Effect of electric Field on the electronic states of parabolic CdS/CdZnS quantum dots

M.Balakumari[1], A. Milton Franklin Benial[2], and P.Elangovan[3]
[1]Department of Physics, M.K.U College, Aundipatti -625512, India
[2]Department of Physics, N.M.S.S.V.N. College, Madurai- 625019, India
[3] PG and Research Department of Physics, Pachaiyappa's College, Chennai -600030,India

Abstract :Using a variational method within the frame work of effective mass approximation ,the binding energy of shallow hydrogenic impurities in parabolic CdS/CdZnS quantum dots is calculated as a function of dot radius in the influence of electric field. An infinite and finite confining potential well with depth is determined by the discontinuity of the band gap in the quantum dot and the cladding. The results show that the impurity binding energy (i) increases as the dot radius decreases, (ii) decreases in an electric field – this decrease is more prominent for wider dots whereas for narrow dots the electric field seems to be unimportant. These results are compared with the existing literatures.

Index terms: quantum dot, binding energy, electric field, variational method .

1. INTRODUCTION

With the development of experimental techniques and an- alytical methods, there has been a considerable amount of work devoted to the study of the states of hydrogenic impurities in low-dimensional semiconductor heterostructures such as quantum wells (QWs), quantum-well wires (QWWs) and quantum dots (QDs)[1–6]. The effects of external perturbation such as magnetic fields, hydrostatic pressure or electric fields on the physical properties of low-dimensional systems constitute a subject of considerable interest from both theoretical and technological points of view, due to the importance of these systems in the development of new semiconductor devices and applications. The study of semiconductor quantum dots (QDs) and nano crystals have been of a great interest from the experimental and theoretical point of view in recent years [7]. The origin of the interest lies in the size of quantization in solids and in those objects. The electron spectrum of an ideal QD comprises a set of discrete levels. This makes the semiconductor quantum dots very important in the applications of optical and transport properties of semiconductors. Bose et al., [8] have obtained the binding energies of hydrogenic donor impurity states in a spherical QD using variational and perturbative approaches with finite and infinite barriers. The results show that as the dot radius decreases, the impurity binding energy increases for the infinite barrier case. On the other hand, for the finite potential it reaches a peak value and then diminishes to a limiting value corresponding to the radius for which there is no bound state in the dot. Rapid progress in semiconductor technology is being made in the fabrication of self assembled quantum dots [9] leading to the possibility of controlling their shapes and dimensions, the number of confined electrons and the structure of energy levels. Due to their reduced dimensionality, these structures exhibit some physical properties such as optical and electrical transport characteristics that are more pronounced than those of bulk semiconductor constituents [10,11]. It is expected that the fabrication of semiconductors with zero dimensions will show exotic electronic behaviour such as the observation of discrete electronic states in GaAlAs/GaAs nanostructures [12] and the photoluminescence of overgrown GaAlAs/GaAs quantum dots [13] due to the electronic confinement. The impurity plays a fundamental role in some physical properties such as optical and transport phenomena at low temperature. The binding energy and the density of states of shallow impurities in cubic [14] and in spherical quantum dot [15] have been calculated as a function of dot size. The study of impurity states in semiconductor states is imperative as the addition of impurities can change the properties of any quantum device dramatically. Using the variational method, Porras-Montenegro et al., [16] studied a hydrogenic impurity in spherical QD systems with both infinite and finite barriers. The results reveal that, as the size of the QD decreases for an infinite barrier, the binding energy of the impurity increases monotonically, and for a finite barrier, the binding energy increases to their maxima and then sharply decreases.

The effect of parabolic confinement on the binding energy of shallow hydrogenic impurities in a spherical quantum dot has been computed as a function of the dot dimension for different impurity positions and also as a function of the impurity position for different dot sizes for the infinite case [17]. They show that the impurity binding energy increases with the reduction in the dot dimension. Also the binding energy is found to depend on the location of the impurity, and the same is the maximum for the on-centre impurity. The quantum dot system also provides a testing ground for calculations involving correlations among electrons. The effect of confinement can be seen either by varying the barrier height or by varying the dot size. Since in semiconductor applications dopants are used it is also of interest to see how a hydrogenic donor will behave under confined geometries. A harmonic oscillator like potential has been used for confinement in few other investigations [18].

