Hydrogenic impurities in quantum wires in the presence of a magnetic field

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We report a calculation of the binding energy of the ground state of a hydrogenic donor in a quantum wire in the presence of a uniform magnetic field applied parallel to the wire axis. We assume that the impurity ion is located at the axis of the wire. The quantum wire is assumed to be a cylinder of GaAs material surrounded by $Ga_{1-x}Al_xAs$. The calculations have been performed by using suitable variational wave functions for infinite and finite confinement potentials. For a given value of the magnetic field, the binding energy is found to be larger than the zero-field case.

I. INTRODUCTION

In the past 20 years, quasi-two-dimensional semiconductor structures (quantum wells) have been studied extensively both theoretically and experimentally, and applied to various electronic and photonic devices. The interest in the quantum size effects present in the low-dimensional structures has been primarily motivated by the fact that the optical and electronic properties of these structures are improved by the reduction of dimensionality. It is expected that the same properties are further improved by the reduction of dimensionality to quasi-one-dimensional quantum wires (QW's). In the past few years, fabrication of quantum wire structures by microfabrication methods such as molecular-beam epitaxy and metal-organic chemical vapor deposition and experimental studies of their properties have been reported.[1-6] In addition, theoretical studies on transport properties,[7-12] optical properties,[13-18] electronic structure,[19-27] and excitonic[28-36] and impurity levels[37-45] in quantum wires have been published.

An understanding of the physics of impurity states in semiconductor QW structures is an important problem in semiconductor physics for various reasons: the reduction of dimensionality in QW's can be controlled by changing the radius of the wire. An electron bound to an impurity at the center of a QW never "sees" the surface of the wire in a very wide wire, and behaves as a three-dimensional (3D) electron bound to an impurity in GaAs, in a GaAs-$Al_xGa_{1-x}As$ structure. For intermediate wire sizes (of the order of the electron Bohr radius), the electron confinement due to the potential barrier can be greater than the confinement due to the impurity, and the electron behaves as a quasi-one-dimensional system. For very thin wires, the finite potential barrier cannot effectively confine the bound electrons which leak out as 3D electrons in $Al_xGa_{1-x}As$ bound to the impurities and weakly perturbed by the potential wall, while for an infinite barrier model, the electrons bound to the impurity ion stay inside the wire, thus increasing the binding energy relative to its bulk value. Furthermore, it is well known that the reduction of dimensionality increases the effective strength of the Coulomb interaction. The binding energy of the ground state of a hydrogenic impurity E_b in D dimensions is given by[46] $E_b=[2/(D-1)]^2 \times R_B m_e/\varepsilon_0^2$, where $R_B=m_0e^4/2\hbar^2$ is the Rydberg constant (13.6 eV), m_e is the electron effective mass (in units of the free-electron mass m_0), and ε_0 is the static dielectric constant. In the 2D case, the binding energy increases four times relative to the 3D case, while in the 1D case, the increase is infinite. Even though this result is somewhat misleading,[47,48] since the infinite bound state is not a formal solution of the strictly 1D problem as it is approached from the quasi-one-dimensional case, this ambiguity does not change the essential picture for quasi-one-dimensional systems; namely, the binding energy of the ground state is greatly enhanced and the effective Coulomb interaction is considerably stronger. This can be understood by the following argument: an electron in a system of reduced dimensionality can move only in a smaller space and spends most of its time close to the impurity. Therefore the binding of the electron should be larger in lower dimensions.

Extensive theoretical work on hydrogenic impurity states in QW's has been reported. Lee and Spector[37] studied the hydrogenic impurity binding energies in QW's by using a variational approach. The binding energy was calculated as a function of wire radius, for infinite confining potential. They compared their results for the binding energies with those obtained by Bastard,[49] for impurities confined in a quasi-two-dimensional well. Bryant[38] studied the effect of changing the cross-sectional form of the QW on the impurity's binding energy for infinite and finite potential barriers and found that in the case of wires with the same cross-sectional area, the binding energies were nearly equal for the cylindrical and rectangular QW's provided that the rectangular form did not deviate too much from the square shape. The impurity ion was positioned at the axis of the wire. Brum[39] studied the same problem, for wires with rectangular cross sections, for infinite confining potential, and for different impurity positions. Brown and Spector[40] calculated the impurity binding energies using infinite and finite cylindrical confining potentials for arbitrary impurity positions. Recently, Weber, Schulz, and Oliveira,[41] Cho and Prucnal,[42] Ferreira da Silva,[43] and Montenegro,

López-Gondar, and Oliveira[44,45] have focused their interest on the density-of-states calculations of hydrogenic impurities in QW's, as a function of impurity position, wire radius, wire cross section, and impurity disorder, using variational procedures within the effective-mass approximation.

