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1997 J. Phys.: Condens. Matter 9 5977

(http://iopscience.iop.org/0953-8984/9/27/023)

J. Phys.: Condens. Matter **9** (1997) 5977–5987. Printed in the UK PII: S0953-8984(97)81609-8

Effects of an applied electric field on the binding energy of shallow donor impurities in GaAs low-dimensional systems

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Received 5 February 1997, in final form 4 April 1997

Abstract. Using a variational procedure within the effective-mass approximation we calculate the binding energy of a shallow donor impurity in cylindrical GaAs low-dimensional systems, under the action of an electric field applied in the axial direction, and considering an infinite confinement potential. We calculate the dependence of the binding energy on the system geometry, the applied electric field, and the donor-impurity position. Our results for small fields and large radius as well as for length greater than the radius coincide quite well with previous results in quantum wells, quantum-well wires, and quantum dots. We find that a proper knowledge of the impurity distribution inside the GaAs low-dimensional system is of relevance in a qualitative comparison between theoretical and experimental results concerning the binding energy of shallow impurities under the action of an applied electric field.

1. Introduction

In the last two decades, with the development of experimental techniques such as molecular beam epitaxy, metal–organic chemical-vapour deposition, and electron beam lithography combined with reverse mesa etching, there has been a lot of interest in the study of the states of hydrogenic impurities in low-dimensional semiconductor heterostructures such as quantum wells (QWs), quantum-well wires (QWWs), and quantum dots (QDs). The effects of applied electric fields on the physical properties of low-dimensional systems constitute a subject of considerable interest from both the theoretical and technological point of view, due to the importance of these systems in the development of new semiconductor devices. In particular, the application of an electric field in the growth direction of the heterostructure gives rise to a polarization of the carrier distribution and to an energy shift of the quantum states. Such effects may introduce considerable changes in the energy spectrum of the carriers, which could be used to control and modulate the intensity output of optoelectronic devices.

Bastard [1] calculated the binding energy of the ground state of a hydrogenic impurity in a QW finding a strong dependence of the energy on the impurity position when it moves along the growth axis of the system. Brown and Spector [2] calculated the binding energy of hydrogenic impurities in cylindrical, infinite-length, GaAs–(Ga, Al)As quantum-well wires for finite and infinite confinement potential. They found for a finite confinement potential that the binding energies coincide for small radius of the QWW for different values of the impurity position along the radial direction. Porras-Montenegro *et al* [3] calculated the ground state energy, the binding energy, and density of states for shallow hydrogenic impurities in cylindrical, infinite-length, GaAs–(Ga,Al)As quantum-well wires.

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In an experimental work Méndez *et al* [4] have found that the application of an electric field may induce a semiconductor–semimetal transition in multiple heterostructures. Using the infinite-confinement potential model, the effects of a longitudinal applied electric field on the density of states and optical-absorption spectra of shallow impurities implanted in a QW have been calculated by Weber [5]. The main feature found was a quenching of one of the peaks due to interface impurities at moderate electric fields. López-Gondar *et al* [6] and Santiago *et al* [7] have shown the electric-field effects on shallow impurity states in GaAs–(Ga, Al)As quantum wells, finding that the density of impurity states as well as the 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 quantum well and at the position at which the binding energy has a maximum. The effects of electric and magnetic fields on the confined impurities in selectively donor-doped QWs have been studied in some detail by Yoo *et al* [8]. They observed that the sensitivity of the absorption-line profile to the impurity distribution increases as the electric-field strength increases, and the impurity distribution is strongly reflected in the absorption-line shape. Latgé *et al* [9–11] studied the effects of both the electric and magnetic fields on the binding energy of donor impurity states in GaAs–(Ga, Al)As QWs finding that a detailed study of the intradonor absorption spectra together with a proper consideration of the impurity doping profile are necessary for a qualitative understanding of the experimental results. Klepfer *et al* [12] have calculated excitonic nonlinear optical processes in GaAs quantum-well wires of rectangular geometry with L and W cross-sectional dimensions in the range of 25–300 Å.

