COULOMB INTERACTION ENERGY AND DIAMAGNETIC SUSCEPTIBILITY OF TWO DONORS IN A QUANTUM DOT

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Abstract: The energy spectra of two interacting donors confined in a spherical quantum dot have been investigated using variational method under the influence of magnetic field. The magnetic field induced binding energy of two donors as a function of dot radius has been calculated within the frame work of single band effective mass approximation. We also computed the coulomb interaction energy of two donors as a function of inter– donor distances for different magnetic field and for various dot radius. The results show that the binding energy of two donors increases with the magnetic field and the diamagnetic susceptibility of two donors increases with the increment in magnetic field and decrement in dot radius. The coulomb interaction energy is only appreciable when inter donor distances approaching nearby or lesser than the effective Bohr radius.

IndexTerms **- variational method, coulomb interaction energy, quantum dot**

I. INTRODUCTION

With the modern crystal growth techniques, it is possible to construct few - electron quantum dots in semiconductors [1, 2]. Isolated quantum dots with only a few electrons can be called as artificial atoms. Due to their δ like function of density of states, the quantum dots are used in optoelectronic devices. Besides, the localization of electrons is determined by the profile of the potential confining the electrons within the quantum dots [3] and the interaction between electrons depends on the shape of the confinement potential. The "atomic" spectra of quantum dots (QDs) are determined by the intricate interplay between the binding forces due to confinement and the repelling Coulomb interaction between the electrons.

Studies on the donor problem in a QD are a useful tool for understanding the electronic and optical properties of impurities. Since, the problem of an electron bound to a hydrogenic impurity in the presence of external factors plays a fundamental role in studying the optical properties of impurities. At first, Bryant [4] reported that the Coulomb interaction energy of two donors in a ultra small Quantum well boxes and showed that electron – electron interactions are dominant in larger boxes and in small boxes subband spacing becomes dominant thus kindling the interest in impurity states. For the past few decades, several theoretical work has been devoted to study two donor [5,6] two acceptor[7,8] in low dimensional semiconductor structures with and without magnetic fields[9,10].

This paper explores the diamagnetic susceptibility of two interacting donors in a Gaussian confining potential under the influence of a magnetic field. The magnetic field induced binding energy of two donors as a function of quantum dot radius has been investigated. The calculations are carried out within the single band effective mass approximation using variational method. Our investigations include Zeeman effect in the Hamiltonian. The technique followed is presented in Section 2 while the results and discussion are presented in Section 3. Finally, we abridge the main conclusions obtained in this paper in the last Section.

II. THEORY AND MODEL

The Hamiltonian for two donor in the quantum dot system within the effective mass approach when the magnetic field is applied is given by

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

where g is the effective Lande factor; μ_B is the Bohr magneton; S_z is the z-component of the total spin, ε_o 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 and m* denotes the effective mass of the electron.

For a zinc blende phase the band gap difference between GaN and $Al_xGa_{1-x}N$ is given by[11]

$$E_{g,Al_xGa_{1-x}N}(x) = (1-x)E_{g,GaN} + xE_{g,AlN} + bx(x-1) \quad (2)$$

$E_{g,Al_xGa_{1-x}N}$, $E_{g,GaN}$ and $E_{g,AlN}$ are the $Al_x Ga_{1-x} N$, GaN and AlN gap energy in axis which passes through Γ point[12,13]. 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 GaN.

$$H_D = -\nabla^2 + \frac{\gamma^2}{4} r^2 \sin^2 \vartheta + \gamma L_z + \frac{V_D}{R^*} + \frac{2}{r_{12}} + \frac{g^* \mu_B B S_z}{R^*} \quad (3)$$

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

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

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

.

Where N_1, and N_2, 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

$$\alpha_1 R + \beta_1 R \tan(\alpha_1 R) = 0 \text{ For s-states} \quad (7)$$

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 Eq. (4&5).