Extensive experimental and theoretical investigations of the behavior of energy levels of shallow impurities in bulk semiconductors and their heterostructures such as quantum wells in the presence of a magnetic field have been carried out during the past 40 years. These studies have been primarily responsible for our current understanding of the nature of these impurities states. The application of the magnetic field modifies the symmetry of these states as well as the nature of the wave functions. The study of the transitions between the energy levels of these impurities leads to the determination of the binding energies, oscillator strengths, and other properties of these levels. Such studies, however, have not yet been performed in quantum wires. As in the case of bulk semiconductors and quantum wells, the study of the behavior of shallow-impurity states in quantum wires in the presence of a magnetic field will lead to a better understanding of their properties.

In this paper we report a calculation of the binding energy of the ground-state of a hydrogenic impurity located at the wire axis, in the presence of constant magnetic field, applied parallel to the wire axis using a variational approach. We have calculated the impurity binding energy for infinite and finite confinement potentials as a function of the wire radius and magnetic field. We use a variational method in which the trial wave function contains a hydrogenic part, and by taking into account the electron confinement and the appropriate confluent hypergeometric functions ${}_1F_1(a,c;x)$ and $U(a,c;x)$.[50] ${}_1F_1(a,c;x)$ is the radial solution of an electron in an infinite potential cylindrical wire, in the presence of a magnetic field, applied parallel to the wire axis, with the appropriate boundary conditions at the wire surface[51] (see Appendix A), while ${}_1F_1(a,c;x)$ and $U(a,c;x)$ are the corresponding solutions for the finite potential cylindrical wire case (see Appendix B). The shape of the wire was chosen to minimize the mathematical difficulties; we chose circular cross section. The wire is sufficiently long so that the motion along the wire's axis is translationally symmetric; the confining potential is a function of radial coordinate only, while the magnetic field being parallel to the wire axis conserves the rotational symmetry of the problem.

II. THEORY

A. Infinite potential barrier case

The Hamiltonian of a system consisting of an electron bound to a donor ion, inside a cylindrical wire of radius R, with infinite potential barrier at the surface, in the presence of a magnetic field parallel to the wire axis, is given by

$$H=\left[\mathbf{p}+\frac{e}{c}\mathbf{A}\right]^2\Big/2m^*-\frac{e^2}{\varepsilon_0|\mathbf{r}-\mathbf{r}_0|}+V(\rho,\phi)\ , \tag{1}$$

where $|\mathbf{r}-\mathbf{r}_0|=[\rho^2+\rho_0^2-2\rho\rho_0\cos(\phi-\phi_0)+z^2]^{1/2}$, ε_0 is the dielectric constant of GaAs material inside the wire, m^* is the effective electron mass, and $\mathbf{r}_0$ is the impurity ion position. The z coordinate gives the relative separation of the electron from the impurity ion along the wire axis. $\mathbf{A}(\mathbf{r})$ is the magnetic-field potential, and $V(\rho,\phi)$ is the confining potential,

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

For an impurity ion located at the wire axis, we write $\rho_0=0$. For a uniform magnetic field we can write $\mathbf{A}(\mathbf{r})=(\mathbf{B}\times\mathbf{r})/2$, where $\mathbf{B}=B\hat{\mathbf{z}}$; in cylindrical coordinates the magnetic-field potential becomes $A_\rho=A_z=0$, $A_\phi=B\rho/2$. The inclusion of the impurity potential leads to a nonseparable differential equation which cannot be solved analytically. Therefore it is necessary to use a variational approach to calculate the eigenfunctions and eigenvalue spectra of the Hamiltonian, especially for the ground state.

Following Brown and Spector,[40] we take into account the cylindrical confining symmetry, the presence of the magnetic field, and the hydrogenic impurity potential, by choosing a trial wave function for the ground state which can be written as a product of a hydrogenic part and the radial solution of an electron in a cylindrical wire in the presence of a magnetic field,

$$\psi(\mathbf{r})=\begin{cases}N\exp[-\xi/2]\,{}_1F_1(-a_{01},1;\xi)\\ \times\exp[-\lambda(\rho^2+z^2)^{1/2}], & 0\le\rho\le R\\ 0, & \rho>R\ .\end{cases} \tag{3}$$

In Eq. (3) the variable $\xi=\rho^2/2\alpha_c^2$, where $\alpha_c=(\hbar c/eB)^{1/2}$ is the cyclotron radius, N is the normalization constant, and λ is a variational parameter. Equation (3) satisfies the boundary condition that $\psi(\rho=R)=0$, while a_{01} is the eigenvalue for the ground state of the problem in the absence of the Coulomb term, being calculated numerically from the boundary-condition eigenvalue equation [Eq. (A7) in Appendix A]. N is given by

$$N^{-2}=-2\pi\frac{dA}{d\lambda}\ , \tag{4}$$

with

$$A=\int_0^R d\rho\,\rho\exp[-\rho^2/2\alpha_c^2]\times{}_1F_1^2(-a_{01},1;\rho^2/2\alpha_c^2)K_0(2\lambda\rho)\ , \tag{5}$$

where K_0 is the modified Bessel function of the second kind of order zero.