At the moment no results about the effects of applied electric fields on the binding energy of shallow impurities in GaAs–(Ga, Al)As QWWs and QDs have been reported. It is for this reason that in this work we calculate the binding energy of hydrogenic impurities in a low-dimensional system (LDS) under the action of an electric field applied in the axial direction of a finite cylindrical geometry, that could be more appropriate to compare theoretical with experimental results due to the lateral confinement we are considering, and which in the limiting cases reproduces quite well the results for QWs, QDs, and infinite-length QWWs. Furthermore, we think that due to the chosen geometry our results are of importance in the understanding of actual experimental results. In this calculation we work within the effective-mass approximation and adopting a variational envelope wave function for the donor electron. Despite the fact that GaAs–(Ga, Al)As microstructures have wells surrounded by barriers of finite height, in our calculations we use the infinite-confinement-potential model because of computing facilities and because for concentrations of Al $0.3 < x < 0.45$ and for radius of the structure greater than ~ 100 Å the differences with respect to the finite model are not substantial [2, 13]. In section 2 we present the theory of the problem. Our results are presented and discussed in section 3, and our conclusions are given in section 4.

2. Theory

The physical system that we consider is a cylindrical finite-length GaAs LDS surrounded by $Ga_{1-x}Al_xAs$ in which the frame of reference is fixed in its centre and the z axis is defined to be the growth direction of the quantum structure coincident with the axis of the cylinder. For the reasons mentioned before and computational facilities, we use the infinite-model approximation for the confinement potential.

In the effective-mass approximation, the Hamiltonian of a hydrogenic donor impurity in a GaAs–(Ga, Al)As LDS, such as that described above, and in the presence of an electric

field, F, applied in the z direction, may be written as:

$$H = H_0 - \frac{e^2}{\varepsilon r} \tag{1}$$

with

$$H_0 = \frac{p^2}{2m^*} + |e|Fz + V(\rho, z) \tag{2}$$

where $r = ((\rho - \rho_i)^2 + (z - z_i)^2)^{1/2}$ is the distance from the carrier to the impurity site, m^* is the donor impurity effective mass, ε is the static dielectric constant, and $V(\rho, z)$ is the well potential, defined as:

$$V(\rho, z) = \begin{cases} 0 & \rho < R, |z| < L/2 \\ \infty & \rho \geqslant R, |z| \geqslant L/2 \end{cases} \tag{3}$$

where R and L are the wire radius and length, respectively.

In our calculations we use for the donor effective mass $m^* = 0.0665m_0$, where m_0 is the free electron mass.

Our equations and some results, for donor impurities, are given in reduced atomic units which correspond to a length unit of one effective Bohr radius, $a^* = h^2\varepsilon/4\pi^2 m^* e^2 \cong 100$ Å, and an energy unit of one effective Rydberg, $R^* = 2\pi^2 m^* e^4/h^2\varepsilon^2 \cong 5.72$ meV.

In this work we are interested in the calculation of the ground state (this corresponds to a 1s-like state) of a shallow donor impurity in the system described above and we assume the envelope trial wave function as:

$$\Psi(\rho, \varphi, z) = N\Phi(\rho, z)\varphi_\lambda(\rho, \varphi, z) \tag{4}$$

where $\Phi(\rho, z)$ is the eigenfunction of (2) and $\varphi_\lambda(\rho, \varphi, z)$ is the ground state hydrogenic part. The function $\Phi(\rho, z)$ is given by

$$\Phi(\rho, z) = \begin{cases} J_0(\beta)Z(\zeta) & \rho < R, |z| < L/2 \\ 0 & \rho \geqslant R, |z| \geqslant L/2 \end{cases} \tag{5}$$

and the ground state hydrogenic part is:

$$\varphi_\lambda(\rho, \varphi, z) = \exp(-\lambda r) \tag{6}$$

where λ is a variational parameter, $J_0(\beta)$ is the ordinary Bessel function of order zero, and $Z(\zeta)$ is a linear combination of Airy functions:

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

The arguments of the Bessel and Airy functions are:

$$\beta = B_{10}\rho/R \tag{8}$$

and

$$\zeta = a_c\frac{z}{L} - \frac{(E_0 - (B_{10}a^*/R)^2)}{w_c} \tag{9}$$

where B_{10} is the first zero of the Bessel function, $w_c = (|e|Fa^*/R^*)^{2/3}$ and $a_c = (w_c)^{1/2}L/a^*$.

