Stark effect of shallow donor impurities in HgS Inhomogeneous Quantum Dots

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Abstract. Using the variational method, within the effective mass approximation, we have calculated the binding energy and the Polarizability of a shallow donor confined to move in [CdS/HgS/CdS] Inhomogeneous Quantum Dots, in the presence of a uniform electric field. We consider an infinitely deep well and we present our results as function of the size of the well and for several values of the electric field strength: (i) The Polarizability decreases when the electric field increases. We find that the Polarizability it is more influenced by the quantum confinement than by the electric field. (ii) The binding energy depends on the inner and the outer radius of the IQD, decrease when the electric field increases and depends strongly on the donor position, (iii) We have demonstrated the existence of a critical value of radius ratio which can be used to distinguish the tree dimension confinement from the spherical surface confinement.

1. Introduction

In the past ten years, studies on the impurity states in semiconductors nanostructures, such as quantum well (QW), quantum well wire (QWW) and quantum dots (QD), have become subjects of extensive investigations both in basic and applied researches [1-5]. Recently, a new class of quantum dots called Quantum-Dots Quantum-well (QDQW) or Inhomogeneous quantum dots (IQD), have been studied both theoretically and experimentally [6-9]. IQD are composed of two semiconductor materials one of which, with the smaller band gap, is embedded between a core and outer shell of the material with the larger band gap. El Ghazi et al [10] have used the variational approach within the framework of the effective mass approximation to calculate the ground-state Hydrogenic shallow-donor binding energy in InGaN/GaN SQD-QW as a function of the ratio of the inner and the outer radius. The effect of electric field is investigated for two confinement regimes. Rezaei et al [11] have calculated the binding energy and self-polarization of hydrogenic impurity confined in a finite confining potential square well wire, under the action of external electric field and hydrostatic pressure. In a previous work, Zounoubi et al [5] have calculated the binding energy and the polarizability of shallow donor impurity in cylindrical QD under applied magnetic field. The ground electron state and the binding energy of a shallow donor impurity in a ZnS/CdSe core–shell QD under applied electric fields were calculated by Cristea et al [12] taking into account the dielectric mismatch at the dot interface.

In the present work, we use a variational method to calculate the shallow donor binding energy in IQD. We will examine the effects of the donor position, the electric field on the binding energy and
polarizability. This paper is organized as follows: in section 2, we present the general formalism; we deduce the analytical values of the binding energy and polarizability as a function of the radius of IQD. The numerical results and discussions are presented in section 3.

2. General formalism
We consider a shallow donor located at the position \( r_0 \) in a Inhomogeneous Quantum Dots made out of \([\text{CdS (Core)}/\text{HgS (Well)}/\text{CdS (Shell)}]\). In the effective mass approximation, the Hamiltonian of the system is written as:

\[
H = -\nabla^2 + \frac{2}{|r-r_0|} + f(r \cos \theta - r_0) + V(r)
\]

Where the confining potential \( V(r) \) is assumed to an infinitely deep well:

\[
V(r) = \begin{cases} 
0, & R_1 < r < R_2 \\
\infty, & r < R_1 \text{ and } r > R_2
\end{cases}
\]

And

\[
|\vec{r} - \vec{r}_0| = \sqrt{r^2 + r_0^2 - 2rr_0 \cos \theta}
\]

R_1 and R_2 are the inner and the outer radius of the IQD respectively. We use the effective Bohr radius \( a^* = \frac{\hbar^2\varepsilon_0}{m^*e^2} \) and the effective Rydberg \( R^* = \frac{m^*e^4}{2\hbar^2\varepsilon_0^2} \) as the units of length and energy (respectively). \( \varepsilon_0 \) is the dielectric constant, \( m^* \) is the electron band effective mass and \( f = \frac{e\alpha^*F}{R^*} \) is a dimensionless measure of the electric field \( F \). We use a variational method approach to determine the ground state, we adopt the wave function given by:

\[
\psi(\vec{r}) = \psi_0(\vec{r}) \left[ 1 + \beta f(r \cos \theta - r_0) \right]
\]

Where \( \beta \) is a variational parameter which takes into account the presence of the electric field and \( \psi_0(\vec{r}) \) is the wave function in the absence of the electric field \( (f = 0) \) given by:

\[
\psi_0(\vec{r}) = \frac{\sin[K(r-R_1)]}{r} e^{-\alpha|\vec{r} - \vec{r}_0|}
\]