At the present work, calculations of binding energies of the donor impurities in CdS quantum dot with the barrier of CdZnS, placed at the centre are performed using the effective mass approximation within a variational scheme. The effect of electric field on the binding energies of shallow donors in the CdS quantum dot with $Cd_{1-x}Zn_xS$ barriers is investigated. A systematic study of variation of electric field as the function of dot size has been attempted with a parabolic confinement of a quantum dot. The

results are then compared with the existing data available. The method followed is presented in the Section 2.2 while the results and discussion are provided in the Section 3.

2. THEORY

The Hamiltonian of the hydrogenic donor impurity, in the effective mass approximation, in a CdS / $Cd_{1-x}Zn_xS$ quantum dot, in the influence of electric field is given by

$$H = -\frac{\hbar^2}{2m*}\nabla^2 - \frac{e^2}{\bar{\varepsilon}(r)r} + |e|Fz + V_D \qquad (2.1)$$

where m* is the electronic effective mass, $\bar{\varepsilon}(r)$ the dielectric function of the QD material, and $V_D = \frac{V_o r^2}{R^2}$ for $|r| \le R$ and Vo for $|r| > R$ where Vo is the barrier that binds the carrier in the dot for finite barrier problem, and $V_0 = \infty$ for infinite barrier problem when $|r| > R$ whose value depends upon the Zn concentration (x) in $Cd_{1-x}Zn_xS$ which is the barrier medium in which we have assumed to have embedded the CdS dot.

Using for the band gap difference, Eg = 2.38+0.68x + $0.85x^2$ (eV) and assuming 60% contribution to the conduction band, for x=0.2, the value of V_o turns out to be 19.176 meV.The units of length and energy used throughout are the effective Bohr radius $R* = \hbar^2\varepsilon_o / m*e^2$ and the effective Rydberg $R_y^* = m*e^4 / 2\varepsilon_o^2\hbar^2$ where ε_o is the dielectric constant and m* is the effective mass of electron in the conduction band minimum of CdS.

In these units, the Hamiltonian given in Eq.(2.1), becomes,

$$H = -\nabla^2 - \frac{2}{r} + \frac{|e|R*Fr\cos\theta}{R_y^*} + \frac{V_D}{R_y^*} \qquad (2.2)$$

V_D is the parabolic confinement.

2.1 Finite barrier Problem

The ground state energy of an electron in a parabolic quantum dot is with electric fields is estimated by variational method. We have assumed the trial wave function

$$\psi_{in}(r) = N_2 e^{-\xi r^2}(1 + \nu Fr\cos\theta) \qquad r \le R$$
$$\psi_{out}(r) = N_3 \frac{e^{-\delta r}}{r}(1 + \nu Fr\cos\theta) \qquad r > R \qquad (2.3)$$

Where N2, N3 are normalization constants. By matching the wave functions and their derivatives at the boundaries of the QD, along with the normalization, we fix the values of N2, N3 and $\xi = 1/R(1/R + \delta).$ we take δ and ν as the variational parameters.

Since the inclusion of impurity potential leads to a nonseparable differential equation which cannot be solved analytically it is necessary to use a variational approach to calculate the eigen function and eigen value of the Hamiltonian for the ground state. Taking into account the parabolic confining geometry and the hydrogenic impurity potential, we use a trial wave function for the ground state with the impurity present is taken as

$$\psi_{in}(r) = N_4 e^{-\xi r^2}(1 + \nu Fr\cos\theta)e^{-\alpha_1 r} \qquad r \le R$$
$$\psi_{out}(r) = N_5 \frac{e^{-\delta r}}{r}(1 + \nu Fr\cos\theta)e^{-\alpha_1 r} \qquad r > R \qquad (2.4)$$

where α_1 and ν are the variational parameter and N_4, N_5 are normalization constants.
The ionization energy is given by

$$E_{ion} = E_{sub} - \langle H \rangle_{\min,} \tag{2.5}$$

Thus the ionization energy is obtained, varying α_1 for different dot sizes.

