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Effect of magnetic field on the impurity binding energy of the excited states in spherical quantum dot

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Abstract. The effect of external magnetic field on the excited state energies in a spherical quantum dot was studied. The impurity energy and binding energy were calculated using the variational method within the effective mass approximation and finite barrier potential. The results showed that by increasing the magnetic field, the energy would be increased. The results obtained by this method were compared with the previous investigations.

Keywords. Impurity energy; turning point; binding energy.

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1. Introduction

Because of the recent advances in nanofabrication technology, it is possible to produce quantum dots whose characteristic dimensions are comparable with the electronic de Broglie wavelengths. The quantum mechanical nature of the electrons therefore plays a dominant role over the optoelectronic properties of the structure [1,2]. A doped hydrogenic impurity in a quantum dot influences both the electronic mobility and its optical properties because of the Coulomb interaction between the electron and the impurity ion. The three-dimensional confinement, depending on the size of the dot, causes the electron to move near the impurity ion which enhances the binding energy because of the increasing interaction strength. The transport mechanism in a semiconductor heterostructure at low temperatures is thus characterized by ionized impurities [3,4]. Numerous theoretical works were published on the bound states of a hydrogenic impurity in spherical quantum dots. The location and strong spatial confinement of the impurity in these quantum dots reflect themselves in the energy levels and in the impurity binding energy [1–10].

Magnetic field has become an interesting probe for studying the physical properties of low-dimensional structures, from both the theoretical and technical points of view. Akbas *et al* [10] studied the problem of an electron bound to an impurity, located at the centre of a spherical quantum dot with infinite potential barriers in a uniform magnetic field. They used a variational method in which the trial wave function contained a Gaussian function. When most of the previous investigations were restricted to the evaluation of the binding energies associated with the lowest 'subband' of the dot [7–15], the impurity binding energy of the excited states in the spherical quantum dot was calculated by Daries Bella *et al* [15]. Whereas the total potential of an electron inside the dot deviates from Coulombic nature, the accidental degeneracy associated with the $n = 2$ states splits up resulting in $2s$ and $2p$ states with different energies. The degeneracy associated with the $l = 1$ state, however, remains because of the central nature of the potential [15].

In the present work, the impurity binding energy of the excited states, located at the centre of a spherical quantum dot, is determined in the presence of a magnetic field applied parallel to the z-axis. A variational scheme was employed within the effective mass approximation. The impurity energy and impurity binding energy of the excited states for finite confinement potential as a function of dot radius and magnetic field for GaAs/$Ga_{1-x}Al_xAs$ structures were calculated. The method followed is presented in §2 while the discussion of the results is given in §3.

2. Theory

In the absence of an impurity, within the effective mass approximation, the Hamiltonian is given by

$$H_0 = -\frac{\hbar^2}{2m^*}\nabla^2 + V(r), \tag{1}$$

where m^* is the effective mass of the electron at the conduction band minimum. The confining potential $V(r)$ is given by

$$V(r) = \begin{cases} 0 & r \leq R \\ V_0 & r \geq R \end{cases}, \tag{2}$$

where V_0 is the barrier height given by $V_0 = Q_\mathrm{c}\Delta E_g(x)$ and Q_c is the off-set parameter of the conduction band. The eigenfunction for the lowest-lying state within the spherical dot of radius R is given by

$$\psi_0(r) = \begin{cases} N_1(\sin(\alpha r)/r) & r \leq R \\ N_1 \sin(\alpha R)\exp(\beta R)(\mathrm{e}^{-\beta r}/r) & r \geq R, \end{cases} \tag{3}$$

where N_1 is the normalization constant and α and β are given by $\alpha = \sqrt{2m^* E_0/\hbar^2}$ and $\beta = \sqrt{2m^*(V_0 - E_0)/\hbar^2}$. Matching the wave functions and their derivatives at the boundary $r = R$, we get

