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Diamagnetic Susceptibility and Donor Binding Energy of Impurity States in Zinc Blende AlGaN/GaN Quantum Dot

Research Article

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Abstract. In the frame work of effective mass approximation, we have determined the donor binding energies of the most minimal donor states, $1s$, $2p_0$ and $2p_\pm$, in zinc blende AlGaN/GaN Quantum dot in the impact of the magnetic field along the development(growth) directions. The calculations are performed utilizing variational method. The calculations are performed using variational method. As a function of the quantum dot radius and the applied magnetic field, the donor binding energies and diamagnetic susceptibilities are obtained. The oscillator quality of the potential transitions between the donor states is then figured by displaying them as the conditions of a two-level atom. Our outcomes demonstrate that (i) the donor binding energy is appreciable for smaller dot radii and magnetic field effect is predominant for larger dot radii, (ii) the diamagnetic susceptibility increases with applied magnetic field and is appreciable only for larger dot radii, (iii) The oscillator quality of the potential transitions between the donor states is not pronounced for smaller dot size radii and plays a significant role in larger dot radii.

Keywords. Quantum dot; Binding energy; Nanoparticles; Variational method

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1. Introduction

The investigation of low dimensional semiconductor structures has been the exciting subject of exploration since the start of quantum hypothesis. The enthusiasm for the investigation of

the physical properties of low dimensional semiconductor structures, for example, quantum wells, wires, and dots, has expanded theoretically [1, 2] and experimentally [3, 4], with the ongoing advances in semiconductor nanotechnology [5–7]. A comprehension of the idea of impurity states in semiconductor structures is one of the imperative issues in semiconductor material science because impurities can drastically alter the properties and execution of a quantum device. Electronic excitation comprises of an approximately limited electron-hole pair (the Mott-Wannierexciton), as a rule delocalized over a length any longer than the lattice constant.

As this exciton Bohr radius reaches the size of the semiconductor crystallite, its electronic properties are beginning to change. This is the so called quantum size effect, which in the optical band gap of exciton energy can be observed as a blue shift. It is only recently, due to advances in the synthesis of materials, can semiconductors be systematically studied [8]. Including impurities has played an important role in low-dimensional semiconductor structures in recent years because the optical and transport properties of devices made from these materials are greatly affected by the presence of shallow impurities. Only with impurities, the devices, such as diodes, transistors can be successfully made [9]. An important aspect to which many theoretical and experimental works have been dedicated the study of impurity states in heterostructures [10–12].

As wide band gap nitride semiconductors, GaN, AlN and their related compounds have attracted considerable interest in recent years, mainly due to their good optical properties and high potential uses in opto-electronics. Group III nitride materials play an important role in the manufacture of high-performance *light-emitting diodes* (LEDs) and lasers that emit in the visible system are increasingly prevalent in medical, security and solid-state lighting applications [13–15].

Due to spontaneous and piezo-electrical polarization, the properties of the wartziteGaN material are strongly affected by the internal field [16], whereas the zinc blend GaN structure, with less band gap, is not strongly built in the internal field due to high crystal symmetry [17]. There has been a lot of work devoted to understanding of hydro-genic impurity in ZB GaN quantum dots and quantum wire [18–21]. In these devices, if the barrier height or the thickness of the barrier is decreased, the wave function will penetrate more into the neighboring quantum dots. A variational method has been used to calculate the binding energy of a hydrogen impurity in Zinc-Blende(ZB) GaN/AlN coupled quantum dots (QDs) [22]. They found that the binding energy increases when the width of quantum well decreases and the impurity's binding energy depends upon its position within the well.

In the present work, we have observed ground and the first excited donor states binding energies to the lowest sub-band within the Zinc-Blende AlGaN / GaN quantum dot. Calculations of the oscillator strength for the transitions between donor states have been presented. Even, in the Zinc Blende quantum dot, we observed the diamagnetic susceptibility of the donor.

2. Model and Theory

Within the framework of effective mass approximation, the Hamiltonian for an electron in the ZB GaN/ AlGaN Quantum dots can be written under the influence of the magnetic field applied along the z axis,

$$H = \frac{1}{2m^*}\left[\vec{p} - \frac{e\vec{A}}{c}\right]^2 + V_D + H_{\text{zee}}, \tag{1}$$

where $V_D = \frac{V_0(B)r^2}{R^2}$ for $-r < R$, $V_0(B)$ for $-r \geq R$, where $V_o(B)$ is the height of the barrier of the quantum dot which is taken to be 70% of the difference in the band gap between ZB GaN/ AlGaN and m^* denotes the effective mass of the electron. H_{zee} denotes the Zeeman term.

