# SPIN - ORBIT COUPLING OF A HYDROGENIC DONOR IN ZINC BLENDE GaN /$Al_X$ $Ga_{1-X}$ N PARABOLIC QUANTUM DOT

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***Abstract : Using variational method, a theoretical study has been carried out on conventional spin – orbit interaction of a donor in GaN/AlGaN quantum dot as a function of quantum dot radius and magnetic field. We computed the donor binding energy with and without inclusion of spin orbit interaction energy with different high intense magnetic field for 2p0 state. Our results show that spin orbit interaction energy is insignificant for quantum dots of all radii. Though the contribution of spin orbit splitting is very small, significantly it enhances the binding energy of the system. Our results are good in agreement with existing literatures.***

## 1.Introduction

The study of low dimensional semiconductor structures has been the interesting subject of investigation since the beginning of quantum theory. The interest in the study of the physical properties of low dimensional semiconductor structures such as quantum wells, wires, and dots, has increased theoretically[1,2] and experimentally[3,4] ,with the recent progress in semiconductor nanotechnology [5-7]. An understanding of the nature of impurity states in semiconductor structures is one of the crucial problems in semiconductor physics because impurities can dramatically alter the properties and performance of a quantum device. It is only recently, due to the advance in materials synthesis, that semiconductors in this size regime can be systematically studied[8].In recent years, addition of impurities plays an important role in the low dimensional semiconductor structures because the optical and transport properties of devices made from these materials are strongly affected by the presence of shallow impurities. Only with impurities, the devices, such as diodes, transistors can be successfully made [9]. The study of impurity states in heterostructures is an important aspect to which many theoretical and experimental works have been devoted [10-12].

The spin –orbit interaction otherwise known as spin orbit coupling plays an important role in devices,which exploit spin transport.This branch of semiconductor physics has come to be known as spintronics[13-14]. Spintronics is a new field of research exploiting the influence of electron spin on the electrical conduction (or current is spin dependent). In hybrid spintronics the data storage and data communication is done by charge only (either electron or hole), but its effect is augmented by the presence of spin. Spin plays a secondary role and influences how charge stores or manipulate information [15]. In present work, We computed the donor binding energy with and without inclusion of spin orbit interaction energy with different high intense magnetic field for 2p0 state.

## 2.Model and Theory

The Hamiltonian for an electron in the ZB GaN/ AlGaN quantum dots under the influence of applied magnetic field along the z direction within the framework of effective mass approximation may be written as

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

Where $V_D = \frac{V_0(B)r^2}{R^2}$ $for - r\langle R$

And $V_0(B)\, for - r \geq R$ 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 [16] the band gap difference between GaN and Al $_x$Ga$_{1-x}$N is given by

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

Where, b is the bowing coefficient, which is equal to 0.53ev for zinc -blende phases. $E_{g,Al_xGa_{1-x}N}$, $E_{g,GaN}$ and $E_{g,AlN}$ are the $Al_x$ $Ga_{1-x}$ N, GaN and AlN gap energy in axis which passes through Γ point[17,18].

In order to calculate the ground state energy of the electron in a ZB GaN quantum dot under the influence of magnetic field, the variational technique is used, and for this the trial wave function is taken as

$$\psi_{in}(r) = A_{in}\frac{Sin(\xi.r)}{r}.e^{-\lambda r^2} \qquad r\langle R$$

$$\psi_{out}(r) = A_{out}\frac{e^{\zeta.r}}{r}.e^{-\lambda r^2} \qquad r \geq R \tag{3}$$

Where $A_{in}$ and $A_{out}$ are normalization constants. We will fix the value of the given normalization constants by matching the wavefunctions and their derivatives at the boundaries of the quantum dot. 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 centre of GaN quantum dot in the presence of magnetic field applied along the growth direction is given 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

$$\Psi_{in}(r) = \psi_{in}(r).\zeta(r) \qquad \text{for } r\langle R$$

$$\Psi_{out}(r) = \psi_{out}(r).\zeta(r) \qquad \text{for } r \geq R \tag{5}$$

Table .1 Hydrogenic functions for the states $2p_0$

| State | $\zeta(r)^*$ |
|---|---|
| $2p_0$ | $r\cos\theta.\exp(-\lambda_2.r)$ |

* $\lambda_i$ are the variational parameters

The ionization energy of the donor in the presence of magnetic field is computed using the following equation .