The binding energy $E_b(R,B)$ of the hydrogenic impurity is defined as the ground-state energy of the system in the absence of the Coulomb term, minus the ground-state energy $\langle H(R,B)\rangle$ in the presence of the Coulomb term; i.e.,

$$E_b(R,B)=\hbar\omega_c(a_{01}+\tfrac{1}{2})-\langle H(R,B)\rangle \ , \tag{6}$$

where $\omega_c=\hbar/m^*\alpha_c^2$ is the cyclotron frequency while the binding energy defined in this way is a positive quantity.

The ground-state energy $\langle H(R,B)\rangle=\langle T\rangle+\langle V\rangle$ is found after tedious algebra. The expressions for $\langle T\rangle$ and $\langle V\rangle$ are

$$\langle T\rangle=\hbar\omega_c(a_{01}+\tfrac{1}{2})+\frac{\hbar^2}{2m^*}\lambda^2 \tag{7}$$

and

$$\langle V\rangle=-\frac{4\pi e^2}{\varepsilon_0}N^2A \ . \tag{8}$$

Therefore

$$E_b(R,B)=-\frac{\hbar^2}{2m^*}\lambda^2-\frac{2e^2}{\varepsilon_0}\frac{A}{dA/d\lambda} \ . \tag{9}$$

For computational purposes, we normalize the expression for the binding energy $E_b(R,B)$ [Eq. (9)] in units of impurity Rydberg: $R_B=m^*e^4/2\varepsilon_0\hbar^2=e^2/2\varepsilon_0 a_B$, where $a_B=\varepsilon_0\hbar^2/m^*e^2$ is the electron Bohr radius, and define $\gamma=\hbar\omega_c/2R_B$. In addition, we transform the integral for A in a dimensionless form by letting $\rho=tR$; the expressions for $\langle H(R,B)\rangle$ and $E_b(R,B)$ are then written as follows:

$$\langle H(R,B)\rangle=\gamma(1+2a_{01})+(\lambda a_B)^2+4a_B\frac{C}{dC/d\lambda} \ , \tag{10}$$

$$E_b(R,B)=-(\lambda a_B)^2-4a_B\frac{C}{dC/d\lambda} \ , \tag{11}$$

where

$$C=\int_0^1 dt\ t\exp[-t^2\xi_R]\,{}_1F_1^2(-a_{01},1;t^2\xi_R)K_0(2\lambda Rt) \ , \tag{12}$$

while $\xi_R=R^2/2\alpha_c^2$.

We use a variational method, and search for the minimum of $\langle H(R,B)\rangle$ with respect to λ, in order to obtain a lower bound of the binding energy. The radial integration for the expression C is performed numerically since there is no analytical method to do it.

B. Finite potential barrier case

For the finite potential barrier case, the potential in the Hamiltonian [Eq. (1)] is taken as zero for $\rho<R$ and V_0 for $\rho>R$. All the other assumptions remain the same. Furthermore, we assume that the electron mass is constant across the barrier. Again, following Brown and Spector's procedure,[40] we take into account the cylindrical confining symmetry, the presence of the magnetic field, and the hydrogenic impurity potential by choosing a trial wave function for the ground-state case which can be written as a product of a hydrogenic part and the radial solution of an electron in a cylindrical wire in the presence of the magnetic field, parallel to the wire axis,

$$\psi(\mathbf{r})=\begin{cases} N\exp[-\xi/2]\,{}_1F_1(-a_{01},1;\xi)\exp[-\lambda(\rho^2+z^2)^{1/2}], & 0\le\rho\le R \\ N\dfrac{{}_1F_1(-a_{01},1;\xi_R)}{U(-a'_{01},1;\xi_R)}\exp[-\xi/2]U(-a'_{01},1;\xi)\exp[-\lambda(\rho^2+z^2)^{1/2}], & \rho>R \ . \end{cases} \tag{13}$$

Equation (13) satisfies the boundary condition ($\partial\Psi_{\rm in}/\partial\rho=\partial\Psi_{\rm out}/\partial\rho$ at $\rho=R$), while a_{01} and a'_{01} are the eigenvalues for the ground state of the problem inside and outside the wire, respectively, being calculated numerically from the relations in Eqs. (B5) and (B6) (see Appendix B). N is given by

$$N^{-2}=-2\pi\frac{d}{d\lambda}[K+M] \ , \tag{14}$$

with

$$K=\int_0^R d\rho\,\rho\exp[-\rho^2/2\alpha_c^2]\times{}_1F_1^2(-a_{01},1;\rho^2/2\alpha_c^2)K_0(2\lambda\rho) \tag{15}$$

and

$$M=\frac{{}_1F_1^2(-a_{01},1;\xi_R)}{U^2(-a'_{01},1;\xi_R)}\times\int_R^\infty d\rho\,\rho\exp[-\rho^2/2\alpha_c^2]\times U^2(-a'_{01},1;\rho^2/2\alpha_c^2)K_0(2\lambda\rho) \ . \tag{16}$$

