta + H_T, \qquad (6)$$

where H_{QD-DBH} is the Hamiltonian from the device *QD-DBH*, H_β for the leads and H_T is the coupling between the leads and *QD-DBH*.

$$H_{QD-BDH} = \sum_{n,s} \varepsilon_n d_{ns}^\dagger d_{ns} + \sum_{m,n} \left[t_{mn}^{SO} d_{m\downarrow}^\dagger d_{n\uparrow} + H.c \right], \qquad (7)$$

$$H_\beta = \sum_{ks} \varepsilon_{k\beta} a_{k\beta s}^\dagger a_{k\beta s}, \qquad (8)$$

$$H_T = \sum_{k,s} \left[t_{LDBH} a_{Lks}^\dagger d_s + t_{RDBH} e^{-isK_R L} a_{Rks}^\dagger d_s + H.c \right], \qquad (9)$$

The amount $\hat{n}_{ns} = d_{ns}^\dagger d_{ns}$ is the number operator, $s = \uparrow$ o $\downarrow$ is the spin index, in which it describes the spin state for the state with spin-up and spin down, respectively. *n* is quantum number for the eigenstates of the single-particle

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Hamiltonian (1), at the isolated QD region with eigenenergy $\varepsilon_n = \langle n | H | n \rangle$. The second equation term (7) is the Rashba H_{R2} interaction in the second quantitation with t_{mn}^{SO} intensity are the elements form the non-diagonal matrix that takes into account the transition process among levels when $(n_\uparrow) \rightarrow (m_\downarrow)$ for $n \neq m$. $k\beta$ is the quantum index for β lead with eigenenergy $\varepsilon_{k\beta} = \langle k\beta | H | k\beta \rangle$. In (9) is the Rashba interaction in the second quantization that gives place to a spin dependent phase factor $-is K_R L$ with $\left(K_R = \alpha \frac{m^*}{\hbar^2} \right)$

where m^* is the effective mass and L is the dimension of our double-barrier system DBH potential in the z-direction.

The quantum transport in the DBH device is solved using the standard Green functions method proposed by Keldysh [13]. The electron current with spin up or spin down in our quantum device can be derived as:

$$I = \frac{2e}{\hbar} \int \frac{d\omega}{2\pi} \text{Re}[t_{LDBH} G_{DBHL}^<(\omega) + t_{RDBH} G_{DBHR}^<(\omega)] \quad (10)$$

where the Green Keldysh function $G^<(\omega)$ is the transform Fourier of $G^<(t)$ that allows to perform the calculations of our quantum model considering the frequency spectrum or the quantized energies of the system.

To solve $G^<$, first we calculate the retarded Green function G_s^r using the Dyson equation:

$$G_s^r = g_s^r + g_s^r \Sigma_s^r G_s^r, \quad (11)$$

where $g_s^{r,a}$, is the retarded (advanced) Green function of the system without coupling between the contacts and the DBH (i.e. $t_{LDBH} = t_{RDBH} = 0$) and Σ_s^r is the self-energy that takes into account the electronic occupation number in the different quantum dot geometries used here.

After solving $G_s^r(\omega)$, the Green function $G_s^<(\omega)$ can be obtained from the standard Keldysh equation,

$$G_s^< = \left(1 + G_s^r \Sigma_s^r\right) g_s^< \left(1 + \Sigma_s^a G_s^a\right) + G_s^r \Sigma_s^< G_s^a \quad (12)$$

$$G_s^< = G_s^r g_s^{r-1} g_s^< g_s^{a-1} G_s^a + G_s^r \Sigma_s^< G_s^a. \quad (13)$$

For our case, $\Sigma_s^< = 0$ and $g_s^{r-1} g_s^< g_s^{a-1}$ is diagonal, with $g_{\beta\beta s}^{r-1} g_{\beta\beta s}^< g_{\beta\beta s}^{a-1} = 2i f_\beta(\omega) / \pi\rho$ $(\beta = L, R)$, and $g_{DBHs}^{r-1} g_{DBHs}^< g_{DBHs}^{a-1} = 0$, where $f_\beta(\omega)$ $f_\beta(\omega)$ is the Fermi distribution function in the contacts β and ρ is the leads density of states.

