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OFF-CENTER DONOR FRACTAL-DIMENSION IN GRADED QUANTUM-WELL WIRES

J. Sierra[1] Ortega , R. A. Escorcia, S. T. Pérez-Merchancano*
Departamento de Física, Universidad del Magdalena
A.A. 731 Santa Marta, Colombia
*Departamento de Física, Universidad del Cauca
Popayan, Colombia

ABSTRACT

A simple method for calculating the ground-state binding energy of an off-center donor impurity in a quantum-well wire (QWW) is presented. A differential equation for the electron-ion correlation function, which coincides with the Schrödinger equation for a hydrogen atom in an effective isotropic and non-homogeneous space, is deduced. This method is used for calculating the ground-state binding energy of a donor in a GaAs-(Ga, Al)As QWW, as a function of the wire radius and the donor position. The effect produced by a graded increasing of the *Al* concentration at the heterostructure interface on the donor binding energy is analyzed. In the particular case of the rectangular potential, our results are in a good agreement with previous variational calculations.

INTRODUCTION

In the last decade, the crystal-growth technology has been improved enough to lead to the fabrication of high quality one-dimensional (1D) semiconductor heterostructures such as quantum-well wires (QWWs) [1, 2]. A large variety of new electrical and optical properties could be found in such low-dimensional systems [3]. Numerous theoretical and experimental works has been done to study the electronic spectra of donor impurities in quantum wires [4-8]. In the most theoretical studies, is used the approximation of ideal interfaces in the heterojunction with a rectangular potential to describe the confinement of electrons as well as the variational method, which generally implies tedious calculations to obtain with reasonable accuracy the donor binding energies. Recently a simple fractal dimension method has been proposed [9] to calculate the ground state energy of a donor centered in QWW by reducing the problem of a donor in the heterostructure to a simple problem of a hydrogen atom in an isotropic and non-homogeneous space with variable dimension, which depends on the electron-ion separation. In this work we extend this method to calculate the ground state binding energy of an off-center donor in a QWW. We apply our procedure to analyze the effect of graded interfaces in the heterostructure, considering different models of the confining potential.

THEORY

Introducing the effective Bohr radius (a_0*) and the Rydberg (Ry^*), as units of length and energy respectively and placing the coordinates origin at the impurity ion position $\mathbf{r}_i$, the dimensionless Hamiltonian for a neutral donor impurity in a cylindrical QWW within the parabolic effective-mass approximation can be written as [4]:

[1] Email jcsierra@b-manga.cetcol.net.co

$$H = H_0(\mathbf{r} + \mathbf{r}_i) - 2/|\mathbf{r}|, \quad H_0(\mathbf{r}) = -\nabla^2 + V(\mathbf{r}) \qquad [1]$$

where $V(\mathbf{r})$ is the confinement potential with axial symmetry and H_0 is the Hamiltonian for an unbound electron in the wire, whose eigenfunction f_0, and eigenvalue E_0, for the ground state can be found exactly by solving the problem:

$$H_0 f_0(\mathbf{r}) = E_0 f_0(\mathbf{r}) \qquad [2]$$

To calculate the donor ground state energy binding, we choose a trial wave function as a product of the anisotropic three-dimensional wave function of the unbound electron with an arbitrary one-dimensional function $\Phi(r)$ that depends only on electron-ion separation and describes the correlation of the electron-ion motion in the QWW

$$\Psi(\mathbf{r}) = f_0(\mathbf{r} + \mathbf{r}_i)\Phi(r) \qquad [3]$$

Starting from the variational principle one can obtain the following Euler–Lagrange equation for the correlation function:

$$-\frac{1}{S_0(r)}\frac{d}{dr}\left[S_0(r)\frac{d\Phi(r)}{dr}\right] - \frac{2}{r}\Phi(r) = -E_b\Phi(r), \; \boldsymbol{E_b = E_0 - E} \qquad [4]$$

where E_b and E are the donor binding and ground state energies respectively. Here S_0 is the volume measure function in an isotropic and non-homogeneous space given by the radial probability density for an unbound electron in QWW, calculated over the sphere of the radius r with center in the ion position $\mathbf{r}_i$:

$$S_0(r) = \overline{|f_0(\mathbf{r} + \mathbf{r}_i)|^2} = \int_{|\mathbf{r}|=r} |f_0(\mathbf{r} + \mathbf{r}_i)|^2 \, d\mathbf{r} \qquad [5]$$

