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

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Abstract

A systematic study of the binding energy of the ground state of a hydrogenic donor in a cylindrical quantum wire is calculated in the presence of a uniform magnetic field applied parallel to the wire axis. Calculations are performed within the effective mass approximation using the variation procedure considering both infinite and finite potentials. We assume that the impurity ion is located at the axis of the wire. The quantum wire is assumed to a cylinder of GaAs material surrounded by $Ga_{1-x}As_xAs$. The binding energy is calculated as a function of the radius of the wire and the applied magnetic field. For the infinite potential well model, the binding energy continues to increase as the radius of the wire decreases whereas in the finite case, the binding energy reaches a peak value as the wire radius decreases to a value characteristic of the cladding. For a given value of the magnetic field, the binding energy is found to be larger than the zero field case. The results are compared with available data in the literature.
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1. Introduction

It is possible to fabricate high quality semiconductor nanostructure with good electronic and optical properties due to the recent development of experimental crystal growth techniques. These physical properties are improved by the reduction of dimensionality to quasi one-dimensional quantum well wires (QWWs). In the last two decades, fabrication of QWW structures by microfabrication methods such as molecular-beam epitaxy and metal–organic chemical vapour deposition and experimental studies of their properties have been reported [1–3]. In the past few years, several theoretical [4,5] and experimental [6,7] studies on electronic structure [8,9], transport properties [10,11], excitonic [12,13] and impurity levels and impurity binding energies [14,15] in QWWs have been performed.

Lee and Spector [16] studied the hydrogenic impurity binding energies in QWWs using a variational approach. The binding energy was calculated as a function of wire radius, for infinite confined potential. Bryant [17] studied the effect of changing the cross-sectional form of the QWW on the impurity's binding energy and found that in the case of wires with the same cross sectional area, the impurity binding energies were nearly equal for the cylindrical and rectangular QWW's provided that the rectangular form did not deviate too much from the square shape. The impurity ion was positioned at the axis of wire. Brum [18] observed the same problem, for wires with rectangular cross sections, for infinite confining potential and for different impurity positions. Brown and Spector [19] calculated the impurity binding energies for arbitrary impurity positions using infinite and finite cylindrical confining potentials. Porras-Montenegro et al. [20] have calculated the binding energies and density of impurity states for donor and acceptor impurities in cylindrical QWWs and determined the impurity-related optical absorption and photoluminescence spectra in GaAs/GaAlAs QWWs.

Magnetic field has become an interesting probe for studying the physical properties of low-dimensional structures, both

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from the theoretical and technical point of view. During the past decade, there has been a considerable amount of work, devoted to the study of the behaviour of energy levels of shallow impurities in QWWs [21–23] in the presence of a magnetic field. Branis et al. [24] treated a problem of the bound electron to an impurity, located on the axis of the wire, in a cylindrical quantum wire with infinite and finite potential barriers in the presence of uniform magnetic field as a function of the width of the quantum wire. They have used a variational method in which the trial wave function contains a hypergeometric function. This confluent hypergeometric function is the radial solution of an electron in an infinite potential cylindrical wire, in the presence of any magnetic field applied along the wire axis with appropriate boundary conditions on the wire surface.

At the present work, the binding energy of the impurity, located at the wire axis, is determined in the presence of magnetic field applied parallel to the wire axis. A variational scheme is employed within the effective mass approximation. We have calculated the impurity binding energy for infinite and finite confinement potentials as the function of wire radius and magnetic field for GaAs/GaAlAs structures. We employ the variational wave function containing a hydrogenic part and, to incorporate the carriers in the wire, the appropriate Bessel functions. The method followed is presented in Section 2 while the discussion of the results is provided in Section 3.

2. Theory

2.1. Infinite potential barrier case

In the frame work of an effective mass approximation, the Hamiltonian for a hydrogenic donor in a cylindrical wire of radius R and length L, in the presence of a magnetic field parallel to the wire axis, for the infinite potential case, is given by

$$H = \frac{1}{2m^*}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 - \frac{e^2}{\varepsilon_0\sqrt{\rho^2+z^2}} + V(\rho), \tag{1}$$

where ε_0 is the dielectric constant of GaAs material inside the wire, m^* is the effective electron mass, $\vec{A}(\rho)$ is the potential vector of the magnetic field and $V(\rho)$ is the confining potential given by

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

By introducing the effective Rydberg $R_B = m^*e^4/2\hbar^2\varepsilon_0^2$ as the unit of energy and the effective Bohr radius $a_B = \hbar^2\varepsilon_0/m^*e^2$ as the length unit, for GaAs these quantities are $R_B = 5.8\,\text{meV}$ and $a_B = 98.72\,\text{Å}$. The Hamiltonian given in Eq. (1) can be written in cylindrical coordinates and in reduced units as

$$H(\rho,\phi,z) = H(\rho,\phi) + H(z) - \frac{2}{\sqrt{\rho^2+z^2}} + \frac{V(\rho)}{R_B}, \tag{3}$$

where

$$\begin{aligned} H(\rho,\phi)\psi_{nlk}(\rho,\phi) = & -\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right]\psi_{nlk}(\rho,\phi) \\ & + \frac{\gamma^2\rho^2}{4}\psi_{nlk}(\rho,\phi) + \gamma L_z\psi_{nlk}(\rho,\phi) \\ = & E_1\psi_{nlk}(\rho,\phi), \end{aligned} \tag{4}$$

$$H(z)\psi_{nlk}(z) = -\left[\frac{\partial^2}{\partial z^2}\right]\psi_{nlk}(z) = E_2\psi_{nlk}(z), \tag{5}$$

where L_z is the z component of the angular momentum operator in units of $\hbar$, and γ is the dimensionless measure of the magnetic field, defined as

$$\gamma = \frac{\hbar eB}{2m^*cR_B}. \tag{6}$$

The Hamiltonian of the system in the absence of the impurity is given by

$$H(\rho,\phi,z) = H_0(\rho,\phi,z) + V', \tag{7}$$

where

$$H_0(\rho,\phi,z) = -\nabla^2 + \gamma L_z + V(\rho), \tag{8}$$

and

$$V' = \tfrac{1}{4}\gamma^2\rho^2. \tag{9}$$

The eigenfunctions of the Hamiltonian H_0 in the absence of a magnetic field and the impurity are

$$\psi_{nlk}(\rho,\phi,z) = \begin{cases} N_1 e^{ikz} e^{\pm il\varphi} J_{|l|}(k_{nl}\rho), & \rho < R, \\ 0, & \rho > R. \end{cases} \tag{10}$$

In terms of Ref. [25], the eigenfunction of Eq. (7) which satisfies the transformation in the strong perturbation procedure can be obtained as

$$\psi_{nlk}(\rho,\phi,z) = \begin{cases} N_1 e^{ikz} e^{\pm il\varphi} J_{|l|}(k_{nl}\rho)\, e^{-(1/4)\gamma\rho^2}, & \rho < R, \\ 0, & \rho > R. \end{cases} \tag{11}$$

where N_1 is the normalization constant of the trial wave function, and J_l is a Bessel function. The quantities k_{nl} are given as solutions of the following equation:

$$J_l(k_{ln}R) = 0, \tag{12}$$

where n is the serial number of the root of the Bessel function for a given value of l. The effects of the confining potential and the magnetic field are automatically included in the trial wave function. The ground state energy is estimated using the trial wave functions given in Eq. (11).

While the influence of the coulomb interaction between the impurity ion and the electron is taken into account, the trail wave function for calculating the ground state energy

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