\( \alpha \) is a variational parameter and \( K = \frac{\pi}{R_2-R_1} \). The exponential factor \( \exp(-\alpha|\vec{r} - \vec{r}_0|) \) describes the Coulomb spatial interaction. The energy is obtained by the minimization with respect to the variational parameter \( \alpha \). The binding energy \( E_b \) of the donor is defined as the ground state energy of the system without Coulomb term minus the ground state energy in the presence of the Coulomb term:

\[
E_b = E_{\text{Sub}} - E_i
\]

The Polarizability can be calculated from the dipole moment and is defined as:

\[
\alpha = \frac{p}{F}
\]

Where the dipole moment is given as:

\[
p = -e(\langle |\vec{r} - \vec{r}_0| \rangle_{f=0} - \langle |\vec{r} - \vec{r}_0| \rangle_{f=0})
\]
3. Results and discussion
In this section we will discuss the results obtained by applying the direct variational method for calculating the binding energy of a shallow donor impurity in the absence and presence of an electric field in IQD and the Polarizability by the formula dipole moment P. Numerical calculations are applied to a Inhomogeneous Quantum Dots made out of [CdS/HgS/CdS]. The physical parameters characterizing the system are given in the table 1:

| Material | m*/m₀ | ε₀ | εₓ | a*(Å°) | R*(eV) | Eg(eV) |
|----------|-------|----|----|--------|--------|-------|
| Cds      | 0.2   | 9,1| 5,5| 5,818  | 3,65   | 2,5   |
| HgS      | 0,036 | 18,2| 11,36| 5,851  | 5,0    | 0,5   |

3.1 Absence of the electric field
In Figure 1 (a) and (b), we plot the variations of the donor binding energy $E_b$ as a function of the ratio $R_1/R_2$ and for different values of the outer radius $R_2$. The ratio $R_1/R_2$ varies between 0 and 1. First, we analyze the two particular cases, $R_1/R_2$=0 and $R_1/R_2$ ≈ 1. In the first case ($R_1/R_2 = 0$), the situation correspond to a HQD. In Figure 1 (a) we present the variations of the binding energy $E_b$ of a donor placed in the center of a spherical layer, as a function of the ratio $(R_1/R_2)$ and for different values of the outer radius $R_2$>0.7a*. We remark that when the ratio $R_1/R_2$ tend to 1, the donor binding energy tends to the limit of $4R^*$ which represents the well-known tow dimensional donor binding energy. We also remark that the binding energy $E_b$ presents a minimum for a critical value of the ratio $(R_1/R_2)_{crit}$ depending of the value of $R_2$. For $R_1/R_2$ equal to zero, $E_b$ recovers the limit corresponding to a HQD. When the core radius $R_1$ increases, the donor is confined to hollow nanosphere, its confinement becomes less important and its binding energy decreases to a minimal value. For a critical value $(R_1/R_2)_{crit}$ there is equilibrium between the surface confinement effects and the tree dimensional confinement effects. For one value of the ratio $R_1/R_2$ greater than $(R_1/R_2)_{crit}$, the surface confinement effects becomes predominant and the binding energy increases. We also notice that the minimum of the binding energy moves toward small values of $R_1/R_2$ when the size $R_2$ of the dot increases and vanishes for large values of $R_2$. This situation is explained by the fact that in the limit $R_2 → \infty$, the quantum dot behavior is similar to the bulk case. When $R_1/R_2$ increases from 0 to 1, the binding energy increases monotonously from the value corresponding to the bulk (3D) to the value corresponding to the surface (2D). In Figure 1(b), we plot the variations of the donor binding energy $E_b$ against the ratio $R_1/R_2$ for different values of the outer radius $R_2$<0.8 a*. We see that the binding energy decreases monotonously when the ratio $R_1/R_2$ increasing from 0 to 1. Indeed, when the inner radius $R_1$ increases, the donor binding energy moves from the HQD situation where the kinetic energy is dominating to a small spherical surface where the coulomb energy prevails. We note that all the curves tend to the values which are in good agreement with the results obtained in reference [7]. The second cases ($R_1/R_2 = 1$) correspond to a narrow HgS well.
Figure 1. Variations of the binding energy $E_b$ as a function of the ratio $R_1/R_2$ for different values of the outer radius of the IQD, (a) $R_2 = 0.4, 0.5, 0.6, 0.7$ and $0.8 \, a^*$ and (b) $R_2 = 1, 2, 3, 4$ and $5 \, a^*$. 

\[ r_0 = \frac{(R_1 + R_2)}{2} \]
In Figure 2, we fix the outer radius at $R_2 = 3\ a^*$ and we plot the variations of the donor binding energy $E_b$ as a function of the donor position $r_0$ and for different values of the inner radius $R_1$ ($R_1 = 0.5\ a^*,\ 1\ a^*,\ 1.5\ a^*,\ 2\ a^*$). We remark that the binding energy presents a maximum when the donor is placed on the center of the spherical layer $r_0 = \frac{R_1+R_2}{2}$. When the donor is placed at the center of the spherical layer, the orbital electronic presents the spherical symmetry, the energy is maximal and decreases when the donor moves toward extremities of the spherical layer. This behavior had been reported for HQD [13].