III. RESULTS

For our DBH of *GaAS-(Ga,Al)As* we consider the effective electronic mass for the GaAs of $m^* = 0.067 m_0$, m_0 is the free electron mass, the Fermi level $E_F = 100 meV$, the barrier height $\Delta E = 300 meV$, the band offset between the BDH and the QD is $\Delta E_1 = 262 meV$ and the width of the barrier (*B*) and the well (*W*) of 80Å and 100Å, respectively.
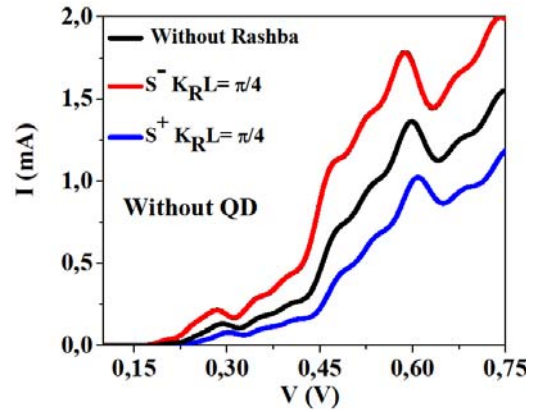

Fig. 2 Current as a function of the applied voltage for our DBH model without *QD* for two different Rashba effect values $K_R L = \frac{\pi}{4}$ y $\frac{3\pi}{4}$ and one without Rashba effect, with spin up (S$^+$) and spin down (S$^-$). The barriers and the well have a width of 80Å and 100 Å. $\Delta E = 300 meV$ corresponding to a concentration of Al of $x = 0.4$

Fig. 2 shows current vs. voltage characteristic for two different Rashba effect values, without *QD* and with S$^-$ spin y S$^+$ spin. It is observed that the current increases in function of the applied voltage in the DBH device presenting certain current peaks for certain voltage values. This happens when an electron in the sea of Fermi in the emitter enters in resonance with a bounded level in the *QW*. Also, as the applied voltage continues increasing, the electron is no longer in resonance with the bounded level in the QW generating a negative differential current, if the applied voltage continues increasing, this direct current will continue growing in the system, showing resonance behavior for higher voltage values. In addition, it is also observed in Fig. 2 that the peaks with S$^-$ go first into resonance with a greater intensity compared to the peaks with S$^+$ and without Rashba effect, showing fundamentally that with this type of polarity (spin down) it improves the electronic flow in the system.

Fig. 3 shows the current characteristic curve vs. voltage for a *QD* in the form of a 50 Å radius lens embedded in a DBH, with S$^+$ spin, S$^-$ spin and with two Rashba interaction values $K_R L = \frac{\pi}{4}$ y $\frac{3\pi}{4}$. It is observed that the current in function of the applied voltage changes significantly when it is compared to the results obtained in Fig. 2. In this figure, it is shown that due to the *QD* presence in lens form, there is a higher concentration of resonant states for certain voltage values. It is also recognized that the current behavior is of

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lower intensity in the DBH for the spin down case in the phase $K_R L = \pi/4$ that in $K_R L = 3\pi/4$, for example for voltage values close to 0.6 V, in the same way, when analyzing the spin up case for the two phases quoted above, it is observed that the noticeably lower current intensity values when the system has embedded a lens in the confinement well as expected in the DBH in the presence of EQDs. In this context, a higher number of peaks in certain voltage values are also determined, which implies a greater tunneling of carriers when comparing Figs. 2 and 3.
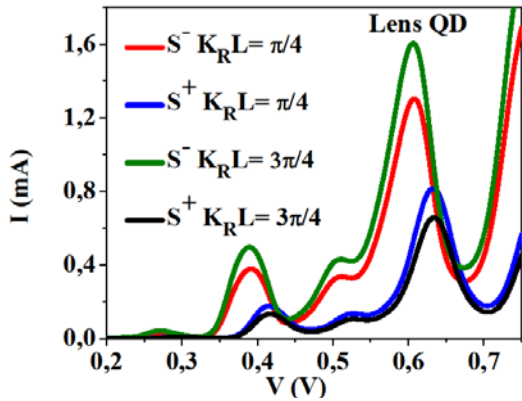
Fig. 3 Current vs. Voltage for a *QD* in the form of a lens with radius 50 Å embedded in a *DBH* with spin up (S^+) and spin down (S^-) and for different values of the Rashba interaction $K_R L = \pi/4$ y $3\pi/4$

In Fig. 3, it is observed that the current is of greater intensity for electrons with S^- spin compared with those of S^+ spin, presenting a movement of the spikes with S^- spin to lower voltage values, this is because the *2D* gas electrons first tunnel into the emitter of the device, when they are in resonance with the states bounded in the *QD* and then in resonance with the bounded states in the *QW*. In the 0.25-0.45 V voltage range, these tunneling peaks are associated to the *QD* linked levels, and between 0.45-0.7 V these tunneling peaks are associated with the confined levels in the *QW*. In addition, it is observed that the Rashba effect has a significant influence on the tunneling current, presenting a higher peak for the interaction $K_R L = \frac{3\pi}{4}$ than for interaction $K_R L = \frac{\pi}{4}$ when the electrons have S^-; and for S^+ electrons the current intensity behavior is inversed, being the greatest peak the one with interaction $K_R L = \frac{\pi}{4}$ compared to the curve with $K_R L = \frac{3\pi}{4}$ interaction.