Equations (4) and (5) describe the problem of a hydrogen atom in a space with variable dimension D^*. The relation between the volume measure function (5) and the fractal dimension [10] is given by the formula $S_0(r) \approx r^{D^*(r)-1}$. As the electron-ion distance is very small the integral (5) is proportional to r^2 and the effective space is three-dimensional. As the electron-ion distance increases the wave function in the wire interfaces vanishes, the integral (5) becomes independent of the sphere radius and the volume measure function $S_0(r)$ tends to a constant value, which is typical for one-dimensional effective space. To obtain an explicit expression for S_0, one can take into account that the unbound electron wave function f_0 has axial symmetry, and for a very long wire depends only on the electron distance from the axis of symmetry, $f_0(\mathbf{r}) \equiv f_0(\rho)$. By using spherical coordinates with the origin placed at the ion position $\mathbf{r}_i$ the formula (5) for a cylindrical QWW is reduced to:

$$S_0(r) = r^2 \int_0^{2\pi} d\varphi \int_0^{\pi} f_0^2\left(\sqrt{r^2 \sin^2\theta - 2r\rho_i \sin\theta \sin\varphi + \rho_i^2}\right) \sin\theta d\theta \qquad [6]$$

where ρ_i is the ion distance from the axis of symmetry.

To analyze the effects of a graded interface on the donor binding energy, we consider cylindrical QWW of radius *R*, for a confinement potential in (1) with soft-edge barrier given by the relation:

$$V(\rho) = V_0 \frac{1 - \exp(-\rho/\xi)}{1 + \exp[-(\rho - R)/\xi]} \qquad [7]$$

where ξ is the interface thickness in the transition region of the heterostructure. The potential $V(\rho)$ increases smoothly from 0 at the axis of the wire ($\rho \to 0$), up to V_0 in the barrier as (ρ -*R*)/ $\xi \gg 1$. For $\xi \to 0$ expression (7) a simple square-well potential is obtained with a potential jump at the interface.

RESULTS AND DISCUSSION

To check the accuracy of the numerical procedure, we first calculated the donor ground state binding energies as a function of the impurity position ρ_i for a model of a GaAs/$Ga_{0.7}Al_{0.3}$As cylindrical QWW with square-well potential, which was analyzed previously by using the variational method [5].

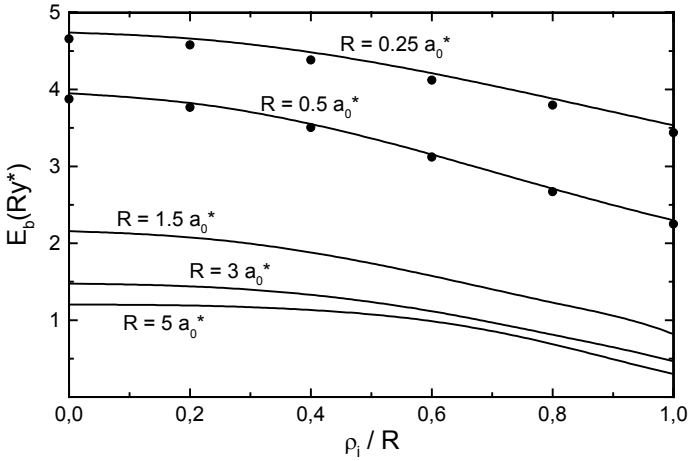

Figure 1. Binding energies for the ground state of a donor in a GaAs/$Ga_{0.7}Al_{0.3}$As cylindrical QWW, as a function of the impurity position ρ_i and for various wire radius. The solid circles present results of the variational calculations from Ref. [5].

