Electronic properties of $Hg_{1-x}Cd_xSe$ lens-shaped quantum dots under external fields

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Abstract. $Hg_{1-x}Cd_xSe$ are II-VI semiconductors alloys with optoelectronic properties that depend upon the molar fraction $x$, which can be further controlled by nanostructuring. In this work one electron confined in a zero-dimensional lens-shaped nanostructure of $Hg_{1-x}Cd_xSe$ surrounded by a matrix of different molar fraction is analyzed and its electronic properties are studied under external magnetic and electric fields. Our system was modeled by means of the 3D Schrödinger equation in the framework of the effective mass approximation, which was solved using a finite element method. The model is described by a discontinuous space with Ben Daniel-Duke boundary conditions. We calculated the energy spectrum and the corresponding probability density of the electron for some low-lying energy levels as a function of: electric field strength on plane and magnetic field strength applied along the growth direction. Also, the effect of finite confinement potential was studied in presence of a uniform magnetic field. Our results shown that the electronic properties of $Hg_{1-x}Cd_xSe$ quantum dots are highly sensitive to a threading magnetic field because the degenerate energy levels are split. On the other hand, the effect of electric and magnetic fields applied simultaneously on a quantum dot can increase the system stability against external perturbation, e.g. thermal interactions.

1. Introduction
The recent interest in semiconductor nanostructured systems has grown side by side with the expansion of technological boundaries and the search of small, light and economic electronic devices, which are used on a wide spectrum of applications. This has lead to the study of material that show interesting opto-electronic properties, such as $Hg_{1-x}Cd_xSe$ alloys. They detect electromagnetic radiation from the infrared to the visible spectrum through molar fraction variations. Also, this alloy can be fabricated with fewer defects than the more known and studied $Hg_{1-x}Cd_xTe$ alloys [1].

The study of this alloy started in the 70s [2] and has attracted the attention of military contractors for the study and future development of infrared detection devices [1]. Recent experimental and theoretical studies on the $Hg_{1-x}Cd_xSe$ alloy showed its potential in the development of new opto-electronic technologies [3–8].

The electronic band structure of $Hg_{1-x}Cd_xSe$ alloys was calculated by [9], and it shows a strong dependence on the molar fraction. When $x = 0$ it behaves like a semi-metal, in $x \approx 0.1$ it suffers an inversion between the conduction and valence bands, and for $x \gtrsim 0.1$ is a semiconductor.
The effective mass of the alloy was given by \[2\], where it is shown that its effective mass is given by a relation with the energy gap. This relation makes it interesting to analyze the semi-conductor alloy with values close to \(x \approx 0.1\), in this case the effective mass has a very small value, which translates in a strong quantum behavior.

2. Theoretical basis
Due to the huge amount of atoms which compose a Quantum Dot (QD), it will be difficult to calculate the interaction of the electrons with each one of the atoms that compose the lattice. We considered a single interaction of the band structure between the valence and conduction band, the effective mass approximation. Under this approximation the Hamiltonian describes the quantum behavior of an electron confined inside a tridimensional QD under the influence of magnetic and electric fields

\[
\hat{H} = \frac{1}{2m^*} \left[ \vec{p}(x,y,z) - e\vec{A}(x,y,z) \right]^2 + eFx + V(x,y,z). \tag{1}
\]

The Coulomb gauge \(\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})\) was used to express the magnetic potential \(\vec{A}\) in terms of the magnetic field. This gauge is essential to properly describe the charge interaction with the magnetic field and is used in semiclassical calculations. The possible energy levels of the system are the eigenvalues of the Hamiltonian. Considering an oriented magnetic field on a \(\theta\) angle relative to the direction of growth and an oriented electric field along the QD plane, we obtain the dimensionless equation of Schrödinger-Pauli

\[
\begin{aligned}
&\left\{ -\nabla^2 - i\gamma \left[ y \left( \cos \theta \frac{\partial}{\partial z} - \sin \theta \frac{\partial}{\partial x} \right) + (x \sin \theta - z \cos \theta) \frac{\partial}{\partial y} \right] + \\
&\quad \frac{\gamma^2 \left[ y^2 + (x \sin \theta - z \cos \theta)^2 \right]}{4} + \alpha Fx + V(x,y,z) \right\} \psi_n(x,y,z) = E_n \psi_n(x,y,z).
\end{aligned} \tag{2}
\]