$$\alpha R + \beta R \tan(\alpha R) = 0. \tag{4}$$

By solving this transcendental equation, the confined particle energy, E_0, can be obtained. The Hamiltonian for a shallow impurity located on the centre of a spherical quantum dot of radius R, in the presence of magnetic field, can be given as

$$H_{\mathrm{IB}} = \frac{1}{2m^*}\left(\bar{p} - \frac{e}{c}\bar{A}\right)^2 - \frac{e^2}{\varepsilon r} + V(r), \tag{5}$$

where ε, e and $\bar{r}$ are the dielectric constant, electron charge and the position vector, respectively. $\bar{A}$ is the vector potential of the magnetic field, $\bar{B} = \nabla \times \bar{A}$. For a homogeneous magnetic field $\bar{B}(0,0,B)$ and along the z-axis, the vector potential is given as $\bar{A} = (\bar{B} \times \bar{r})/2$. Using the effective Rydberg constant $R^* = m^* e^4/2\hbar^2\varepsilon^2$ as the unit of the energy and the effective Bohr radius $a^* = \hbar^2\varepsilon/m^* e^2$ as the unit of the length, eq. (5) becomes

$$H_{\mathrm{IB}} = -\Delta - \frac{2}{r} + \frac{\gamma^2}{4} r^2 \sin^2\theta + \gamma L_z + \frac{V(r)}{R^*}, \tag{6}$$

where $\gamma = \hbar\omega_{\mathrm{c}}/2R^*$ is the dimensionless parameter depending on magnetic field and $\omega_{\mathrm{c}} = eB/m^* c$ is the cyclotron frequency. There is to no exact solutions to the impurity states in quantum dot and therefore, the impurity energy in the presence of magnetic field is calculated by traditional variational method. The following trial wave function is adopted for the excited impurity states in spherical quantum dot [12,13]:

$$\psi_{\mathrm{IB}}(r) = \begin{cases} A_1(\sin(\alpha r)/r) f(r) \mathrm{e}^{-\lambda r^2} & r \le R \\ A_1 \sin(\alpha R)\exp(\beta R)(\mathrm{e}^{-\beta r}/r) f(r)\mathrm{e}^{-\lambda r^2} & r \ge R \end{cases}, \tag{7}$$

where A_1 and λ are the normalization constant and the variational parameter to be determined and $f(r)$ are hydrogenic functions given as [15]

$$f(r) = R_{nl}(r) Y_{lm}(\theta,\phi) = \begin{cases} (2-\gamma_1 r)\exp(-\gamma_1 r) & 2s \\ r\exp(-\gamma_2 r)\cos(\theta) & 2p_0 \\ r\exp(-\gamma_3 r)\sin(\theta)\mathrm{e}^{(\pm i\phi)} & 2p_\pm \end{cases}, \tag{8}$$

The impurity energy E_{IB}, under the magnetic field, is obtained by

$$E_{\mathrm{IB}} = \min_{\gamma,\lambda} \frac{\langle \psi_{\mathrm{IB}} | H_{\mathrm{IB}} | \psi_{\mathrm{IB}} \rangle}{\langle \psi_{\mathrm{IB}} | \psi_{\mathrm{IB}} \rangle}. \tag{9}$$

The influence of magnetic field on the energy levels of electron in the spherical quantum dot is determined by

$$E_{\mathrm{B}} = \min_{\kappa} \frac{\langle \psi_{\mathrm{B}} | H_{\mathrm{B}} | \psi_{\mathrm{B}} \rangle}{\langle \psi_{\mathrm{B}} | \psi_{\mathrm{B}} \rangle}, \tag{10}$$

where the Hamiltonian and the trial wave function are given as

$$H_{\mathrm{B}} = -\nabla^2 + \frac{\gamma^2}{4} r^2 \sin^2\theta + \frac{V(r)}{R^*} \tag{11}$$

