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The effect of first order magnetic field in a GaAs/AlAs spherical quantum dot with hydrogenic impurity

M. Abdollahi
M. A. Talebian Darzi[*]
H. Hoseinkhani
H. Baghbani Rizi

Department of physics, Faculty of science, I.H.U Tehran, Iran.

ABSTRACT

In this research, the effect of the first order magnetic field on the ground-state of a centered hydrogenic donor impurity in a GaAs/AlAs spherical quantum dot has been calculated. The perturbation method has been used within the framework of effective mass approximation for these calculations. Overall, the analysis shows that a proper choice of quantum dot radius and magnetic field can significantly change the normalized binding energy. The concluded information may be used to calculate the small changes in quantum dot radius and thus detect different magnetic field strengths.

Keywords: *Hydrogenic impurity; Perturbation method; Spherical quantum dot; Turning point*

* Corresponding author:
M. A. Talebian Darzi
Department of physics, Faculty of science, I.H.U Tehran, Iran.
Tel +98 9111121447
Fax +98 2177104938
Email mtalebiand@yahoo.com

INTRODUCTION

In recent years, the effect of quantum dot size in low dimensions has been extensively investigated. Quantum dots are zero-dimensional nanostructures which have become the focus of intense (extensive) research, and the discovery of their wide applications in industry, medicine, agriculture, and… has intensified scientific interest in this miniscule particle. Interest in studying the effects of magnetic field on the quantum dots stems from its use in electronic and optical devices and its extensive applications in many other areas. The difference between quantum dots and other quantum systems (quantum wires and wells) is that the energy levels in the quantum dots are completely discrete. Using modern methods of quantum dot growth, quantum dots of different geometrical sizes and shapes such as spherical, cylindrical, and ellipsoidal have been obtained. A considerable amount of electronic and optical work done on the spherical quantum dot have been cited in the references [1−12].

The key problem in these works is the absence of information regarding energy levels of the confined carriers, and the lack of understanding concerning how the one-electron levels and consequently the size and shape of quantum dots are to be treated.

Numerous theoretical works have been published on the bound states of a hydrogenic impurity in spherical quantum dots. The location and absolute spatial confinement of the impurity in these quantum dots reflect themselves in the ground state energy and the impurity binding energy. The ground state and binding energy is larger for a completely confined (infinite potential) spherical quantum dot compared to a finite confined (finite potential) one, and is maximized for an on-centre impurity [3-5]. Hence, the change in the binding energy may serve as a clear signal for variation in the effective radius of the spherical quantum dot. On the other hand, one can obtain further insight by making use of a perturbing force such as an external constant magnetic field. In case of an on-centre donor, the magnetic field enhances the binding energy [2]. So far, shifts in binding energies due to impurity in spherical quantum dots in the presence of a magnetic field have been estimated using variation methods.

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To enhance the binding energy in this work, the normalized binding energy is used - the normalized binding energy is defined as the ratio of the binding energy to the hydrogenised donor impurity energy which is used in the theoretical description of the behavior of an on-center donor in a spherical quantum dot with infinite potential barrier in the presence of the magnetic field. Using normalized binding energy will lead to a better understanding of the properties of the quantum dot. In the present work, employing a perturbation procedure within the effective-mass approximation, the binding energies of an impurity located at the centre of a spherical GaAs/AlAs quantum dot has been calculated in the presence of an infinite confining potential. Normalized binding energies are calculated as a function of radius of quantum dots and a uniform magnetic field strength.