Where \(\gamma = \frac{eB}{2m^* R_y}\) is the dimensionless coefficient of the magnetic field, that is present in the second and third term as the paramagnetic and diamagnetic parts, \(\alpha = \frac{e a_0}{R_y}\), the dimensionless coefficient of the electric field, \(a_0 = \frac{\hbar}{m^* e}\), the effective Böhr radius, \(R_y = \frac{e^2}{2 m^* \hbar^2}\), the effective Rydberg and \(V(x,y,z)\) represents the structural confinement potential

3. Modeling and simulation by finite elements
Two models were used to perform calculations. In the first model, the QD was considered isolated, with infinite confinement potential outside the QD and zero inside the QD, as can be seen in Fig. 1.

\[
V(x,y,z) = \begin{cases} 
0 & \text{Inside the QD} \\
\infty & \text{Outside the QD}
\end{cases} \tag{3}
\]
In the second model a finite confinement potential was considered. In this model the nanostructure is surrounded by an alloy with different molar fraction. Two zones are defined, the first one representing the QD of $Hg_{1-x}Cd_xSe$, molar fraction $x = 0.14$, and the second one representing the matrix that covers the QD, with a different molar fraction $Hg_{1-x_0}Cd_{x_0}Se$, $x_0 = 0.18$, this zone is simulated by a cylinder.

The problem was solved in a discontinuous space meshed of tetrahedral finite elements, the shape function used to interpolate over the space is a Lagrange polynomial of third degree. The meshing parameters were calculated by a convergence criteria which assures three significant figures; their values were chosen based on [10].

Due to the fact that the confinement potential is finite there is a possibility of finding the electron outside the QD; a very fine mesh was used in the matrix zone that is closer to the QD. This helps in the optimization of calculation time based on the criteria that are more important the QD domain and its surroundings. A representation of this can be seen in Fig. 2.

The confinement potential is given by Eq. 4, the potential in the matrix is calculated as the 60% of the difference between the energy gap of the QD and the energy gap of the matrix.

$$V(x, y, z) = \begin{cases} 0 & \text{Inside the QD} \\ V = 39 \text{ meV} & \text{Inside the matrix} \\ \infty & \text{Otherwise} \end{cases}$$ (4)

The effective mass of the electron inside the QD has a value $m^{*}_{QD}$, on the matrix its value is given by $m^{*}_X$.

$$m^{*} = \begin{cases} m^{*}_{QD} = 0.08m_e & \text{Inside the QD} \\ m^{*}_X = 0.51m_e & \text{Inside the matrix} \end{cases}$$ (5)

The wave function that describes the electron needs to be continuous over the space, however, the properties that describe the behavior of this electron are different in each alloy. An appropriate boundary condition is the Ben Daniel-Duke condition [11], which is used to ensure continuity in the interface between the QD and the matrix. The following equation takes into account the change of effective masses on this boundary

$$\frac{1}{m^{*}_{QD}} \nabla \psi(x, y, z) \cdot \vec{n} = \frac{1}{m^{*}_X} \nabla \psi(x, y, z) \cdot \vec{n}.$$ (6)

On the boundaries, when the confinement potential is infinite, the wave function takes null values; in such points the Dirichlet boundary condition is imposed

$$\psi = 0.$$ (7)
4. Numerical results and discussions

In order to study the effect due to the application of external magnetic and electric fields on the electronic properties of a confined electron inside a QD, the energy levels calculations were performed to the first and second models described in the previous section. The calculation includes energy spectrum as a function of the magnetic field intensity over the growing direction and electric field along the plane of the QD, as a function of the angular orientation of the magnetic field between the growing direction and along QD plane. The probability density for the lowest states was calculated to 3D, however a 2D representation were obtained by the integration along the growing axis.