and

$$\psi_{\mathrm{B}}(r) = \psi_0(r)\mathrm{e}^{-\kappa r^2} \tag{12}$$

for s states, and

$$\psi_{\mathrm{B}}(r) = \begin{cases} B_1[\frac{\sin(\alpha_2 r)}{(\alpha_2 r)^2} - \frac{\cos(\alpha_2 r)}{(\alpha_2 r)}] \cos\theta e^{-\kappa r^2} & r \leq R \\ B_2[\frac{1}{\beta_2 r} + \frac{1}{(\beta_2 r)^2}]\mathrm{e}^{-\beta_2 r} \cos\theta \mathrm{e}^{-\kappa r^2} & r \geq R \end{cases} \tag{13}$$

with

$$B_2 = B_1 \left(\frac{\beta_2}{\alpha_2}\right)^2 \left(\frac{\sin(\alpha_2 R) - \alpha_2 R \cos(\alpha_2 R)}{\beta_2 R + 1}\right) \mathrm{e}^{\beta_2 R} \tag{14}$$

and

$$\frac{\cot(\alpha_2 R)}{\alpha_2 R} - \frac{1}{(\alpha_2 R)^2} = \frac{1}{\beta_2 R} + \frac{1}{(\beta_2 R)^2} \tag{15}$$

for the p states [15].

3. Results and discussion

The magnetic field-dependent binding energy, $E_{\mathrm{b}} = E_{\mathrm{B}} - E_{\mathrm{IB}}$, was calculated for GaAs/$\mathrm{Ga}_{1-x}\mathrm{Al}_x$As spherical quantum dot as a function of the magnetic field strength and the radius of the dot.

The parameters used in the calculations are [16]: $m^* = 0.067 m_0$, $\varepsilon = 13.1$, when $x = 0.2$, $Q_{\mathrm{c}} = 0.685$ and the barrier potential becomes $V_0 = 161.73$ meV. The effective Rydberg constant $R^* = 5.31$ meV, and the effective Bohr radius $a^* = 103.43$ Å.

The donor binding energy (E_{b}) and the impurity energy (E_{I}) of the excited states as a function of dot radius are shown in figure 1. According to this figure, the excited energies of impurity ($E_{\mathrm{I}}^{2s}, E_{\mathrm{I}}^{2p}$), are high for small R and decrease as the radius increases. It is interesting to note that the impurity energy becomes negative when the dot radius is larger than $1.653a^*(4.912a^*)$ for $2s$ ($2p$) state. This value of the dot radius, at which the impurity energy changes from positive to negative, is known as the turning point. The calculated value by Akbas *et al* [10] $1.852a^*$ for $1s$ state. The difference is due to the finite potential barrier and different eigenstates. The binding energy for $2s$ state increases, attains a maximum value, and then decreases as the dot radius increases. When the dot radius is extremely large, the confining potential has a small influence on the impurity and the wave function approaches the corresponding state of a free space hydrogen atom. As can be seen, the variations of binding energy of the $2p_{\pm}$ states are different from that of the $2s$ state. The negative binding energy shows that the $2p$ states are unbound except for dots of larger radii because the eigenfunction for $2p$ states vanishes at the donor site. The results obtained are similar to those of the Daries Bella's work [15].

To investigate the effect of magnetic field on the energy levels, the energies of the excited state of electron, with no impurity, vs. γ for different dot radii (turning points) in finite quantum dot are shown in figure 2. It can be seen that the energy levels E_{B} of the electron depend on both the magnetic field strength γ and the radius of the dot, such that for a given radius, the energy of the electron increases as B increases.

