# Impurity Binding Energy in Spherical Quantum Dot in the Presence of an Electric field

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**Abstract**

**Introduction:** Semiconductor nanostructures have attracted much attention due to its application in the development of optoelectronic devices. In these structures the electron spectrum comprises a set of discrete levels. On the other hand, donor impurity in quantum dots can alter the properties of a quantum devices.

**Aim:** Study of the effect of external electric field on the impurity binding energy in a spherical quantum dot.

**Materials and Method:** The energy levels are investigated using variational method within the effective mass approximation and finite barrier potential**.**

**Results:** The energy of impurity and binding energy are calculated in terms of radius of quantum dot. The binding energy is reduced with increases the radius of dot. The ground state energy of electron, impurity energy, and normalized binding energy versus electric field for different dot radii in finite quantum dot are also calculated.

**Conclusion:** The results show the energies decrease with increases the strength of electric field.

***Keywords*:** Impurity energy, Spherical dot, Turning point, Normalized binding energy

## Introduction

The study of semiconductor quantum dots and nanocrystals have been of a great interest from the experimental and theoretical point of view in recent years.[1] The origin of the interest lies in the size of quantization in solids and in those objects. The electron spectrum of an ideal quantum dot comprises a set of discrete levels. This makes the semiconductor quantum dot very important in the applications of optical and transport properties of semiconductors. The physical properties of the controlling quantum dot is attractive not only from the fundamental scientific point of view, but also because of its potential application in the development of semiconductor optoelectronic devices. [2]

Impurities in semiconductors can affect the electrical, optical, and transport properties. Understanding the nature of impurity states in semiconductor structures is a crucial problem. With characteristic dimensions comparable to the de Broglie wavelength of electron, these structures are particularly sensitive to atomic scale variations in geometry. Thus, impurity can dramatically alter the properties of a quantum device.[3] In order to understand how a hydrogenic donor impurity affects the spectrum of a single electron in low-dimensional

semiconductor structures, many researchers focused their attention on energy quantized states of the charged carriers. The study of the impurity states in semiconductor nanostructures was initiated only in the pioneering works of Bastard. [4] In spite of the growing interest in the topic of impurity doping in nanocrystallites, most of the theoretical works carried out on shallow donors in spherical quantum dots employ variational approaches,[5] or alternatively, perturbation methods limited to the strong confinement regime[6,7], while exact solution has been obtained only for centered impurities.[8,9] Bose et al. obtained the binding energy of a shallow hydrogenic impurity in a spherical quantum dot with a parabolic potential shape[10] and square-well barriers,[6,7] respectively. Additionally, a computational scheme yielding exact (numerical) wave functions and energies of a spherical nanocrystallite, with a shallow donor impurity located anywhere inside, is presented by Movilla and Planelles.[11] For simplicity and to protect the symmetric situation the impurity can be located at the center of the dot. An electron bounded to an impurity located at the center of quantum dot behaves like a bounded three-dimensional electron when the radius of the dot is very large. [12] However, as the dot radius is reduced, spatial confinement becomes very important.

On the other hand, the effect of the external electric field on the binding energy and wave functions play a significant role in the quantum dots. In a study conducted by Dane et al.[13], the binding energy of impurity under uniform electric field in the infinite quantum dot has been calculated. In the present work, the Schrodinger equation in finite spherical quantum dot is analytically solved, and the ground state energy and wave function are calculated by applying the boundary conditions at the interfaces, then using the variational method, the impurity binding energy in spherical quantum dot under a constant uniform electric field with finite confining potential is calculated.