The binding energy $E_b(R,B)$ is defined as before [Eq. (6)], where $\langle T\rangle$ and $\langle V\rangle$ are now given as

$$\langle T\rangle=-2\pi N^2\left[\hbar\omega_c(a_{01}+\tfrac{1}{2})\frac{dK}{d\lambda}+\hbar\omega_c(a'_{01}+\tfrac{1}{2})\frac{dM}{d\lambda}\right]+\frac{\hbar^2}{2m^*}\lambda^2 \tag{17}$$

and

$$\langle V\rangle=-\frac{4\pi e^2}{\varepsilon_0}N^2[K+M]-2\pi V_0N^2\frac{dM}{d\lambda} \ . \tag{18}$$

Therefore

$$E_b(R,B)=-\frac{\hbar^2}{2m^*}\lambda^2-\frac{2e^2}{\varepsilon_0}\frac{[K+M]}{d[K+M]/d\lambda} \ . \tag{19}$$

We normalize the expression for the binding energy $E_b(R,B)$, in units of impurity Rydberg R_B,

$$\langle H(R,B)\rangle=\gamma(1+2a_{01})+(\lambda a_B)^2+4a_B\frac{[Q+P]}{d[Q+P]/d\lambda} \ , \tag{20}$$

$$E_b(R,B)=-(\lambda a_B)^2-4a_B\frac{[Q+P]}{d[Q+P]/d\lambda}\ , \tag{21}$$

where

$$Q=\int_0^1 dt\ t\exp[-t^2\xi_R\,]_1F_1^2(-a_{01},1;t^2\xi_R)K_0(2\lambda Rt) \tag{22}$$

and

$$P=\frac{{}_1F_1^2(-a_{01},1;\xi_R)}{U^2(-a'_{01},1;\xi_R)}\int_0^1 dt\ t\exp[-t^2\xi_R\,]\times U^2(-a'_{01},1;t^2\xi_R)K_0(2\lambda Rt)\ . \tag{23}$$

III. RESULTS AND DISCUSSIONS

We have calculated the values of the binding energy E_b of a donor where the impurity ion is located on the axis of the QW ($\rho_0=0$) in the presence of a uniform magnetic field applied along the axis of the quantum wire. The values of the physical parameters pertaining to the material GaAs in the QW's used in our calculations are $m^*=0.067m_0$ and $\varepsilon_0=12.5$.

For the case of an infinite potential barrier, the binding energy diverges as $R/a_B\to 0$, for any magnetic-field strength. In Fig. 1 we plot the binding energy versus the wire radius for different magnetic fields. For very small wire radii, the binding energy is relatively insensitive to the magnetic fields used here since the electron is strongly confined in a small volume by the infinite potential barrier. For wire radius $R\approx a_B$ the different magnetic-field curves tend to deviate from each other reaching asymptotically the bulk case values, for $R\approx 10a_B$. Increasing magnetic field decreases the cyclotron radius for the electron relative to the wire radius, and increases the binding energy. In this limit of large wire radius, the binding energy for $B=0$ approaches the bulk case result: the Rydberg constant R_B. For magnetic fields up to $B=400$ kG, the binding energy converges asymptotically to bulk case results, studied by Aldrich and Greene.[52] In addition, our results in the zero-field case agree with those of Brown and Spector.[40]

In Fig. 2 we plot the binding energy versus the magnetic field for different wire radii. For $R<a_B$ the binding energy is totally insensitive to the increase of the magnetic field for the values used here, while for $R>a_B$ the binding energy is smaller for larger wire radii, a situation that disappears when the magnetic field goes beyond 200 kG. For small values of the magnetic field, the change in the binding energy is somewhat complicated, whereas for large values of the magnetic field, it tends to be linear as