Figure 3 shows the impurity energies of the $2s$ and $2p$ excited states as a function of the magnetic field strength for different dot radii. As can be seen, the impurity

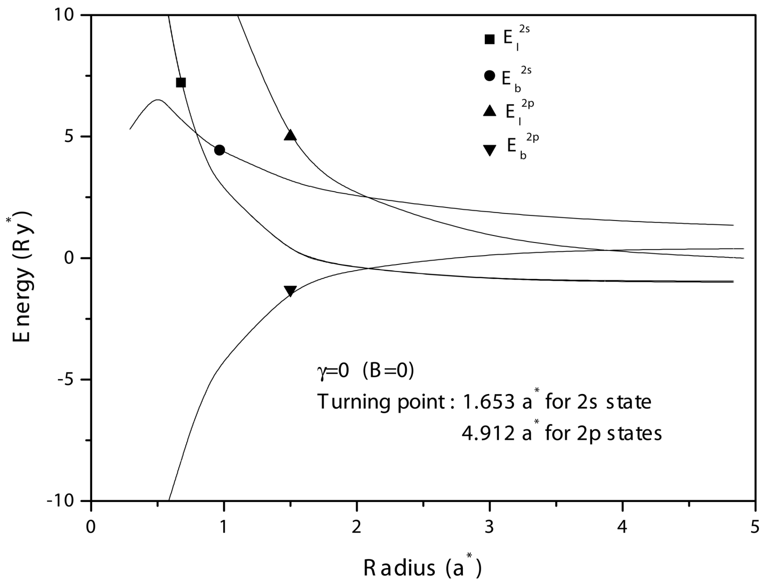

Figure 1. The impurity energy (E_{IB}) and the binding energy (E_{b}) of the excited states vs. the radius of the finite GaAs/$Ga_{0.8}Al_{0.2}$As quantum dot.

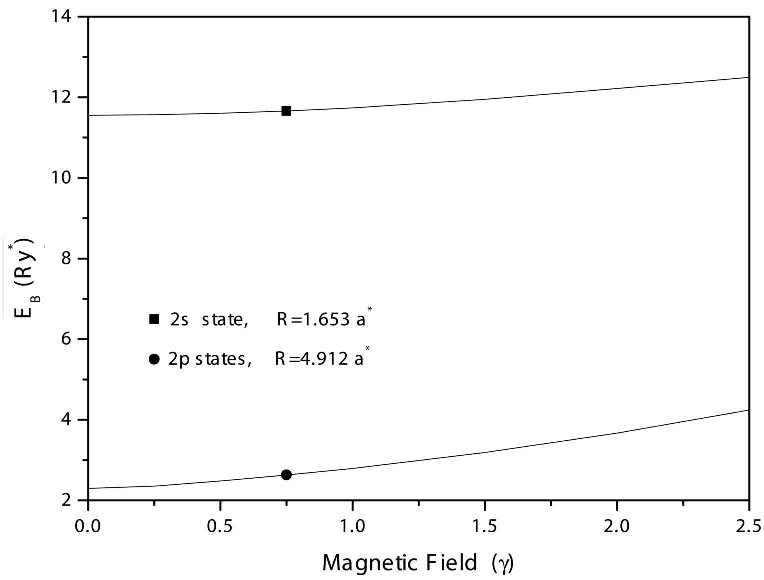

Figure 2. Excited state energy of the electron in terms of the magnetic field for different dot radii.

