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Shallow impurity states and transition energies in cylindrical GaAs–Ga_{0.6}Al_{0.4}As quantum well wires under applied magnetic fields

Pablo Villamil¹, Carlos Cabra¹ and N Porrás-Montenegro²

¹ Departamento de Matemáticas y Física, Universidad de Sucre, AA 406, Sincelejo, Colombia

² Departamento de Física, Universidad del Valle, AA 25360, Cali, Colombia

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Abstract

In this work, using the effective-mass approximation within a variational approach, we have studied the behaviour of the binding and transition energies of a donor shallow impurity in a cylindrical GaAs–Ga_{0.6}Al_{0.4}As quantum well wire (QWW) as a function of the wire radius, the impurity position and the applied magnetic field. The QWW is of infinite length with a finite radial confining potential and the magnetic field is applied parallel to the wire axis. In our calculations we have considered the 1s-, 2p_±- and 3p_±-like impurity states. We have found that for the 1s-like state the impurity binding energy increases with the magnetic field for impurity positions close to the centre of the wire, but diminishes for on-edge impurities, highlighting the competition between the geometrical and magnetic confinement. Also, we have observed that the energy of the 2p_±- and 3p_±-like excited states is greater than the energy of the electron ground state without the presence of the impurity for small radius of the QWW, a result which is more pronounced for higher magnetic fields. Our results are in good agreement with previous theoretical reports, with lower binding and transition energies than those which use infinite confinement potential, as expected.

1. Introduction

The great progress in the last years of modern technologies in crystal growth have allowed the production of a high quality of various low-dimensional systems such as quantum wells, QWs (2D), quantum well wires, QWWs (1D), and quantum dots, QDs (0D), where the quantum mechanical nature of the carriers plays an important role, and it has motivated an increasing interest in the studies of their optical and electrical properties [1–7].

A great many theoretical and experimental investigations on these systems in the presence of shallow impurities have been published [8–18]. The scientific community has the necessity of understanding the behaviour of shallow impurities in quantum semiconductor devices since

they can drastically alter the physical properties of these quantum systems. Although magnetic field effects seem to have less technological significance, they provide a far richer insight into semiconductor physics than what is possible by studying electron states under the action of applied electric fields. Magnetic fields have become crucial ingredients of characterization techniques used to evaluate semiconductor physics. The magnetic field greatly alters the nature of the electronic states, which manifest themselves in magneto-optic or magneto-transport phenomena.

Since the pioneer work of Bastard on hydrogenic impurity states in QWs [19] a great many theoretical works in QWWs have been reported. Many authors have worked on the measurements and calculation of the binding energies, density of impurity states, transition energies and photoluminescence spectra associated with shallow impurities in GaAs–Ga_{1-x}Al_xAs QWWs using different techniques, methods and geometries [20–28]. Polaron correction to donor states in a single quantum well has been investigated by several groups [29–31]. Also, polaron correction to the transition energies of shallow donor impurities in GaAs superlattices in the presence of a magnetic field has been studied [32, 33] within second-order perturbation theory in which only the 3D-bulk phonon modes of GaAs were included. In previous works Villamil *et al* [22, 23] have calculated the binding energy of the ground and some excited states as well as some allowed transition energies of an *on-centre* impurity in GaAs–Ga_{1-x}Al_xAs QWWs, using a radial *infinite* confinement potential and under the action of a magnetic field applied in the axial direction. To our knowledge, up to now there are no reports on this subject using a *finite* radial confinement potential in cylindrical GaAs–Ga_{1-x}Al_xAs QWWs, not only for the impurity ground state but for its excited states, and as a function of the impurity position along the wire radius under the action of applied magnetic fields.

In this work we consider a shallow impurity inside an infinite length QWW with finite radial confining potential and in the presence of a uniform magnetic field applied in the axial direction. We use the effective-mass approximation within the variational approach to calculate the binding energy and the transition energies associated with the 1s-, 2p_±- and 3p_±-like states of a hydrogenic impurity in a GaAs–Ga_{1-x}Al_xAs QWW as a function of the wire radius, the impurity position inside the wire and an applied magnetic field. In section 2 we present the theory followed for this calculation. Our results and discussions are presented in section 3, and conclusions in section 4.

