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Density of shallow-donor impurity states in rectangular cross section GaAs quantum-well wires under applied electric field

A Montes†, C A Duque† and N Porras-Montenegro‡

† Departamento de Física, Universidad de Antioquia, A A 1226, Medellín, Colombia
‡ Departamento de Física, Universidad del Valle, A A 25360, Cali, Colombia

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Abstract. We calculate the binding energy and the density of states of a hydrogenic shallow donor impurity in quantum-well wires with rectangular cross section using a variational procedure within the effective-mass approximation under the influence of a constant electric field applied perpendicular to the axes of the wire. Calculations were performed as functions of the position of the impurity in a quantum-well wire of infinite depth and for various sizes of the wire cross section. The binding energy and the density of impurity states are analysed and compared with their quantum-well wire counterparts. Our results indicate that a proper consideration of the density of impurity states when electric fields are applied in the structure may be of relevance in the interpretation of future experimental data on optical phenomena related to shallow impurities in quantum-well wires.

1. Introduction

Since Bastard [1] calculated for the very first time the hydrogenic impurity states in quantum wells (QWs) many works on this subject have been published. Variational calculations for $n = 1$ levels in QWs with electric fields were performed by Bastard *et al* [2] and for the binding energies of shallow impurities by Brum *et al* [3]. Oliveira and Falicov [4] have calculated the density of impurity states (DOIS) within a variational calculation in the effective-mass approximation. Calculations were performed for simple neutral and double singly ionized impurities in a GaAs QWs of infinite depth. They gave a correct description of the experimental results. Weber [5] and López-Gondar *et al* [6] have calculated the DOIS and optical absorption spectra of shallow impurities in QWs under the influence of a longitudinal electric field and considering infinite and finite confinement potential. They found that, as a general feature, the DOIS and impurity-related optical absorption for finite electric fields exhibit three Van Hove-like singularities corresponding to the binding energies associated with impurities at the two edges of the QW and at the position at which the binding energy has a maximum. Additionally, they showed that the lack of symmetry around the $z_i = 0$ (z_i, impurity position) position when $F \neq 0$, is reflected in *one* additional peak in the DOIS.

The binding energies and DOIS in spherical GaAs–(Ga,Al)As quantum dots (QDs) have been calculated by Porras-Montenegro *et al* [7]. They observed that for small radii of the structure the DOIS presents one structure associated with on-edge donors, while for large radii it shows two structures associated with on-centre and with on-edge donor positions

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that may be important in the understanding of optical experiments of doped QDs. Along the same lines, Ribeiro and Latgé [8] have performed a comparative study of impurities in cubic and spherical GaAs QDs. They showed that for QDs with similar volumes, the results for the impurity-binding energies and the shapes of the DOIS do not depend on the geometric details of the quantum systems.

In the last two decades, some electron and impurity properties have been calculated in quantum-well wires (QWWs). Brown and Spector [9] have obtained the binding energy of hydrogenic impurities in cylindrical, infinite-length, GaAs–(Ga Al)As QWWs for finite and infinite confinement potential. They found that for a finite confinement potential the binding energies curves coincide for small radius of the QWW and for different values of the impurity position along the radial direction. Porras-Montenegro *et al* [10] calculated the ground state energy, the binding energy and the DOIS of shallow hydrogenic impurities in cylindrical GaAs–(Ga Al)As QWWs. They found, as a general feature, that the DOIS presents two structures associated with impurities on-centre and on-edge in the QWW. Weber *et al* [11] have calculated the DOIS and energy spectra of hydrogenic impurities in rectangular cross section QWWs without considering the effects of external fields. Their calculations indicate that the DOIS of the impurity band becomes richer in structure as soon as some symmetry is lost, and concluded that one should therefore be cautious in analysing experimental results on QWWs (e.g. photoluminescence and absorption spectra on doped QWWs). The effects of an applied electric field on the binding energy of shallow donor impurities in rectangular cross section GaAs QWWs was presented by Montes *et al* [12], considering an infinite confinement potential and using a variational scheme. For wires with the same transversal section as those of Brown and Spector [9] they observed the same behaviour for the impurity binding energy.