![Figure 2](image)

**Figure 2.** Variations of the binding energy $E_b$ as a function of the donor position $r_0$ for different values of the inner radius of the IQD: $R_1 = 0.5, 1, 1.5$ and $2\ a^*$ where $R_2 = 3\ a^*$.

### 3.2 Presence of the electric field

In Figure 3, we present the binding energy $E_b$ as a function of the ratio $R_1/R_2$ for two different confinement regimes $R_2 = 1\ a^*$ and $R_2 = 2\ a^*$ and for two several values of the electric field $f = 0, 0.4$ and 0.8. We remark that when the electric field increases the binding energy decreases and the effect of the electric field becomes more important when the ratio $R_1/R_2$ offers toward 1 or the outer radius of the IQD increases. We can explain this result by the fact that the confinement decreases. In Figure 4, we fix the outer and the inner radius of the IQD respectively at $R_2 = 3 \ a^*$ and $R_1 = 1 \ a^*$ and we plot the binding energy $E_b$ as a function of the donor position $r_0$ for two different values of the electric field $f = 0$ and 0.4. We notice that the electric field reduced the binding energy. Its effect is more pronounced when the impurity is placed on the center of the spherical layer ($r_0 = \frac{R_1+R_2}{2}$) and decreases when the donor moves toward extremities of the spherical layer.
Figure 3. Variations of the binding energy $E_b$ as a function of the ratio $R_1/R_2$ for two different values of the outer radius of the IQD, $R_2 = 1\, a^*$ and $2\, a^*$ and two values of the electric field $f = 0.4$ and $0.8$. The solid curve corresponds to the binding energy variation in the absence of electric field.

Figure 4. Variations of the binding energy as a function of the impurity position for two different values of the electric field (IQD).

We present in figure 5, the Polarizability of a donor placed in a HQD as a function of the dot radius $R_2$ and for different values of the electric field. We note that the Polarizability decreases with increasing the intensity of the electric field. We remark also that the Polarizability decreases with the size of the quantum dot. The results show that the Polarizability decreases as the radius of the dot decreases for both cases. For larger quantum dots, the electronic confinement is negligible and therefore the results tend to the case of HgS bulk. The Polarizability decreases when the intensity of the electric field increases.

The Polarizability of a donor as a function of the position of $r_0/R_2$ HQD is plotted in figure 6. We show that the Polarizability increases with the position until it reaches the report $r_0/R_2 \approx 0.5$. For $r_0/R_2 > 0.5$ Polarizability decreases with increasing the size of the dot. This implies that the
The confinement effect is more significant than the effect of the electric field. Its effect is more pronounced when the impurity is placed between $r_0/R_2 ≈ 0.5$ to 0.7 and decreases as the donor moves to the ends of the dot. We also note that the Polarizability increases when we increase the electric field.

**Figure 5.** Polarizability of an impurity function of the radius $R_2$ for different values of the electric field $f = 0.1, f = 0.16, f = 0.18$ et $f = 0.2$

**Figure 6.** Polarizability of an impurity donor function deposition $r_0/R_2$ for two values of the electric field.

4. Conclusion
In conclusion, we have studied the donor binding energy and the Polarizability in IQD. The calculation was performed within the effective mass approximation and using the variational method.
The results show that (i) The Polarizability decreases when the electric field increases. We find that the Polarizability is more influenced by the quantum confinement than by the electric field. (ii) The binding energy depends strongly on the core and the shell radius, we have illustrate the existence of a critical value which may be important for the nanofabrication techniques. This value may also be used to distinguish the three dimensional confinement from the spherical surface confinement. (iii) The binding energy depends strongly on the donor position. We demonstrated that it is maximal when the donor is placed in the center of the HQD or IQD and the effect of the electric field reduces the binding energy. The calculations of the Polarizability of a donor in Inhomogeneous quantum dots IQD are in progress.

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