Fig. 4 shows the current characteristic curve vs voltage for a *QD* in the form of a ring with internal radius $R_{int} = 30$ Å, and external radius $R_{ext} = 50$ Å embedded in a DBH, with spin up and spin down and with two values of Rashba interaction $K_R L = \pi/4$ y $3\pi/4$. In this figure, a higher number of peaks are observed than in previous results for similar voltage values, indicating a higher concentration of resonant states favoring quantum electron tunneling. This is due to the change of geometry in the EQD in the DBH, which indicates that our system is sensitive to the geometric change of dots. It is

observed that the current changes its behavior when the S^+ spin and S^- spin cases with phases $K_R L = \pi/4$ y $3\pi/4$ are studied. This behavior is similar to the one observed in Fig. 3 only that due to the morphology of the EQD, the current behavior shows higher values for spin down with a phase $K_R L = \frac{3\pi}{4}$ than for a phase $K_R L = \frac{\pi}{4}$ showing again an improvement of tunneling when the system is polarized with spin down.
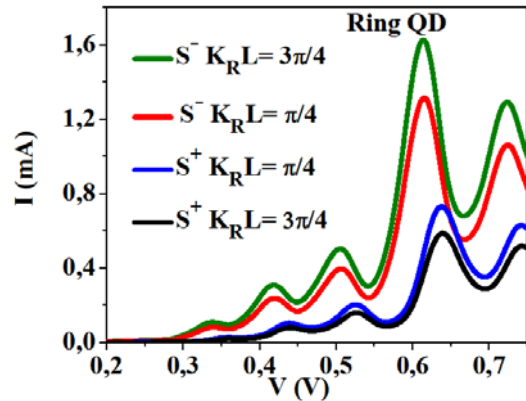

Fig. 4 Current vs. Voltage for *QD* in the form of a ring of internal radius $R_{int} = 30$ Å y $R_{ext} = 50$ Å embedded in a DBH with spin up (S^+) and spin down (S^-) and for different values of the Rashba interaction $K_{RL} L = \pi/4$ y $3\pi/4$

Fig. 5 shows similar behaviors of the current intensity in function of voltage as in Figs. 3 and 4, but they show a greater system efficiency when the EQD geometry is changed allowing to conclude in these cases, that the concentration of these resonants is higher when the confinement increases and the EQDs morphology changes.
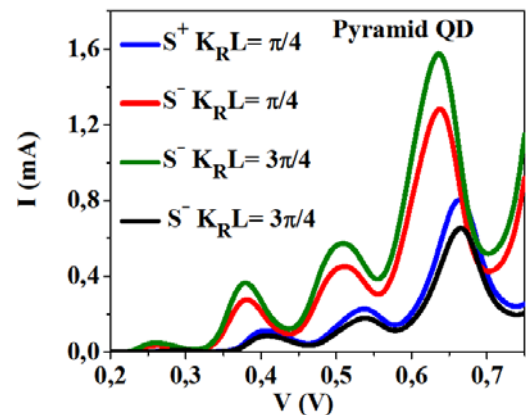

Fig. 5 Current vs Voltage for two *QDs* in the form of a pyramid embedded in a DBH with spin up (S^+) and spin down (S^-) and for different values of the Rashba interaction $K_R L = \pi/4$ y $3\pi/4$

