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Binding energy of impurity states in an inverse parabolic quantum well under magnetic field

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Abstract

We have investigated the effects of the magnetic field which is directed perpendicular to the well on the binding energy of the hydrogenic impurities in an inverse parabolic quantum well (IPQW) with different widths as well as different Al concentrations at the well center. The Al concentration at the barriers was always $x_{max} = 0.3$. The calculations were performed within the effective mass approximation, using a variational method. We observe that IPQW structure turns into parabolic quantum well with the inversion effect of the magnetic field and donor impurity binding energy in IPQW strongly depends on the magnetic field, Al concentration at the well center and well dimensions.

1. Introduction

In recent years, the study of confined hydrogenic systems in quantum well heterostructures (QWHs) has been a subject of great interest and an enormous amount of literature has been devoted to this field ([1–8] and references therein). However, there is still interest in studying some original QWHs with a wide variety of confining potential shapes such as parabolic, half parabolic, graded and V-shaped quantum wells [6,9–12]. As known, with atomic layer-by-layer deposition such as molecular-beam epitaxy (MBE), it is possible to fabricate a QWH having any desired potential shape. Two kinds of growth techniques, digital [9] and analog [13] have been used in the fabrication of nonsquare quantum wells. An inverse parabolic quantum well (IPQW) was fabricated experimentally in Refs. [14,15]. Envelop function calculations of energy levels were also presented in these papers.

In this work, we report the effects of the magnetic field on the binding energy of the hydrogenic impurities in an IPQW with different widths as well as different Al concentrations at the well center. The Al concentration at the barriers was always $x_{max} = 0.3$. The potential profile of IPQW is given in Fig. 1.

2. Theory

We define the z-axis to be along the growth axis, in order to see the effect of the magnetic field on the spatial confinement of the donor electron, magnetic field is applied perpendicular to the growth direction i.e. $\vec{B} = (B, 0, 0)$. We choose a vector potential **A** written in the form $\vec{A} = (0, -Bz, 0)$ to describe the applied magnetic field. Parallel magnetic field has a small quantitative impact on the quantum well's energy spectrum. If a magnetic field perpendicular to the quantum well plane is applied, however energy spectrum is changed considerably. This fact directly influences the nature of electronic and optical properties in these structures.

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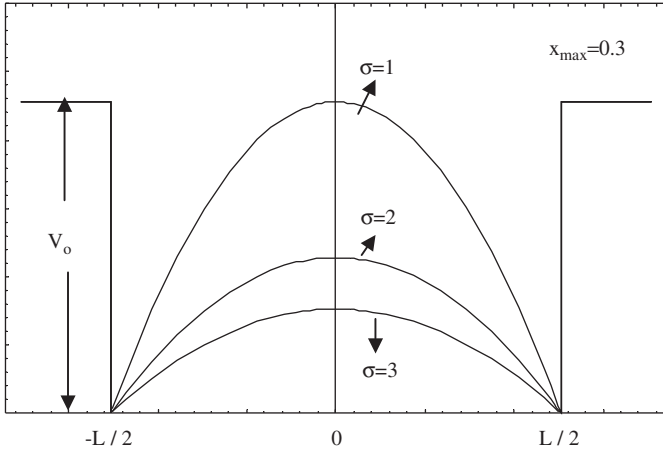E-mail address: ekasap@cumhuriyet.edu.tr (E. Kasapoglu).

Fig. 1. The schematic representation of IPQW for different Al concentration values at the well center.

Within the framework of an effective-mass approximation, the Hamiltonian of a hydrogenic donor impurity in a GaAs/Ga$_{1-x}$Al$_x$As IPQW in the presence of magnetic field, can be written as

$$H = \frac{1}{2m_e}\left[\vec{p}_e + \frac{e}{c}\vec{A}(\vec{r}_e)\right]^2 + V(z_e) - \frac{e^2}{\varepsilon_o|\vec{r}_e - \vec{r}_i|}, \quad (1)$$

where m_e is the effective mass, e the elementary charge, $\vec{p}_e$ the momentum, ε_0 the dielectric constant, $\vec{r}(=\vec{r}_e - \vec{r}_i)$ the distance between the carrier and the donor impurity site and $V(z_e)$ the confinement potential profile for the electron in the z-direction.