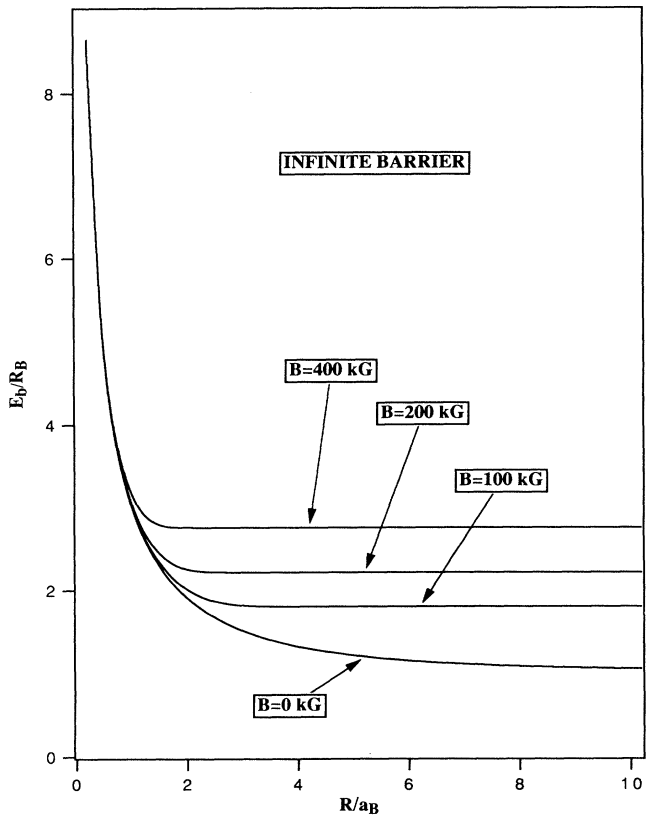

FIG. 1. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic Rydberg (R_B) in GaAs (5.8 meV) as a function of the radius of the wire (R) expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å) for several values of the magnetic field.

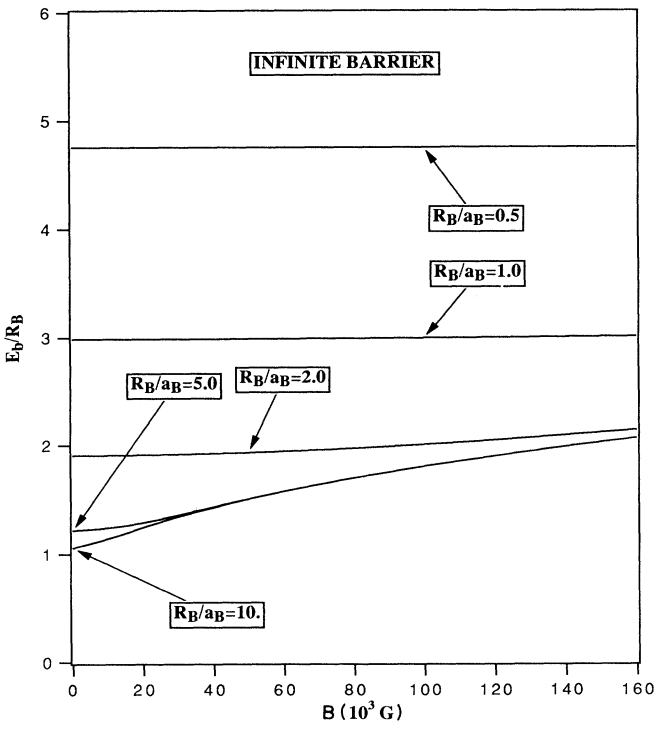

FIG. 2. Variations of the binding energy of a donor (E_b), expressed in terms of a hydrogenic Rydberg (R_B) in GaAs (5.8 meV) as a function of the magnetic field for several values of the radius of the wire expressed in terms of the Bohr radius (a_B) in GaAs ($\sim$98 Å).

expected. Very high magnetic fields confine the electron close to the wire axis, increasing in effect the binding energy.

For the case of the finite potential barrier, the values of the physical parameters pertaining to GaAs in the QW's in our calculations remain the same as before and the electron mass and the dielectric constant are assumed to have the same values across the barrier. The finite potential barrier is taken as $V_0 = Q_e\ (1.36x + 0.22x^2)$ (eV),[53] where $Q_3 = 0.6$ and x is the Al concentration. Our results, in the zero magnetic-field case, agree with those of Brown and Spector.[40]

In Fig. 3 we display the variation of the binding energy as a function of the radius of the wire for an impurity ion located at the axis of the wire for several values of the magnetic field. The Al concentration in the barrier materials is assumed to be $x = 0.4$. For a given value of the magnetic field, the binding energy increases 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 material as the wire radius goes to zero. This is due to the fact that as the wire radius is decreased the electron wave function is compressed thus leading to the enhancement of the binding energy. However, below a certain value of R, the leakage of the wave function into the barrier region becomes more important and thus the binding energy starts decreasing until it reaches a value which is characteristic of the barrier material as $R \to 0$. For a given value of R the binding energy increases as a function of the magnetic field due to the increasing compression of the wave function with magnetic field.

In Fig. 4, we plot the variation of the binding energy as a function of the magnetic field for several values of the wire radius. We find that for small values of R/a_B (≤ 0.2) the change in the binding energy with magnetic field is similar to that in the case of bulk GaAs as most of the wave function resides in the barrier. For intermediate values of R/a_B (~ 0.2–2.0) the variation of the binding energy with magnetic field is considerably smaller as the electron wave function is highly confined by the barrier potential. For larger values of R/a_B (≥ 2.0) the binding energy varies with magnetic field essentially the same way as it does in bulk GaAs.