The presence of an external electric field in rectangular cross section QWWs modifies the impurity band due to the fact that the field breaks the energy degeneracy for symmetrical impurity positions along the transversal section of the wires. This is reflected in additional peaks for the impurity DOIS and in the absorption and photoluminescence spectra. In the present work we extend the analysis of Weber *et al* [11] and Montes *et al* [12] by considering the effect of an applied electric field on the shallow donor impurities implanted in rectangular cross section GaAs–(Ga Al)As QWWs. The dimensions and the geometry of the system that we have considered can be considered quite realistic due to the increasing maturity of the *nm*-structuring processes (see, for example, Schweizer *et al* [13]). We present results for the binding energy and the DOIS in the effective-mass approximation, using a variational scheme, and in the infinite-confinement potential model. The effect of a finite potential well and the resulting leaking of the wave functions into the embedding material can approximately be accounted for by introducing an effective well–wire transversal area, A_{eff}, which is slightly larger than the actual area A [14].

2. Theory

In the effective-mass approximation, the Hamiltonian for a hydrogenic donor impurity in a rectangular cross sectional area and infinite-length GaAs QWW under an electric field, F, applied perpendicular to the axes of the wire and along the x-direction is

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x, y) + |e|Fx - \frac{e^2}{\varepsilon r} \tag{1}$$

where $r = [(x - x_i)^2 + (y - y_i)^2 + z^2]^{1/2}$ is the distance between the carrier and the impurity site, $m^* = 0.0665\ m_0$ is the donor-impurity effective mass (with m_0 being the free-electron

mass), $\varepsilon = 12.58$ is the static dielectric constant and $V(x, y)$ is the infinite confinement potential. As a trial wave function for the ground state of the impurity we have used

$$\psi(r) = N\varphi(x, y)\,\mathrm{e}^{-\lambda r} \tag{2}$$

where λ is a variational parameter and $\varphi(x, y)$ is the usual wave function for an unperturbed QWW:

$$\varphi(x, y) = \cos\left(\frac{\pi x}{L_x}\right)\cos\left(\frac{\pi y}{L_y}\right) \tag{3a}$$

without electric field and

$$\varphi(x, y) = \varphi(\xi)\cos\left(\frac{\pi y}{L_y}\right) \tag{3b}$$

when we consider the applied electric field. Here L_x and L_y are the dimensions of the rectangular cross-section of the QWW, and $\varphi(\xi)$ is a linear combination of Airy functions:

$$\varphi(\xi) = B_i(+)A_i(\xi) - A_i(+)B_i(\xi) \tag{4}$$

where ξ reads

$$\xi = a_c\frac{x}{L_x} - \frac{E_0 - (\hbar^2\pi^2/2m^*L_y)}{\hbar\omega_c} \tag{5}$$

with $\omega_c = (eF)^{2/3}/(2m^*\hbar)^{1/3}$ and $a_c = (2m^*\omega_c/\hbar)^{1/2}L_x$.

In (4), one has

$$A_i(\pm)[B_i(\pm)] = A_i[B_i]\left(\pm\frac{a_c}{2} - \frac{E_0 - (\hbar^2\pi^2/2m^*L_y)}{\hbar\omega_c}\right) \tag{6}$$

where E_0 is the eigenvalue for the ground state of the system without impurities, obtained as the first root of the transcendental equation:

$$B_i(+)A_i(-) - A_i(+)B_i(-) = 0. \tag{7}$$

The trial impurity ground-state energy $\langle\psi|H|\psi\rangle$ has to be minimized with respect to λ. The impurity binding energy $E_i \equiv E(L_x, L_y, x_i, y_i)$ is calculated with respect to the bottom of the QWW conduction band.

If the transversal section of the QWW is not too small, one may treat the impurity position as a continuous random variable and, provided that there is no intentional doping, the density of impurity states [1] per unit energy, $g_{L_xL_y}(E_i)$, can be defined as

$$g_{L_xL_y}(E_i) = \frac{1}{L_xL_y}\int_{S(E_i)}\frac{\mathrm{d}s}{|\nabla(E_i)|} \tag{8}$$

where $S(E_i)$ is the surface of constant energy $E = E_i$ and ∇ is the gradient with respect to the impurity position. In the case of a rectangular GaAs QWW the DOIS was obtained via a histogram method [11] for a mesh of points uniformly distributed along the irreducible part of transversal section of the QWW.

In the next section, our results for donor impurities are given in reduced atomic units that correspond to a length unit of one effective Bohr radius, $a^* = \hbar^2\varepsilon/m^*e^2 \cong 100$ Å and an energy unit of one effective Rydberg, $R^* = m^*e^4/2\hbar^2\varepsilon \cong 5.72$ meV.

