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Energy Spectra of CdS/Cd1-xZnx S Nano Dot Under the Influence of Magnetic field

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Abstract

We present a theoretical study on shallow donor binding energies of CdS/ CdZnS nano dot as a strength of applied magnetic field along Z direction for various Zn concentration. Calculations are carried out by using the technique of variational ansatz within the frame work of effective mass approximation. Our results show that the binding energies are drastically affected by the dot radius, the strength of magnetic field and concentrations.

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1. Introduction

In the last few decades, a proper quantitative understanding of low dimensional semiconductor systems, such as nano wells (NWs), nano dots, nano wires and super lattices has been of great interest in experimental and theoretical point of view,due to their importance for potential applications in electronic and optoelectronic devices[1,2]. Nano dots[NDs] are devices in which charge carriers are confined in all the dimensions. They are very interesting for optoelectronic and magnetic devices due to their singular nature of density of electrons. It is possible to fabricate NDs containing a number of electrons with recent advances in nanofabrication technology. A perceptive nature of impurity states in semiconductor nano dots is one of the crucial problems in semiconductor physics because impurities can dramatically alter the properties and performance of a quantum device [3-6]. Semiconductors composed of II–VI materials having wide band gap with the impurity, with larger sizes of NDs are achievable. The binding energy of the impurity increases as the size of the confining region is of the order of the Bohr radius.

`NDs are observed to have a series of different ground states as the magnetic field is increased experimentally [7]. Understanding their nature is still one of the major theoretical goals in this field though many properties of the states can be measured. There has been considerable progress in the fabrication of NDs during the last few years, which has stimulated an increasing interest in investigating the properties of such systems. One of the major theoretical goals is to understand the nature of the many-body ground states for various magnetic field strengths [8-10].

In the present work, we have considered a CdS nano dot embedded in a $Cd_{1-x}Zn_xS$ matrix with finite barriers. The barrier height depends on Zn concentration x. We estimate the total energy of the system variationally, assuming parabolic well potential for confinement for a finite barrier height. The energy levels of the low-lying states are calculated as a function of magnetic field. Calculations are made by using variational ansatz within the effective-mass approximation.

2. Theory

Our system consists of a parabolic nano dot (depth VD, and radius R) containing a donor impurity inside the ND of the magnetically non-uniform “spin-doping” super lattice system with CdS nano dot embedded in a $Cd_{1-x}Zn_xS$ matrix with a finite barrier. Consider electron is moving in a ND each having an effective mass m*, which is $0.19m_o$ for CdS. The Hamiltonian in the system within the effective mass approach when the magnetic field is applied is given by

$$H = \frac{1}{2m^*}(\vec{P} + \frac{e}{C}\vec{A})^2 + V(\rho) + \frac{e^2}{\varepsilon_o r} + g^*\mu_B B S_z \qquad (1)$$

where ρ refers to theposition vector of an electron in two dimensions, $\vec{P}$ is the corresponding momentum operator, m* is the electron effectivemass and $\vec{A}$ is the vector potential corresponding to the magneticfield B which has been applied in the z direction. .g is the effective Lande factor; μ_B is the Bohr magneton; S_z is the z-component of the total spin, ε_o is the effective dielectric constant of the ND, and $V_D = \frac{V_{0B} r^2}{R^2}$ *for* $|r| \le R$ *and* $V_D = V_{0B}$ *for* $|r| > R$ $V_{OB}(\bar{r})$ is the barrier height given by $V_{OB}(\bar{r}) = Q_c \Delta E_g(x)$. Q_c is the conduction band off-set parameter, which is taken to be 0.658 and the band gap difference between CdS and $Cd_{1-x}Zn_xS$ is given by [11]

$$\Delta E_g(x) = 2.38 + 0.68x + 0.85x^2 \quad eV. \qquad (2)$$

The units of length and energy used throughout the present paper are the effective Bohr radius $R^* = \hbar^2 \varepsilon_o / m^* e^2$ and $R_y^* = m^* e^4 / 2\varepsilon_o^2 \hbar^2$ where ε_o is the static dielectric constant of CdS.

$$H_D = -\nabla^2 + \frac{\gamma^2}{4} r^2 \sin^2\vartheta + \gamma L_z + \frac{V_D}{R^*} + \frac{2}{r} + \frac{g^*\mu_B B S_z}{R^*} \qquad (3)$$

where L_z is the total orbital angular momentum along in the z-direction and γ is the measure of magnetic field.