EXPERIMENTAL

In effective mass approximation, the Hamiltonian of a hydrogenised impurity located at the center of a spherical quantum dot of radius, a, in the absence of external magnetic field, can be written as:

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\varepsilon \vec{r}} + V(\vec{r}) \qquad (1)$$

Where m^* the electron isotropic effective mass, ε is the dielectric constant of the material inside the quantum dot, e and $\vec{r}$ are the electron charge and position vector, respectively.
The confining potential defined by

$$V(\vec{r}) = \begin{cases} 0 & r < a \\ \infty & r > a \end{cases} \qquad (2)$$

The Hamiltonian of a hydrogenised impurity located at the center of a spherical quantum dot in the presence of an external magnetic field B can be written as

$$H = \frac{1}{2m^*}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{e^2}{\varepsilon \vec{r}} + V(\vec{r}) \qquad (3)$$

Where $\vec{A}$ is the potential vector derived from the magnetic field, $\vec{B} = \vec{\nabla} \times \vec{A}$ and the equation (3) can be rewritten, as:

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\varepsilon \vec{r}} - \frac{e}{2m^*c}|B|(L_z + 2S_z) + \frac{e^2}{8m^*c^2}B^2(x^2 + y^2) + V(\vec{r}) \qquad (4)$$

Due to the weak field, the influence of quadratic magnetic field, $(\frac{e^2}{8m^*c^2}|B|^2(x^2 + y^2))$, is to be ignored.

Here, the effective radius, $a^* = \dfrac{\varepsilon \hbar^2}{m^* e^2}$ is used as a unit of length, the effective Rydberg, $R^* = \dfrac{e^2}{2\varepsilon a^*}$ is used as a unit of energy and the parameter $\beta = \dfrac{\hbar \omega_c}{2R^*}$ with $\omega_c = \dfrac{eB}{m^* c}$ is used as a unit of dimensionless magnetic field; consequently the Hamiltonian can be written as following:

$$H = -\nabla^2 - \frac{2}{r} - \frac{\beta}{\sqrt{2m^*}}(L_z + 2S_z) + \frac{V(r)}{R^*} \tag{5}$$

The ground-state wave function and energy of an electron confined in the unperturbed spherical quantum dot of radius, a, are given by

$$R_0 = \begin{cases} A_0 J_0(kr) & r < a \\ 0 & r > a \end{cases} \tag{6}$$

where

$$A_0 = \frac{1}{\sqrt{\int_0^a J_0(Kr)J_0(K'r)r^2 dr}}$$

and

$$E_{100} = R^*(a^* \frac{\pi}{a})^2 \tag{7}$$

Using the perturbation method, the disturbed wave function in the presence of the magnetic field is:

$$\psi_n = \phi_n + \sum_{n \neq n'} \frac{\langle \phi_{n'} | H_B | \phi_n \rangle}{E_n^0 - E_{n'}^0} | \phi_{n'} \rangle \tag{8}$$

or

$$\psi_n = \left\{ \begin{aligned} &\left(1 \pm \sum_{n'=2}^{\infty} \frac{a^2 \gamma}{a^{*2} \pi^2 (1 - n'^2)} A_0^2 \int_0^a J_0(K'r)J_0(Kr)r^2 dr \right) \\ &\times \left(1 - \sum_{n'=2}^{\infty} \frac{2a^2}{a^* \pi^2 (1 - n'^2)} A_0^2 \int_0^a J_0(K'r)J_0(Kr)r dr \right) \times A_0 |Y_0^0 J_0(K'r)\rangle \end{aligned} \right\} \tag{9}$$

And disturbed ground state energy in the presence of a magnetic field is obtained from the following equation:

$$E_{n'} = \Delta E^{(1)} + E_{100} \tag{10}$$

The $\Delta E^{(1)}$ is the first order energy change in the presence of the magnetic field.

$$\Delta E^{(1)} = \beta R^* \times \left(1 - \sum_{n'=2}^{\infty} \frac{2a^2}{a^{*2} \pi^2 (1 - n'^2)} A_0^2 \int_0^a J_0(k'r)J_0(Kr)r dr \right)^2 A_0^2 \int_0^a J_0(k'r)J_0(Kr)r^2 dr \tag{11}$$

The normalized binding energy is as following:

$$NE_{B1} = \frac{E_{100c}}{E_{n'}} - 1 \tag{12}$$

where E_{100c} is ground state energy including the Coulomb interaction.

