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Barrier height effect on binding energies of shallow hydrogenic impurities in coaxial GaAs/$Al_xGa_{1-x}As$ quantum well wires under a uniform magnetic field

H.D. Karki[a], S. Elagoz[a,*], P. Baser[a], R. Amca[a], I. Sokmen[b]

[a] *Cumhuriyet University, Department of Physics, Sivas, Turkey*
[b] *Dokuz Eylul University, Department of Physics, Izmir, Turkey*

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Abstract

The ground state binding energies of axial hydrogenic impurities in a coaxial cylindrical quantum well wire are reported as a function of the barrier height and the radius of wire in the presence of a uniform magnetic field applied parallel to the wire axis. The quantum well wire (QWW) is assumed to be an infinitely long cylinder of GaAs material surrounded by $Al_xGa_{1-x}As$ (for finite case and vacuum for infinite case). Binding energy calculations were performed with the use of a variational procedure in the effective mass approximation. We observed that the binding energy is sensitive to well radius only for both larger R values and small magnetic fields. We also compared the infinite and finite case binding energies and showed that increasing the Al concentration in the finite barrier case, binding energies are increased as expected. Our results are in good agreement and complementary with the previous theoretical works.

Keywords: Quantum well wire; Impurity; Binding energy; Magnetic field

1. Introduction

In the past 30 years, modern growth techniques such as molecular beam epitaxy (MBE), chemical vapour deposition (CVD) and metal organic chemical vapour deposition (MOCVD) and advanced lithography techniques have made possible the realization of

* Corresponding address: Cumhuriyet University, Fen Edebiyat Fakultesi, Fizik Bolumu, 58140 Sivas, Turkey. Tel.: +90 3462191010/1411.
E-mail address: elagoz@cumhuriyet.edu.tr (S. Elagoz).

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high quality semiconducting heterostructures consisting of layers of different semiconductors with sharp interfaces and controlled layer thicknesses. The unique physics character of the electronic–optical properties of semiconducting superlattices and heterostructures and the wide range of potential device applications associated with these systems resulted in a great deal of work devoted to the understanding of the nature of the impurity, electronic and excitonic states in semiconducting heterostructures [1–18]. It is very well known that GaAs/$Al_xGa_{1-x}As$ structures have been the subject of research for the following technological reasons. Firstly, GaAs and $Al_xGa_{1-x}As$ both posses a direct gap band structure (most attention has been focused on the system with aluminum concentration x of $Al_xGa_{1-x}As$ less than 0.45 in this concentration range band gap is direct at the Γ point); second, in single crystal heterostructures of the GaAs/$Al_xGa_{1-x}As$, the lattice constant of GaAs and $Al_xGa_{1-x}As$ are nearly identical so that they are closely lattice matched and last one, abrupt spatial transitions in the energy gap are possible. In particular work on impurity properties in quantum wells (QWs) was pioneered by Bastard [2], with several other more detailed investigations performed by others [3–13], in which impurity levels in quantum well wires (QWW) and the energy spectrum of the ground state and binding energy of impurities in GaAs/$Al_xGa_{1-x}As$ QWWs was studied taking into consideration the infinite and finite size of the barrier potential effects, etc. Many authors also have worked out in detail for cylindrically shaped QWWs with or without magnetic field effects [13–25].

In this work, we report the calculation of the ground state binding energy of an on-centre hydrogenic impurity in GaAs/$Al_xGa_{1-x}As$ QWWs by using the effective mass approximation for different aluminum concentrations. The binding energy–well radius as well as binding energy–magnetic field value dependency is investigated. The calculations are made for a QWW constructed as a core wire made of GaAs embedded in $Al_xGa_{1-x}As$. The barrier height V between GaAs and $Al_xGa_{1-x}As$ is taken as $V = Q(1.36x + 0.22x^2)$ eV where $Q = 0.6$ is a fixed ratio of the band gap and x is the Al concentration [7]. All results are presented in reduced effective atomic units of length and energy, which are given by Bohr radius a_B ($m^*e^4/2\varepsilon_o^2\hbar^2$) and effective impurity Rydberg R_B ($\varepsilon_o\hbar^2/m^*e^2$) for GaAs. Namely, $a_B = 98$ Å and $R_B = 5.78$ meV for hydrogenic donors in GaAs/$Al_xGa_{1-x}As$ QWWs. Where m^* and ε_o are the effective electron mass and the static dielectric constant of GaAs which are taken equal to $0.067m_o$ and 12.5 for wire and barrier.