In (7)

$$A_i(\pm)[B_i(\pm)] = A_i[B_i]\left(\pm a_c/2 - \frac{(E_0 - (B_{10}a^*/R)^2)}{w_c}\right) \tag{10}$$

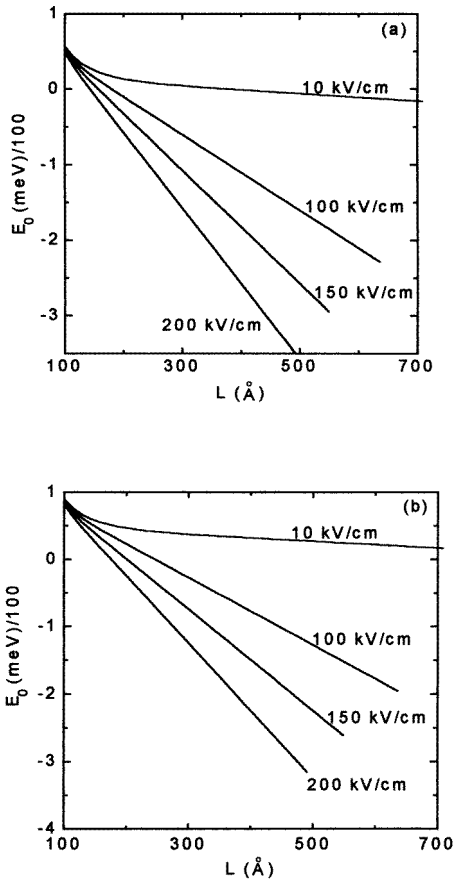

Figure 1. Energy of the ground state of a cylindrical GaAs low-dimensional system with radius of 3000 Å (a) and 100 Å (b) as a function of the system length and for different values of the applied electric field.

and E_0 is the eigenvalue for the Hamiltonian of (2), which is obtained as the first root of the transcendental equation:

$$B_i(+)A_i(-) - A_i(+)B_i(-) = 0. \tag{11}$$

The ground state energy, E_i, of a hydrogenic impurity in a GaAs–(Ga, Al)As LDS with an applied electric field, F, is given by

$$E_i = E_0 - (\lambda a^*)^2 + 2(\lambda a^{*2} - a^*)N^2P + 2\lambda a^{*2}B_{10}N^2G + 2\lambda a^{*2}a_cN^2H \tag{12}$$

where

$$P = \int_0^{2\pi}\int_0^{R}\int_{-L/2}^{L/2}\left(|Z(\zeta)|^2|J_0(\beta)|^2\frac{\exp(-2\lambda r)}{r}\right)\mathrm{d}v \tag{13}$$

$$G = \int_0^{2\pi}\int_0^{R}\int_{-L/2}^{L/2}\left((\rho-\rho_i\cos(\varphi))|Z(\zeta)|^2|J_0(\beta)|\left|\frac{\mathrm{d}J_0(\beta)}{\mathrm{d}\beta}\right|\frac{\exp(-2\lambda r)}{Rr}\right)\mathrm{d}v \tag{14}$$

$$H = \int_0^{2\pi}\int_0^{R}\int_{-L/2}^{L/2}\left((z-z_i)|Z(\zeta)|\left|\frac{\mathrm{d}Z(\zeta)}{\mathrm{d}\zeta}\right||J_0(\beta)|^2\frac{\exp(-2\lambda r)}{Lr}\right)\mathrm{d}v \tag{15}$$