3. RESULTS AND DISCUSSION

Our numerical computation is carried out for one of the typical II – VI semiconducting materials, CdS, as an example with the material parameters shown in the following: ε_o =5.7 ; and m* = 0.19m_e; where m_e is the single electron bare mass.

Fig.1 shows the variation of donor binding energy with dot size for the infinite barrier with and without electric field. The binding energy decreases when dot size increases in both cases. The decrease in ionization energy with the increase of well width is a common feature [19]. It does not show much variation when an electric field is applied, unlike in the case of quantum well [20] and the binding energy increases monotonically for the dot radius when R< 5a*. This situation is clearly brought out in Fig. 2 where the binding energy decrease with increase of electric field. The binding energy is higher for smaller dot radii due to the quantum confinement effect.

The donor binding energy as a function of dot radius with and without the electric field for finite barrier is shown in Fig.3. The binding energy decreases for applied field. The decrease is more for wider dots . For narrow dots, the electric field seems to be unimportant. This is attributed to the fact that the quantum confinement effects are appreciable for smaller dots. As the applied electric field is increased the electron is pulled towards one side of the quantum dot as a result the binding energies decreases as a function of applied electric field.

An Interesting features that is seen in Fig.4 is that for dot radius ≤ 45 a*, the binding energies in strong electric field ≥ 1 X 10^5 V/m becomes negative. The reason being enhanced tunneling due to asymmetry of the well in strong electric fields working against the impurities binding[21]. In Fig.5 displays that the influence of electric field on the binding energy of the quantum dot system. It clearly shows that the binding energy of the system reduced abruptly by applied strength of electric field and tunneling comes to play . The lowest binding energy with electric field is show in Fig 6. It strongly suggest that the electric field reduces the binding energy of the system and enhances the play of tunneling is shown by the negative value of binding energy.

In conclusion, the binding energy of hydrogenic impurities in quantum dots with parabolic confinement decreases as the electric field increases and the relative reduction gets smaller with decreasing strength of the confining potential . The electric field seems to be unimportant for smaller dots and the tunneling comes to play for high electric field.

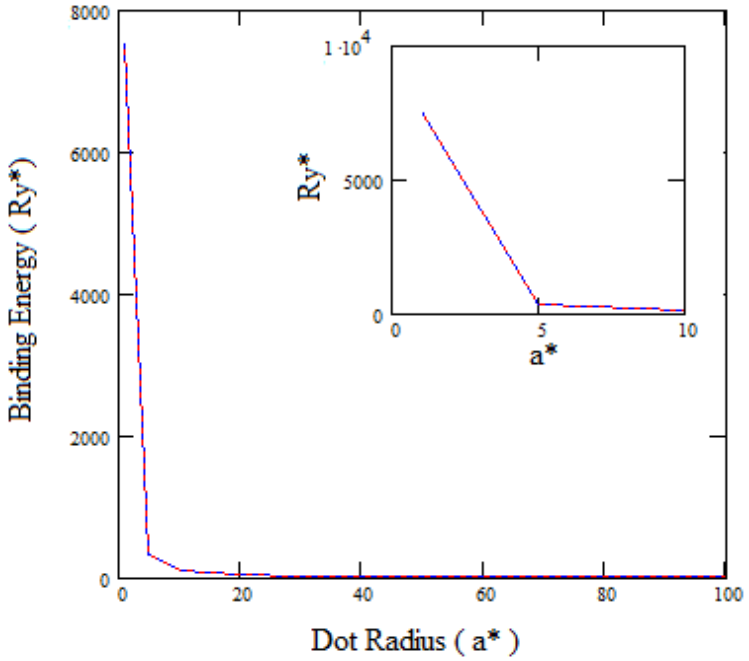

Figure 1 Variation of Binding energy with dot radius with and without electric field for infinite barrier. Inset diagram shows monotonic increase of binding energy for R ≤ 5a*.