2. Theory

In the effective mass approximation the Hamiltonian of a hydrogenic impurity at the centre of a cylindrical wire of radius R in presence of a magnetic field applied parallel to the wire axis is given by:

$$H = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m^*} - \frac{e^2}{\varepsilon_o\,|\mathbf{r} - \mathbf{r_o}|} + V(\rho, \phi) \tag{1}$$

where $|\mathbf{r} - \mathbf{r_o}| = \sqrt{(\boldsymbol{\rho} - \boldsymbol{\rho_o})^2 + (\mathbf{z} - \mathbf{z_o})^2}$, ε_o is the dielectric constant of GaAs material inside the wire, m^* is the effective electron mass and $\mathbf{r_o}$ is the impurity ion position.

2.1. Infinite potential barrier case

In this case the confinement potential is chosen as,

$$V(\rho, \phi) = \begin{cases} 0, & \rho \le R \\ \infty, & \text{elsewhere.} \end{cases} \tag{2}$$

For the system with an externally applied uniform magnetic field $\mathbf{B} = B_o\hat{z}$, we choose the magnetic field potential as $\mathbf{A} = \frac{1}{2}\rho B_o\hat{\phi}$. For the impurity ion positioned at the axis of wire axis, $\rho_0 = 0$ and $z_0 = 0$ are taken. In cylindrical coordinates, we can write the Hamiltonian of the system as:

$$H = -\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right] - \frac{\mathrm{i}\hbar}{2}\omega\frac{\partial}{\partial\phi} + \frac{1}{8}m^*\omega^2\rho^2 - \frac{e^2}{\varepsilon_o\sqrt{\rho^2+z^2}} + V(\rho) \tag{3}$$

where ω is cyclotron frequency and defined as $\frac{eB}{m^*c}$. The inclusion of the impurity potential leads to a non-separable differential equations which cannot be solved analytically. Therefore following in the footsteps of Brown and Spector [4], we use a variational approach, namely a trial wave function which is the product of a variational term such as $\mathrm{e}^{-\lambda\sqrt{\rho^2+z^2}}$, where λ is variation parameter, and the wave function without Coulombic interaction which is written as $\Psi(\rho,\phi,z) = R(\rho)\mathrm{e}^{\mathrm{i}m\phi}\mathrm{e}^{\mathrm{i}k_z z}$ where, $R(\rho)$ and $\mathrm{e}^{\mathrm{i}m\phi}$ $(m = 0, \pm1, \pm2, \ldots)$ are the radial and angular parts of the electron wave function. The ground state trial wave function $(m = 0, l = 1)$ is taken as:

$$\Psi(\rho,z) = \begin{cases} N\mathrm{e}^{-\frac{\xi}{2}}\,{}_1F_1(-a_{0,1},1,\xi)\mathrm{e}^{-\lambda\sqrt{\rho^2+z^2}}, & 0 \le \rho \le R \\ 0, & \rho > R \end{cases} \tag{4}$$

where $\xi = \frac{\rho^2}{2\alpha_c^2}$ is a dimensionless variable, $\alpha_c = \sqrt{\frac{\hbar c}{eB}}$ is the cyclotron radius and ${}_1F_1(-a_{0,1},1,\xi)$ is Kummer confluent hypergeometric function. Eq. (4) satisfies the boundary condition that $\underset{\rho\to R}{\Psi(\rho)} = 0$, while $a_{0,1}$ is the eigenvalue for the ground state of the system in the absence of the Coulomb term. Finally, N is the normalization constant and it is given by:

$$\frac{1}{N^2} = -2\pi\frac{\mathrm{d}A}{\mathrm{d}\lambda} \quad \text{and} \quad A = \int_0^R \rho\mathrm{e}^{-\frac{\rho^2}{2\alpha_c^2}}\,{}_1F_1^2(-a_{01},1,\xi)K_0(2\lambda\rho)\,\mathrm{d}\rho \tag{5}$$

where K_0 is modified Bessel function of the second kind of order zero. The binding energy of the hydrogenic impurity E_b is defined as the energy difference between the energy of the system with and without the Coulomb term. That is

$$E_b(R,B) = \hbar\omega_c\left(a_{01}+\frac{1}{2}\right) - \min_{\lambda}\langle T+V\rangle = -\frac{\hbar^2}{2m^*}\lambda^2 - \frac{2e^2}{\varepsilon_o}\frac{A}{\mathrm{d}A/\mathrm{d}\lambda}. \tag{6}$$

For numerical calculations; we use normalized binding energy $\tilde{E}_b = E_b/R_\mathrm{B}$ and all lengths are scaled by Bohr radius. After some algebra and setting $\rho = Rt$ we obtain:

$$\tilde{E}_b = -(\lambda\tilde{a}_B)^2 - 4\tilde{a}_B\frac{C}{\mathrm{d}C/\mathrm{d}\lambda} \tag{7}$$

where:

$$C = \int_0^1 t\mathrm{e}^{-t^2\frac{R^2}{2\alpha_c^2}}\,{}_1F_1^2\left(-a_{01},1,t^2\frac{R^2}{2\alpha_C^2}\right)K_0(2\lambda Rt)\mathrm{d}t. \tag{8}$$

We use a variational method and search for the minimum of $\min_\lambda \langle \mathbf{T} + \mathbf{V} \rangle$ with respect to λ, in order to obtain a lower bound of the binding energy. The radial integration for the expression C in performed numerically since there is no analytical method with which to do it.

2.2. Finite potential barrier case

In the finite potential barrier case, the potential $V(\rho, \phi)$ in the Hamiltonian (Eq. (1)) is taken as:

$$V(\rho, \phi) = \begin{cases} 0, & \rho \le R \\ V_o, & \rho > R. \end{cases} \tag{9}$$

All the other assumptions in the infinite potential barrier case remain the same. Both the differences of the effective electron mass and the dielectric constant between GaAs and $Al_xGa_{1-x}As$ are ignored; similar calculation for this case is made as before. The ground state trial wave function is

$$\Psi(\rho, z) = \begin{cases} N e^{-\frac{\xi}{2}} {}_1F_1(-a_{01}, 1, \xi) e^{-\lambda\sqrt{\rho^2+z^2}}, & 0 \le \rho \le R \\ N \dfrac{{}_1F_1(-a_{01}, 1, \xi_R)}{U(-a'_{01}, 1, \xi_R)} e^{-\frac{\xi}{2}} U(-a'_{01}, 1, \xi) e^{-\lambda\sqrt{\rho^2+z^2}}, & \rho > R \end{cases} \tag{10}$$

where $U(-a'_{01}, 1, \xi)$ is confluent hypergeometric function. The eigenvalues of the ground state wave function a_{01} and a'_{01} are derived by the boundary conditions. Similar to the infinite potential barrier case we obtain:

$$\frac{1}{N^2} = -2\pi \frac{\mathrm{d}}{\mathrm{d}\lambda}[Q + P], \tag{11}$$

with

$$\begin{aligned} Q &= \int_0^1 t e^{-t^2 \frac{R^2}{2\alpha_c}} {}_1F_1^2\left(-a_{01}, 1, t^2 \frac{R^2}{2\alpha_c}\right) K_0(2\lambda R t)\mathrm{d}t \quad \text{and} \\ P &= \frac{{}_1F_1^2\left(-a_{01}, 1, \frac{R^2}{2\alpha_c}\right)}{U^2\left(-a'_{01}, 1, \frac{R^2}{2\alpha_c}\right)} \int_1^\infty t e^{-t^2 \frac{R^2}{2\alpha_c}} U^2\left(-a'_{01}, 1, t^2 \frac{R^2}{2\alpha_c}\right) K_0(2\lambda R t)\mathrm{d}t \end{aligned} \tag{12}$$

and the normalized binding energy is:

$$\tilde{E}_b(R, B) = -(\lambda \tilde{a}_B)^2 - 4\tilde{a}_B \frac{Q + P}{\mathrm{d}(Q + P)/\mathrm{d}\lambda}. \tag{13}$$

As we did for the infinite case, we use a variational method to obtain $\min_\lambda \langle \mathbf{T} + \mathbf{V} \rangle$ with respect to λ, in order to obtain a lower bound of the binding energy.