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

$$H_{ID} = H_D - \sum_{i=1,2} \frac{e^2}{\varepsilon r_i} \quad (8)$$

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

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

. (9)

where ζ_1 and ζ_2 are the variational parameter. 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 by

$$E_{ion} = E_D + \gamma - \langle \psi | H_{ID} | \psi \rangle_{\min} \quad (10)$$

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

$$H_{IE} = \left\langle \Psi_{1s}(\vec{r}_1, \vec{r}_2) \left| \frac{2}{|\vec{r}_1 - \vec{r}_2|} \right| \Psi_{1s}(\vec{r}_1, \vec{r}_2) \right\rangle \quad (11)$$

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 quantum dot is given as [14]

$$\chi_{dia} = -\frac{e^2}{6m^* \varepsilon_0 c^2} \left\langle (\vec{r} - \vec{r}_0)^2 \right\rangle \quad (12)$$

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

III. RESULTS AND DISCUSSION

In our calculations, the values of physical parameters pertaining to GaN/AlGaN quantum dots are $m_{GaN}^* = 0.19m_0$, $\varepsilon = 9.5$, the effective Bohr radius is $a_B^* = 26.45A^0$ and an effective Rydberg is $R_y^* = 28.644meV$ and γ = 1 for 90.4 T

Fig.1 shows the variation of two donor binding energy as a function of dot radius in the presence and in the absence of magnetic field strengths. It clearly shows that the binding energy increases with the decrease of dot radius. There is a "turn over" that the binding energy is maximum at R = 20A°, is due to the donor is approaching the limit of effective Bohr radius of the given system. As the quantum dot radius approaches zero, the quantum confinement becomes negligibly small, and the tunneling comes to play in the finite barrier problem. Due reason, the binding energy again decreases drastically. For all the dot radius, there is an enhancement in the binding energy with and without magnetic field strengths. This is a well known result in all quantum well structures [15]. The binding energy is appreciable for smaller dot radii due to the confinement, and the magnetic field effects are prominent for small-size dots.

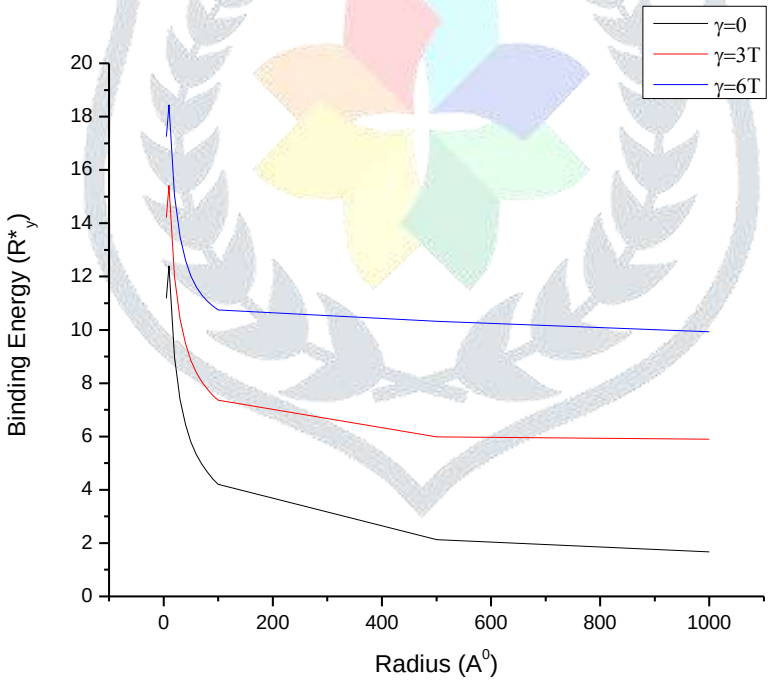

Figure.1 Variation of binding energy with the dot radius for different magnetic field

The computed values of diamagnetic susceptibility of two donors for different values of magnetic field are presented in **Fig. 2.** It is observed that the variation of diamagnetic susceptibility is not prominent for smaller dot radii due to the domination of geometrical confinement. On the other hand, the diamagnetic susceptibility increases with the magnetic field; this is because the magnetic field induced geometrical confinement is dominant beyond the radius of 90 Å in which the electron wave function is localized more around the impurity ion