The eigen functions for the lowest states within the dot are given by

$$\psi_{1s}(\bar{r}) = \begin{cases} N_1 \dfrac{\sin(\alpha_1 r)}{r} e^{-\delta r^2}, & r \le R, \\ N_2 \dfrac{e^{-\beta_1 r}}{r} e^{-\delta r^2}, & r > R \end{cases} \quad (4)$$

.

where N_1, N_2, N_3 and N_4 are normalization constants α_1 and β_1 are given by

$$\alpha_1 = \sqrt{2m^* E_1} \text{ and } \beta_1 = \sqrt{2m^*(V_D - E_1)} \quad . \quad (5)$$

Matching the wave functions and their derivatives at the boundary r = R, the energy eigen values are determined by imposing the boundary conditions,

$$-\frac{i\hbar}{m^*}\frac{\partial \psi}{\partial r}(r < R)\Big|_{r=R} = -\frac{i\hbar}{m^*}\frac{\partial \psi}{\partial r}(r \ge R)\Big|_{r=R} \quad (6)$$

Using Eqs.(4) –(6), we obtain

$$\alpha_1 R + \beta_1 R \tan(\alpha_1 R) = 0 \quad (7)$$

The ground state energy of the conduction electron in a parabolic ND in an external magnetic field, E_D, is obtained by minimizing the expectation value of H_D with respect to the trial wave functions given in Eq. (4).

The Hamiltonian for a donor situated at the center of the parabolic dot in the presence of external magnetic field applied along the growth direction, in the unit of effective Rydberg and effective Bohr radius, is

$$H_{ID} = -\nabla^2 + \frac{\gamma^2}{4} r^2 \sin^2 \vartheta + \gamma L_z + \frac{V_D}{R^*} - \frac{2}{r} + \frac{g^* \mu_B B S_z}{R^*} \quad (8)$$

The ground state energy of the donor in the presence of magnetic field is obtained by the variational method using the trial wave functions, Eqn.(4) with $e^{-\alpha r}$, where α is the variational parameter. The ground state energy is estimated by minimizing the expectation value of H_{ID} with δ *and* α as the variational parameters with respect to the above trial wave functions.

The ionization energy is obtained by

$$E_{ion} = E_D + \gamma - \langle \psi | H_{ID} | \psi \rangle_{\min} \quad (9)$$

The confining potential energies of a donor is calculated using the Hamiltonian (Eq.(8)) and the wave functions Eqs.(4) for various concentrations and different magnetic field.

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3. Results and Discussion

Our numerical computation is carried out for one of the typical semiconducting materials, CdS, as an example with the material parameters shown in the following: ε_o =5.7; and m* = 9m_e; where m_e is the single electron bare mass.

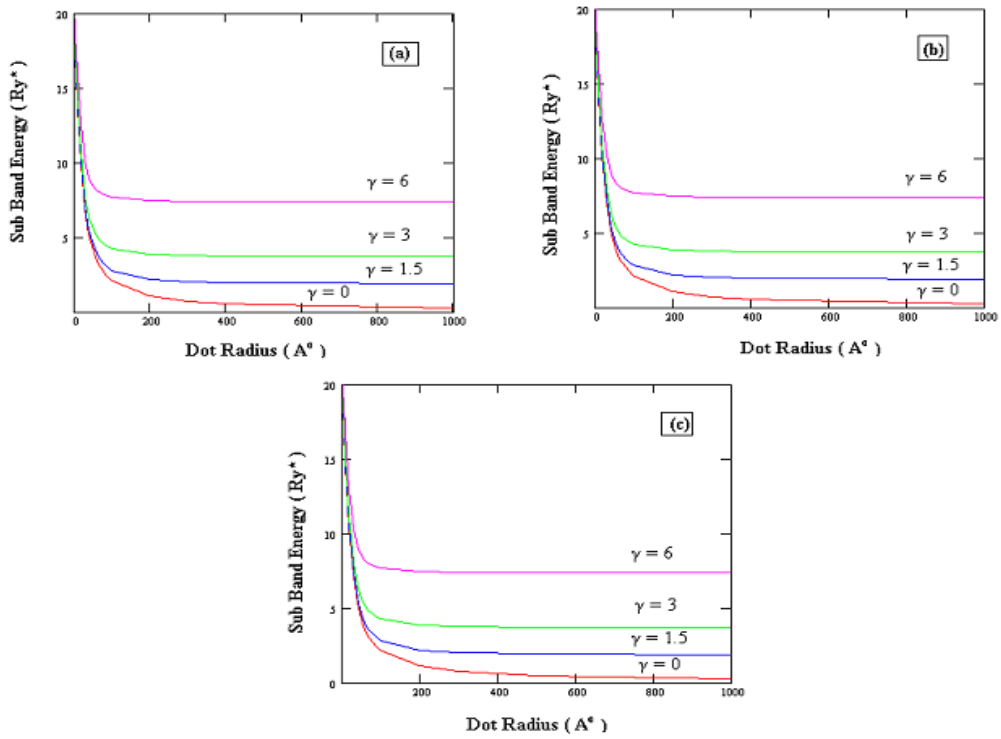

Fig .1. (a, b, c) Sub band energy as a function of dot radius with different magnetic field strength for different concentrations (a) x = 0.1 (b) x = 0.2 and (c) x = 0.3

In Fig.1, we have displayed the variation of the lowest sub band energy of carriers for different field strengths as a function of the dot radius. The results show that (i) the binding energy decreases as dot radius increases for the all concentrations (ii) the binding energy increases in a magnetic field for all dot sizes and. In general, in all nano well structures the magnetic field increases with the binding energy [12,13].