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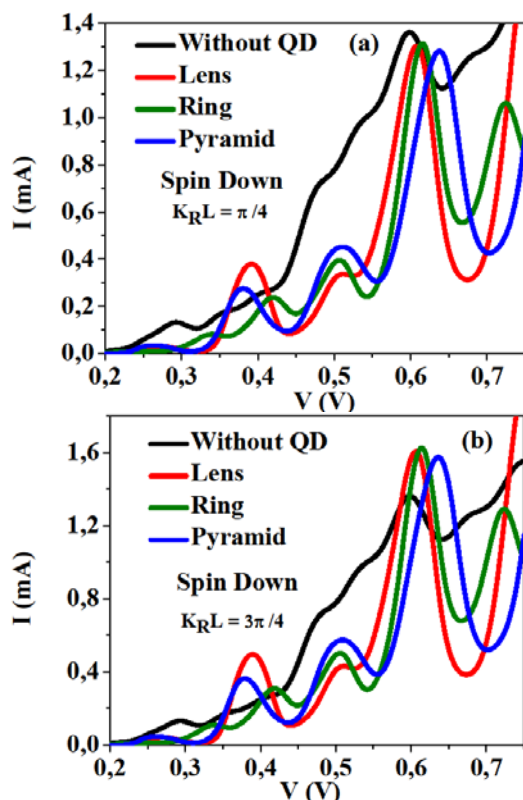
Fig. 6 Current vs Voltage for three EQDs of different geometries in a DBH with spin down (S⁻) and for different values of the Rashba interaction $K_R L = \pi/4$ y $3\pi/4$
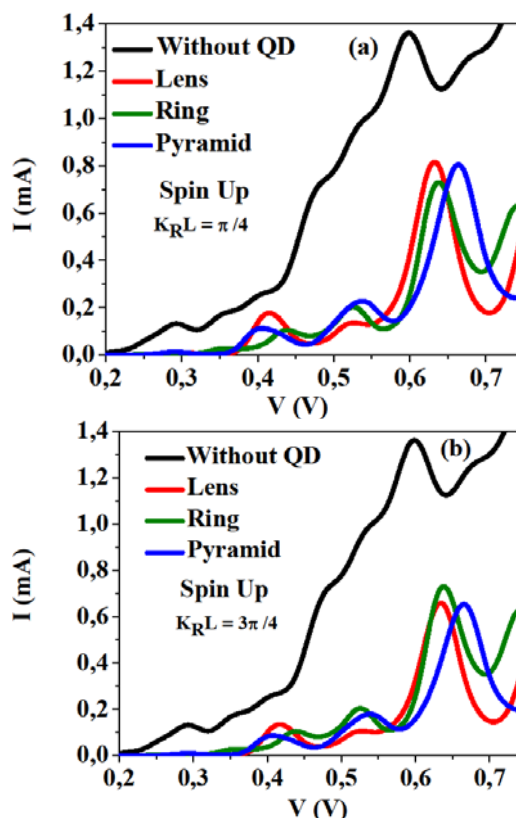

Fig. 7 Current vs Voltage for three EQDs in the form of a lens, ring and pyramid in a DBH with spin up (S⁺) and for different values of the Rashba interaction $K_R L = \pi/4$ y $3\pi/4$

In Figs. 6 and 7, we present the current vs voltage for three *QDs* of different shape as lens, ring, and pyramid embedded in the *QW* of our quantum mechanical model (DBH) and a graph without EQD, for two values of the Rashba interaction $K_R L = \pi/4$ y $3\pi/4$. In these two graphs, it is observed that the case with spin down favors the electron quantum tunneling, and the intensity of the resonance peaks is higher compared with spin up. It is observed that for certain values of the applied voltage in the heterostructure, the intensity of the resonant peaks in the current increases showing the predominance of the geometric confinement for certain *QD* morphology, and for other voltage values the Rashba effect predominates. For example, in these figures it is observed that the peaks located between 0.25 and 0.45 V are more intense for the *QD* in the lens than for the pyramid and the ring forms, this is due to a higher confinement. The bound levels in the *QW* of the heterostructure are more energetic in the ring form compared to the pyramid and the lens form [14], then the first resonant level encountered by the electron is the ring, then the lens and finally the pyramid. For voltage values between 0.6 and 0.7 V, a decrease in the intensity of the resonant peaks and a movement of the peaks to high voltage values are noticed, and being the highest peak of the *QD*, the one with the ring form, compared to the quantum dots lens and pyramid form, this happens due to the spin orbit effect included in the system.

IV. CONCLUSION

In this work, we have studied the behavior of current as a function of voltage for a double potential barrier system (DBH) that has EQDs of different geometry. The study of current intensity was conducted using a Hamiltonian from the system in the formalism of the second quantization where we included among others, the spin-orbit coupling. Here it was highlighted that the interacting spin orbits Rashba type, that is dominant throughout the DBH generates spin-flip between levels allowing the Zemman effect to change the current intensity behavior when spin-up or down states are taken into account, indicating that the spin polarization changes. Likewise, we observe that the current intensity in our DBH is susceptible to the presence of EQDs and that it is significantly modified when the morphology of the *QDs* changes.

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