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

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

*2.2. Effect of SOI*

The Hamiltonian for the conventional Spin Orbit interaction is given by

$$H_{so} = \xi(r)L.S \tag{7}$$

Where $\xi(r) = 1/(2m^2C^2r)dV_c(r)/dr$ , wherein C is the velocity of light.

By Using $V_c(r) = -1/r$ , we get

$$H_{so} = B/r^3 \tag{8}$$

Where $B = [j(j+1) - l(l+1) - 3/4]/(4m^2C^2)$

There is no spin orbit interaction for 1s and 2s state.

The first order perturbation leads to

$$\Delta E_{so} = \langle\Psi|H_{so}|\Psi\rangle \tag{9}$$

In a hydrogen atom, the spin orbit interaction energy is given by [19]

$$E_{so} = \frac{c\hbar z^4\alpha^2 R[j(j+1) - l(l+1) - s(s+1)]}{2n^3 l[l+1/2][l+1]} \tag{10}$$

Where $\hbar$ is the Planck's constant and $R = 2\pi^2 me^4 / C\hbar^3$, is the Rydberg constant. In an atomic units α =1/C

**3.Results and discussion**

We present the results of our calculations in Fig 1-7. In our present work, we are limited to 2p states as the 1p state have larger SOI energy than other states such as 1d state and it is in the order of $10^{-4}$ meV. In general, for p states, the possible values of j are 3/2 and 1/2. Fig 1shows the binding energy as a function of dot radius for different magnetic field with and without spin orbit interaction energy for j=3/2.We observe that in all the cases the donor binding energy increases as the dot radius decreases. This is a well known result in nanostructures, so called quantum confinement effect. Influence of magnetic field also increases the donor binding energy. Spin orbit interaction energy is appreciable for dots of radius $\geq 50A^0$. The spin orbit interaction energy is insignificant for smaller dot radius in both cases for j = 3/2 and j = 1/2 as shown in Fig.2. The physics behind that peculiar behavior is the play of confinement is predominant over the magnetic field and SOI.

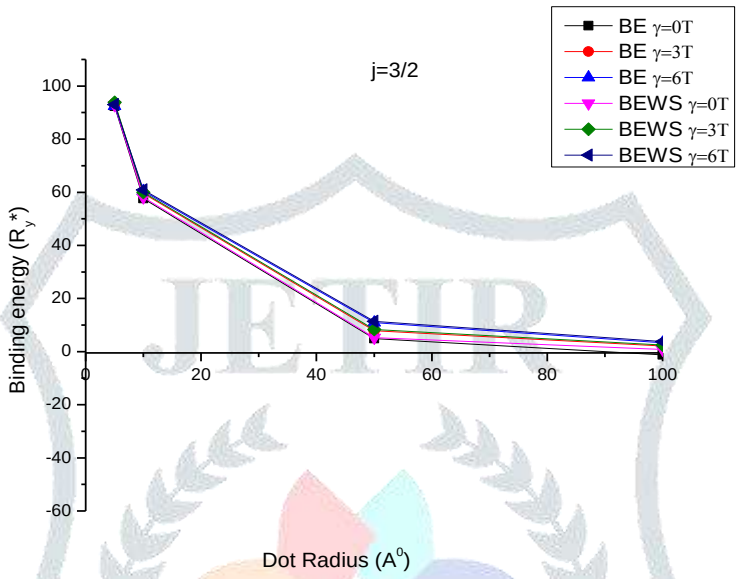


**Fig 1 Variation of binding energy as a function of dot radius for different magnetic field with and without spin orbit interaction energy for j = 3/2**