The donor ionization energy as a function of dot radius is given in Fig.2. As expected, the ionization energy decreases with an increase of dot radius, reaching the bulk value for large dot radii. Also we observe an enhancement in the binding energy in a magnetic field. As the dot radius approaches zero the confinement becomes negligibly small, and in the finite barrier problem the tunneling becomes huge. So the ionization energy again approaches the bulk value. Hence the variation of ionization energy with dot radius shows a peak around 1R* for all the magnetic fields. This is a well known result in all quantum well structures [14].

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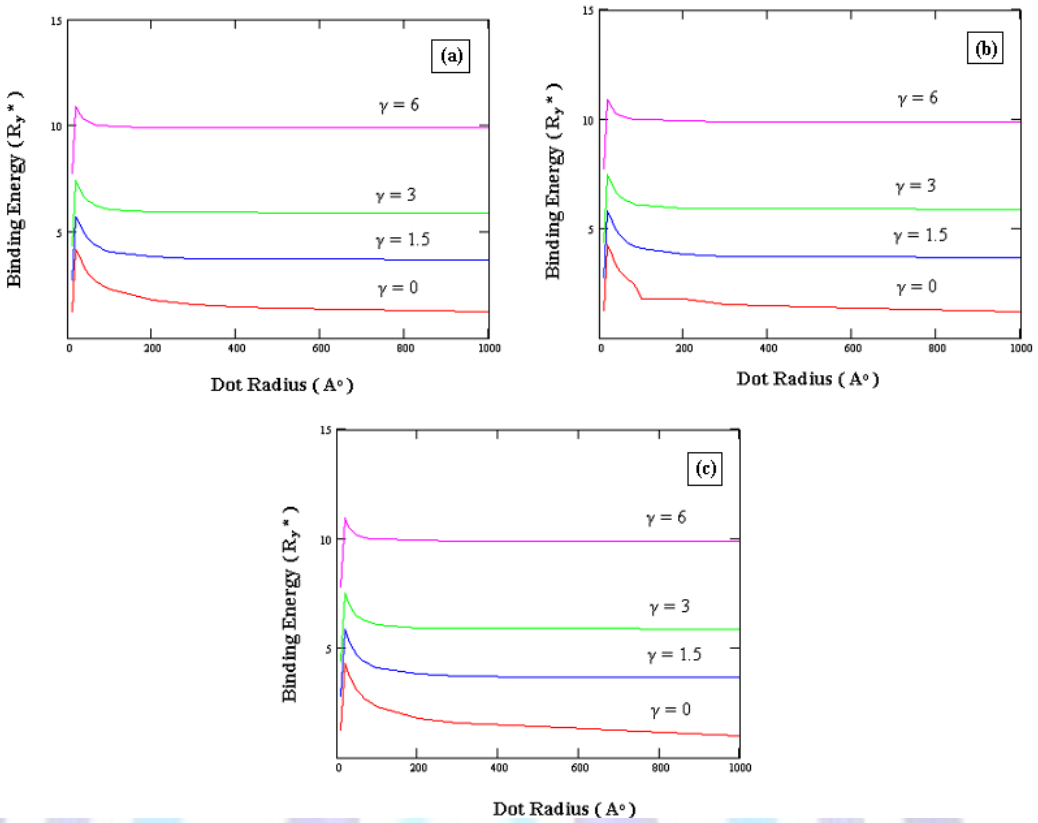

Fig .2. (a, b, c) Binding energy as a function of dot radius with different magnetic field strength for different concentrations (a) x = 0.1 (b) x = 0.2 and (c) x = 0.3

