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Density of impurity states of hydrogenic impurities in an inverse parabolic quantum well under the magnetic field

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Abstract

We investigated the effects of the magnetic field on the density of impurity states in a GaAs/GaAlAs inverse parabolic quantum well (IPQW) for different Al concentrations at the well center. The calculations were performed within the effective mass approximation, using a variational method. We report in this paper the effects of the magnetic field, well width and the Al concentration at the well center on the density of states and the binding energies of the donor impurities.

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1. Introduction

The understanding of the electronic structure, transport, excitonic and impurity properties of semiconducting heterostructures such as quantum wells (QWs), quantum well wires (QWWs) and quantum dots (QDs) is a problem of considerable importance from both theoretical and technological point of view. Since Bastard [1] studied for the very first time the problem of hydrogenic impurities in infinite-barrier QWs by analyzing the binding energy, density of impurity states and the optical and photoluminescence spectra of shallow donor and acceptors, many works on this subject were published. Mailhot et al. [2] and Greene and Bajaj [3] improved the performance by calculating the ground state and the first excited states of hydrogenic impurities for QWs of finite depth. The density of impurity states and a correct interpretation of the obtained results were given by Oliveira and Falicov [4]. Weber calculated the densities of states and the optical absorption spectra of shallow donors and acceptors in quantum wells under the influence of a constant electric field [5]. The binding energies and density of impurity states of hydrogenic impurities in both infinite and finite GaAs/Ga,AlAs QWWs area calculated by Porras-Montenegro et al. [6] as a function of the wire radius and of the impurity location in the well . They found that as a general feature, the density of impurity states presents two structures associated with impurities at the center and at the edge of the QWW that may be important in the understanding of the absorption and luminescence experiments of the doped GaAs/Ga, AlAs QWW. Density of shallow-donor impurity states in rectangular cross-section GaAs QWWs under applied electric field were calculated by Montes et al. [7]. Their results indicate that a proper consideration of the density of impurity states, when electric field is applied in the structure may be of relevance in the interpretation of the future experimental data on optical phenomena related to shallow impurities in QWWs. Along the same lines, they also calculated density of states of a donor impurity in a GaAs quantum box under the action of an applied electric field [8].

Most of the work were concentrated on square QWs but it is certain that this is the best structure for devices

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based on the low-dimensional semiconductor heterostructures. With atomic layer-by-layer deposition such as molecular-beam epitaxy (MBE), it is possible to fabricate a QW structure having any desired potential shape. Chen et al. [9] have successfully grown an inverse parabolic QW by MBE using a digital compositional grading superlattice composed of $Ga_{0.64}Al_{0.36}As/GaAs$. They found large Stark shift and amplitude reduction 1e–1hh exciton resonance under applied electric field in the photoluminescence spectra, which are substantially larger than the conventional square QW.

In this work, we present results for the hydrogenic impurity binding energy and density of impurity states in an inverse parabolic QW under the influence of the magnetic field. The magnetic field is an important additional parameter, since it can be applied experimentally in a well-controlled way and modifies fundamentally the electronic and optical properties of the low-dimensional semiconductor heterostructures.

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 is written form $\vec{A} = (0, -Bz, 0)$ to describe the applied magnetic field. If a magnetic field perpendicular to the QW plane is applied, energy spectrum is changed considerably. This fact directly influences the nature of electronic and optical properties in these structures.

Within the framework of an effective-mass approximation, the Hamiltonian of a hydrogenic donor impurity in an inverse $GaAs/Ga_{1-x}Al_xAs$ parabolic quantum well (IPQW) in the presence of magnetic field can be written as

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

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

The functional form of the confinement potential is given as

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

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

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

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

where the term $\rho = \sqrt{(x_e - x_i)^2 + (y_e - y_i)^2}$ is the distance between the electron and impurity in the $(x–y)$ plane, the location of the hydrogenic donor in the structure is denoted as $(0,0,z_i)$.

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

$$\phi(r) = \psi(z)\frac{1}{\lambda}\left(\frac{2}{\pi}\right)^{1/2}e^{-\rho/\lambda}, \tag{4}$$

where the wave function-$\Psi(z)$ is exactly obtained from the Schrödinger equation in the z-direction, second part is the wave function in the $(x–y)$ plane and it is chosen to be the wave function of the ground state of a two-dimensional hydrogen-like atom [1,10], λ is a variational parameter.

This separable trial wave function is well suited for narrow well structures as the z localization is provided by the free-particle carrier functions. In the range where most structures the quantum size effects are important the separable wave function gives almost the same results as the nonseparable wave function [11].

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:

$$E_b = E_z - \min_{\lambda}\langle\phi|H|\phi\rangle, \tag{5}$$

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

If the quantum well is not too thin, one may treat the impurity position as a continuous random variable and, provided that there is no intentional doping, one can define a density of the impurity states (DOIS) per unit energy $g(E_i)$ as [1,5]

$$g(E_i) = \frac{1}{L}\sum_{\{z_i\}}\left|\frac{\partial E_i}{\partial z_i}\right|^{-1}, \tag{6}$$

where $\{z_i\}$ are all impurity positions with the same impurity binding energy E_i. Our results are presented in reduced atomic units (a.u.*), which correspond to a length unit of an effective Bohr radius $a_o = \hbar^2\varepsilon_o/m_ee^2$, and an energy unit of an effective Rydberg, $R_o = m_ee^4/2\hbar^2\varepsilon_o^2$.

3. Results and discussion

For numerical calculations, we take $m_e = 0.067m_o$ (where m_o is the free electron mass), $\varepsilon_o = 12.5$ and the