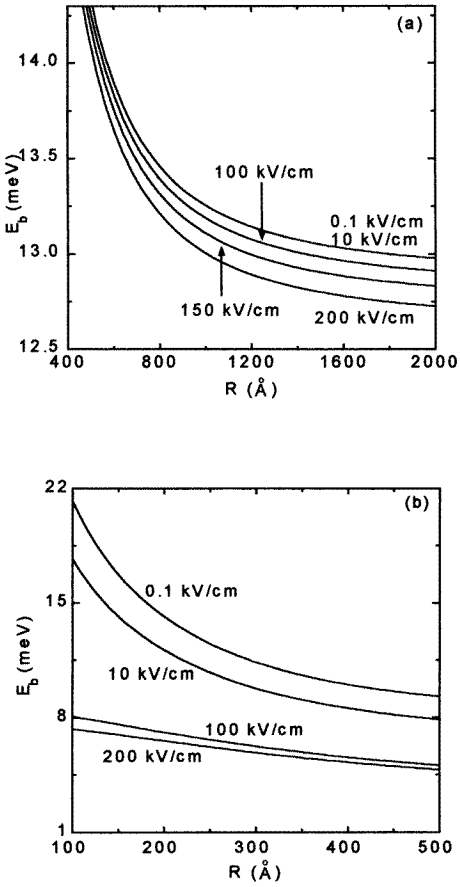

Figure 2. Binding energy of a donor impurity located at the centre of a cylindrical GaAs low-dimensional system, for a length of 100 Å (a) and 400 Å (b), as a function of the radius of the structure and for different values of the applied electric field.

and

$$1/N^2 = \int_0^{2\pi} \int_0^R \int_{-L/2}^{L/2} \left(|Z(\zeta)|^2 |J_0(\beta)|^2 \exp(-2\lambda r) \right) \mathrm{d}v. \tag{16}$$

The binding energy is obtained from the definition:

$$E_b = E_0 - E_i|_{\lambda_0} \tag{17}$$

where λ_0 is the value of λ which minimizes E_b.

With the above equations we calculate the binding energy as a function of the cylinder geometry, applied electric field, and impurity position.

3. Results

In figure 1 we present the energy of the ground state for a LDS without the impurity, for radius of 3000 Å (a) and 100 Å (b) as a function of the length of the cylinder and for different values of the electric field. We observe that the energy diminishes as the length

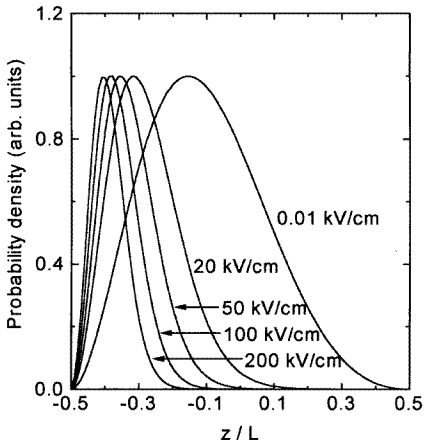

Figure 3. Probability density for the 1s-like donor state in a GaAs low-dimensional system of 100 Å radius and 400 Å length for an impurity position of −200 Å on the axis of the structure and with different values of the electric field.

of the structure is increased and this behaviour is stronger as the magnitude of the electric field is augmented. In comparing the results in the (a) and (b) cases, they show that the effect of the electric field depends entirely on the geometry and has the same behaviour, corresponding to a rigid shift along the energy scale of about 28.6 meV. However the differences in the value of the energy are determined by the radial confinement. In case (b), we practically are in the presence of a QD, while in (a) the system is like a QW.

In figure 2 we display the binding energy for a LDS, for lengths of 100 Å (a) and 400 Å (b) as a function of the structure radius, for different values of the electric field and with the impurity located at the centre of the cylinder. In (a) we observe that for an electric field less or equal than 10 kV cm^{-1}, the effect on the binding energy its not appreciable. For electric fields larger than 10 kV cm^{-1}, in contrast the effect of the electric field on the binding energy is notorious, showing a decrease in its magnitude. When the radius of the cylinder is increased the geometric confinement of the electron is diminishing and for this reason we observe a decreasing binding energy. This effect is larger for radius less than 1200 Å. However, due to the small value of length, 100 Å, the binding energy keeps high values larger than 12.54 meV. The interpretation for this behaviour is that the small length imposes a high axial confinement on the electron wave function. In (b), for a length of 400 Å, we notice that for weak electric fields, less than or equal to 10 kV cm^{-1}, we obtain an appreciable effect of the electric field on the binding energy. For higher values of the field, equal or larger than 100 kV cm^{-1}, the effect of the electric field is small due to the concentration of the electronic probability density close to negative values in the axial direction, see figure 3. For electric fields of 0.1 kV cm^{-1} and 10 kV cm^{-1}, when the radius of the system is increased, the binding energy decreases rapidly to 8.55 meV (1.5 R^*). This value is slightly higher than the similar one in the bulk of GaAs, 5.7 meV (1.0 R^*), due the effect of geometric confinement. However for higher electric fields, 100 kV cm^{-1} and 200 kV cm^{-1}, we obtain the same behaviour but softer and with values lower than in the bulk limit, due precisely to the action of the electric field.