And finally, we would like to mention that we have tested the accuracy of our variational approach by considering the case in which the applied magnetic field is very small and the potential barriers are infinite, using a first-order perturbation approach. Our unperturbed wave function corresponds to the situation where the magnetic field is zero and thus is identical to that used in Ref. 40. Using the magnetic-field term, i.e., $m^*\omega_c^2\rho^2/8$, as perturbation we find that the change in the binding en-

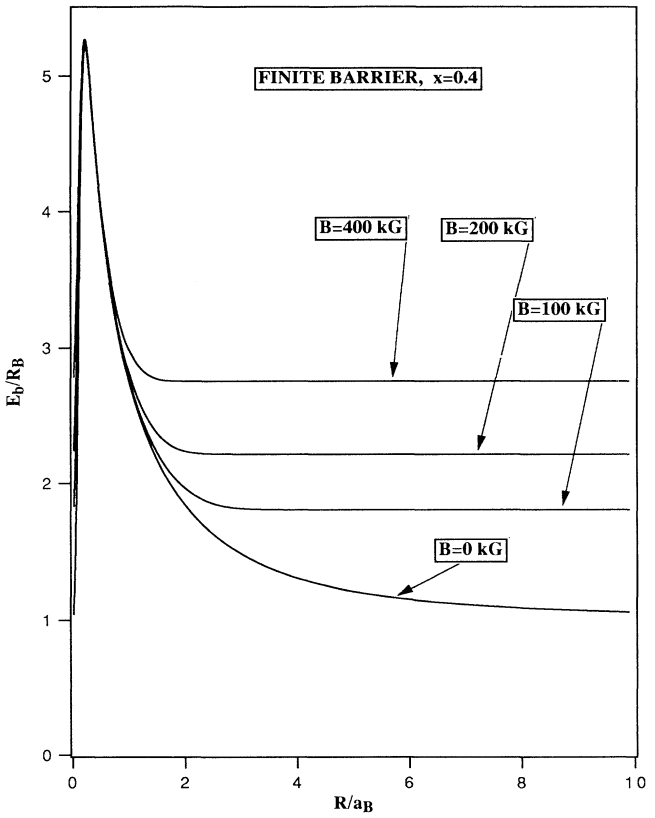

FIG. 3. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic Rydberg (R_B) in GaAs (5.8 meV) as a function of the radius of the wire (R) expressed in terms of the Bohr radius (a_B) in GaAs (~ 98 Å) for several values of the magnetic field.

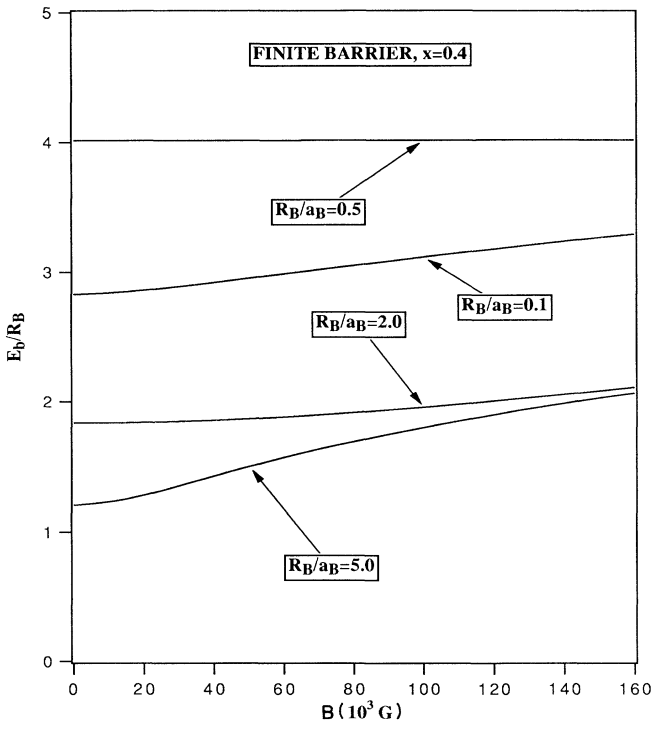

FIG. 4. Variation of the binding energy of a donor (E_b), expressed in terms of a hydrogenic Rydberg (R_B) in GaAs (5.8 meV) as a function of the magnetic field for several values of the radius of the wire expressed in terms of the Bohr radius (a_B) in GaAs (~ 98 Å).

ergy thus obtained is within a few percent of that calculated using our variational approach for small values of γ ($\gamma \leq 0.1$). In our calculations we have considered both an infinite and a finite barrier case. In the case of infinite barriers the calculations are much simpler and lead to results which for intermediate and large wire radii ($R/a_B > 1$) agree fairly well with those in the finite barrier case with commonly used values of Al concentration. Though the infinite barrier case, strictly speaking, does not have a physical relevance; for material systems, not considered in this work, the results obtained in an infinite barrier case can be applied to those systems as long as the wire sizes are not too small, namely, $R/a_B > 1$.