RESULTS AND DISCUSSION

A considerable amount of work has been invested in deciphering the binding energies of a hydrogenic impurity in a spherical GaAs/AlAs quantum dot. The parameters $m^* = 0.067m_0$ and $\varepsilon = 13.1$ are used in the calculations. The resulting effective Rydberg is $R^* = 5.31meV$ and the effective Bohr radius is 103.43A°. For these values of material parameters, the value of the magnetic strength ($\beta = 0.1$) corresponds to a magnetic field of 0.614852T.

Figure 1 shows the calculated perturbed energy, $E_{n'}$ as a function of the dot radius in the absence of a magnetic field. When the dot radius is larger than $2.093a^*$, the perturbed energy, $E_{n'}$, becomes negative. This value of the dot radius at which the energy $E_{n'}$ changing from positive to negative is known as the turning point (a_t). The small differences observed at the turning point between previous reports and the present study [1] can be attributed to the different methods employed here.
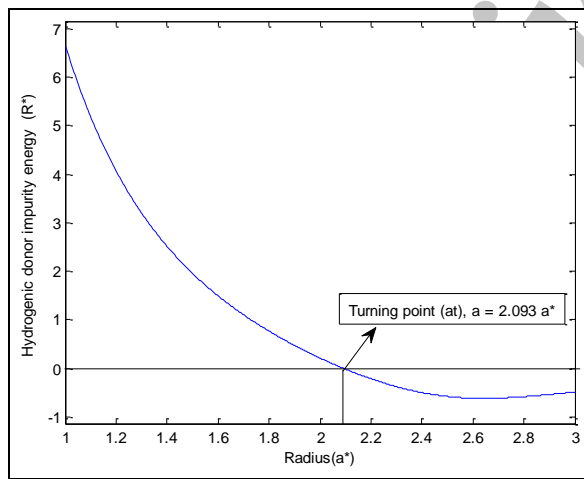

Fig. 1. The hydrogenic donor impurity energy, $E_{n'}$, as a function of radius of the spherical quantum dot in the absence of magnetic field.

For each dot radius, there is the magnetic field strength β_0 for which $E_{n'}$ has its zero value. Figure 2, is showing the magnetic field strength changes with respect to the dot radius, $a > a_t$. The value β_0 increases and the slope of the β_0 decreases with increasing dot radius.
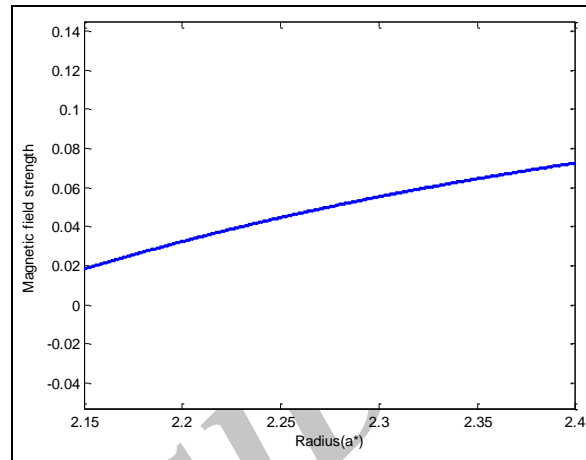

Fig. 2. Variation of the magnetic field strength versus dot radius.