3. Results and discussion

The results for the infinite potential barrier case are shown in Fig. 1(a) and (b). Fig. 1(a) presents the ground state binding energy of a hydrogenic impurity located on the axis of a cylindrical wire versus the wire radius for different magnetic fields. For a very small wire radius ($R < a_B$), the binding energy is relatively insensitive to the externally applied magnetic fields because no matter how high the B field strength is the electron cannot get any closer to impurity

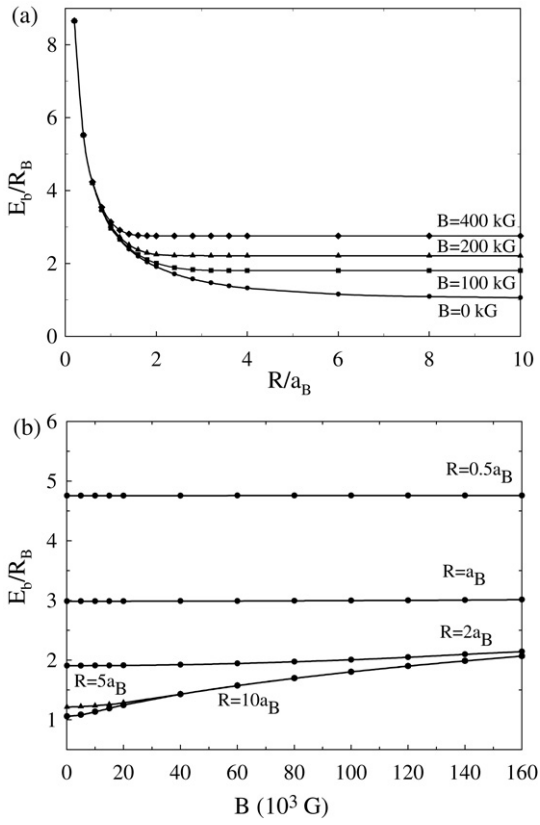

Fig. 1. Ground state binding energy of hydrogenic impurity (a) as a function of the wire radius for different externally applied magnetic field, (b) as a function of externally applied magnetic field for different wire radius in infinite potential barrier case.

due to the infinite potential barrier. At this region changing B values has no effect on the ground state binding energy. For wire radius $R \approx a_B$ the curves tend to deviate from each other and reach steady values as the wire radius increases for any B values. While the wire radius becomes very large ($R \gg a_B$), the ground state binding energy converges to the corresponding bulk values because the electron no longer interacts with the wire boundary, i.e. the impurity behaves like a free hydrogen atom. For a large value of the wire radius, the ground state binding energy for $B = 0$ approaches to the bulk case result, namely the Rydberg constant R_B as confirmed by similar works in literature. For $R \geq a_B$, the ground state binding energy is larger for increasing magnetic fields as expected.

In Fig. 1(b) we plot the binding energy versus the magnetic field for different wire radius. The ground state binding energy increases as wire radius decreases. The ground state binding energy is totally insensitive to the increase of the magnetic field for $R \leq 2a_B$. In large values of the wire radius and in small values of the magnetic field, the ground state binding energy is slightly complicated. The variation of ground state binding energy is much more pronounced due to the stronger confinement effect of the magnetic field and the spatial confinement. To illustrate this point we look at the percentile change in binding energy; for $R = 0.5a_B$ the change is % 0.2 while for $R = 5a_B$ this change is % 47 for $B = 20$–100 kG.