4.1. First model: infinite potential

The lowest energy levels of one-electron QD as a function of the magnetic field intensity are shown in Fig. 3. The observed behavior in the energy levels shows several features: crossing points between different levels, energy levels monotonically growing, initially increase and then decrease of energy levels. Such behavior can be understood as the superposition of the two terms due to the interaction of the electron with the magnetic field. The paramagnetic term defines the coupling between the magnetic field and the permanent magnetic moment of the rotating electron that is linear and can be positive or negative depending on if its clockwise or counterclockwise direction. The diamagnetic term is always positive, quadratic and increases the kinetic energy of the electron.

The lens axial symmetry promotes degeneration in the energy system, which is evident in the number of crosses between energy levels, in the low field intensity regime the structural and the magnetical components of the confinement are comparable. It is also observed how the levels that were degenerate in the absence of magnetic field are now unfolded under the effect of an external field, analogous to the Zeeman effect which is observed in atoms, giving more accessible states to the electrons. Furthermore, as the magnetic field increases the spectral structure acquires a Landau levels type configuration associated to a dominant magnetic confinement.

The energy levels in absence of external field are similar to the quantum harmonic oscillator. This is explained by the similarity in the shape of the confinement potential that acts over the electron. In the Fig. 3 is shown how the upper energy levels lose their degeneracy.

![Figure 3: Energy levels for a lens-shaped QD under external magnetic field $B$ on the growing direction with infinite potential confinement.](image1)

![Figure 4: Energy levels for a lens-shaped QD under external magnetic field $B$ on the growing direction and electric field on the plane direction with infinite potential confinement.](image2)
The lowest energy levels for a QD as a function of the magnetic field intensity with constant electric field are shown in the Fig. 4. The lens has a low height, an additional confinement in the direction of growth does not generate changes in energy spectra; so the field direction was simulated in the plane of the QD. An additional confinement due to the electric field, which greatly increases the energy of all levels, is observed. In the other hand, the states are unfolded in absence or for weak magnetic fields because the electrical confinement breaks the rotational symmetry of the lens. When the magnetic field contribution to the energy is greater than the electrical contribution, the energy levels behave in a similar way to what is seen in Fig. 3.

4.2. Second model: finite potential
In Fig. 5 the lowest energy levels for the lens-shaped model with finite barriers are shown. A limit on the number of located states within the structure is appreciable, and is given by the confinement potential between the two alloys and the magnetic confinement. Higher energy levels than this confinement extend the probability of finding the electron over the matrix and behave quasi-continuously because in the simulation this matrix has a finite dimension. If the nanostructure was embedded in an infinite crystal no quantum effects would be observed for the electron and the energy levels would be continuous.

Figure 5: Energy levels for a lens-shaped QD under an external magnetic field $B$ on the growing direction with finite potential confinement.

In Fig. 6 the probability density in the $xy$ plane, in the $xz$ plane and the probability percentage of finding the electron inside the QD for the first five energy levels is shown. The results reveal that the electron has a significant probability of being found outside the nanostructure; even if its energy is less than to the potential barrier, this behavior shows that the confined electron is tunneling. For large magnetic fields confinement increases towards the center of the QD, which translates in a slight increase in the probability of finding it in the structure.

It is useful to clarify that the molar fractions were selected to allow the confined electron to have an appreciable tunneling to the matrix and a limit on the number of possible states, this happens in a confining potential of only a few meV. When calculating the confinement potential equation in a molar fraction of $x = 1$, i.e. $CdSe$, a confinement potential of approximately 1eV is obtained; with this kind of confinement results are very similar to those found with an infinite potential barrier, except for a slight decrease in energy levels.
Figure 6: Probability distribution on the planes $xy$, $xz$ and the probability of finding the electron inside the QD.

5. Conclusions

The results obtained for the case of an electron confined in a zero-dimensional nanostructure $Hg_{1-x}Cd_xSe$, show that the electronic properties of such systems are highly sensitive to the intensity of external fields applied. Another feature that might have great applicability is simultaneous action of magnetic and electric fields on the lens. This is of great importance because the increased energy at all levels ensures a greater system stability against external perturbation. Finally, the simulation with finite potential confinement showed tunneling effects and a limited number of states in the QD, which is what is expected for a real nanostructure.

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