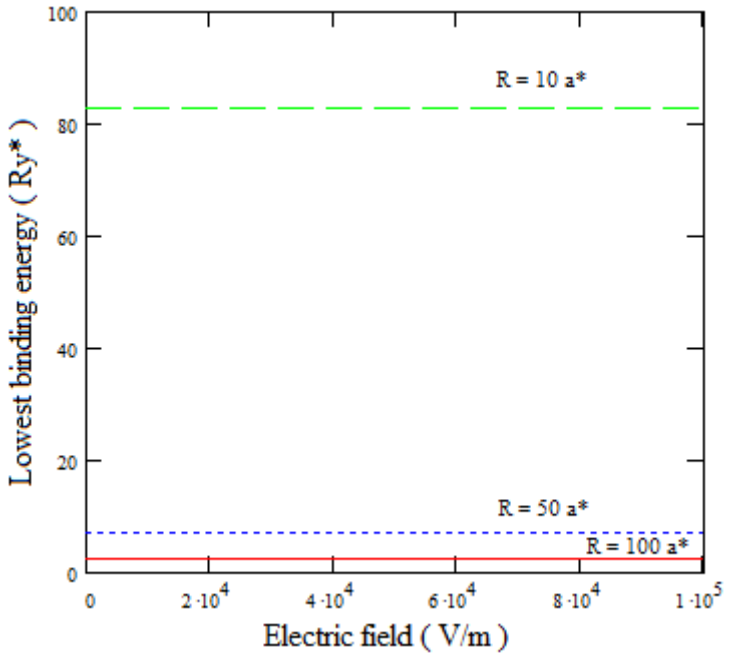

Figure 2 Variation of the lowest binding energy with Electric Field for different dot radii. The upper set of lines indicates for the dot radius, 10a* and the lower set of lines indicates for the dot radius, 100a*.

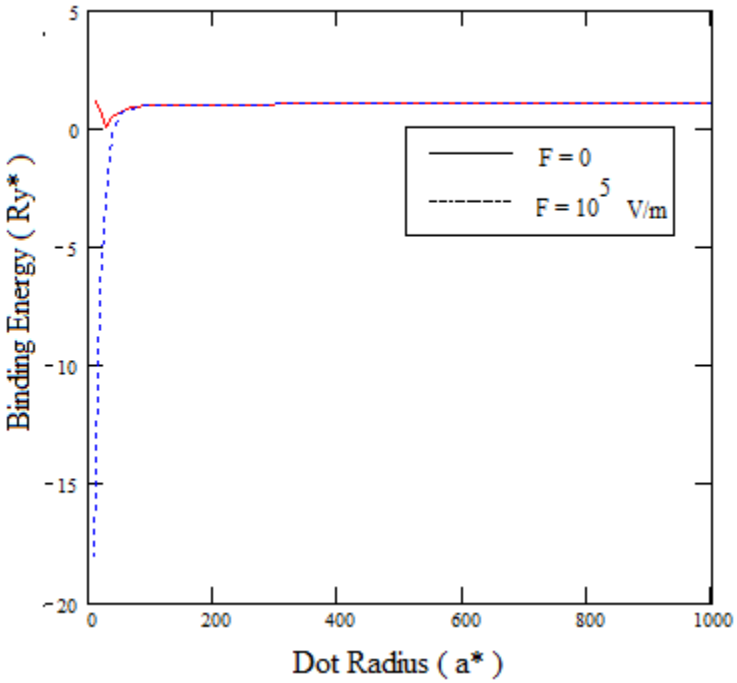

Figure 3 Variation of binding energy with Dot Radius with and without the electric field.