## Materials and Method

### Experimental

In the absence of any impurity, within the effective mass approximation, the Hamiltonian is given by:

$$H_0 = -\frac{\eta^2}{2m^*}\nabla^2 + V(r) \tag{1}$$

where $m^*$ is the effective mass of the electron at the conduction band minimum. The confining potential $V(r)$ is given by:

$$V(r) = \begin{cases} 0 & r \le R \\ V_0 & r > R \end{cases} \tag{2}$$

where $V_0$ is the barrier height given by $V_0 = Q_c \Delta E_g(x)$ and $Q_c$ is the conduction band off-set parameter. The eigenfunction for the lowest lying state within the dot is:

$$\psi_0(r) = \begin{cases} N_1 \dfrac{\sin(\alpha r)}{r} & r \le R \\ N_2 \dfrac{e^{-\beta r}}{r} & r > R \end{cases} \tag{3}$$

where $N_1$ and $N_2$ are normalization constants and $\alpha$ and $\beta$ are given by:

$$\alpha = \sqrt{2m^* E_0 / \eta^2} \quad \text{and} \quad \beta = \sqrt{2m^*(V_0 - E_0)/\eta^2}$$

Matching the wave function and their derivatives at the boundary $r = R$, we get:

$$N_2 = N_1 \sin(\alpha R) e^{\beta R} \tag{4}$$

and,

$$\alpha R + \beta R \tan(\alpha R) = 0 \tag{5}$$

Solving this transcendental equation, Eq.(5), the confined particle energies, $E_0$, are obtained. The Hamiltonian for a shallow impurity located at the center of a spherical quantum dot of a radius $R$, in the presence of electric field can be written as:

$$H_{IF} = \frac{-\eta^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon r} + e\vec{F}\cdot\vec{r} + V(r) \qquad (6)$$

where $\varepsilon, e$ and $\vec{r}$ are dielectric constant, electron charge and the position vector, respectively. The external uniform electric field $\vec{F}$ is applied in $z$ – direction. Using the effective Rydberg constant $R^* = m^* e^4 / 2\eta^2 \varepsilon^2$ as the unit of the energy and the effective Bohr radius $a^* = \eta^2 \varepsilon / m^* e^2$ as the unit of the length, Eq. (6) becomes:

$$H_{IF} = -\nabla^2 - \frac{2}{r} + \eta r\cos\theta + V(r) \qquad (7)$$

where $\eta = ea^* F / R^*$ is the dimensionless measure of the electric field. The impurity energy in the presence of electric field is calculated by a traditional variational method, due to no exact solutions to the impurity states in quantum dot. The following trial wave function is adopted for ground impurity state in spherical quantum dot:

$$\psi_{IF}(r,\theta) = \begin{cases} A_1 \dfrac{\sin(\alpha r)}{r} e^{-\gamma r} e^{-\lambda r\cos\theta} & r \le R \\ A_2 \dfrac{e^{-\beta r}}{r} e^{-\gamma r} e^{-\lambda r\cos\theta} & r > R \end{cases} \qquad (8)$$

where $A_1$, $A_2$, $\gamma$, and $\lambda$ are the normalization constants and the variational parameters to be determined. The energy $E_{IF}$ is obtained by

$$E_{IF} = \min_{\gamma,\lambda} \frac{\langle \psi_{IF} | H_{IF} | \psi_{IF} \rangle}{\langle \psi_{IF} | \psi_{IF} \rangle} \qquad (9)$$

The influence of the electric field on energy levels of electron in spherical quantum dot is determined by

$$E_F = \min_{\kappa} \frac{\langle \psi_F | H_F | \psi_F \rangle}{\langle \psi_F | \psi_F \rangle} \qquad (10)$$

where the Hamiltonian and trial wave function are given as

$$H_F = -\nabla^2 + \eta r\cos\theta + V(r) \qquad (11)$$

and

$$\psi_F(r,\theta) = \begin{cases} B_1 \dfrac{\sin(\alpha r)}{r} e^{-\kappa r\cos\theta} & r \le R \\ B_2 \dfrac{e^{-\beta r}}{r} e^{-\kappa r\cos\theta} & r > R \end{cases} \qquad (12)$$

To better understand of behaviour of binding energy, normalized binding energy, $NE_{bF}$, that is defined as the ratio of the binding energy to the ground energy of spherical quantum dot without impurity, is also calculated.

$$NE_{bF} = 1 - \frac{E_{IF}}{E_F} \qquad (13)$$

**Results and discussion**

The normalized binding energy and electric field-dependent binding energy, $E_{bF} = E_F - E_{IF}$, are calculated for $GaAs/AlAs$ spherical quantum dot as a function of the electric field strength and the radius of dot.