Our results displayed in Fig. 1 for R = 0.25 a_0* and R = 0.5 a_0* are in a good agreement with those obtained in Ref. [5] (solid circles). It is seen from Fig.1 that the donor binding energy decreases monotonically as the donor position displaces from center to

QWW edge due to the variation of the symmetry of the ground state wave function from the symmetry typical for 1s-like orbit to the 2p-like orbit. The symmetry variation provides the increasing of the mean distance between electron and ion and therefore the decreasing of the donor binding energy. As the confinement is weak (see curve for R = 0.5 a_0* in Fig.1), the binding energy of a donor placed in the QWW center approaches to the 1s-like state value in bulk (~1 *Ry**) meanwhile the correspondent value for a donor placed in the edge of the QWW approaches to 0.25 *Ry**, value corresponding to 2p-like donor orbit in bulk.

In Fig. 2 we plot the binding energies dependencies on QWW radius for a donor placed at the middle position between the center and edge in a GaAs/$Ga_{0.6}Al_{0.4}$As cylindrical QWW for two models, with interface thickness ξ/R = 0.001, 0.3 in the transition region, corresponding to almost rectangular potential, and very smooth edge-barrier one, respectively (see inset of Fig. 2). Our results for the rectangular potential (solid lines) are in a good agreement with those obtained in Ref. [6] (open circles).

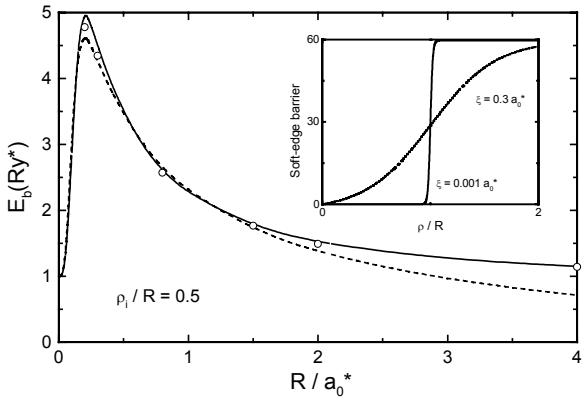

Figure 2. Binding energies of a donor in a GaAs/$Ga_{0.6}Al_{0.4}$As cylindrical QWW with soft-barrier potential, as a function of the wire radius for the models with the square-well and soft-edge barrier confining potentials.

The binding energies of a donor in a GaAs/$Ga_{0.7}Al_{0.3}$As cylindrical QWW as a function of the impurity position ρ_i are presented in Fig. 3 for three different interface thickness values: ξ/R = 0.001, 0.1, 0.3, corresponding to almost rectangular, smooth and very smooth edge-barrier potential, respectively.

It is seen from Fig.3 that the order of the curves in the upper group for wire radius R = 1.0 a_0*, as the confinement is intermediate is opposite to one in the lower group for R = 0.25 a_0* as confinement is very strong. This is due to the fact that in the first case the electron energy levels are situated closely to the bottom of the conduction band, the electronic orbital confinement in this region for the smooth potential is stronger than for rectangular one, and the potential shape corresponding to ξ/R = 0.3 gives the largest binding energy, followed by the ξ/R = 0.1, whereas the ξ/R = 0.001 present the smallest confinement and binding energy. As the QWW radius decreases, the energy level rises to the upper part of the conduction band where, on the contrary, the electronic orbital confinement is stronger for the rectangular potential.

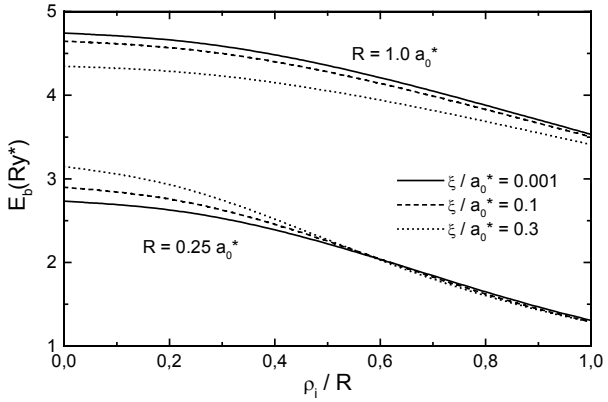

Figure 3. Binding energies of a donor in a $GaAs/Ga_{0.7}Al_{0.3}As$ cylindrical QWW as a function of the impurity position ρ_i for a model with soft-edge barrier potential for different interface thickness values and different wire radii.

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