IV. SUMMARY

We have presented a calculation of the binding energy of a hydrogenic impurity in a quantum wire with infinite and finite potential barriers, in the presence of a uniform magnetic field, as a function of the width of the quantum wire, for the case of an impurity located on the axis of the wire. The magnetic field is assumed to be parallel to the axis of the wire. The calculations have been performed by using a suitable variational wave function, which takes into account the confinement (either infinite and finite) of the carriers in the wire, and the influence of the Coulomb interaction between the impurity ion and the electron. The binding energy continues to increase as the radius of the wire decreases for the infinite potential barrier case, while in the presence of a magnetic field, additional increases for the binding energy are reported, especially for larger wire radii. In the case of finite potential barriers and for a specific value of the magnetic field, the binding energy has a maximum for a certain value of the wire radii. In quantum wires with very small and very large radii, the binding energy as a function of the magnetic field behaves essentially the same way as it does in bulk GaAs.

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APPENDIX A: ELECTRON IN A CYLINDRICAL WIRE IN A MAGNETIC FIELD: INFINITE BARRIER CASE

The problem of an electron in a cylindrical QW, in the presence of a uniform magnetic field applied parallel to the axis of the wire for an infinite potential barrier case, was solved by Rensink.[51] Even though it was a significant contribution, it has not been frequently cited in the physics literature. In the following, we briefly summarize Rensink's analysis and results.

The Hamiltonian of an electron in a magnetic field and confined inside a cylindrical wire of radius R with an infinite potential barrier is

$$H=\left[\mathbf{p}+\frac{e}{c}\mathbf{A}\right]^2\Big/2m^*+V(\rho,\phi)\ , \tag{A1}$$

where $V(\rho,\phi)$ is the confining potential,

$$V(\rho,\phi)=\begin{cases}0, & 0\leq\rho\leq R\\ \infty, & \rho>R\ .\end{cases} \tag{A2}$$

For a uniform magnetic field applied along the z axis we can write the Schrödinger equation as

$$H\psi=-\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\right]+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right]\psi$$

$$+\frac{m^*\omega_c^2}{8}\rho^2\psi+\frac{\hbar\omega_c}{2i}\frac{\partial}{\partial\phi}\psi+V(\rho,\phi)\psi=E\psi\ , \tag{A3}$$

for $0\leq\rho\leq R$. The Hamiltonian has rotational symmetry around the z axis, and translational symmetry along the z axis; the eigenfunctions are written as follows:

$$\psi(\rho,\phi,z)=\frac{N}{\sqrt{2\pi L}}\exp[im\phi]\exp[ik_z z]\exp[-\xi/2]$$

$$\times\xi^{|m|/2}{}_1F_1(-a_{|m|l},|m|+1;\xi)\ , \tag{A4}$$

while the eigenvalues are given by

$$E=\frac{p_z^2}{2m^*}+\hbar\omega_c\left[a_{|m|l}+\frac{m}{2}+\frac{1}{2}+\frac{|m|}{2}\right]\ , \tag{A5}$$

where $m=0,\pm1,\pm2,\ldots$, $l=1,2,3,\ldots$, L being the length of the wire ($L\gg R$), $p_z=\hbar k_z$, and

$$N^{-2}=\alpha_c^2\int_0^{\xi_R}d\xi\exp[-\xi]\xi^{|m|}{}_1F_1^2(-a_{|m|l},|m|+1;\xi)\ . \tag{A6}$$

In Eq. (A4), ${}_1F_1(-a_{|m|l},|m|+1;\xi)$ is the general form of the confluent hypergeometric function,[50,54] which remains finite at $\xi=0$.

The value of $a_{|m|l}$ is determined by the boundary condition that the wave function vanish at the surface of the wire ($\rho=R$),

$${}_1F_1(-a_{|m|l},|m|+1;\xi_R)=0\ , \tag{A7}$$

where $\xi_R=R^2/2\alpha_c^2$. For the eigenvalue equation, $a_{|m|l}$ is the lth zero of ${}_1F_1(-a_{|m|l},|m|+1;\xi_R)$.

The energy spectrum here differs from the usual spectrum of an electron in a uniform magnetic field in free space,[55] because the $a_{|m|l}$ are no longer integers. However, Rensink[51] has shown that when the magnetic field becomes very strong, so that the radius of the cylinder R is large compared to the cyclotron radius α_c, the eigenvalues $a_{|m|l}$ closely approach non-negative integers, so that the wave function is finite everywhere. The eigenfunctions and the eigenvalues for very large magnetic fields are

$$\psi(\rho,\phi,z)=\frac{1}{\sqrt{2\pi L}}\exp[im\phi]\exp[ik_z z]\frac{1}{\alpha_c|m|!}\times\left[\frac{(N_p+|m|)!}{N_p!}\right]^{1/2}\times\exp[-\xi/2]\xi^{|m|/2}{}_1F_1(-N_p,|m|+1;\xi)\ , \tag{A8}$$

$$E=\frac{p_z^2}{2m^*}+\hbar\omega_c\left[N_p+\frac{m}{2}+\frac{1}{2}+\frac{|m|}{2}\right]\ , \tag{A9}$$

where $a_{|m|l}=N_p$, $N_p=0,1,2,\ldots$.