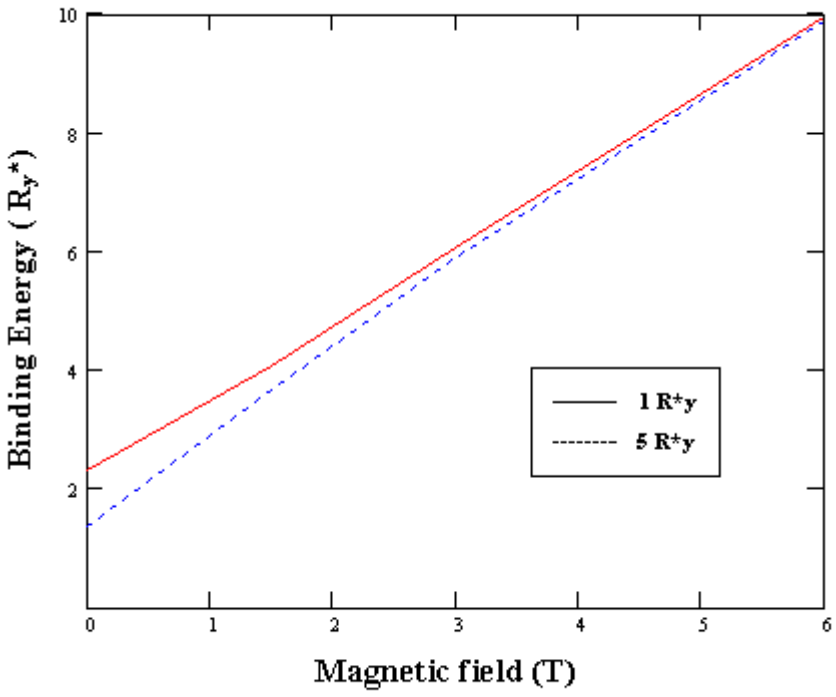

Fig. 3. Binding energy as a function of Magnetic field strength for particular concentration x = 0.3

We have taken the dot radius R=15R* (i.e., strong confinement) and R=5R* (weak confinement) and plotted the variation of energy spectra with a measure of magnetic field for x = 0.3 in Fig. 3. It is clearly seen that lower magnetic field

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has great influence on strong confinement and also it depicts that there is no appreciable change in binding energy even increasing the magnetic field for strong confinement as well as weak confinement. Such magnetic field induced angular momentum (and spin) transitions have been observed experimentally [14, 15] for dots with parabolic-like confinement earlier.

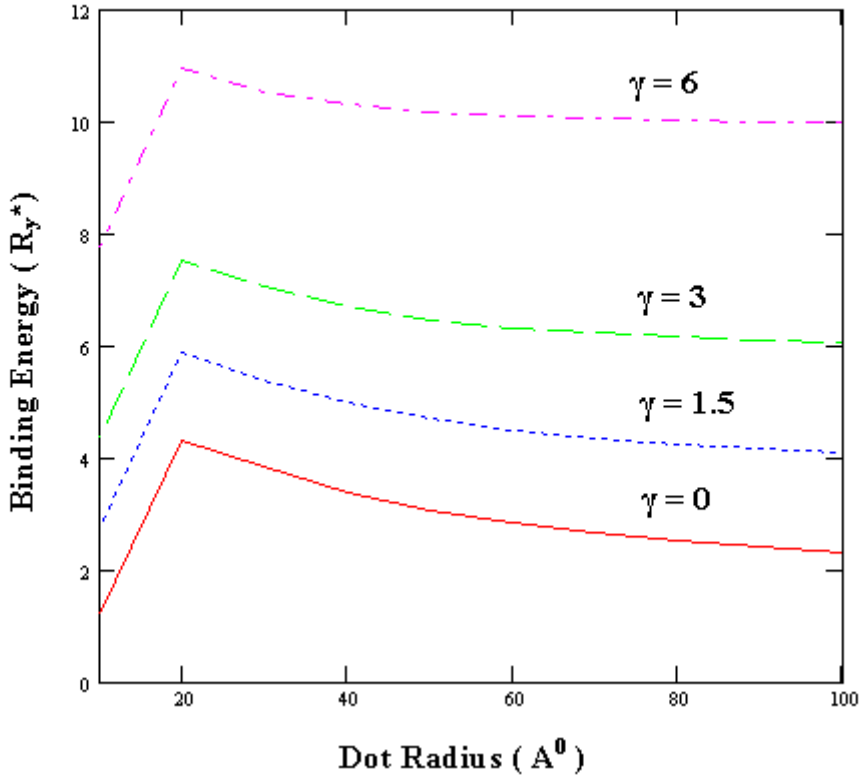

Fig . 4. Binding energy as a measure of dot radius for quantum confinement region(R<100 A^o)

Fig.4 displays the binding energy as a function of dot radius for different magnetic field strength for nano region such as R<100 A^o for particular Zn concentration x = 0.3. As the magnetic field increases the binding energy of the nano dot system. Which strongly suggest that the tunability of band gap using strong magnetic field.

In conclusion, when a electron is introduced into the nano dot, we have estimated the energy levels of the nano dot system as a function of magnetic field. Calculations are made by using variational ansatz within the effective-mass approximation. We found that the band gap tunability is achieved by doping and external fields such as magnetic field[16,17]. The influence of magnetic field has great influence on the nano dot system rather than its Zn composition. The present results are helpful to realize the magnetic and optical properties of QD material. We hope that the present work would stimulate further experimental activities on impurity states in quantum dots.

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