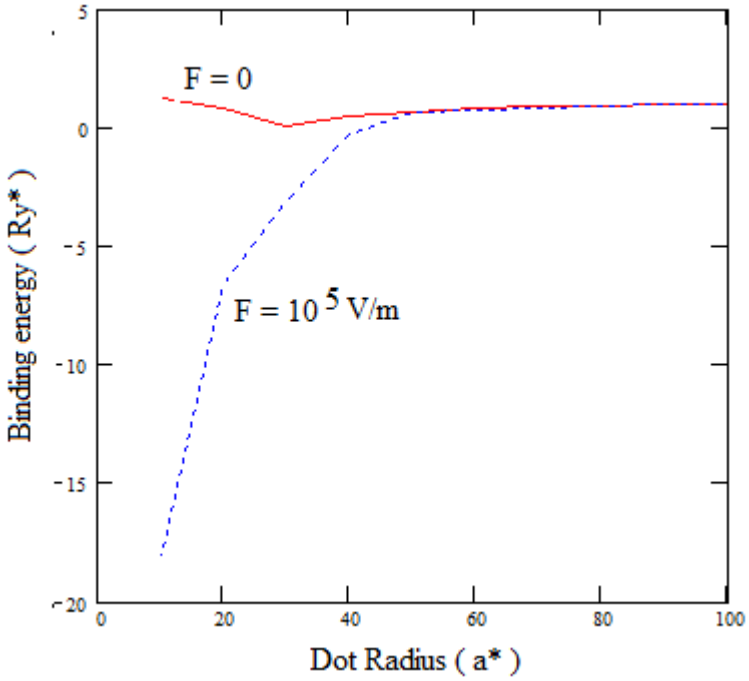

Figure 4 Variation of binding energy with Dot radius with and without the electric field