3. Results

In figure 1 we present the binding energy, for shallow donor impurities, as a function of the impurity position along the transversal section in a rectangular cross section GaAs QWW with $L_x = 200$ Å and $L_y = 100$ Å. In figures 1(a) and 1(c) we do not consider the effect of external electric field, whereas in figures 1(b) and 1(d) an external electric field of 150 kV cm^{-1} is applied to the systems in the x-direction. In cases 1(a) and 1(b) we consider three fixed values for the impurity in the y-direction and the impurity moves along the x-direction. The opposite situation occurs for figures 1(c) and 1(d). In figures 1(a) and 1(c), where we do not consider external fields, we observe that the binding energy is degenerate for symmetrical positions with respect to the centre of the transversal section of the wire. This degeneracy is broken in figure 1(b) due to the presence of the external electric field applied in the x-direction. In figure 1(d) where the system is under an external electric field, we observe degeneracy in the binding energy, due to the fact that the field is perpendicular to the direction corresponding to the different impurity locations. In comparing figures 1(a) and 1(b) we observe that for impurity positions close to the right

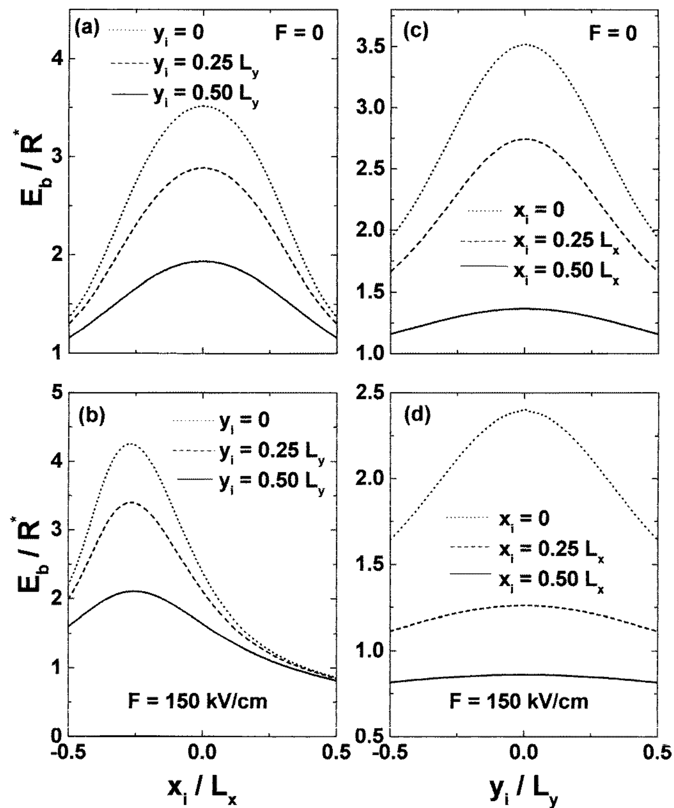

Figure 1. Binding energies for shallow donor impurities, as a function of the impurity position along the x- and y-directions on the transversal section in a rectangular cross section GaAs QWW with $L_x = 200$ Å and $L_y = 100$ Å. In (a) and (c) we do not consider the effect of external electric field. In (b) and (d) the system is under the effect of an electric field of 150 kV cm^{-1}, applied in the x-direction.

