JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **11** No 3, 03006(4pp) (2019)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **11** № 3, 03006(4cc) (2019)

Effects of High Magnetic Field on the Energy Spectra of Two Donors in a Strained Zinc Blende Quantum Dot

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(Received 04 February 2019; revised manuscript received 11 June 2019; published online 25 June 2019)

The electronic states of two donors in a strained quantum dot (QD) under the influence of high magnetic field have been investigated. Numerical calculations are carried out using variational principle within the single band effective mass approximation by means of magnetic field strength through energy dependent effective mass. Studies on the donor problem in a QD are a useful tool for understanding the electronic and optical properties of impurities. The study of two donor impurities in low dimensional semiconductor structures with and without magnetic fields is performed. We will adopt to calculate the binding energy in zinc blende QD. Our investigations include Zeeman Effect in the Hamiltonian. The magnetic field induced diamagnetic susceptibility of two donors is computed as a function of QD radius. The variation of two-donor binding energy as a function of dot radius for different magnetic field strength applied with and without field is conducted. The results show that the binding energy increases with the decrease of dot radius, reaching a maximum value, and then decreases when the dot radius still decreases. The contribution of diamagnetic susceptibility to the donor binding energy is the measure of spatial extension of the ground state. The inter-donor distance is the measure of Coulomb interaction energy of the two donor systems. The Coulomb interaction energy is only appreciable when inter-donor distances approach nearby or lesser than the effective Bohr radius. Our results show that the high magnetic field, the QD radius and Coulombic interaction energy have a remarkable influence on the electronic states of two donors in a strained QD. The results seem good and in better agreement with other literatures.

Keywords: Strained quantum dot, Variational method, Coulomb energy.

DOI: 10.21272/jnep.11(3).03006 PACS numbers: 73.21.Fg; 73.21.La

1. INTRODUCTION

In recent years, III-V wide band gap semiconductors of nitride groups and their binary and ternary compounds have attracted much attention. GaN and its related semiconductor alloys are most promising for potential application in optical, optoelectronic, and electronic devices [1]. For low-dimensional heterostructures, many theoretical and experimental investigations have been performed on the issue of binding energy of an electron to a donor impurity [2]. The understanding of the electronic and optical properties of impurities in such systems is important because the optical and transport properties of devices made from these materials are strongly affected by the presence of shallow impurities [3]. The nitride-based materials have good performances, possess high speed operation and are highly reliable [4]. The properties of wurtzite GaN based quantum heterostructures are strongly affected by the built-in electric field [5]. Zinc blend GaN structure, having less band gap, does not have strong built-in internal field due to high crystal symmetry.

Understanding the performance of optical devices is important in this area.

GaN based quantum dots (QD) have also shown to be a promising candidate for quantum computing [6, 7]. The study of two donor [8] and two acceptor [9] impurities in low dimensional semiconductor structures with and without magnetic fields is done.

In the present work, the calculations are performed by variational method using the single band effective mass approximation by the magnetic field strength. We will adopt to calculate the binding energy in zinc blende QD. Our investigations include Zeeman Effect in the Hamiltonian. The effect of magnetic field on variational parameter and diamagnetic susceptibility of a strained GaN/AlGaN QD is investigated with and without the effect of field. The magnetic field induced binding energy of two donors as a function of quantum dot radius has been investigated. In Section 2, a theoretical calculation of the problem is given. The result and discussion are presented in Section 3. Finally, the main conclusions are presented in the last Section.

2. THEORY

The Hamiltonian for two donors in the QD system within the effective mass approach, when applying magnetic field, is given by

$$H = \sum_{j=1}^{2}\left[\frac{1}{2m(E)^*}\left(\bar{p}_j + \frac{e}{c}\bar{A}_j\right)^2 + V_D(\bar{r}_j)\right] + \frac{e^2}{\varepsilon_o r_{12}} + g^*\mu_B B S_z, \quad (1)$$

where g is the effective Lande factor; μ_B is the Bohr magneton; S_z is the z-component of the total spin, ε_0 is the effective dielectric constant of the QD, 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 0.70.

Due to large influence on the electronic energy lev-

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els in a semiconductor QD, we have used the material dependent effective mass in our calculations.
The energy dependent effective mass is given by:

$$\frac{1}{m(E)}=\frac{1}{m(0)}.\frac{E_g(E_g+\Delta)}{(3E_g+2\Delta)}.\left[\frac{2}{E+E_g}+\frac{1}{E+E_g+\Delta}\right], \quad (2)$$

where ε is the dielectric constant of GaN, E_g is the energy band gap, Δ is the spin-orbit band splitting, and E denotes the conduction band energy of the electron, $m(0)$ is the conduction band effective mass.

$$g(E)=2\left[1-\frac{m_0}{m(E)}.\frac{\Delta}{3(E_g+E)+2\Delta}\right], \quad (3)$$

where m_0 denotes the free electron mass.