For a ZB phase [12] the band gap difference between GaN and $Al_xGa_{1-x}N$ is given by

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

where b is bowing coefficient which is equal to 0.53 eV for Zinc-Blende phases. $E_{g,Al_xGa_{1-x}N}$, $E_{g,\text{GaN}}$ and $E_{g,\text{AlN}}$ are the $Al_xGa_{1-x}N$, GaN and AlN gap energy in axis which passes through Γ point [23, 24].

To measure the electron's ground-state energy in a ZB GaN quantum dot under magnetic field effect, the variational technique is used and for this the trial wave function is taken as,

$$\begin{aligned}
\psi_{\text{in}}(r) &= A_{\text{in}}\frac{\sin(\xi\cdot r)}{r}\cdot e^{-\lambda r^2}, \quad r < R, \\
\psi_{\text{out}}(r) &= A_{\text{out}}\frac{e^{\zeta\cdot r}}{r}\cdot e^{-\lambda r^2}, \qquad r \geq R,
\end{aligned} \tag{3}$$

where A_{in} and A_{out} are normalization constants. By matching the wave-functions and their derivatives at the quantum dot boundaries, we will fix the value of the given normalization constants. Here $\xi = \sqrt{\frac{2m^*E}{\hbar^2}}$ and $\zeta = \sqrt{\frac{2m^*(V-E)}{\hbar^2}}$ and λ is the variational parameter.

2.1 Donor Ionization Energy

The Hamiltonian for a hydrogenic donor placed at the center of the GaN quantum dot in the presence of a magnetic field applied along the direction of growth by

$$H_D = H - \frac{e^e}{\varepsilon_0 r}. \tag{4}$$

By employing the following trail wave function with α as the variational parameter,

$$\begin{aligned}
\Psi_{\text{in}}(r) &= \psi_{\text{in}}(r)\cdot\zeta(r) \qquad \text{for } r < R, \\
\Psi_{\text{out}}(r) &= \psi_{\text{out}}(r)\cdot\zeta(r) \quad \text{for } r \geq R.
\end{aligned} \tag{5}$$

Table 1. Hydro-genic functions for the states 1s, $2p_0$ and $2p_\pm$

State	$\zeta(r)^*$
$1s$	$\exp(-\lambda_1\cdot r)$
$2p_0$	$r\cos\theta\cdot\exp(-\lambda_2\cdot r)$
$2p_\pm$	$r\sin\theta\cdot\exp(-\lambda_3\cdot r)\cdot\exp(i\phi)$

*: λ_i are the variational parameters

The donor's ionizing energy is assessed using the following equation in the presence of the magnetic field:

$$E_{ion} = \langle\psi|H|\psi\rangle_{\min} - \langle\Psi|H_D|\Psi\rangle_{\min}, \tag{6}$$

where $\langle\Psi|H_D|\Psi\rangle_{\min}$ and $\langle\psi|H|\psi\rangle_{\min}$ represents the energy state of an electron with and without impurity in a quantum dot, respectively.

2.2 Diamagnetic Susceptibility

The hydro-genic donor's diamagnetic susceptibility in the quantum dot was investigated by variationally solving the Schrodinger equation to find the functions of the ground state wave functions. The diamagnetic susceptibility is the testing tool to check the accuracy of the wave-function chosen in the variational approximation of the ground state energy. It is well known that the error involved in the measurement of any physical property other than energy is the square root of the error involved in the energy estimate. The following eqn. (7) is used to calculate the diamagnetic susceptibility

$$\chi_{dia} = \frac{e^2}{6m^*\varepsilon_0 c^2}\langle r^2\rangle, \tag{7}$$

where c is the velocity of light and $\langle r^2\rangle$ mean square distance of the electrons from the nucleus.

3. Results and Discussion

The values of the GaN/AlGaN quantum dot physical parameters used in our calculations are $m^*_{\mathrm{GaN}} = 0.19m_0$, $\varepsilon = 9.5$, the effective Bohr radius is $a^*_B = 26.45$ Å and an effective Rydberg is $R^*_y = 28.644m$ eV.