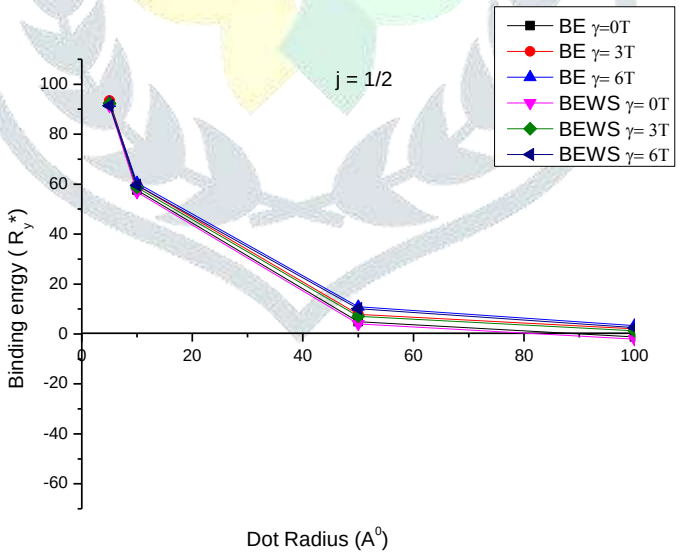


**Fig 2 Variation of binding energy as a function of dot radius for different magnetic field with and without spin orbit interaction energy for j = 1/2**

Fig. 3 displays the spin orbit interaction energy as a function of dot radius. In general, for 2p0 states the value of l is 1 and if l is different from 0 then j can be either l+s or l-s. So the SOI energy splits up into two components one corresponding to j = 3/2 and another one corresponding to j = 1/2. It is also interesting to note that spin orbit splitting energy is constant for all radius of quantum dots which is in contrast to quantum well cases [20]. It is due to addition of confinement brought out in quantum dot.

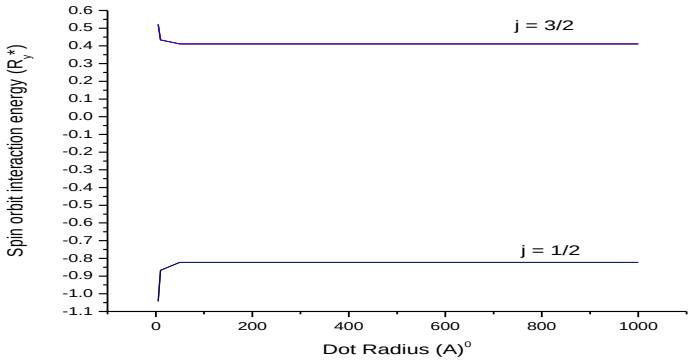


**Fig 3. Quantum dot radius with spin orbit interaction energy for 2p0 states for different magnetic fields.**

Fig 4 and Fig 5 shows that the spin orbit interaction energy as a function of magnetic field for two different dot radius. We observe that the effect of magnetic field is insignificant for these two cases. SOI is constant for various magnetic field. This is a consequences of additional confinement in a quantum dot. E. A de Andrada et al [21] reported that the magnitude of SOI of GaAs heterostructures is less than 1mev. But, for GaSb/InSb heterostructures, the zero filed spin splitting is 10meV.