In figure 3 we present the electronic probability density, in the z direction, for the 1s-like state in a GaAs LDS of radius 100 Å and length 400 Å. The impurity is positioned at −200 Å on the z axis of the system and different values of the electric field are applied in the

axial positive direction (in all curves the maxima of the probability density are normalized to unity). We observed that the maximum of the probability density is shifted to the left side as the field increases. For electric fields less than 20 kV cm^{-1} the shift is larger than for higher fields, a situation in which there is a strong concentration of the electronic probability density at the left edge of the structure, and consequently the binding energy remains almost constant in this limit.

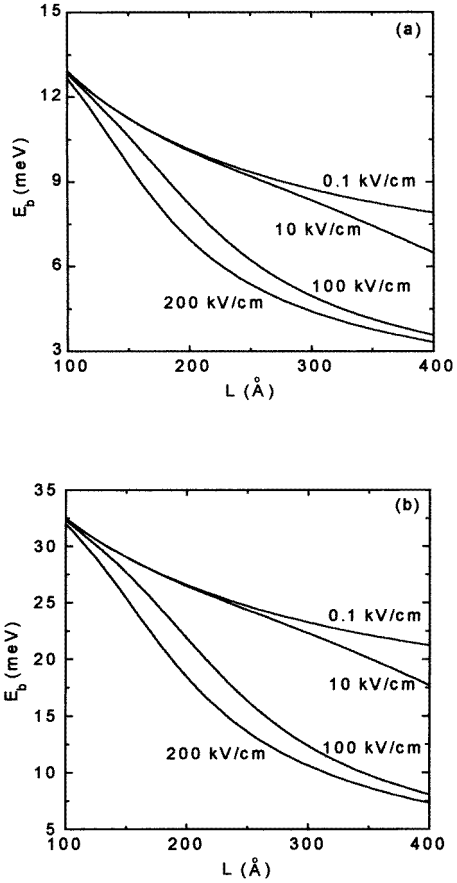

Figure 4. Binding energy of a donor impurity located at the centre of a cylindrical GaAs low-dimensional system as a function of the length, for structures of radius 3000 Å (a) and 100 Å (b), and for different values of the electric field.

The binding energy of a donor impurity located at the centre of the structure as a function of length, and for different values of the electric field, is shown in figure 4, (a) and (b), for cylinders of radius 3000 Å and 100 Å, respectively. We observe that the behaviour of the binding energy is quite similar in both cases, diminishing as the length and the electric field increase. However, for every value of the applied electric field the variation of the binding energy is larger in (b) than in (a) due to the higher geometric confinement in the radial direction, which is in correspondence with the results presented in figure 1.

In figure 5 we show the binding energy of a donor impurity located at the centre of the LDS as a function of the applied electric field for different geometries of the system. We observe that in cases for which there is a high geometric confinement in the axial

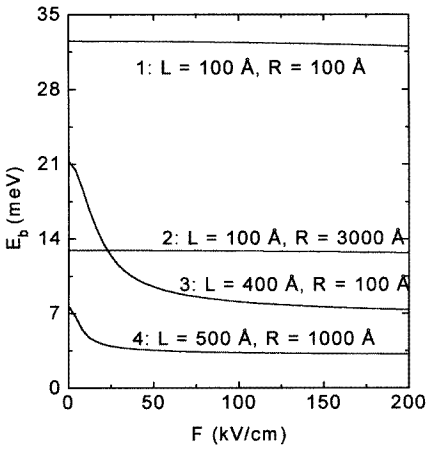

Figure 5. Binding energy of a donor impurity in a cylindrical GaAs low-dimensional system located at the centre of the structure as a function of the applied electric field and for different dimensions of the cylinder.

