Polarizability and binding energy of a shallow donor in spherical quantum dot-quantum well (QD-QW)

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Abstract. The polarizability and the binding energy is estimated for a shallow donor confined to move in inhomogeneous quantum dots (CdS/HgS/CdS). In this work, the Hass variational method within the effective mass approximation in used in the case of an infinitely deep well. The polarizability and the binding energy depend on the inner and the outer radius of the QDQW, also it depends strongly on the donor position. It’s found that the stark effect is more important when the impurity is located at the center of the (QDQW) and becomes less important when the donor moves toward the extremities of the spherical layer. When the electric field increases, the binding energy and the polarizability decreases. Its effects is more pronounced when the impurity is placed on the center of the spherical layer and decrease when the donor move toward extremities of this spherical layer. We have demonstrated the existence of a critical value which can be used to distinguish the tree dimension confinement from the spherical surface confinement and it’s may be important for the nanofabrication techniques.

1. Introduction
In this last decade the advances in nanofabrication technology have made it possible to manufacture low-dimensional semiconductor materials such as quantum well (QW), quantum well wire (QWW) and finally quantum dots (QDs) structure where the electron is confined in three directions. With their reduced dimensionality, new effects can be observed and studied. In particular, the binding energies of shallow donors are expected to become important while they are known to be low in bulk materials [1-2]. The semiconductor quantum dots (QDs) structure, often called artificial atoms, have great potential for device applications in the nanometer scale [3]. Therefore, in recent years, both experimental and theoretical studies of the electronic and optical properties of homogenous quantum dots (QDs) have attracted the considerable attention of many scientists in condensed matter physics and applied sciences [4-6]. In this structure, a new type of quantum dot (QD) structure, called a quantum dot-quantum well (QDQW) or inhomogeneous quantum dots (IQD), has been fabricated and studied. Theses structures experimentally 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.
Nowadays, a synthesized inhomogeneous spherical quantum dot with a central core and one or several layers of shells (such as CdSe/ZnS, InAs/ZnSe, CdS/PbS) called core–shell structure quantum dot or quantum dot–quantum well (QDQW) attracts many scientists’ interests [7,8]. Xi Zhang and al [9] studied the third-order nonlinear susceptibilities associated with intersubband transition are theoretically calculated for ZnS/CdSe cylindrical quantum dot quantum well. X.N.Li and D.Z.Yao [10] interested on the study for nonlinear optical properties of the CdSe/ZnS quantum dot quantum well (QDQW). Xing and al. [11] focus problem of bound polarons in quantum dot quantum well (QDQW) structures is studied theoretically. For more details on the chemical fabrication of this new artificial structure, we refer to references: CdSe/ZnS/CdSe/ZnS [12], In(Ga)As/GaAs [13] and InAs/ZnSe [14].

Understanding the Impurity states in these structures is an important problem in semiconductors technology. Many works have been devoted to the studies of impurity states in the quantum well, quantum wire and quantum dots. Recently, J.Silva and al [15] have calculated the donor binding energy as a function of the donor position in QD with an infinite spherical well and for different radius of the structure. They found that the donor binding energy decreases when the donor position increases reaching a minimum, as the donor position is equal to the radius of the QD. Recently the dipole polarizability of the harmonic oscillator of nanodot has been calculated analytically [16-17]. Many theoretical attempts have been made to understand the polarizability [18-20]. For QDQW, to the best of our knowledge no work has been done to treat the polarisability and evaluate the effect of the donors position. The quantum confined stark effect has been the subject of numerous experimental and theoretical investigations [21] which demonstrated that the binding energy are shifted to low energies in the presence of an uniform electric field. The effect of the latter is to change the energy levels in the QD and giving rise to a polarization of the distribution of charge carriers and has other energy transition between quantum state [22]. D Schoss et al are presented a theoretical and experimental study on the inhomogeneous quantum dots (CdS/HgS/CdS) [23].

In this work, we use a variational method to calculate the polarisability and the binding energy of an electron bound to a donor impurity confined to move in inhomogeneous quantum dots (CdS/HgS/CdS) in the strong and the moderate regime of confinement. We will examine the electric field and the position of a donor impurity effects on the binding energy and the polarizability. We will examine the effect of the size of the dots.

![Diagram](image.png)

**Figure 1.** Schematic diagram of quantum dots-quantum well structure. $R_1$ and $R_2$ are the inner and the outer radius of the QDQW respectively.
2. General formalism

We consider a hydrogenic impurity located at the position \( r_0 \) of a quantum dot-quantum wells (QDQW) made from [CdS (Core)/HgS(well)/CdS (Shell)] subjected to the action of an electric field outside F. The confining potential is assumed as a model of an infinite deep well. In the effective mass approximation, the Hamiltonian system is written:

\[
H = H_0 + V(r) + W
\]  

(1)

Where \( V(r) \) is the confining potential. It’s written by:

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

(2)

\( R_1 \) et \( R_2 \) denotes the inside and outside radius of the quantum dot-quantum wells, respectively.