The material parameters used in the calculations are[13,14]: $m^* = 0.067 m_0$, $\varepsilon = 13.1$, and the barrier potential $V_0 = 280\,meV$. The effective Rydberg constant is $R^* = 5.31 meV$, and the effective Bohr radius is $a^* = 103.43\ \mathring{A}$.

The calculated binding energies versus the radius of quantum dot are shown in Fig.1. According to this figure, the energy of impurity ($E_{IF}$), and binding energy are higher for smaller $R$ and decrease as the radius increases. It is interesting to note that the impurity energy becomes negative when the dot radius is larger than $1.720a^*$. This value of the dot radius at which the impurity energy changes from positive to negative is known as turning point. The calculated value by Dane et al.[13] for the turning point is $1.852a^*$. The difference is due to the finite barrier potential. As could be seen, the impurity energy approaches to $-R^*$ as the radius become larger than $4a^*$. The binding energy is reduced with increase the radius of dot, this is because the probability of finding an electron in the central region of the dot decreases, as the dot radius increases. The normalized binding energy increases with radius, and it is equal to $1R^*$ for the turning point. For the sake of comparison, the numerical results of Dane et al.[13] are also shown in these figures, dotted curves. As it is seen, the difference between the two results decrease as the radius of dot increases.

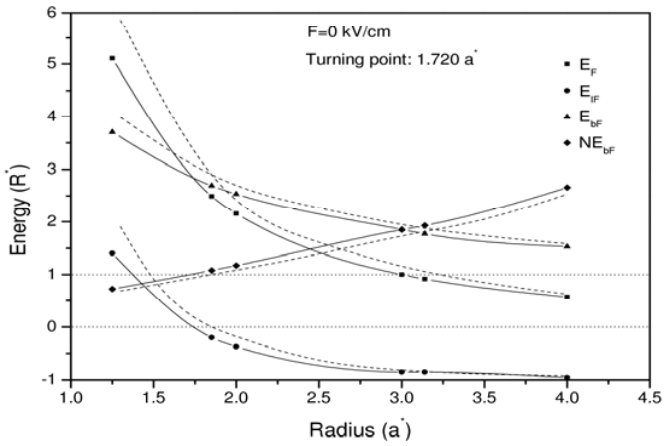


Figure 1- The ground state energy $E_F$, the impurity energy $E_{IF}$, the binding energy $E_{bF}$, and the normalized binding energy $NE_{bF}$ versus the radius of the finite $GaAs/AlAs$ quantum dot.

To investigate the effect of an electric field on the energy levels , the ground state energy of electron versus $F$ for different dot radii in finite quantum dot is shown in Fig.2. It can be seen that the energy levels $E_F$ of electron depend on both the electric field strength $F$ and radius of dot, such that for a given value of radius, the energy of electron decreases as $F$ increase. For comparison the numerical analysis by Dane et al.[13] for infinite barrier potential is also presented , dotted curve. It is also interesting to note that the difference increases with

strength of electric field. The reduction of the energy with respect to infinite barrier potential is due to the penetration of wave functions into the barrier region.

Figure 3 shows the impurity energy as a function of the electric field strength for different dot radii. As could be seen , the impurity energy drop as electric field or the size of quantum dot increases. In the presence of the electric field, the charge distribution is concentrated near the interface of the quantum dot, and therefore the value of $E_{IF}$ increases.