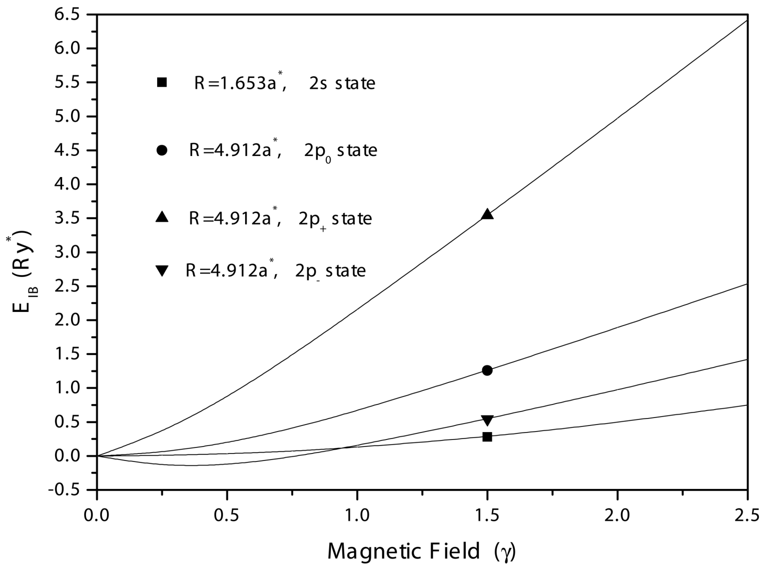

Figure 3. The impurity energy of the excited states ($E_{\rm IB}$) as a function of the magnetic field for various radii.

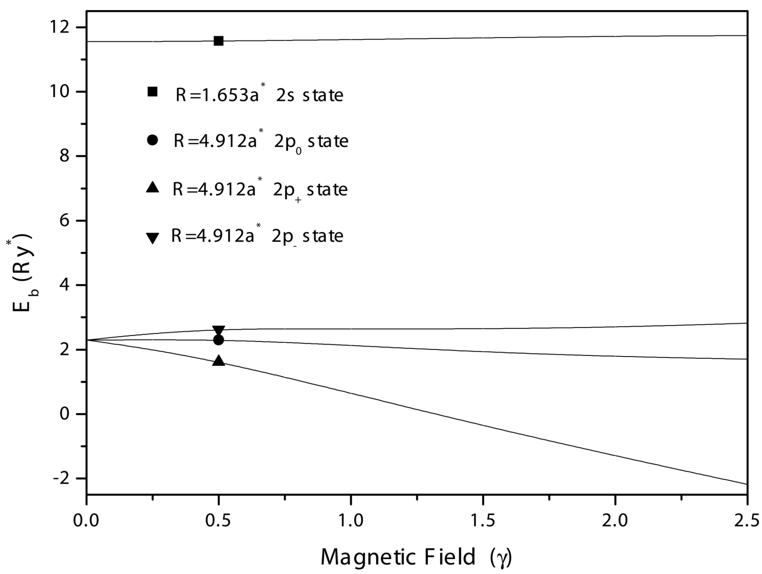

Figure 4. The dependence of binding energy ($E_{\rm b}$) of the excited states vs. magnetic field in finite GaAs/$Ga_{0.8}Al_{0.2}$As spherical quantum dots.

energies increase as the size of the quantum dot increases. The impurity energy also increases with the magnetic field because of the increasing compression of the wave function with the magnetic field. It is interesting to note that the degeneracy of the $2p$ states is broken by applying magnetic field [15]. γ_0 is the magnetic field strength for which $E_{\rm IB}$ is zero. It is clearly seen that γ_0 increases with the increasing dot radius, and $\gamma_0 = 0.06$ for $R = 1.653a^*$ ($2s$ state) and $\gamma_0 = 0.78$ for $R = 4.912a^*$ ($2p$ state).

In figure 4, the dependence of the binding energies on the magnetic field for excited states with $m_l = 0, \pm 1$ are presented for various dot radii. For all values of m_l, as the dot radius increases the binding energy decreases because of the increased electron localization area. It is noteworthy that because of the pronounced influence of the magnetic field onto excited states, the binding energy depends more strongly on the induction of the magnetic field for the state with $m_l = 1$ than for the state with $m_l = 0$. The binding energy of $m_l \neq 0$ states is affected not only by the diminished area of localization due to the growth of γ, but also due to the addition of the positive or negative (for $m_l = \pm 1$) energy of azimuthal motion of the electron in the magnetic field.

In the present study, the impurity energy and binding energy of the $2s$ and $2p$ excited states in the spherical quantum dot with finite barrier potential in terms of strength of magnetic field were calculated. The results clearly showed the effects of the confining potential and B on the energy. The calculated energies for the finite confining potential case were compared with numerical results [10,15,16].

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