\( H_0 \) is the Hamiltonian in the absence of the electric field given by:

\[
H_0 = -\frac{\hbar^2}{2m^*} \Delta - \frac{e^2}{\varepsilon_0 |\vec{r} - \vec{r_0}|}
\]

(3)

Where \( |\vec{r} - \vec{r_0}| = \sqrt{r^2 + r_0^2 - 2rr_0 \cos \theta} \)

\( \varepsilon_0 \) is the dielectric constant and \( m^* \) is the effective mass of the electron in the QDQW.

\[
W = e \cdot f \cdot (r \cos \theta - r_0)
\]

(4)

Thus we introduce the dimensionless parameter characterizing the strength of the electric field

\[
f = \frac{e F}{R^*}.
\]

In a system of reduced units the Hamiltonian of an electron bound to a donor impurity in the dot ball is given by:

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

(5)

The Schrödinger equation expressed in spherical coordinates \((r, \theta, \phi)\) is written as:

\[
H \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)
\]

(6)

We use a variational method approach to determine the ground state binding energy and the polarisability, We adopt the wave function given by:

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

(7)

\( \psi_0 \) is the wave function in the absence of the electric field \((f = 0)\) given by:

\[
\psi_0 = \frac{\sin[K(r - a)]}{r} e^{-a|\vec{r} - \vec{r_0}|}
\]

(8)

Where \( \alpha \) and \( \beta \) are the variationals parameters (which takes into account the presence of the electric field).

The energy is obtained by the minimization with respect to the variationals parameters:

\[
E = \min_{\alpha, \beta} \left\{ \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \right\}
\]

(9)

The binding energy \( E_b \) of the Impurity is given by:

\[
E_b = E_{sub} - E_i
\]

(10)
The electric polarizability of an impurity depending on the position of the electric field increases the confinement of the electron and reduces the polarizability. That we can explain that by the decrease of the geometric dimensions of the quantum dot creates a compression wave function and the electron is closest to the impurity. It is causes the increased binding energy decreases when the dot radii decreases with decreasing the dot radii. It is due to the distribution of the electronic wave function. Therefore, the decrease of the geometric dimensions of the quantum dot creates a compression wave function and the electron is closest to the impurity. It is causes the increased binding energy. Our results are in good agreement with those found by Silva-Valencia and all [2, 25].

In figure 4. In this figure, we show that the electric polarizability increases with the donor position until...
it reaches the report $\frac{r_0}{R_2} \approx 1/2$. For $\frac{r_0}{R_2} > 1/2$ polarizability decreases with increasing the size of the quantum dot. This implies that the confinement effect is more significant than the effect of the electric field in the case of weak non-significant inverse positions in major positions. Its effect is more pronounced when the impurity is placed between the middle of the dot $\frac{r_0}{R_2} \approx 0,4$ to $\frac{r_0}{R_2} \approx 0,8$ and decreases as the donor moves to the ends of the dot. We also note that the electric polarizability decreases as we increase the electric field.

Figure 2. Variations of the donor binding energy $E_b$ as a function of the donor position ($r_0 / R_2$) for different values of the dot radius $R_2 = 1 \, a^*$, $2 \, a^*$, $3 \, a^*$, $4 \, a^*$ and $6 \, a^*$.

Figure 3. Polarizability of an impurity function of the radius $R_2$ for different values of the electric field $f = 0.1$, $f = 0.16$, $f = 0.18$ and $f = 0.2$. 
3.2 Inhomogeneous Quantum Dot ‘‘IQD’’

In figure 5, we present the binding energy $E_b$ as a function the ratio $(R_1/R_2)$ for two different regimes of confinement has $R_2 = 1a^*$ and $R_2 = 2a^*$ and for two values of electric field $f = 0.4$ and 0.8. We see that the binding energy depends strongly of the ratio $\frac{R_1}{R_2}$ increasing from 0 to 1 and presents a minimum $\left(\frac{R_1}{R_2}\right)_{\text{crit}}$ which can be used in nanofabrication of QDQW. When the inner radius $R_1$ a increases, the donor binding energy moves from the ‘’HQD’’ situation $\left(\frac{R_1}{R_2} \rightarrow 0\right)$ where the kinetic energy is dominating to a small spherical layer $\left(\frac{R_1}{R_2} \rightarrow 1\right)$ where the coulomb energy prevails and the donor can be considered as a fixed.

We note that when the electric field increases, the binding energy decreases and we also note that the electric field effect becomes more pronounced when the ratio $(R_1/R_2)$ tend to 1.

We have reported in figure 6, the electric polarizability of the donor impurity according to the ratio $R_1/R_2$ of the quantum dot quantum well (QDQW) for four values of outer radii $R_2$ and for an electric field strength $(f = 0.2)$. This figure illustrates the competition between the geometric confinement (the size of QDQW) and containment of the electric field on the polarizability.

For large values of the ratio $R_1/R_2$ (low spherical layer), the geometric confinement is important and the wave function of the electron is very localized. The electric polarizability of the impurity becomes less important and is relatively insensitive to the outer radii $R_2$ of the QDQW. For low values of the ratio $R_1/R_2$ (large spherical layer), the effect of electric field predominates. The polarizability is strongly depend of the size of quantum dot-quantum well. We note that the polarizability decreases as the $R_1/R_2$ ratio increases.
4. Conclusion

In conclusion, we have studied the polarizability and the binding energy of an impurity located in Inhomogeneous Quantum Dots (IQD) in the presence of an electric field. It’s clear that they strongly depend on the geometric confinement, the impurity position and the electric field.

We have shown the existence of a critical value \( \frac{R_1}{R_2} \) which may be important for the nanofabrication techniques.
We think that the present study will allow a better understanding of the behaviour of these new structures. We believe that our results of the polarisability in IQD will be relevant in the interpretation of experimental results. Unfortunately, we could not compare our results as no explicit experimental data are available in the literature.

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