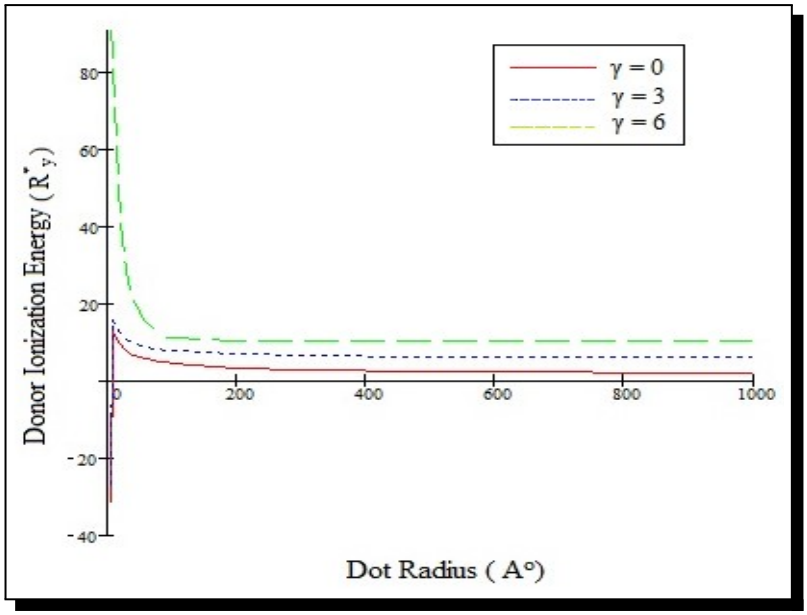

Figure 1. Donor Ionization energy with and without the magnetic field for 1s state

Figure 1 Exhibits the donor ionization energy under the magnetic field effect as a function of the quantum dot radius in 1s state. In all cases, such as with and without the magnetic field,

the binding energy increases as the quantum dot radius decreases and it reaches the maximum and then decreases to negative. Because of the size of the semiconductor crystallite exceeds the effective Bohr radius; the presence of peculiar material begins to change its electronic properties. This is so called as quantum size effect, which can be detected as a blue shift in the optical band gap of exciton energy. In our case, tunneling comes to play if the radius of the quantum dot approaches the effective Bohr radius $R \leq 26.45$ Å. For higher magnetic field; there is a significant shift in the donor ionization energy of the system within nano scale limit.

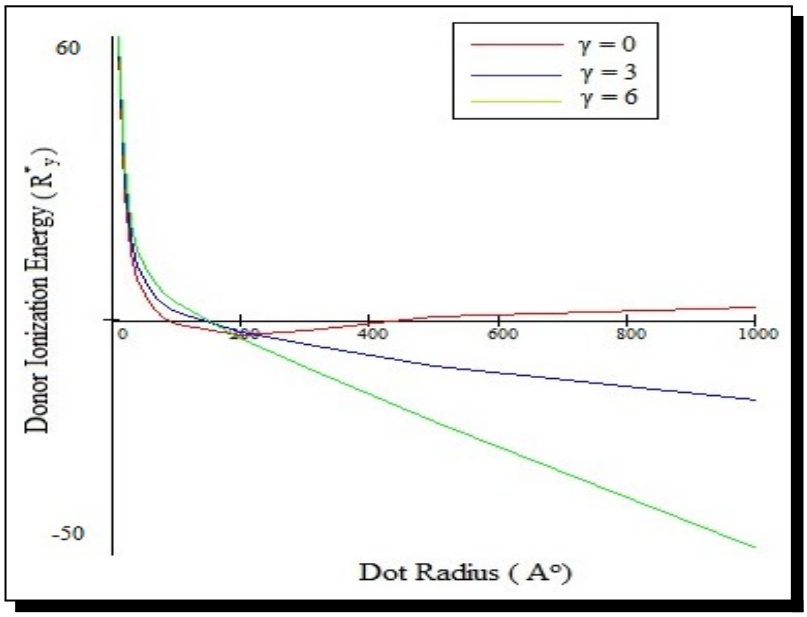

Figure 2. Donor Ionization energy as a function of dot radius with different magnetic field for $2p_0$ state

Donor ionization energy varies with the radius of quantum dot for different magnetic field for $2p_0$ state is as shown in Figure 2. The donor ionization energy is appreciable for smaller dot radii and in this case the effect of the magnetic field is also imperceptible. An increment in quantum dot radius towards bulk limit reveals the existence of this unbound state as depicted in Figure 2. Even for higher magnetic fields, the magnetic field effect is not significant in the nano scale limit. The donor ionization energy for $2p_0$ state as a function of quantum dot radius with varying magnetic field is contrary to the donor ionization energy for $1s$ state as shown in Figure 1.