2. Theory

The Hamiltonian of a donor impurity in a cylindrical GaAs–Ga_{1-x}Al_xAs QWW with radius R , finite radial confinement potential $V(\rho)$ and in the presence of an applied magnetic field, in the effective-mass approximation, can be written as

$$\mathbf{H} = \frac{1}{2m^*} \left[\mathbf{P} + \frac{e}{c} \mathbf{A} \right]^2 - \frac{e^2}{\varepsilon |\mathbf{r} - \mathbf{r}_0|} + V(\rho), \quad (1)$$

where $|\mathbf{r} - \mathbf{r}_0| = \sqrt{(\rho - \rho_0)^2 + z^2}$, \mathbf{r}_0 is the impurity ion position, measured from the centre of wire, the z coordinate is the relative separation of the electron from the impurity ion along the wire axis, ε is the dielectric constant of the GaAs semiconductor inside the wire, m^* is the effective electron mass and $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field. For a uniform magnetic field applied in the wire axis direction, the vector potential can be written as $\mathbf{A}(\mathbf{r}) = 1/2(\mathbf{B} \times \mathbf{r})$, with $\mathbf{B} = B\hat{\mathbf{z}}$, and in cylindrical coordinates becomes

$A_\rho = A_z = 0$, $A_\varphi = (B\rho)/2$. The confining potential $\mathbf{V}(\rho)$ is defined as

$$\mathbf{V}(\rho) = \begin{cases} 0, & 0 \leq \rho \leq R \\ V_0, & \rho > R. \end{cases} \quad (2)$$

The Hamiltonian of the system in cylindrical coordinates and in effective Rydbergs, R^* , becomes

$$\mathbf{H} = -\nabla^2 - i\gamma \left(\frac{\partial}{\partial \varphi} \right) + \frac{\gamma^2 \rho^2}{4} - \frac{2}{r} + \mathbf{V}(\rho). \quad (3)$$

The term $\gamma = e\hbar B/(2m^*cR^*)$ is the electron energy in the first Landau level ($n = 0$) due to the action of the magnetic field. For donor impurities in GaAs, $m^* = 0.065$, $\varepsilon = 12.58$, $a_0 \approx 100 \text{ \AA}$ and $R^* = 5.83 \text{ meV}$.

Following Brown and Spector [12], we assume suitable variational wavefunctions for the different states, as the product of a hydrogenic part Γ_{nlm} and the appropriate confluent hypergeometric functions. The trial wavefunctions for the ground state and some excited states of the impurity are written as

$$\begin{aligned} & \Psi_{nlm}(\mathbf{r}) \\ &= \begin{cases} N_{nlm} \exp\left[-\frac{\xi}{2}\right] 1F1(a_{01}, 1, \xi) \Gamma_{nlm}(\mathbf{r}, \{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}), & \rho \leq R \\ N_{nlm} \frac{1F1(a_{01}, 1, \xi_R)}{U(a'_{01}, 1, \xi_R)} \exp\left[-\frac{\xi}{2}\right] U(a'_{01}, 1, \xi) \Gamma_{nlm}(\mathbf{r}, \{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}), & \rho > R. \end{cases} \end{aligned} \quad (4)$$

In equation (4), N_{nlm} are the normalization constants of the respective nlm states, $1F1(a_{01}, 1, \xi)$, and $U(a'_{01}, 1, \xi)$ are the confluent hypergeometric functions which are the corresponding solutions for the case of finite confinement potential, in the presence of a uniform magnetic field parallel to the wire axis, where $\xi = \frac{eB\rho^2}{2\hbar c} = \frac{1}{2}\gamma\rho^2$, and ξ_R is the ξ variable evaluated in $\rho = R$. a_{01} and a'_{01} are the parameters of the confluent hypergeometric functions for the ground state of the problem inside and outside the wire, respectively, which are calculated numerically by means of the boundary conditions $\frac{\partial \Psi_{nlm}}{\partial \rho}|_{\rho=R} = \frac{\partial \Psi_{nlm}}{\partial \rho}|_{\rho=R}$. Γ_{nlm} are the hydrogenic wavefunctions, corresponding to the nlm states, as was proposed by Latgé *et al* [13]. λ_{nl} , α_{nl} and β_{nl} are variational parameters used by Chaudhury and Bajaj [14] that vary according to λ_{nl} in such a way that the orthogonalization between the states with different nlm sub-indices is preserved.