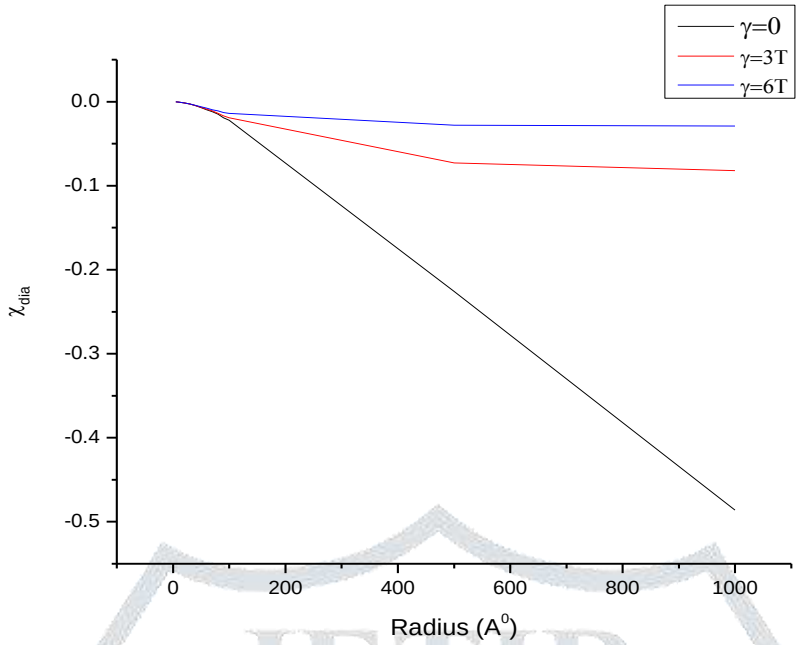

Figure .2 Diamagnetic susceptibility with dot radius for different magnetic field

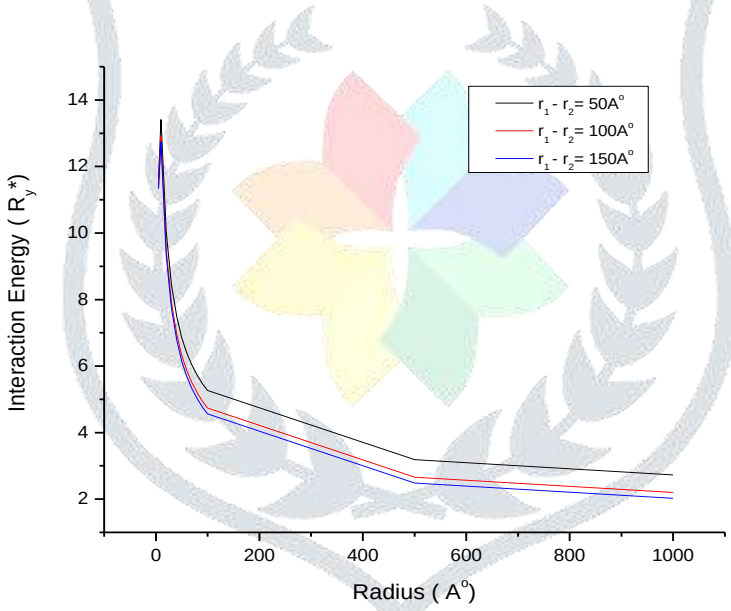

Figure .3 Variation of donor- donor interaction energy with dot radius as a function of inter - donor distances without magnetic field $\gamma = 0$

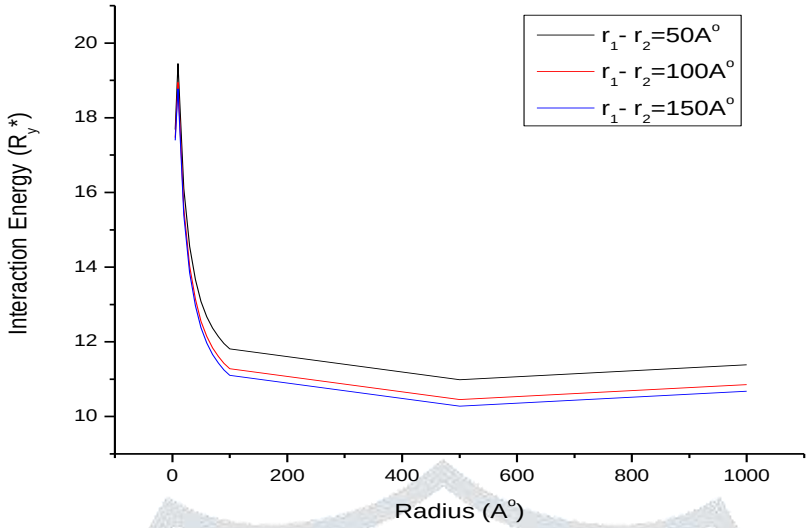

Figure .4 Variation of donor- donor interaction energy with dot radius as a function of inter - donor distances with magnetic field

$\gamma = 6$

Fig.3 shows the variation of interaction energy with dot radius as a function of different inter-atomic distances in the absence of magnetic field strength ($\gamma = 0$) and in the presence of magnetic field strength ($\gamma = 6$) is as shown in **Fig. 4**. It is noticed that interaction energy decreases with the increase in inter-impurity distance. The increase of potential energy with the inter impurity distance and the confinement of dot makes more binding. We also observed that for smaller QD radius the interaction energy reduces as the magnetic field is increased as well as inter atomic distance increased. In addition to that, we are unable to minimize the Hamiltonian for the inter-impurity distance which is less than 50 Å. We believe that when the inter-impurity distance becomes closer and closer the total system becomes cluster in which a single particle variation technique cannot be applied further [16].