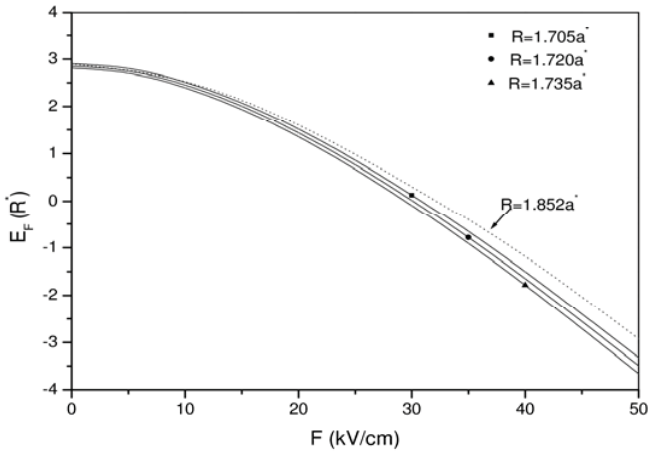


Figure 2- Energy levels ( $E_F$ ) calculated for electron in terms of the electric field strengths for different dot radii.

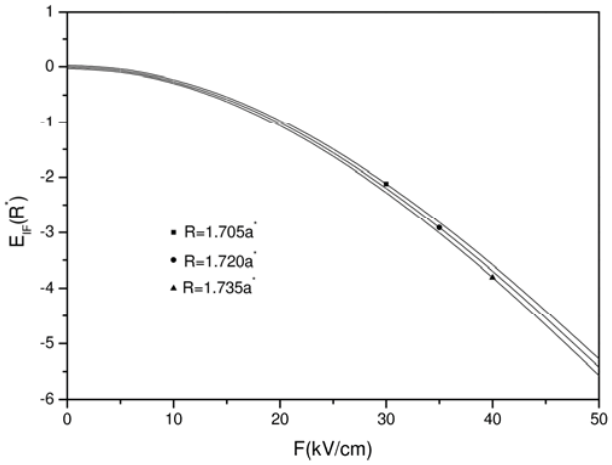


Figure 3- The impurity energy $E_{IF}$ as a function of the electric field strengths

The normalized binding energies in terms of $F$ in a finite quantum dot are shown in Fig.4. Based on this figure, $NE_{bF}$ increases and takes infinity for a given value of electric field $F_0$. $F_0$ is the electric field strength for which the ground state energy ( $E_F$ ) in the

presence of electric field has its zero value. According Fig.2, the value of $F_0$ increases with decreases the radius of dot. For $F < F_0$ $(F > F_0)$ the normalized binding energies are positive (negative), and in the near of the $F_0$ are infinity.

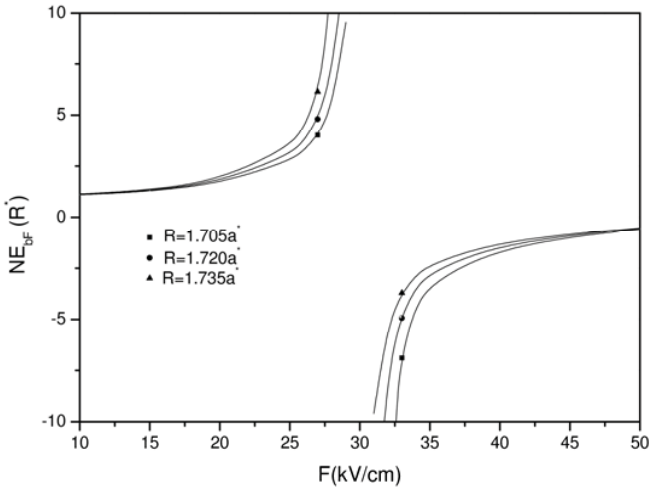


Figure 4-The normalized binding energy $NE_{bF}$ versus electric field strengths in finite $GaAs/AlAs$ spherical quantum dots

**Conclusion**

In the present study, the impurity energy and normalized binding energy in the spherical quantum dot in finite barrier potential in terms of strength of electric field are calculated. The results clearly show the effect of confining potential and $F$ on the energy. The calculated energies for the finite confining potential case are compare with numerical results.[13]

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