In our calculations we take the binding energy of a hydrogenic impurity, $E_{b,nlm}$, of a given like-state Ψ_{nlm} , as the energy necessary to move one electron from the donor level to the first level of the conduction subband and is calculated by means of the equation

$$\begin{aligned} E_{b,nlm} &= E_{10} - \min_{\lambda_{nl}} \langle \Psi_{nlm} | \mathbf{H} | \Psi_{nlm} \rangle \\ E_{10} &= \gamma(1 - 2a_{01}). \end{aligned} \quad (5)$$

E_{10} is the first level of the conduction subband in the absence of the Coulomb term. The term $\min_{\lambda_{nl}} \langle \Psi_{nlm} | \mathbf{H} | \Psi_{nlm} \rangle$ means that the Hamiltonian expected value is minimized with respect to λ_{nl} . The general expression of the Hamiltonian expected value $\langle \Psi_{nlm} | \mathbf{H} | \Psi_{nlm} \rangle$, for all Ψ_{nlm} like-states, in a cylindrical QWW of infinite length is written as

$$\begin{aligned} \Psi_{0i} &= \Psi_{\text{inside}}(\rho) = N_{nlm} \exp\left[-\frac{\xi}{2}\right] 1F1(a_{01}, 1, \xi) \\ \Psi_{0e} &= \Psi_{\text{outside}}(\rho) = N_{nlm} \frac{1F1(a_{01}, 1, \xi_R)}{U(a'_{01}, 1, \xi_R)} \exp\left[-\frac{\xi}{2}\right] U(a'_{01}, 1, \xi) \\ \Psi_{nlm}(\mathbf{r}) &= \begin{cases} \Psi_{\text{inside}}(\rho) \Gamma_{nlm}(\mathbf{r}, \{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}), & \rho \leq R \\ \Psi_{\text{outside}}(\rho) \Gamma_{nlm}(\mathbf{r}, \{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}), & \rho > R \end{cases} \end{aligned} \quad (6)$$

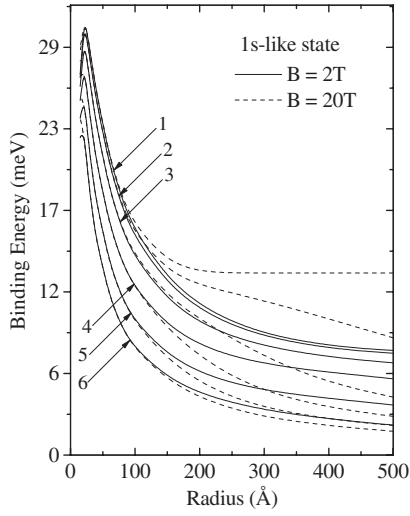


Figure 1. Binding energy as a function of the wire radius, for the 1s-like state of a donor impurity in a cylindrical GaAs–Ga_{0.6}Al_{0.4}As QWW, for two magnetic fields, and different positions of the impurity: 1—($\rho_i = 0$), 2—($\rho_i = R/5$), 3—($\rho_i = 2R/5$), 4—($\rho_i = 3R/5$), 5—($\rho_i = 4R/5$), 6—($\rho_i = R$).