For a zinc blende phase, the band gap difference between GaN and $Al_xGa_{1-x}N$ is given as

$$E_{g,Al_xGa_{1-x}N}(x)=(1-x)E_{g,GaN}+xE_{g,AlN}+bx(x-1), \quad (4)$$

$E_{g,Al_xGa_{1-x}N}$, $E_{g,GaN}$ and $E_{g,AlN}$ are the $Al_xGa_{1-x}N$, GaN and AlN band gap energies on the axis which passes through Γ point. 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_0 is the static dielectric constant of GaN.

The strain-induced potential for the conduction band is given by

$$V_{cstrain}=a_c(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}) \quad (5)$$

where a_c is the deformation potential constant of the conduction band $\varepsilon_{[xx]}=\varepsilon_{[yy]}=(a_0-a)/a$, where a_0 and a are the lattice parameters of bulk GaN and AlN, respectively, and $\varepsilon_{[zz]}=-2\left(\frac{c_{12}}{c_{11}}\right)\varepsilon_{xx}$, where c_{11} and c_{12} are the elastic constants, the values of which are obtained from [10].

The strain-induced potential for the valence band can be written as

$$V_{vstrain}=a_v(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})-\frac{b}{2}(\varepsilon_{xx}+\varepsilon_{yy}-2\varepsilon_{zz}), \quad (6)$$

where a_v and b are the deformation potential constants of the valences band.

$$H_D=-\nabla^2+\frac{\gamma^2}{4}r^2\sin^2\vartheta+\gamma L_z+\frac{V_D}{R^*}+\frac{2}{r_{12}}+\frac{g^*\mu_B BS_z}{R^*}. \quad (7)$$

The ground state energy of an electron in a parabolic QD is estimated by the variational method. We have assumed the trial functions as

$$\psi_{1s}(\vec{r})=\begin{cases}N_1\dfrac{\sin(\alpha_1 r)}{r}e^{-\delta r^2}, r\le R;\\ N_2\dfrac{e^{-\beta_1 r}}{r}e^{-\delta r^2}, r>R.\end{cases} \quad (8)$$

where N_1 and N_2 are the normalization constants and α_1 and β_1 are given by

$$\alpha_1=\sqrt{2m^*E_1},\ \beta_1=\sqrt{2m^*(V_D-E_1)}. \quad (9)$$

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

$$-\frac{i\hbar}{m^*}\frac{\partial\psi}{\partial r}(r<R)\ |_{r=R}=-\frac{i\hbar}{m^*}\frac{\partial\psi}{\partial r}(r\ge R)\ |_{r=R}. \quad (10)$$

Using equations (4)-(6), we obtain for s-states

$$\alpha_1 R+\beta_1 R\tan(\alpha_1 R)=0. \quad (11)$$

The ground state energy of the conduction electron in a parabolic QD 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 equations (4), (5).

The Hamiltonian for two donors situated at the center of the parabolic dot in the presence of an external magnetic field applied along the growth direction, is written as

$$H_{ID}=H_D-\sum_{i=1,2}\frac{e^2}{\varepsilon r_i}. \quad (12)$$

In the presence of a magnetic field, the ground state energy of the donor is obtained by the variational method using the trial wave functions,

$$\Psi_{1s}(\vec{r}_1,\vec{r}_2)=\begin{cases}N_1\dfrac{\sin(\alpha_1 r)}{r}e^{-\delta r^2}e^{-\zeta_1 r_1}e^{-\zeta_2 r_2},\\ N_2\dfrac{e^{-\beta_1 r}}{r}e^{-\delta r^2}e^{-\zeta_1 r_1}e^{-\zeta_2 r_2},\end{cases} \quad (13)$$

where ζ_1 and ζ_2 are the variational parameters. The ground state energy is estimated by minimizing the expectation value of H_{ID} with δ and ζ as the variational parameters with respect to the above trial wave functions. For the sake of mathematical convenience, we consider $r_1 = r_2 = r$.

The ionization energy is obtained as

$$E_{ion}=E_D+\gamma-\langle\psi|H_{ID}|\psi\rangle_{min}. \quad (14)$$

The confining potential energies of two interacting donors are calculated using the wave functions (9) for 1s states is obtained by

$$H_{IE}=\left\langle\Psi_{1s}(\vec{r}_1,\vec{r}_2)\left|\frac{2}{|\vec{r}_1-\vec{r}_2|}\right|\Psi_{1s}(\vec{r}_1,\vec{r}_2)\right\rangle. \quad (15)$$

In the above equation $|\vec{r}_1-\vec{r}_2|$ determines the role of inter-donor distances in the Coulomb interaction energy of two donor systems.