Fig. 5 displays the variation of diamagnetic susceptibility as a function of magnetic field strengths for two different dot radius. The contribution of diamagnetic susceptibility to the donor binding energy is the measure of spatial extension of the ground state. It is observed that the diamagnetic susceptibility is appreciable for smaller dot radius compared to larger dot radius even for higher magnetic field. It is reported that the diamagnetic susceptibility increases when the dot radius decreases for all the magnetic field strengths.

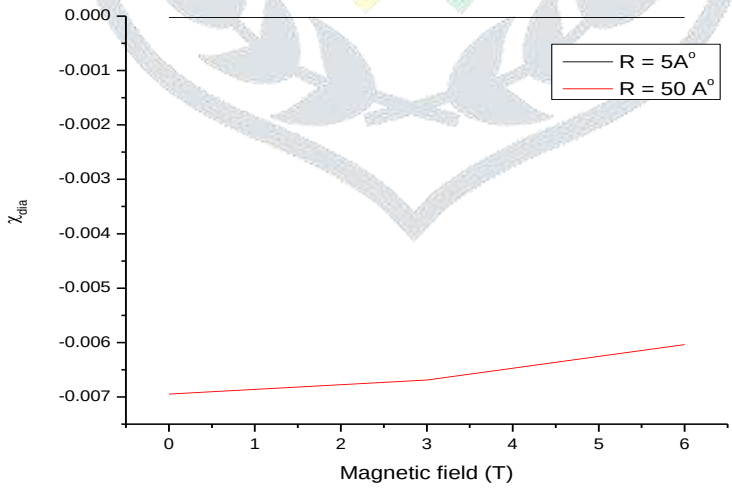

Figure. 5 Variation of diamagnetic susceptibility with magnetic field

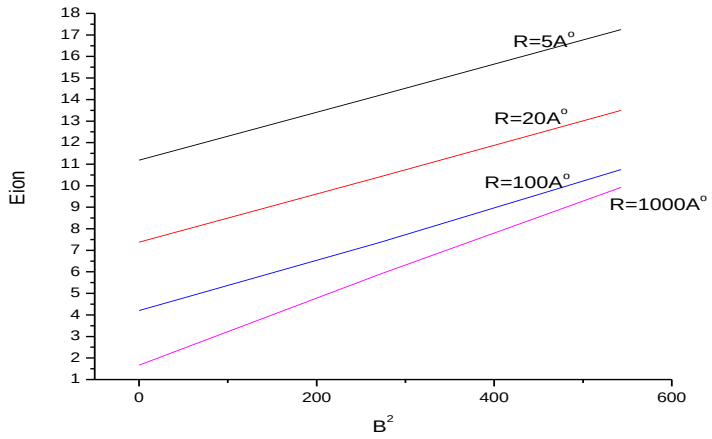

Figure. 6 Variation of donor binding energy with B^2

Fig. 6 shows the magnetic field induced donor binding energy for different quantum dot radius. We observe two important points: (i) the donor binding energy increases with increase in magnetic field (B). It can be interpreted that the orbit radii of the electrons is proportional to the QD size[17]. When the strength of magnetic field (B) increases, the dot size will decrease and the Coulomb attraction will increase. Henceforth, the binding energy of the ground state slowly increases with increasing B. (ii) For smaller dot radius, the donor binding energy is predominant, this is because the magnetic field which reduces the geometrical confinement and aids the repulsive forces of donor. It is well known that in a finite dot, there is a turnover in the binding energy as the system goes from quasi low dimensional to strictly low dimensional indicating a decrease in confinement at a particular radius due to tunneling. Hence, at a lower dot radius the repulsive force gain in strength and causes tunneling which in turn reduce the binding energy. This effect is not due to any interaction of magnetic field with the donor themselves but due to there is a reduction in confinement barrier.

In conclusion, we have investigated the Coulomb interaction energy and the diamagnetic susceptibility of two donors in a Gaussian confining potential quantum dot in the influence of a magnetic field through the trial wave function. The binding energy of two donors as a function of dot radius has been calculated within the single band effective mass approximation. Our results are good in agreement with the existing literatures [18]. It may be important in the quantitative understanding the optical and magnetic properties of the two donor QDs

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