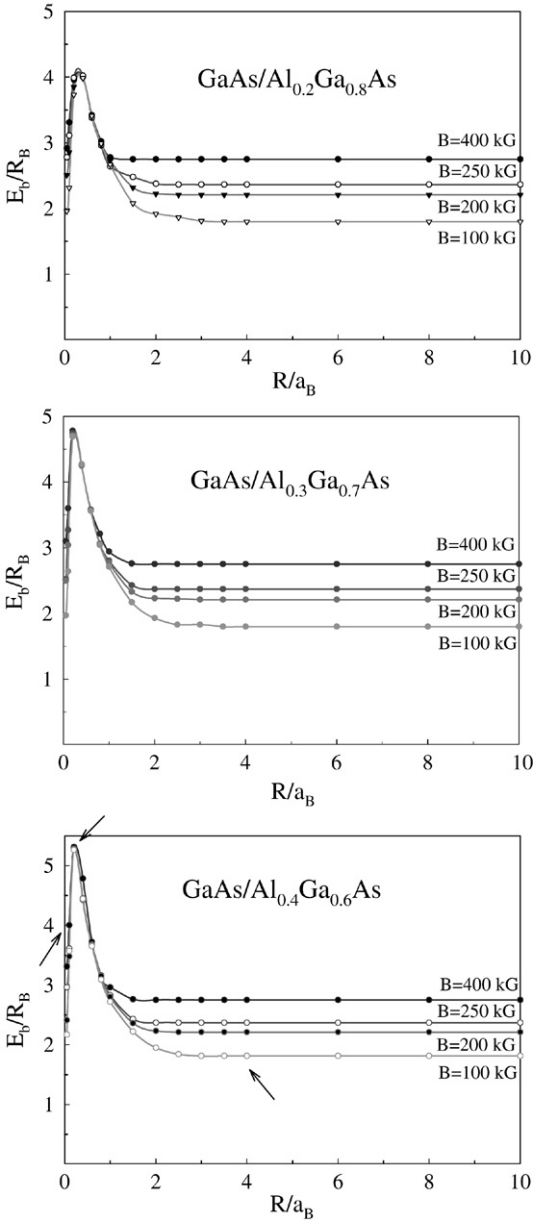

Fig. 2. Ground state binding energy of hydrogenic impurity as a function of the wire radius with aluminum concentration $x = 0.2, 0.3$ and 0.4 for different values of externally applied magnetic field in finite potential barrier case. Arrows are for Fig. 3.

The results of the ground state binding energy in the finite potential barrier case are discussed in this section. Calculations were made for three choices of the alloy composition of $Al_xGa_{1-x}As$ and our results are presented in Figs. 2–5. The well depth is determined by the potential discontinuities of the well and cladding which in turn depends on the Al concentration x in