Figure 3 shows the binding energy as a function of quantum dot radius with different magnetic field for $2p_\pm$ state. The energy of donor ionization decreases as expected with an increase in the radius of quantum dots. With smaller dot radii, the donor binding energy is appreciable. Influence of magnetic field play and significant role in $2p_\pm$ state compared to $1s$ and $2p_0$ state. Donor ionization energy is more for $1s$ state compared to $2p_0$ state and $2p_0$ state have more binding energy compared to $2p_\pm$ state.

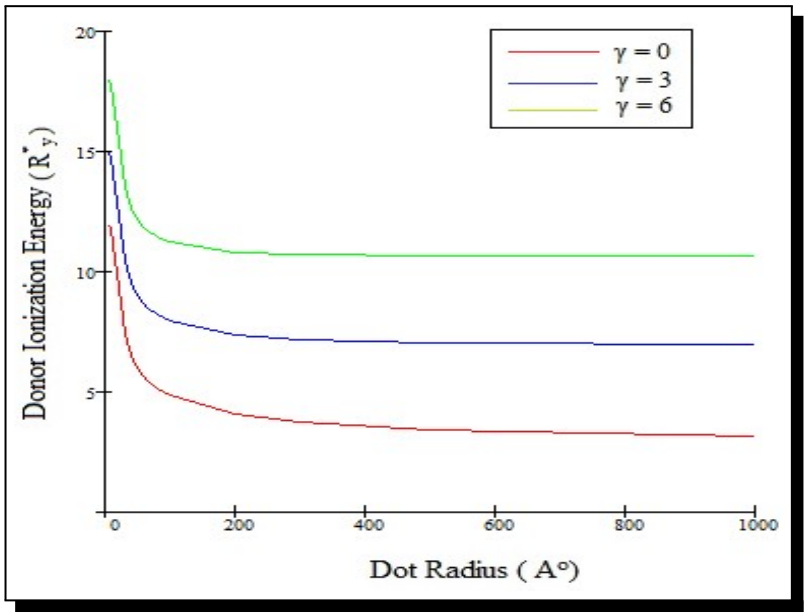

Figure 3. Donor Ionization energy as a function of dot radius with different magnetic field for $2p_{\pm}$ state

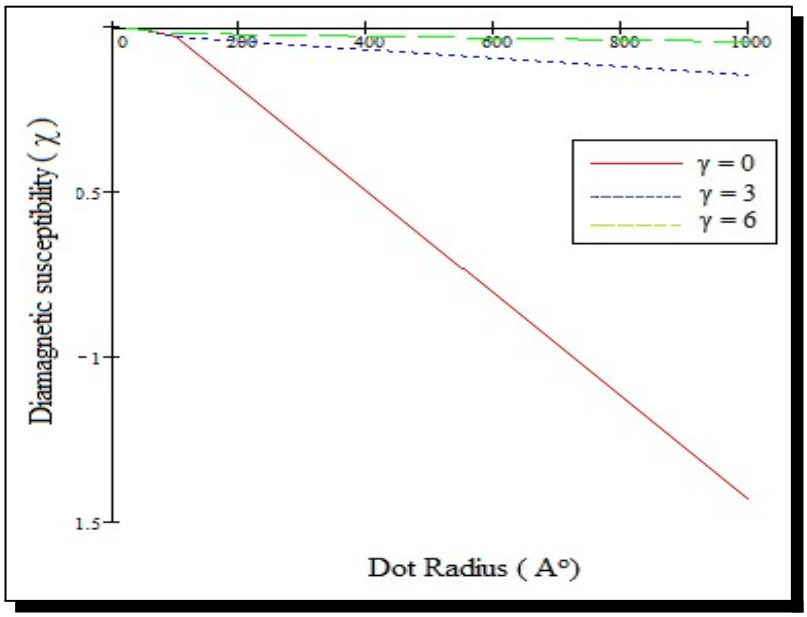

Figure 4. Diamagnetic susceptibility as a result of dot radius with different magnetic field for 1s state

Figure 4, displays the effect of a magnetic field on a donors diamagnetic susceptibility in a quantum dot as a function of the dot radius for 1s state. It is noted that due to the domination of geometric confinement, the variation of diamagnetic susceptibility is not pronounced for radii of smaller quantum dots. On the other hand, the diamagnetic susceptibility increases with the magnetic field; this is because the structural confinement caused by the magnetic field is dominant where the role of the electron wave is more localized around the impurity ion that is also applicable for $2p_0$ state as shown in Figure 5.