In the limit of very small magnetic fields, by expanding Eq. (A4), in terms of Bessel functions,[56] Rensink has shown that one can recover the eigenfunctions and eigenvalue spectrum of an electron inside a cylindrical wire of radius R, in the absence of a magnetic field,[57] i.e.,

$$\psi(\rho,\phi,z)=\frac{1}{\sqrt{2\pi^2LR}}\exp[im\phi]\exp[ik_z z]\times\frac{J_{|m|}(\chi_{|m|l}\rho/R)}{J_{|m|+1}(\chi_{|m|l})}\ , \tag{A10}$$

$$E=\frac{p_z^2}{2m^*}+\frac{\hbar^2\chi_{|m|l}^2}{2m^*R^2}+\hbar\omega_c\frac{m}{2}\ , \tag{A11}$$

where $a_{|m|l}=x_{|m|l}/4\xi_R-|m|/2-\frac{1}{2}$ and $x_{|m|l}$ is the lth zero of the Bessel function $J_{|m|}$ of order $|m|$.

APPENDIX B: ELECTRON IN A CYLINDRICAL WIRE IN A MAGNETIC FIELD: FINITE BARRIER CASE

We extend now the infinite potential barrier results to the case of a finite potential barrier. For $0\le\rho\le R$, the solution must not diverge at $\xi=0$; the eigenfunctions and the eigenvalues of the problem inside the wire are

$$\psi_{\rm in}(\rho,\phi,z)=\frac{N}{\sqrt{2\pi L}}\exp[im\phi]\exp[ik_z z]\exp[-\xi/2]\times\xi^{|m|/2}{}_1F_1(-a_{|m|l},|m|+1;\xi)\ . \tag{B1}$$

Here, the eigenvalues are given by

$$E=\frac{p_z^2}{2m^*}+\hbar\omega_c\left[a_{|m|l}+\frac{m}{2}+\frac{1}{2}+\frac{|m|}{2}\right]\ , \tag{B2}$$

where $\xi_R=R^2/2\alpha_c^2$, and $m=0,\pm1,\pm2,\ldots$, $l=1,2,3,\ldots$. For $\rho\ge R$, the solution must converge at $\xi\to\infty$. The eigenfunctions and the eigenvalues for the electron outside the wire are

$$\psi_{\rm out}(\rho,\phi,z)=\frac{N}{\sqrt{2\pi L}}\frac{{}_1F_1(-a_{|m|l},|m|+1;\xi_R)}{U(-a'_{|m|l}|m|+1;\xi_R)}\times\exp[im\phi]\exp[ik_z z]\times\exp[-\xi/2]\xi^{|m|/2}U(-a'_{|m|l},|m|+1;\xi)\ , \tag{B3}$$

where $U(-a,|m|+1;\xi)$ is the general form of the confluent hypergeometric function,[50,54] which remains finite as $\xi\to\infty$, while the eigenvalues are given by

$$E=\frac{p_z^2}{2m^*}+V_0+\hbar\omega_c\left[a'_{|m|l}+\frac{m}{2}+\frac{1}{2}+\frac{|m|}{2}\right]\ . \tag{B4}$$

The values of $a_{|m|l}$ and $a'_{|m|l}$ are derived as roots of a system of two equations: the matching relation for the derivative of the wave function inside and outside the wire and the relation between eigenvalues $a_{|m|l}$ and $a'_{|m|l}$,

$$\frac{\partial}{\partial\rho}\psi_{\rm in}\bigg|_{(\rho=R)}=\frac{\partial}{\partial\rho}\psi_{\rm out}\bigg|_{(\rho=R)} \tag{B5}$$

and

$$\hbar\omega_c[a_{|m|l}-a'_{|m|l}]=V_0\ . \tag{B6}$$

The normalization constant N is written as follows:

$$N^{-2}=\alpha_c^2\left[\int_0^{\xi_R}d\xi\exp[-\xi]\xi^{|m|}{}_1F_1^2(-a_{|m|l},|m|+1;\xi)+\frac{1F_1^2(-a_{|m|l},|m|+1;\xi_R)}{U^2(-a'_{|m|l},|m|+1;\xi_R)}\times\int_{\xi_R}^{\infty}d\xi\exp[-\xi]\xi^{|m|}\times U^2(-a'_{|m|l},|m|+1;\xi)\right]\ . \tag{B7}$$

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