The diamagnetic susceptibility χ_{dia} of the donor impurity in the QD is given as

$$\chi_{dia}=-\frac{e^2}{6m^*\varepsilon_0 c^2}\left\langle(\vec{r}-\vec{r}_0)^2\right\rangle, \quad (16)$$

where c is the velocity of light, $\left\langle(\vec{r}-\vec{r}_0)^2\right\rangle$ is the mean square distance between electron and nucleus.

3. RESULTS AND DISCUSSION

In our calculations, the values of physical parameters pertaining to GaN/AlGaN QDs are $m_{GaN}^* = 0.19m_0$, $\varepsilon = 9.5$, the effective Bohr radius is $a_B^* = 26.75$ Å and the effective Rydberg is $R_y^* = 28.644$ meV and $\gamma = 1$ for 90.4 T.

Fig. 1 shows the variation of two-donor binding energy as a function of dot radius for different magnetic field strength with and without applied field. In all the cases, it definitely shows that the binding energy increases with the decrease of dot radius, reaching a maximum value and then decreases when the dot radius still decreases. This is due to the fact the QD radius approaches zero, the confinement becomes negligibly small, and the tunneling comes to play in the finite barrier problem. Due to the reason, the binding energy again decreases drastically. This is a well-known result in quantum well structure and nanostructure [11]. It is in agreement with the other investigators [12, 13]. The value of all the magnetic field behavior is observed, and we notice that the binding energy increases with magnetic field for the entire dot radius. There is a "turn over" at $R = 15$Aº where the binding energy is maximum, this is due to the donor approaches the limit of effective Bohr radius of the given system. Moreover, the binding energy is appreciable for smaller dot radius due to the confinement, and the magnetic field effects are prominent for small-size dots. For the entire dot radius, there is an enhancement in the binding energy with and without magnetic field strengths.

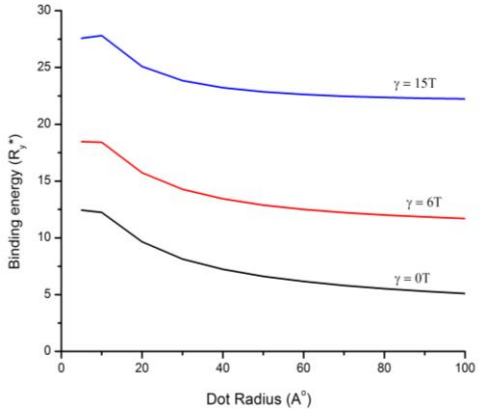

Fig. 1 – Dot radius with binding energy for different magnetic field

Fig. 2 shows the variational parameter as a function of dot radius for different magnetic field strength. We have adopted the variational method to evaluate the ground state energy of the given system. Its central point is the search for an optimum wave-function $\Psi(r)$ that depends on a number of parameters. This is called the trial wave-function. This variational approach consists in varying these parameters in the expression for the expectation value of the energy

$$E = \frac{\int \psi^* H \psi dr}{\int \psi^* \psi dr}$$

until it reaches its minimum value. This value is an upper limit of the energy level pursued. The so-called trial wave function depends on a set of free variational parameters. It is the measure of minimum energy of a system. It is observed that the variational parameter is appreciable only behind the regime of effective Bohr radius even for high magnetic field.

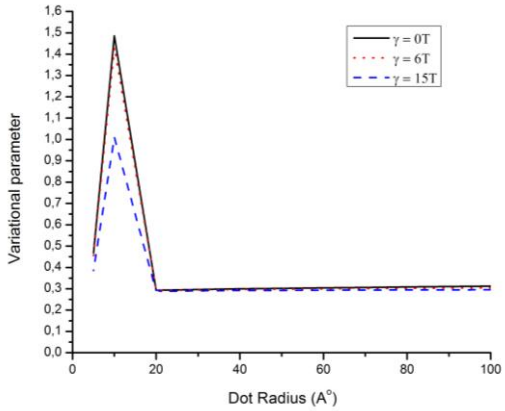

Fig. 2 – Variational parameter as a function of dot radius for different magnetic field