$$\begin{aligned}
 \langle \Psi_{nlm} | \mathbf{H} | \Psi_{nlm} \rangle &= \langle \mathbf{H} \rangle \\
 &= E_{10} - \langle \Psi_{0i}^* \Gamma^* \Psi_{0i} (\nabla^2 \Gamma) \rangle \Big|_0^R - \langle \Psi_{0e}^* \Gamma^* \Psi_{0e} (\nabla^2 \Gamma) \rangle \Big|_R^\infty \\
 &\quad - 2 \left\langle \Psi_{0i}^* \Gamma^* \frac{1}{r} \Psi_{0i} \Gamma \right\rangle \Big|_0^R - 2 \left\langle \Psi_{0e}^* \Gamma^* \frac{1}{r} \Psi_{0e} \Gamma \right\rangle \Big|_R^\infty \\
 &\quad - 2 \langle \Psi_{0i}^* \Gamma^* (\nabla \Psi_{0i}) \cdot (\nabla \Gamma) \rangle \Big|_0^R - 2 \langle \Psi_{0e}^* \Gamma^* (\nabla \Psi_{0e}) \cdot (\nabla \Gamma) \rangle \Big|_R^\infty \\
 &\quad - i\gamma \left\langle \Psi_{0i}^* \Gamma^* \Psi_{0i} \frac{\partial \Gamma}{\partial \varphi} \right\rangle \Big|_0^R - i\gamma \left\langle \Psi_{0e}^* \Gamma^* \Psi_{0e} \frac{\partial \Gamma}{\partial \varphi} \right\rangle \Big|_R^\infty. \tag{7}
 \end{aligned}$$

In equation (7) $\Psi_{\text{inside}}(\rho)$, $\Psi_{\text{outside}}(\rho)$ are the radial parts of the wavefunctions for any state of the system inside and outside the well region. The symbol $\langle \Omega \rangle_a^b$ in equation (7) means the integral of the argument Ω between the limits a and b . Ψ_{0i}^* , Ψ_{0e}^* and Γ^* are the complex conjugates of Ψ_{0i} , Ψ_{0e} and Γ , respectively. When $B = 0$ T, $\gamma = 0$ and therefore the two last terms of the Hamiltonian expected value are zero.

The allowed transition energies are given by

$$E_T(nlm \rightarrow n'l'm') = |E_{b,nlm}(R, B) - E_{b,n'l'm'}(R, B)|, \tag{8}$$

and the selection rules used for the allowed transitions are

$$\begin{aligned}
 \Delta l &= l - l' = \pm 1 \\
 \Delta m &= m - m' = 0, \pm 1. \tag{9}
 \end{aligned}$$

3. Results and discussion

Figure 1 displays the donor binding energy as a function of the wire radius for the 1s-like state of a donor impurity in a cylindrical GaAs–Ga_{0.6}Al_{0.4}As QWW. The donor impurity is placed in different radial positions ($\rho_i = 0, R/5, 2R/5, 3R/5, 4R/5$ and R , corresponding to curves 1, 2, 3, 4, 5 and 6, respectively) and under the action of the applied magnetic fields of 2 and 20 T. We found that for any wire radius and for any magnetic field the binding energy diminishes as the impurity position varies from the centre ($\rho_i = 0$) to the edge ($\rho_i = R$) of the QWW. For a given value of the magnetic field and of the impurity position, the binding energy increases