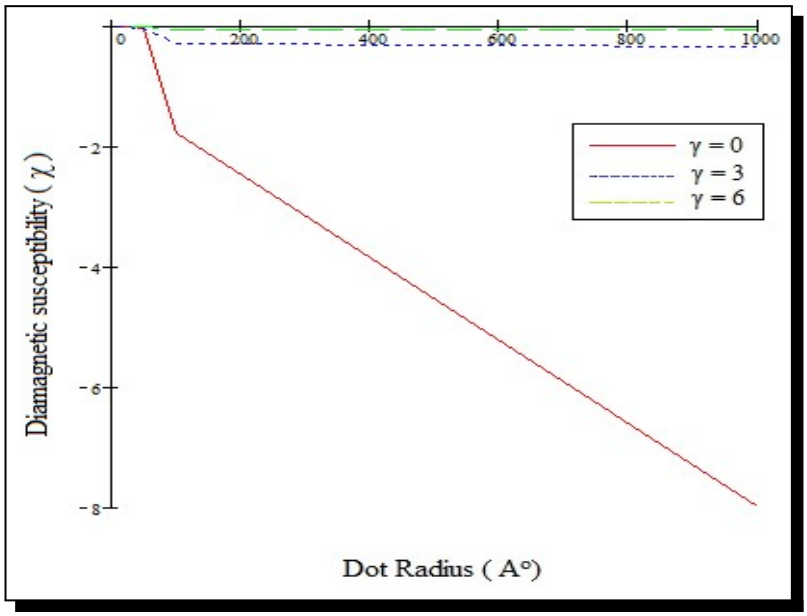

Figure 5. Variation of Diamagnetic susceptibility as a function of different magnetic field with dot radius for $2p_0$ state

Figure 6 shows the magnetic field induced diamagnetic susceptibility of a donor in a quantum dot for $2p_{\pm}$ state. Diamagnetic susceptibility is appreciable with reduction of quantum dot radius and influence of magnetic field is not significant play in $2p_{\pm}$ state compared to the other two states. Diamagnetic susceptibility slowly increases with decrease of QD radius and more pronounced in small dot radii.

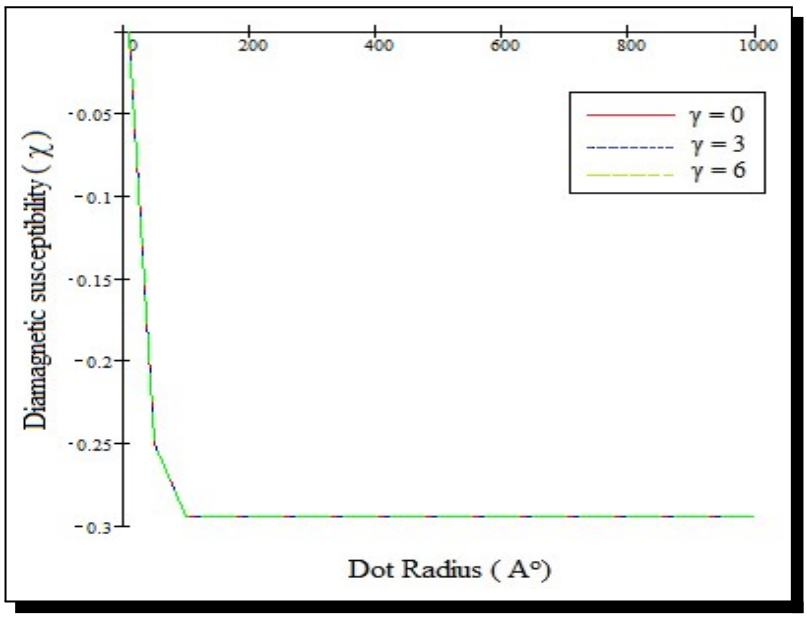

Figure 6. Diamagnetic susceptibility as a function of dot radius with varying magnetic field for $2p_0$ state

4. Conclusion

In conclusion, we calculated the donor binding energy for ground ($1s$) and some low lying excited states ($2p_0$ and $2p_\pm$) of a confined donor in a GaN/AlGaN QD using variational method. Influence of magnetic field on binding energy and diamagnetic susceptibility is of the donor is computed as a function of quantum dot radius. Our results are good in agreement with existing literatures. Our result will light throw some novelty in future electronic and optical studies in quantum structures.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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