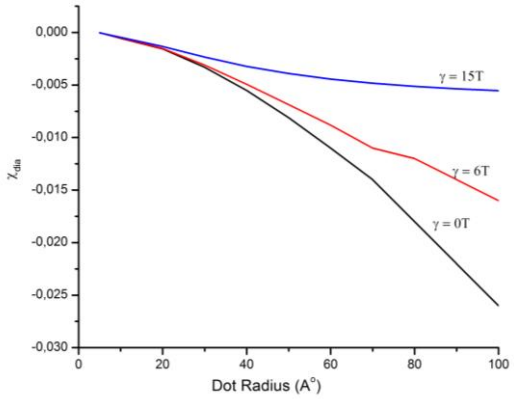

Fig. 3 – Variation of diamagnetic susceptibility as a function of dot radius for different magnetic field

The variation of diamagnetic susceptibility as a function of dot radius for different magnetic field strength is shown in Fig. 3. Diamagnetic susceptibility is a tool to check the accuracy of the wave function selected in variational method. The contribution of diamagnetic susceptibility to the donor binding energy is the measure of spatial extension of the ground state. It is observed that there is an increase in diamagnetic susceptibility when the dot radius decreases for all the magnetic field strengths. Also it is noted that the diamagnetic susceptibility increases with the decrease of quantum dot size and in the smaller size region, reaching a maximum and then decreases, which is very similar to the one observed in the donor binding energy with the dot size. The magnetic field dependence of diamagnetic susceptibility is not prominent for small dot radii due to the domination of geometrical confinement.

Fig. 4 displays the interaction energy as a function of quantum dot radius. The inter-donor distances are the measure of Coulomb interaction energy of the two donor systems. The interaction energy of the system is appreciable when the inter-donor distances reach and beyond the effective Bohr radius such as when the interaction energy starts to decrease. We believe that when

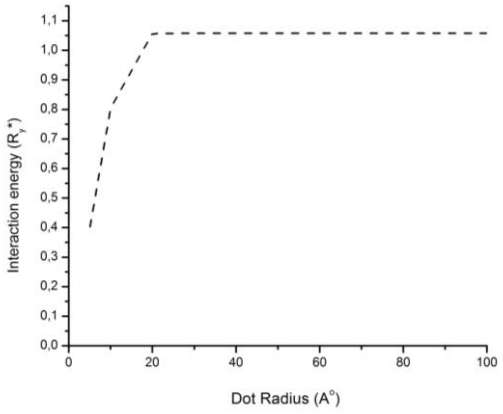

Fig. 4 – Interaction energy with dot radius

the inter-impurity distance becomes closer and closer, the total system becomes a cluster, in which a single particle variation technique cannot be applied further [14]. The increase of potential energy with the inter-impurity distance and the confinement of dot make more binding.

4. CONCLUSIONS

In conclusions, we have investigated the binding energy of two donors confined in a zinc-blende GaN/AlGaN strained QD by means of a variational approach within the framework of single band effective mass approximation. We have demonstrated the magnetic field induced energy spectra of two donors through the energy dependent effective mass with non-zero angular momentum as a function of dot radius. It may be important in the quantitative understanding the optical and magnetic properties of the two donor QDs.

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Вплив сильного магнітного поля на енергетичні спектри двох донорів у сфалеритовій квантовій точці

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Досліджено електронні стани двох донорів у напруженій квантовій точці (КТ) під впливом сильного магнітного поля. Чисельні розрахунки проводяться з використанням варіаційного принципу в межах односмугового наближення ефективної маси за допомогою напруженості магнітного поля через енергозалежну ефективну масу. Дослідження проблеми донора в КТ є корисним інструментом для розуміння електронних і оптичних властивостей домішок. Виконано дослідження двох донорних домішок у низькорозмірних напівпровідникових структурах із і без магнітних полів. Для розрахунку, береться енергія зв'язку у сфалеритовій КТ. Наші дослідження включають ефект Зеемана у гамільтоніані. Індукована магнітним полем діамагнітна сприйнятливість двох донорів обчислюється як функція радіуса КТ. Здійснюється варіювання енергії зв'язку двох донорів як функції радіуса точок для різної напруженості магнітного поля з і без прикладеного поля. Результати показують, що енергія зв'язку зростає зі зменшенням радіуса точки, досягаючи максимального значення, а потім зменшується при зменшенні радіуса точки. Внесок діамагнітної сприйнятливості у донорську енергію зв'язку є мірою просторового розширення основного стану. Міждонорна відстань є мірою енергії кулонівської взаємодії двох донорних систем. Енергія кулонівської взаємодії помітна лише тоді, коли міждонорні відстані наближаються або менші, ніж ефективний радіус Бора. Наші результати показують, що сильне магнітне поле, радіус КТ та енергія кулонівської взаємодії мають значний вплив на електронні стани двох донорів у напруженій КТ. Результати здаються коректними і добре узгоджуються з іншими літературними даними.

Ключові слова: Напружена квантова точка, Варіаційний метод, Кулонівська енергія.