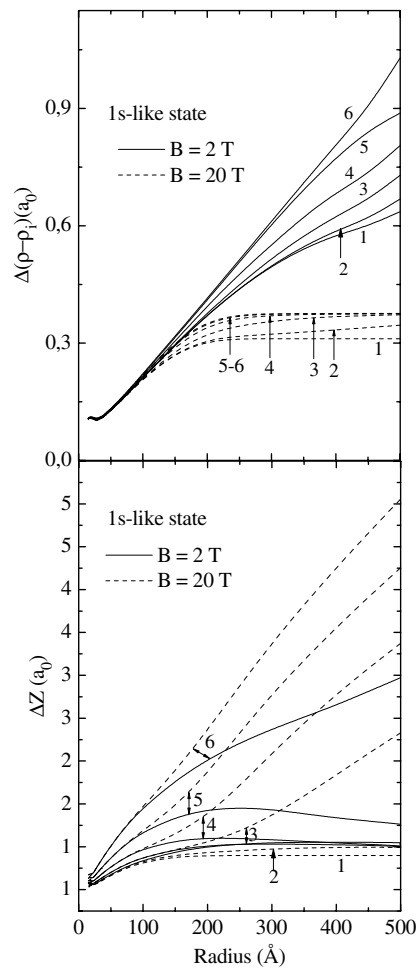


Figure 2. Width of the donor impurity wavefunction, in the 1s-like state, in the radial direction (upper figure) and in the z direction (lower figure) in a cylindrical GaAs-Ga_{0.6}Al_{0.4}As QWW as a function of the wire radius, and for two applied magnetic fields. The impurity is located at 1—($\rho_i = 0$), 2—($\rho_i = R/5$), 3—($\rho_i = 2R/5$), 4—($\rho_i = 3R/5$), 5—($\rho_i = 4R/5$), 6—($\rho_i = R$).

from its bulk value in GaAs as the wire radius is reduced, reaches a maximum value, and then drops to the bulk value characteristic of the barrier potential for wire radius close to zero. For $R > 100 \text{ \AA}$, in curves 3, 4, 5 and 6 we observe that the binding energy with $B = 20 \text{ T}$ (dashed lines) is smaller than the binding energy with $B = 2 \text{ T}$ (solid lines) while in curves 1 and 2 the binding energy presents a different behaviour. This behaviour of the binding energy can be understood observing figure 2. In it, we present the numerical results for the widths, $\Delta(\rho - \rho_i)$ and ΔZ , of the wavefunction for donor positions at $\rho_i = 0, R/5, 2R/5, 3R/5, 4R/5$ and R , and two magnetic fields, $B = 2$ and 20 T . In this figure, we observe that for the two magnetic fields considered the wavefunction is more localized in the radial than in the z direction. Also, the wavefunction is more localized, in the radial and in the z direction, when the donor impurity is located close to the centre of the wire than when it is located close to the border of the wire. On the other hand, in the radial direction, the wavefunction is more localized when the magnetic field is 20 T . In the z direction, the wavefunctions that correspond to curves 3,

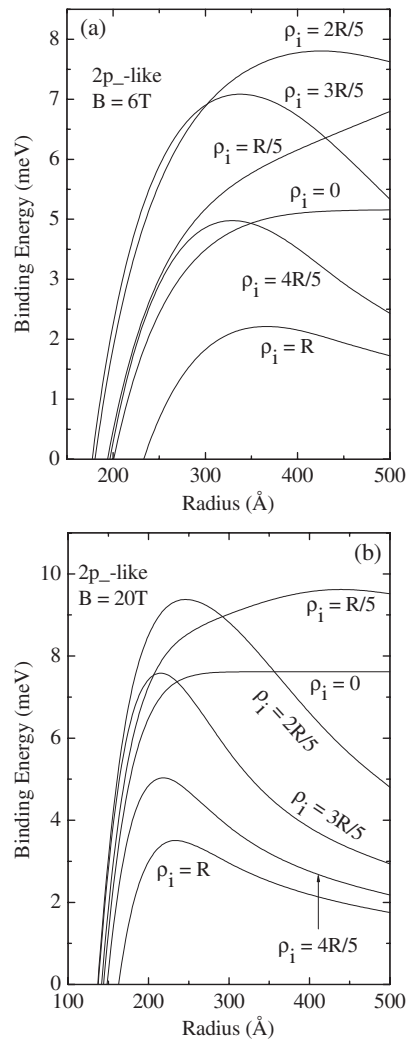


Figure 3. Binding energy as a function of the wire radius for the 2p₋-like state of a donor impurity in a cylindrical GaAs-Ga_{0.6}Al_{0.4}As QWW for two applied magnetic fields, ($B = 2, 20$ T), and for different impurity positions: 1—($\rho_i = 0$), 2—($\rho_i = R/5$), 3—($\rho_i = 2R/5$), 4—($\rho_i = 3R/5$), 5—($\rho_i = 4R/5$), 6—($\rho_i = R$).