direction the binding energy is practically independent of the applied electric field. When this confinement diminishes there is a noticeable decrement of the binding energy for the electric fields up to 75 kV cm^{-1}. This is because the effect of the electric field on the carrier distribution produces a strong shift of the electronic probability density with respect to the impurity (see figure 3). In case 1 where the situation is similar to a QD, in the limit of zero electric field our results are in agreement with those reported by Porras-Montenegro *et al* [14, 15], while in case 2 which corresponds to the QW limit, our results coincide in good agreement with those found by Weber [5] and López Gondar *et al* [6] in the whole range of applied electric fields.

Our calculations for the effect of the electric field on the binding energy of a donor impurity located at different positions on the z axis in LDSs of different geometries are displayed in figure 6. For all cases, when the electric field is close to zero, negative and positive directions on the cylinder are indistinguishable. For this reason the probability density has reflection symmetry in the axial direction for symmetric positions of the impurity with respect to the centre of the structure. As a consequence, for axial symmetric positions of the impurity along the z axis, the binding energy has the same value. In (a) and (b), for $z_i = -L/2$ and $z_i = -L/4$ it is observed that the binding energy increases linearly with the applied electric field, while for the situation in which the impurity is located at the right of the centre, $z_i = L/4$ and $z_i = L/2$, the binding energy decreases linearly with the increase of the applied electric field. This behaviour is because the electric field makes the electron approach (leave) the impurity depending on the impurity position, causing the binding energy to increase (decrease). In figure 6(c), for $z_i = -L/4$, we observe a special behaviour in the binding energy as a function of the applied electric field. Different to the corresponding cases in (a) and (b), the binding energy presents a maximum when the electric field is close to 20 kV cm^{-1}. This is because as the electric field is increased up to this value the electronic probability density around the impurity is enhanced. The opposite situation occurs for higher values of the electric field. Consequently an analogous behaviour is observed in the binding energy.

In figure 7 we present the binding energy of a donor impurity in a cylindrical finite-length GaAs LDS for different values of the electric field as a function of the impurity

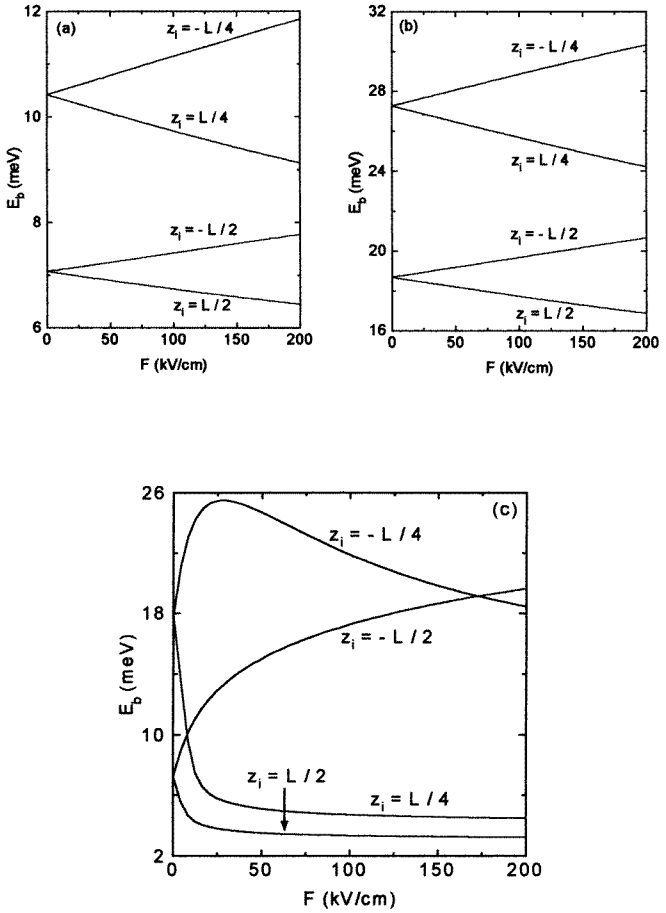

Figure 6. Binding energy of a donor impurity located at different positions along the z axis of a cylindrical GaAs low-dimensional system as a function of the applied electric field for different dimensions of the structure: $L = 100$ Å and $R = 3000$ Å (a), $L = 100$ Å and $R = 100$ Å (b), and $L = 400$ Å and $R = 100$ Å (c).