The functional form of the confinement potential is given as

$$V(z_e) = \begin{cases} \frac{V_o}{\sigma}\left(1 - \left(\frac{z}{L/2}\right)^2\right), & |z| \leqslant L/2, \\ V_o, & |z| > L/2, \end{cases} \quad (2)$$

where $\sigma = x_{max}/x_c$ (x_{max} is the constant Al concentration at the barriers, x_c the Al concentration at the well center), V_o is the band discontinuity for $x_{max} = 0.3$, V_o/σ the maximum value of potential at the center of IPQW and L is the width of IPQW.

By using cylindrical coordinates $x = \rho\cos\phi$, $y = \rho\sin\phi$, we obtained the Hamiltonian as follows.

$$H = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\Phi^2}\right) - \frac{\hbar^2}{2m_e}\frac{d^2}{dz_e^2}$$
$$+ \frac{e^2B^2}{2m_ec^2}z_e^2 + V(z_e) - \frac{e^2}{\varepsilon_o\sqrt{\rho^2 + (z_e - z_i)^2}}, \quad (3)$$

where the term $\rho\left(= \sqrt{(x_e - x_i)^2 + (y_e - y_i)^2}\right)$ is the distance between the electron and impurity in the $(x-y)$ plane and the location of the hydrogenic donor in the structure is denoted as $(0, 0, z_i)$. Eq. (3) does not contain the term $(eB/m_ec)z_ep_y$ because, the expectation value of this term is identically zero for the chosen trial wave function in Eq. (4).

The following trial wave function of the ground impurity state is given as

$$\Psi(r) = \psi(z)\varphi(\rho, \lambda), \quad (4)$$

where the wave function $\psi(z)$ is exactly obtained from the Schrödinger equation in the z-direction, the wave function in the $(x-y)$ plane—$\varphi(\rho, \lambda)$ is chosen to be the wave function of the ground state of a two-dimensional hydrogen-like atom [16,17]:

$$\varphi(\rho, \lambda) = \frac{1}{\lambda}\left(\frac{2}{\pi}\right)^{1/2}e^{-\rho/\lambda}, \quad (5)$$

in which λ is a variational parameter. The ground state impurity binding energy is evaluated by minimizing the expectation value of the Hamiltonian in Eq. (3) with respect to λ.

The ground impurity binding energy is obtained as follows:

$$E_b = E_z - \min_\lambda\langle\Psi|H|\Psi\rangle \quad (6)$$

where E_z is the ground-state energy of electron obtained from Schrödinger equation in the z-direction without impurity.
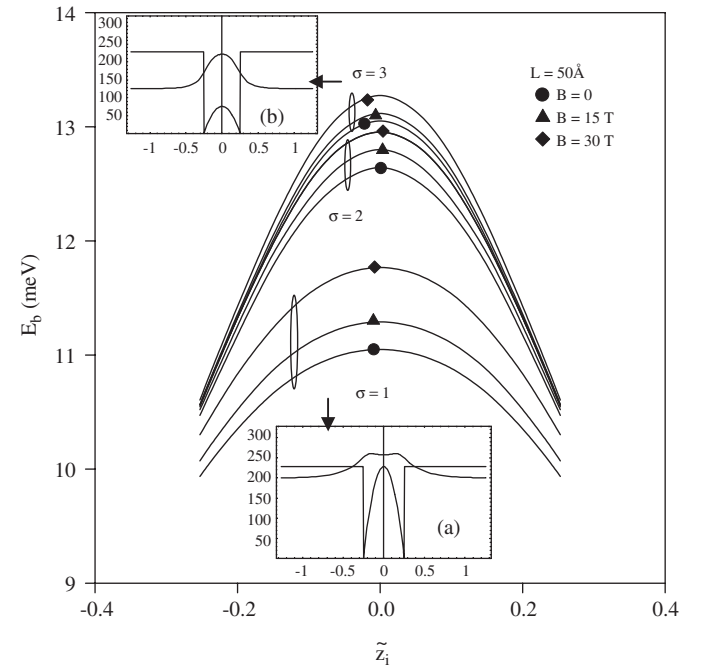

Fig. 2. Variation of the impurity binding energy as a function of the normalized impurity position for different magnetic field values and different Al concentrations at the center of IPQW for $L = 50\,\text{Å}$. The insets show the spatial distribution of the ground state wave function of the electron in the IPQW in the absence of the magnetic field for (a) $\sigma = 1(x_c = x_{max} = 0.3)$ and (b) $\sigma = 3(x_c = 0.1)$, respectively.