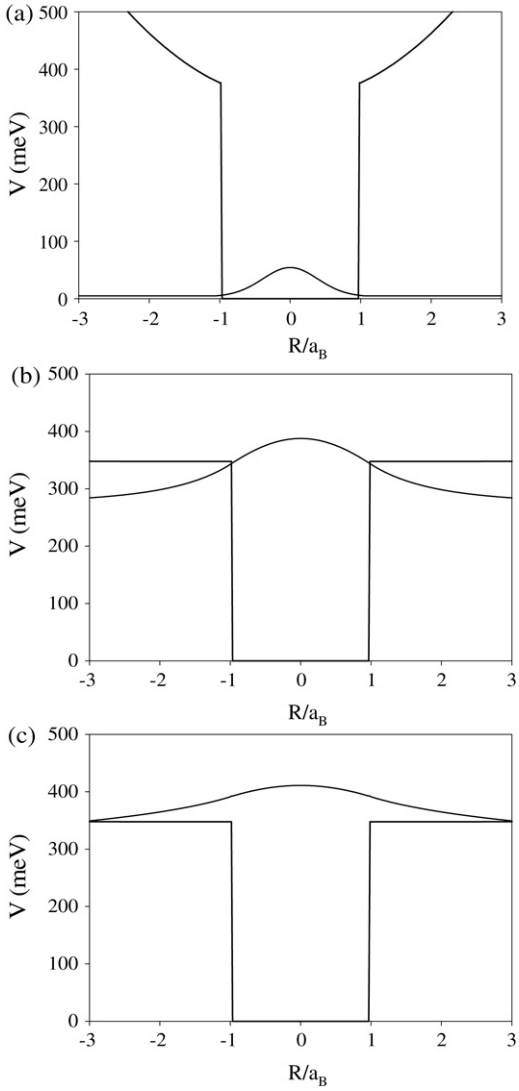

Fig. 3. Ground state localization as a function of ρ with aluminum concentration $x = 0.4$ and $B = 100$ kG for marked points of Fig. 3 plotted on finite potential profile. (a) $R = 3a_B$, (b) $R = 0.2a_B$ and (c) $R = 0.1a_B$. The min. of the probability plots are shifted up an amount equal to the electronic energy for each case.

the cladding. In our calculation, we have considered Al concentration x of 0.2, 0.3, 0.4, which correspond to potential barrier of approximately $V = 168$, 256 and 348 meV.

In Fig. 2, we illustrate how the changeover in ground state binding energy versus the wire radius for different strengths of an applied field with on-centre impurity to be effected by the well depth. The difference between the results for the infinite and finite potential barrier cases is striking when the QWs radius becomes small. In all the other cases, the results for finite potential barrier are nearly identical to the case of infinite potential barrier for any magnetic field strength. As the QW radius becomes very large, the ground state binding energy behaves like in the case of

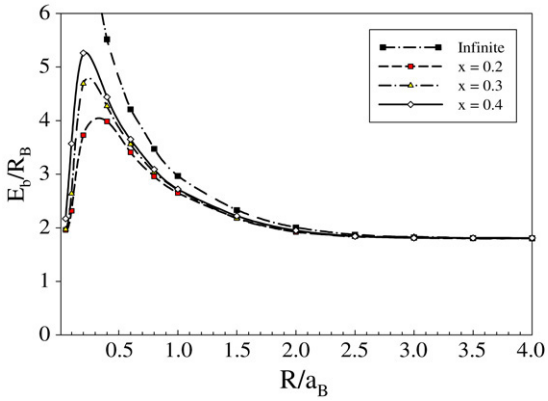

Fig. 4. Ground state binding energy of hydrogenic impurity as a function of wire radius with aluminum concentration $x = 0.2$, 0.3 and 0.4 for different values of magnetic field values in the case of a finite potential barrier.

infinite potential barrier and attains the bulk value of GaAs. For any magnetic field strength, the ground state binding energy increases from the bulk value of GaAs as the wire radius decreases and peaks at a finite value then drops sharply to the bulk value of $Al_xGa_{1-x}As$. This is due to the fact that the kinetic energy of the confined electron becomes larger by the uncertainty principle, and thus increases the probability of the electron leaking outside the wire and then the electron is only weakly affected by the potential barrier. This conclusion is supported by Fig. 3 where localization of charged particle is plotted vs ρ on the potential profile for different points marked in Fig. 2 corresponding to different wire radii. Clearly as we follow through the a, b and c points which b indicates the peak value in the binding energy, and a, b values are taken from the opposite sites of this peak. The particle in a is bounded in the QW and its radius is smaller than the wire radius, so it has a smaller binding energy as QW radius decreased then it started interacting with the boundaries; at this point its radius is comparable with the wire radius therefore it has a skipping orbit type motion and is closest to the impurity so the binding energy is the largest. As wire radius decreases further, the energy of the confined electron becomes larger by the uncertainty principle; thus the electron leaks outside the wire and it is free to move around the impurity or elsewhere, therefore resulting in a lower and not much changing binding energy as seen in point c. The maximum value of ground state binding energy increases while Al content x increases as summarized in Fig. 4.