4, 5 and 6, with $B = 20$ T, are less localized than those curves that correspond to $B = 2$ T. Curves 1 and 2 with $B = 20$ T indicate that the wavefunction is more localized than those curves corresponding to $B = 2$ T. This behaviour of the wavefunction is reflected in the donor binding energy in all curves.

Figures 3(a), (b) present the binding energy as a function of the wire radius for the 2p₋-like state of a donor impurity in a cylindrical GaAs-Ga_{0.6}Al_{0.4}As QWW for different impurity positions and applied magnetic fields. From these results it is observed that for all impurity positions, the wire radius for which the 2p₋-like state is bound (its energy is lower than that of the first electron level of the QWW without the presence of the impurity) diminishes with the magnetic field. Also, it is observed that depending on the impurity position and the strength of the magnetic field the binding energy changes with the radius of the wire. For

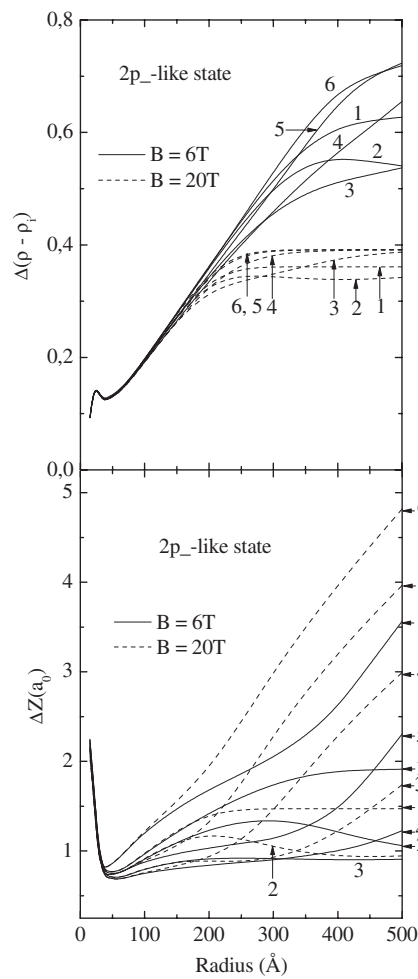


Figure 4. Width of the donor impurity wavefunction, in the $2p_-$ -like state, in the radial direction (upper figure), and in the z direction (lower figure) in a cylindrical GaAs-Ga_{0.6}Al_{0.4}As QWW as a function of the wire radius, and for two applied magnetic fields. The impurity is located at 1—($\rho_i = 0$), 2—($\rho_i = R/5$), 3—($\rho_i = 2R/5$), 4—($\rho_i = 3R/5$), 5—($\rho_i = 4R/5$), 6—($\rho_i = R$).

example, for some curves, the binding energy increases up to a maximum at a given radius and diminishes for higher radii. This behaviour is more evident for $B = 20$ T.

The results for the width of the wavefunction for donor impurity positions along the wire radius, at $\rho_i = 0, R/5, 2R/5, 3R/5, 4R/5$ and R , with B equal to 6 and 20 T, in the radial and z directions, are shown in figure 4 as a function of the wire radius. We observe the following: (i) the wavefunction is more localized in the radial direction than in the z direction for the same magnetic field and ρ_i ; (ii) in the radial direction the wavefunction is more localized with $B = 20$ T than with $B = 2$ T; (iii) for $R < 50$ Å the localization is not sensitive to the magnetic field and the geometric confinement overwhelms the magnetic one; (iv) as the radius of the wire diminishes, the width of the wavefunction reaches a minimum value, that is to say a maximum of localization, and then it increases, reflecting the delocalization of the wavefunction within the GaAs region and its spread-out in the Ga_{1-x}Al_xAs region; (v) the