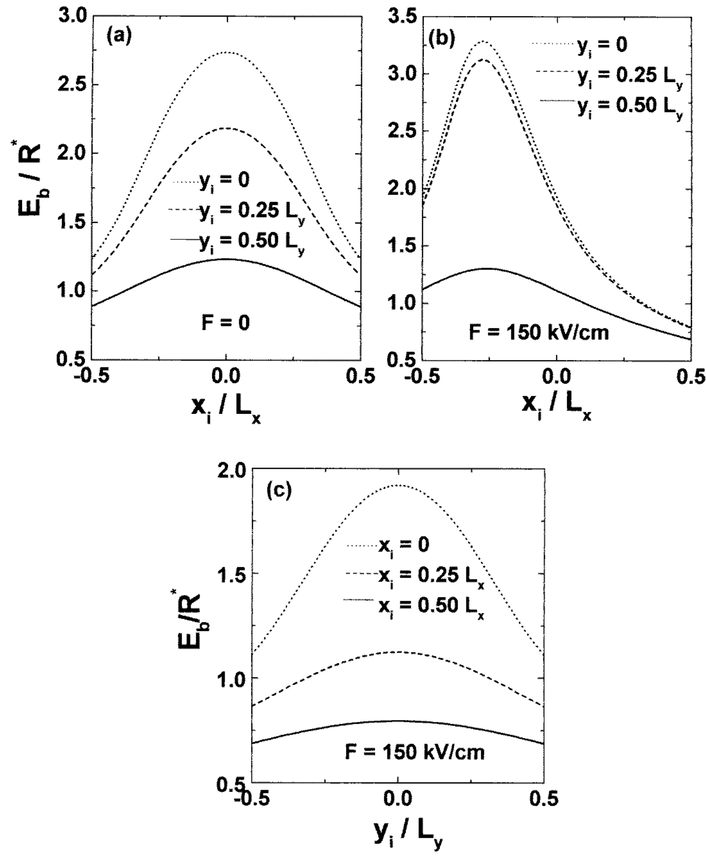

Figure 2. Binding energies for shallow donor impurities, as a function of the impurity position along the x- and y-directions on the transversal section in a square cross section GaAs QWW with $L_x = L_y = 210$ Å. In (a) we do not consider the effect of external electric field. In (b) and (c) the system is under the effect of an electric field of 150 kV cm^{-1}, applied in the x-direction.

(left) edge of the transversal section of the wire the binding is lower (higher) in figure 1(b) than in figure 1(a). For the right edge this situation occurs due to the fact that the electric field moves the electronic probability density away from the impurity, whereas for the left border the electric field and the potential barrier compete in order to bring the electronic probability density near to the impurity. In figure 1(d) all curves are lower than in 1(c) due to the fact than the applied electric field displaces the electronic probability density from the impurity position. In figures 1(a) and 1(c) for curves with the same label the difference in the binding energy is associated with the effects of the potential barriers.

The binding energy as a function of the shallow donor impurity position in a square cross section ($L_x = L_y = 210$ Å) GaAs QWW without and with an applied electric field $F = 150$ kV cm^{-1} is presented in figure 2. In figure 2(a) we consider the impurity position varying along the x-direction for three fixed positions along the y-axis without electric fields. Due to the zero electric field and the geometry of the system, the x- and y-directions for the impurity position are equivalent. In cases 2(b) and 2(c) where the electric field is 150 kV cm^{-1} and the impurity position varies along the x- and y-directions, the physical situation and the analysis are similar to those of figures 1(b) and 1(d), respectively.

For the case 2(a) where the transversal section of the QWW is square it is clear that the DOIS should present two peaks associated with impurities close to the centre and to the edge of the transversal section of the wire, whereas for the rectangular case (figures 1(a) and 1(c)) the DOIS should present three peaks: one associated with impurities at the centre and the two other peaks generated from the lifting of the degeneration for impurities close to the x- and y-borders of the structure. It is clear that the presence of applied electric fields should be reflected in some changes in the structures of the DOIS.

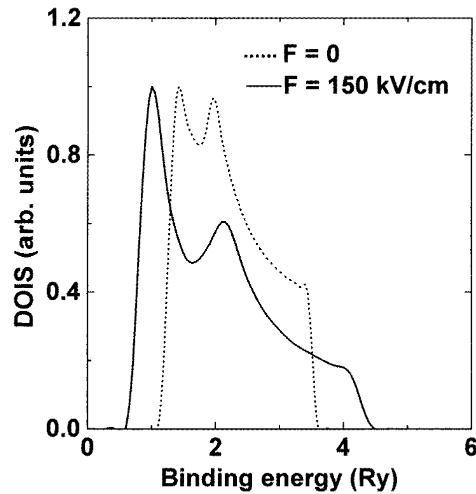

Figure 3. Densities of donor impurity states as a functions of the impurity binding energy, for a QWW with $L_x = 200$ Å and $L_y = 100$ Å, in the presence of an electric field (solid line) and in the absence of an electric field (dotted line).

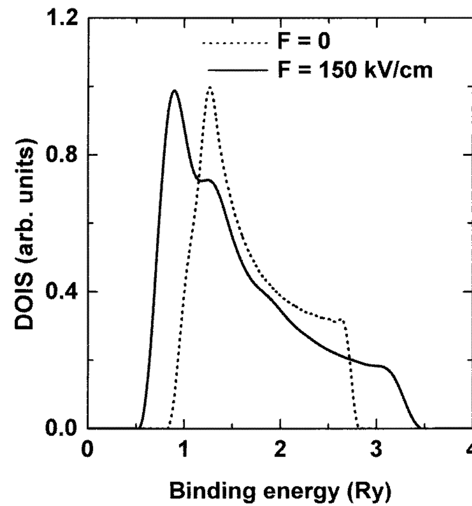

Figure 4. Densities of donor impurity states as a functions of the impurity binding energy, for a QWW with $L_x = L_y = 210$ Å, in the presence of an electric field (solid line) and in the absence of an electric field (dotted line).