position along the cylinder axis and for different geometries. We observe that the binding energy is larger for impurity positions at the left, with respect to the symmetrical position at the right of the centre of the structure, due to the action of the applied electric field which displaces the probability density to the left of the structure (see figure 3). This difference is larger for higher fields. It is important to note that for high electric fields, 100 kV cm^{-1} and 200 kV cm^{-1}, and for large length values, the binding energy is the same when the impurity is close to the right border of the LDS, as shown in figure 7(b). This result is expected due to the high concentration of the probability density at the left of the cylinder.

4. Conclusions

Using the effective-mass approximation and within a variational procedure we have calculated the binding energy of the 1s-like state in cylindrical GaAs–(Ga, Al)As low-dimensional structures (QWs, QWWs, and QDs), within the infinite-confinement-potential

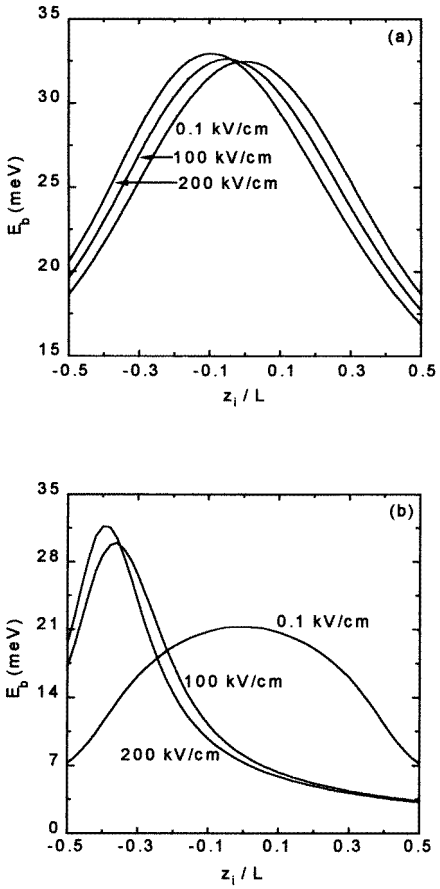

Figure 7. Binding energy of a donor impurity in a cylindrical GaAs low-dimensional system for different values of the electric field, as a function of the impurity position for different dimensions of the system: $R = 100$ Å and $L = 100$ Å (a) and $R = 100$ Å and $L = 400$ Å (b).

model, and axial applied electric field. We found that our results in the limiting cases approximate quite well to those reported by other authors in QDs, QWs, and infinite-length QWWs. The electric field enhances the electronic probability for negative values of the axial direction given a noticeable decrement (increment) in the binding energy for impurities located at the centre and at the positive (negative) part of the LDS axis. For small lengths of the structure, of the order of 100 Å, the binding energy is not sensitive to the variations of the electric field and only depends on the variations of the structure radius, while for LDSs of 500 Å length the binding energy strongly decreases with the increment of the applied electric field up to values of approximately 75 kV cm^{-1}, since for higher values the electronic wave function is concentrated at the negative region of the axial direction. We found that the binding energy depends on the structure geometry and on the impurity position and increases noticeably when its location is shifted in a direction contrary to that of the applied electric field. Our results indicate that a proper knowledge of the impurity distribution inside the structure is of relevance in a quantitative comparison between theoretical and experimental results concerning the binding energy of shallow impurities under the action of an applied electric field.

Acknowledgments

This work was partially financed by the Colombian Scientific Agency Colciencias. CAD is grateful for the hospitality at the Department of Physics of the Universidad del Valle (Cali, Colombia) where part of this work was done. NP-M thanks Dr M Virasoro for his hospitality at the ICTP at Trieste, where part of this work was done.

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