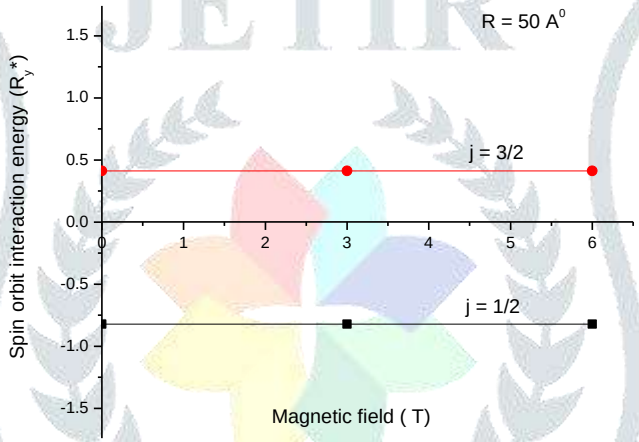


**Fig 4 Spin orbit interaction energy as a function of magnetic field for the dot radius R = 50 A$^0$**

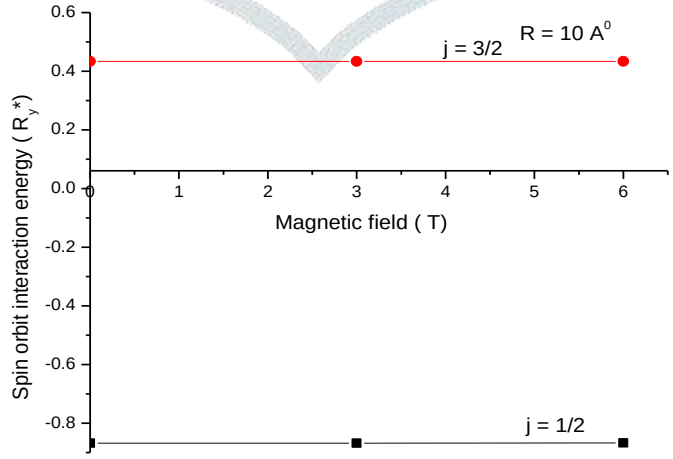


**Fig 5 Spin orbit interaction energy as a function of magnetic field for the dot radius R = 10 A$^0$**

Fig 6 and Fig 7 displays the spin orbit interaction energy for j = 3/2 and j = 1/2 as a function of intense magnetic field for a aot radius r = 10 $A^0$. It is significant to notice that spin orbit interaction energy decreases as magnetic field increases in both cases. It is due to the increase in magnetic field tries to increase the confinement of quantum dot and the confinement predominant over the spin orbit interaction energy. Influence of magnetic field is only appreciable for dots of larger radii.

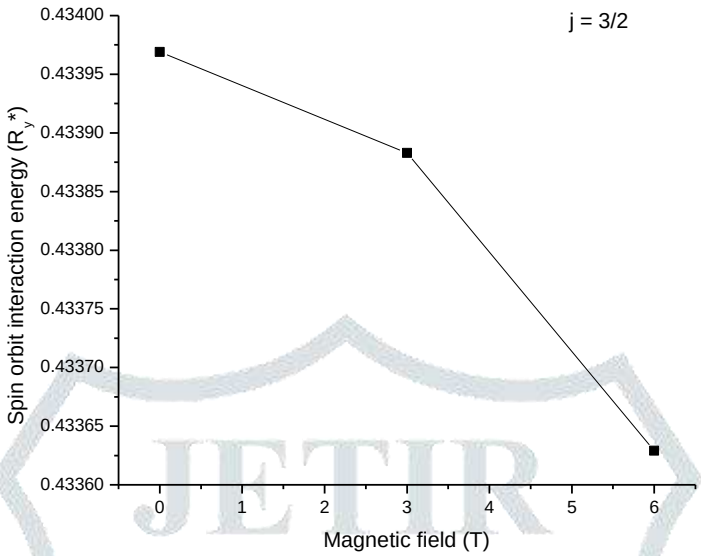


**Fig 6 Spin orbit interaction energy as a function of magnetic field for the dot radius R = 10 $A^0$ for j =3/2**

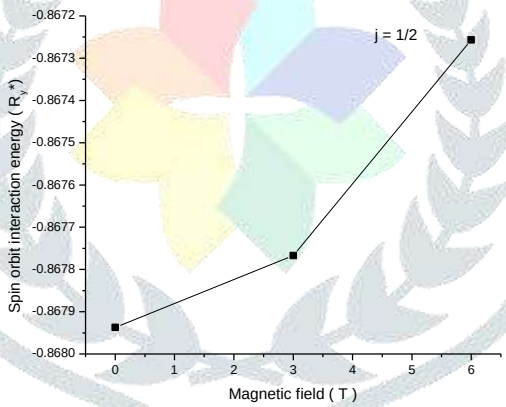


**Fig 7 Spin orbit interaction energy as a function of magnetic field for the dot radius R = 10 $A^0$ for j =1/2**

**Conclusion**

Influence of spin orbit interaction is significant on the study of transport phenomena such as mesoscale transport phenomena, quantum hall effect and Aharonov Bohm effect. We conclude that the contribution of spin orbit coupling $H_{so}$should not be neglected even it is in the order 1- 10meV. It plays a significant role in enhancing the donor binding energy of a quantum dot. Our result should light throw on the studies of far infra red radiation detection and spin filters.

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