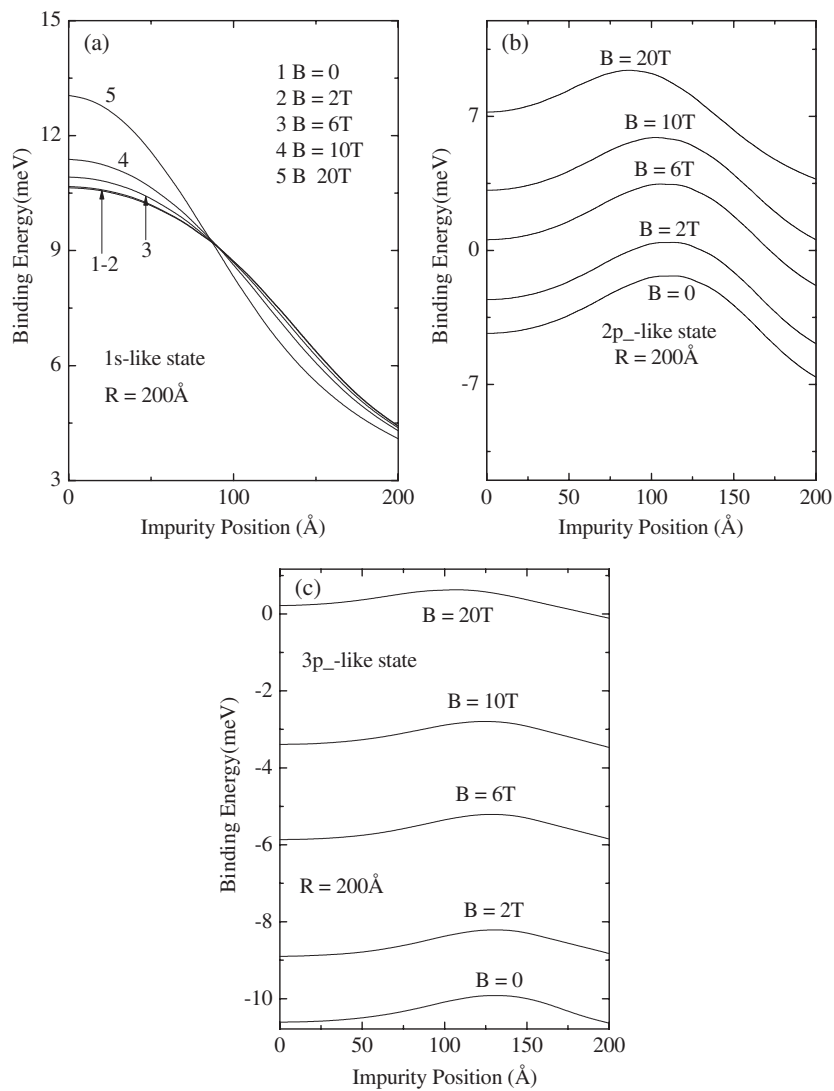


Figure 5. Binding energy of (a) 1s-, (b) 2p₋- and (c) 3p₋-like states of a donor impurity in a cylindrical GaAs–Ga_{0.6}Al_{0.4}As QWW as a function of the impurity position for a 200 Å wire radius and for different magnetic fields: 1—($B = 0 \text{ T}$), 2—($B = 2 \text{ T}$), 3—($B = 6 \text{ T}$), 4—($B = 10 \text{ T}$), 5—($B = 20 \text{ T}$).

behaviour of the wavefunction, in the radial and z directions, corresponds to the behaviour of the binding energy for the same magnetic field and ρ_i ; that is to say, the binding energy increases when the wavefunction is more localized. We have found similar results for the 3p₋-like state.

The binding energies of the ground and some excited states of an impurity in a cylindrical GaAs–Ga_{0.6}Al_{0.4}As QWW as a function of the impurity position for a wire with $R = 200 \text{ \AA}$ and different magnetic fields are presented in figure 5. This figure shows that for the 2p₋- and 3p₋-like states and for every impurity position the binding energy increases with the magnetic field. It is good to notice that the binding energy of the 3p₋-like state is negative, which