In figure 3 we present the shallow donor DOIS for a rectangular cross section GaAs QWW. The dimensions of the systems are the same as in figure 1 ($L_x = 200$ Å and $L_y = 100$ Å). The curves are for zero and 150 kV cm^{-1} electric field, applied in the x-direction, respectively. In both cases, as we discussed above, the DOIS presents *one* structure associated with impurities close to the centre of the transversal section of the wire (3.4 Ryd in the dotted line and 4.05 Ryd in the continuous line). This values are in agreement with those of figures 1(a) and 1(b). For the case with zero electric field the peaks are associated with impurity positions close to the borders of the structure: $|x_i| \sim L_x/2$ with $|y_i| \sim 0$ for the peak at 1.42 Ryd and the other peak at 1.98 Ryd for impurities in the region of $|y_i| \sim L_y/2$ with $|x_i| \sim 0$. The presence of an applied electric field (continuous line) breaks the symmetry of the system along the x-direction and as a consequence the peaks of the DOIS are shifted to lower binding energies. Also, in this case we see a peak with the greater intensity for a binding energy of 1.0 Ryd, associated with impurities located in the region $x_i = L_x/4$ with $|y_i| = L_y/2$. The value of the relative intensity for the peak at 1.0 Ryd is higher than the other peaks due to the low value of the slope of the binding energy as a function of the impurity position. This effect is associated with the shift of the probability electronic density away from the impurity position (see figure 1(b) for $x_i/L_x = 0.25$).

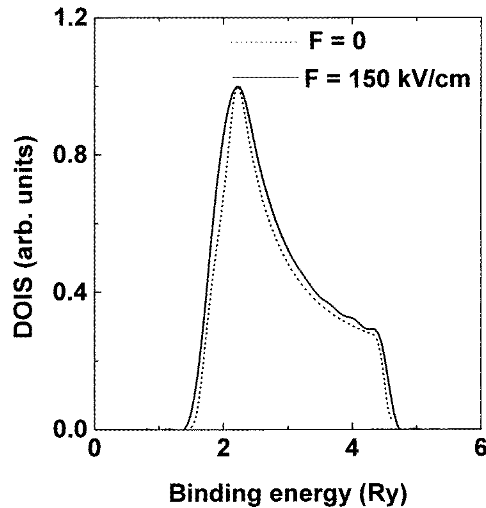

Figure 5. Densities of donor impurity states as a functions of the impurity binding energy, for a QWW with $L_x = L_y = 100$ Å, in the presence of an electric field (solid line) and in the absence of an electric field (dotted line).

In figures 4 and 5 we present our results for the DOIS in square cross section GaAs QWWs, considering the effects of an applied electric field. The dimensions of the QWW are $L_x = L_y = 210$ Å and $L_x = L_y = 100$ Å, respectively. For zero electric field (dotted lines), because of the spatial symmetry of the structures, we observe only two peaks: one, at higher energy, for on-centre impurities and the other, at lower energy, for impurities close to the edges. Due to the applied electric field (continuous lines) the peak with low energy is resolved into two peaks associated with impurities in the regions $x_i = L_x/4$ with $|y_i| = L_y/2$ and the other for $x_i = -L_x/4$ with $|y_i| = L_y/2$. This effect is not observed in figure 5 due to the low dimensions of the structure where the effects of the applied electric field are perceptible [5, 15].

The results we present for the binding energy and the DOIS without considering applied fields are in good agreement with previous reports in GaAs QWs [5] and QWWs [11].

4. Conclusions

We calculated the binding energies and the density of states of hydrogenic shallow donors impurities in quantum-well wires with rectangular cross sections, using a variational procedure within the effective-mass approximation, under the influence of an electric field applied perpendicular to the axis of the wire.

In the absence of an electric field the binding energy is degenerate for symmetrical position of the impurities with respect to the centre of the transversal section of the wire. However, this degeneracy is broken when an electric field is applied in the x-direction. An important effect of the applied electric field is the splitting of the peak into two peaks of smaller intensities in the DOIS when the square symmetry is lost (dotted line in figures 3 and 4). When the electric field is applied in the rectangular cross section (figure 3) we observe that the impurity DOIS is shifted and the shape of the peaks is altered. In conclusion, we found that the electric field and geometric shape of the cross section of QWWs gives interesting features in the DOIS. In particular, our calculation indicates that

the DOIS becomes richer in structure as soon as some symmetry is lost, and when an electric field is applied to the system. Finally, although experimental results for the binding energies of impurities in QWW structures are not yet available, our results indicate that a knowledge of the shape of the DOIS may be of importance in the quantitative understanding of experimental work on shallow impurities in QWW structures.

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