Figure 3, shows the ground state wave function and the disturbed wave function in presence of both first order magnetic field and the coulomb_interaction as a function of quantum dot radius. By applying the magnetic field, one can observe (figure 3) the amplitude of wave function for the spin up is slightly higher than that of the ground state wave function, while the spin down is slightly lower. Consequently, the slope of the wave function for the spin up is slightly sharper than the spin down mode. Depending on the chosen potential (infinite potential), wave functions in all three modes go to zero at the boundary of quantum dot.
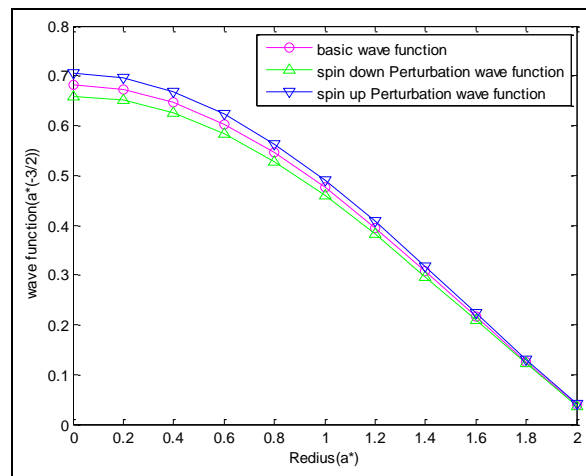
Figure 4 shows the probability of electrons within the quantum dots as a function of quantum dot radius for the ground and the disturbed states in presence of first order magnetic field. As one can see, electron density has the highest value at the center of quantum dot and the lowest value at the boundary.
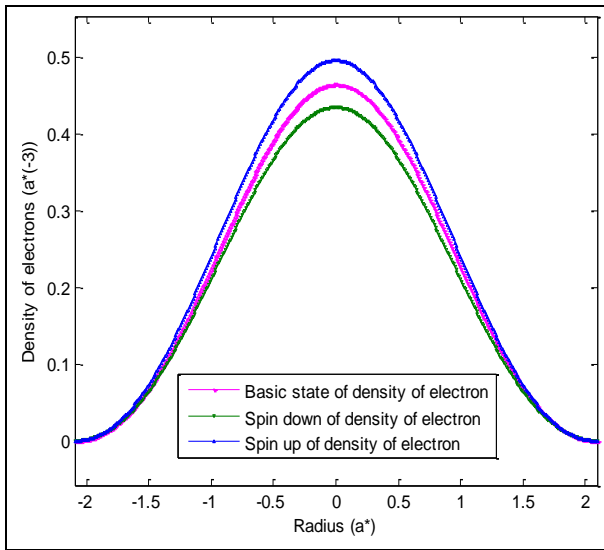

Fig. 4. Density of electrons within the quantum dot as a function of the dot radius

In Figure 5, the results of the normalized binding energy NE_{B1} have been presented as a function of magnetic field strength β for six given values of the dot radius. From this figure, one can see that special values of β (say β_0) has an asymptotic line where the normalized binding energy NE_{B1} for $\beta < \beta_0$ will start from a small negative value and escalate to an infinite negative binding energy NE_{B1} at asymptote β_0. For $\beta > \beta_0$ it will do so as well, however it will start from infinite positive binding energy at asymptote β_0 and progress to a small positive one at a higher magnetic field strength for each value of the quantum dot radius.
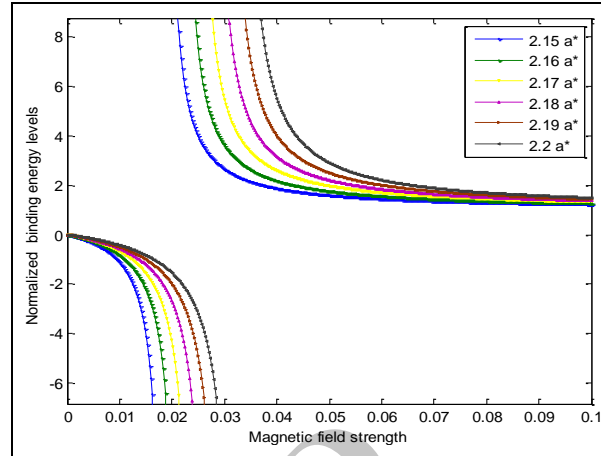

Fig. 5. The normalized binding energy levels, NE_{B1}, as a function of the magnetic field strength β.

CONCLUSION

In conclusion, a proper choice of the quantum dot radius and magnetic field can significantly change the normalized binding energy NE_{B1} of on-center hydrogenic impurity in the infinitely confined spherical quantum dot, GaAs/AlAs, which may be used to calculate the small change in the quantum dot radius. In other words, in the vicinity of a magnetic field β_0, the dramatic change in the energy NE_{B1} may serve as a clear signal for detection of the effective radius (dimension) of the quantum dot in the presence of perturbation fields. The novelty of our work is the utilization of perturbation methods to find the influence of first order, weak magnetic fields on quantum dots [13-15].

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