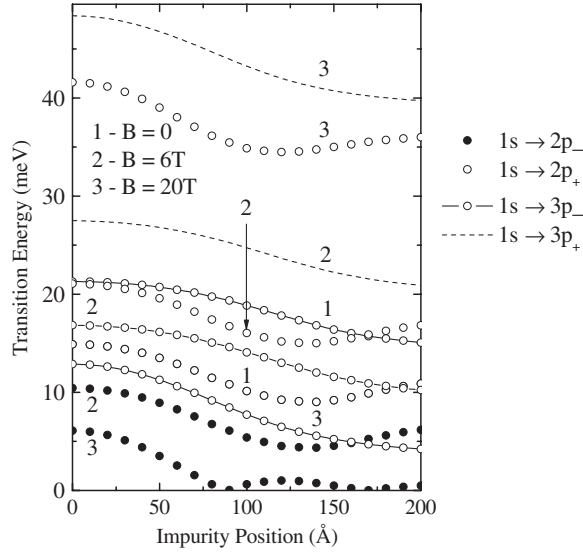


Figure 6. $1s \rightarrow 2p_{\pm}$ and $1s \rightarrow 3p_{\pm}$ infrared transition energies of a donor impurity in a GaAs–Ga_{0.6}Al_{0.4}As QWW 200 Å in radius, as a function of the impurity position along the wire radius for different applied magnetic fields.

according to our definition of binding energy, equation (5), means that this state is not bound; that is, the $3p_{-}$ energy levels are higher than the electron ground state in the well wire without the impurity. For the $1s$ -like state the binding energy decreases as the impurity approaches the edge of the well.

The transition energies $1s \rightarrow 2p_{\pm}$ and $1s \rightarrow 3p_{\pm}$ versus impurity position for a QWW with radius of 200 Å and different magnetic fields are displayed in figure 6. We observe that the $1s \rightarrow 2p_{-}$ and $1s \rightarrow 3p_{-}$ transitions diminish with the magnetic field while $1s \rightarrow 2p_{+}$ and $1s \rightarrow 3p_{+}$ transitions increase with the magnetic field for every impurity position. For $B = 0$, the $1s \rightarrow 2p_{-}$ ($1s \rightarrow 3p_{-}$) and $1s \rightarrow 2p_{+}$ ($1s \rightarrow 3p_{+}$) transition energies coincide and for that reason we only have presented the curve for the transitions $1s \rightarrow 2p_{+}$ and $1s \rightarrow 3p_{-}$. For each magnetic field, the $1s \rightarrow 3p_{-}$ and $1s \rightarrow 3p_{+}$ transition energies diminish when the impurity goes from the centre ($\rho_i = 0$) to the border ($\rho_i = R$) of the wire. On the other hand, the transition energies $1s \rightarrow 2p_{-}$ and $1s \rightarrow 2p_{+}$ for all magnetic fields vary, diminishing up to a certain impurity position and increasing as the impurity approaches the barrier edge. In comparing our results for the transitions $1s \rightarrow 2p_{-}$ and $1s \rightarrow 3p_{-}$ with those reported by Villamil and Porras-Montenegro [22], for the infinite confinement potential, figure 6(a) in this reference, we have found a very good agreement, but with lower values in the present report, as expected, because of the *finite* confinement.

4. Conclusions

In this work, using the effective mass-approximation within the variational approach, we have calculated the binding and the allowed transition energies between the $1s$ -, $2p_{\pm}$ - and $3p_{\pm}$ -like states of a hydrogenic donor impurity in a cylindrical GaAs–Ga_{1-x}Al_xAs QWW, under the action of a magnetic field applied in the axial direction, using a finite confinement potential. Our results are in good agreement with previous theoretical reports, but with lower binding and

transition energies than in those works which use infinite confinement potential, as expected. We have found that the $2p_{\pm}$ - and $3p_{\pm}$ -like excited states are not bounded in a QWW with small radius, a radius which diminishes with the applied magnetic field. We have found that the binding energy of the impurity ground state diminishes when the impurity position varies from the centre to the edge of the QWW. According to our results the impurity position inside the QWW is crucial in understanding the optical responses of these systems associated with impurity states. We believe the present calculation will be of importance in the understanding of future experimental work in this subject.

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