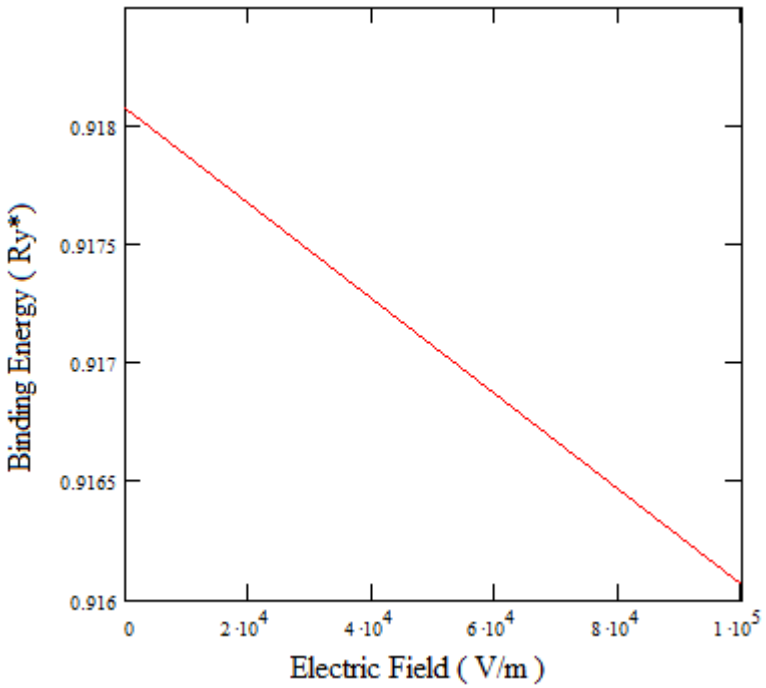

Figure 5 Variation of binding energy with the different electric field

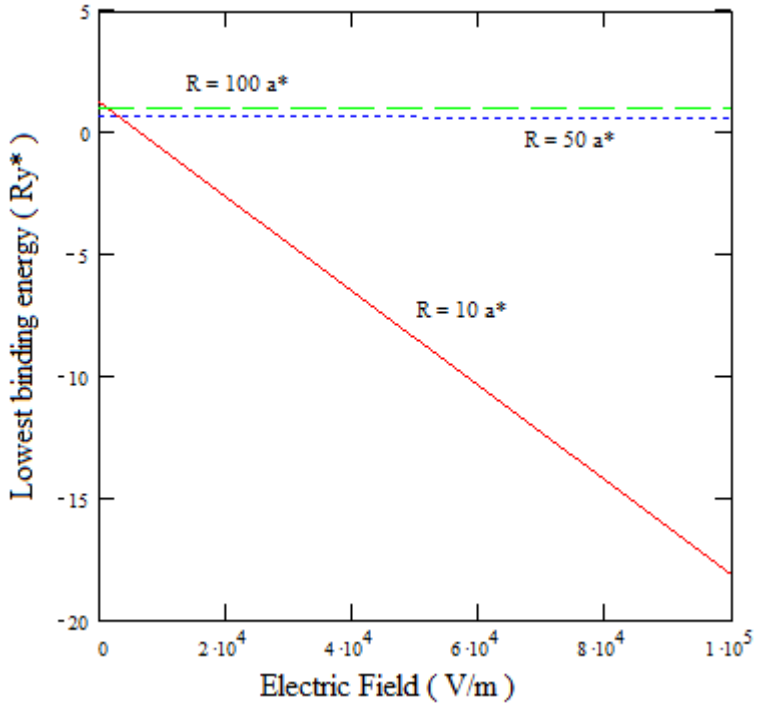

Figure 6 Variation of the lowest binding energy with Electric Field for different dot radii. The upper set of lines indicates for the dot radius, 100a* and the lower set of lines indicates for the dot radius, 10a*.

REFERENCES

[1] Heon Ham and Harold N. Spector, Phys. Rev. B 62, 13599 (2000).
[2] Hong-Jing Xie, Physica E 22, 906 (2004).
[3] R. B. Santiago, L. E. Oliveira, and J. d'Albuquerque e Castro, Phys. Rev. B 46, 4041 (1992).
[4] A. Latg´e, N. Porras-Montenegro, and L. E. Oliveira, Phys. Rev. B51, 2259 (1995).
[5] A.L.Morales,A.Montes,S.Y.L´opez,andC.A.Duque,J.Phys: Condens. Matter 14, 987 (2002).
[6] A. M. Elabsy, J. Phys.: Condens. Matter 6, 10025 (1994), and references therein.
[7] D.Bimberg, Semicond.33, 951 (1999).
[8] C.Bose and Sarkar, Phys. Stat. Sol (b) 218, 461 (2000).
[9]R. C. Ashoori, Nature 379, 413 (1996).
[10] R.Dingle, A.C.Gossard and W.Wiegmann, Phys.Rev.Lett.33,827(1974).
[11]L.L.Chang, L.Esaki and R.Tsu, Appl.Phys.Lett.24,593(1974).
[12]M.A.Reed, J.N.Randall, R.J.Aggarwal, R.J.Matyi, T.M.Moore and A.E.Wetsel, Phys.Rev.Lett.60,535 (1988).
[13]H.E.G.Arnot, M.Watt, C.M.Sotomayor-Torres, R.Glew, R.Cusco, J.Bates and S.P.Beaumont, Superlatt.Microstruct.5,459 (1989).
[14] F.J.Ribeiro and A.Latgé, Phys.Rev. B50, 4913(1994).
[15] J.L.Zhu, J.J.Xiong and B.L.Gu, Phys.Rev. B41, 6001(1990).
[16] N. Porras-Montenegro and S.T.Pérez-Merchancano, Phys. Rev.B46,9780 (1992)
[17] Chayanika Bose, J.Appl.Phys.83,3089 (1998).
[18]H. O. Oyoko, C. A. Duque, N. Porras-Montenegro, J.Appl.Phy. 90, 819 (2001).
[19] G. Bastard, Phys. Rev. B 24 (1981) 4714.
[20] G. Bastard, E.E.Mendez, L.L. Chang and L.Esaki , Phys.Rev.B 28(1983) 3241.
[21] A. John Peter , Physics Letters A 355(2006) 59