For different Al concentrations, the ground state binding energy as a function of the externally applied magnetic field for a selected wire radius is shown in Fig. 5. The most important feature apparent in all plots is the change of the ground state binding energy as Al content x increases. This change occurs because the confining potential height increases as x increases. The ground state binding energy increases with increasing Al concentration; the difference between the curves of the energy levels for a given value of the wire radius increases with increasing Al concentration. The increase in energy spacing between the values of $0.2a_B$ and $0.6a_B$ is larger then others. For small values of $R \leq 2a_B$ the change in the ground state binding energy with applied magnetic field is similar to that in the case of bulk $Al_xGa_{1-x}As$ since the most of the wave function resides in the barrier, particles move in $Al_xGa_{1-x}As$ therefore increasing magnetic field has no effect on binding energy. When the wire radius is increased, the variation of the ground state binding energy with applied magnetic field becomes more effective in this cases the contribution to the ground state binding energy comes both from the spatial confinement and

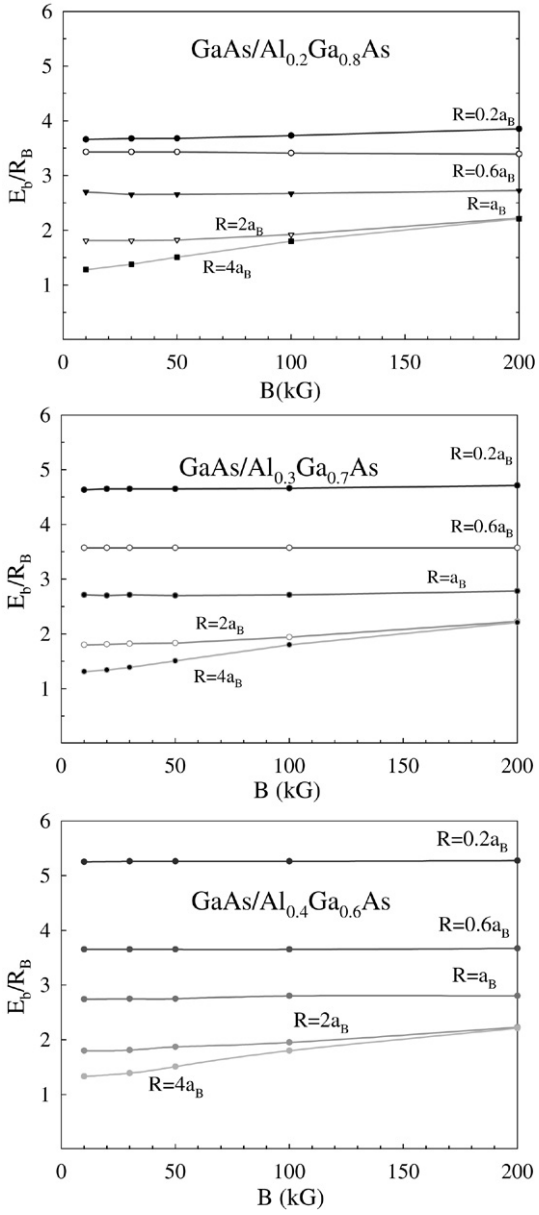

Fig. 5. Ground state binding energy of hydrogenic impurity as a function of the externally applied magnetic field with aluminum concentration $x = 0.2$, 0.3 and 0.4 for different values of wire radius in a finite potential barrier case.

the applied magnetic field confinement. For $R > 2a_B$, the ground state binding energy increases with increasing externally applied magnetic field strength. Since in this case the particle residing in barrier gets pushed toward the well region i.e. to the impurity.

In conclusion, we have studied the ground state binding energy of hydrogenic impurity depending on Al concentration in QWWs structures by using the effective mass approximation in

cylindrical coordinates. We obtained results that are consistent with the previous results obtained by Brown [4], Villamil [24], Karki [25], and Hsieh [20] for Al content $x = 0.4$. The ground state binding energy increases on decreasing the wire radius of QWWs for both infinite and finite potential barrier cases. In contrast to the infinite potential barrier case, the ground state binding energy approaches to a specific value than drops to the bulk value of $Al_xGa_{1-x}As$ as the wire radius decreases. For very large wire radius, the binding energy is also not sensitively dependent on the wire radius and applied magnetic field strength. Finally, increasing Al concentration gives rise to an increase in the binding energy for a very small wire radius.

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