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Binding Energy of the Ground and First Few Excited States of a Shallow-Donor Impurity in Rectangular-Cross-Sectional Area GaAs Quantum-Well Wires under Applied Electric Field

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Using a variational approach within the effective mass approximation we calculate the binding energy of the ground and some excited donor impurity states in quantum-well wires with rectangular and cylindrical transversal sections under the action of applied electric fields. We study the binding energy as a function of the geometry of the system, the applied electric field as well as the impurity position inside the structure. We found that the presence of the electric field breaks down the degeneracy of states for impurities symmetrically positioned within the structure, and that the geometric confinement and the electric field are determinant for the existence of bound excited states in these structures.

Introduction. The development of experimental techniques such as molecular beam epitaxy, metal-organic chemical-vapor deposition, and electron beam lithography combined with reverse mesa etching, has permitted the study of hydrogenic impurity states in low-dimensional semiconductor heterostructures, such as quantum wells (QWs) [1], quantum-well wires (QWWs) [2], and quantum dots (QDs) [3].

Electric fields have become an interesting probe for studying the physical properties of low-dimensional systems, both from the theoretical and technological point view. For example, the application of an electric field in the growth direction of the heterostructure produces a polarization of the carrier distribution and an energy shift of the quantum states. The effects of electric and magnetic fields on the confined impurities in QWs have been studied by some authors [4 to 6], 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. Some works have been reported about the binding energies of the ground and first few excited impurity states in QWs [7, 8] and QWWs [9] heterostructures without applied electric fields. They have shown that for sufficiently small QW widths (or QWW radius) some impurity excited states are not bound. Recently, we have studied the effects of an applied electric field on the binding energy of the ground state of shallow donor impurities in cylindrical finite length GaAs low-dimensional systems (LDS) [10] and in rectangular GaAs QWWs [11]. 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 opposite to that of the applied electric field.

In this paper, we calculate the binding energy for the ground and first few excited states of hydrogenic donor impurities in rectangular and cylindrical transversal section GaAs QWWs under the action of an electric field. In this calculation we work within the effective-mass approximation and adopt a variational envelope-wave function for the electron. 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.

Theoretical Framework. The physical systems that we consider are a cylindrical finite length GaAs LDS and a rectangular transversal section GaAs QWW in which the frame of reference is fixed in its center and the z-axis is defined to be the axis of the cylinder and of the rectangular-sectional wire.

In the effective mass-approximation, the Hamiltonian of a hydrogenic donor impurity in a GaAs–(Ga,Al)As heterostructure, such as those described above, and in the presence of an electric field, F, applied in the z-direction (for cylindrical LDS) or in x-direction (for rectangular QWWs) may be written as

$$H = \frac{p^2}{2m^*} + |e|\, F\xi + V_c - \frac{e^2}{\varepsilon r}\Bigg|, \tag{1}$$

where r is the distance between the carrier and the impurity site, $m^* = 0.0665m_0$ (where m_0 is the free electron mass) is the donor-impurity effective mass, ε is the static dielectric constant, e is the electron charge, and V_c is the confinement potential, which is taken as zero inside the heterostructure and infinite otherwise. In the second term at the right, $\xi = x$ for the rectangular QWWs case and $\xi = z$ for the cylindrical LDS.

In this paper, we are interested in the calculation of the ground and first few excited states of a shallow donor impurity in the system described above and we assume the envelope trial wave functions as

$$\Psi_{nl}(\mathbf{r}) = N_{nl}\Phi(\varrho, z)\, \Gamma_{nl}(\mathbf{r}, \{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}), \tag{2}$$

where N_{nl} are normalization constants, Φ is the eigenfunction of Hamiltonian in Eq. (1) without the impurity-potential term at the right [10, 11], and Γ_{nl} are the hydrogenic wave functions [9, 12]. The numbers n and l are principal and orbital angular momentum quantum numbers. In this work we consider $n = 1, 2, 3$ with $l = 0, 1$. Here the λ_{nl} are variational parameters; we follow the work by Chaudhuri and Bajaj [8] on GaAs–(Ga,Al)As QWs and Latgé et al. [9, 12] on GaAs–(Ga,Al)As infinite QWWs and determine the β_{nl} and α_{nl} by requiring that the Γ_{nl} form a set of orthogonal functions in all space.

The binding energy is calculated from the definition

$$E_b(n, l) = E_0 - E_{nl}|_{\{\lambda_0, \beta_0, \alpha_0\}}, \tag{3}$$

where E_{nl} is the expectation value of the energy corresponding to the Hamiltonian in Eq. (1), $\{\lambda_0, \beta_0, \alpha_0\}$ is the set of variational parameters that minimizes E_{nl}, and E_0 is the eigenvalue for the Hamiltonian (1) without the impurity-potential term.

In the following section, the results for donor impurities are given in reduced atomic units [2].

Results. In Fig. 1 we present the transversal section of the rectangular-cross-sectional area QWW used in our calculations. Special points of the impurity position and the

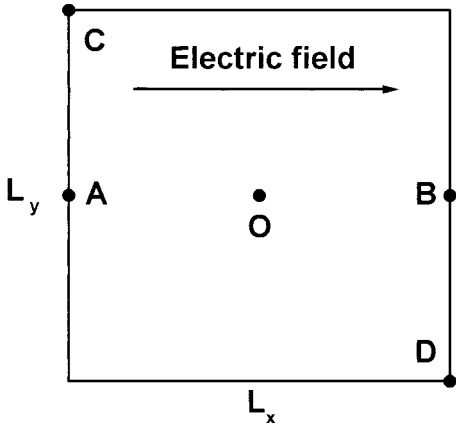

Fig. 1. Cross-sectional area of the GaAs QWW under study, with special points of the impurity position labeled A, B, C, D, and O. For all cases the electric field is applied in the x-direction

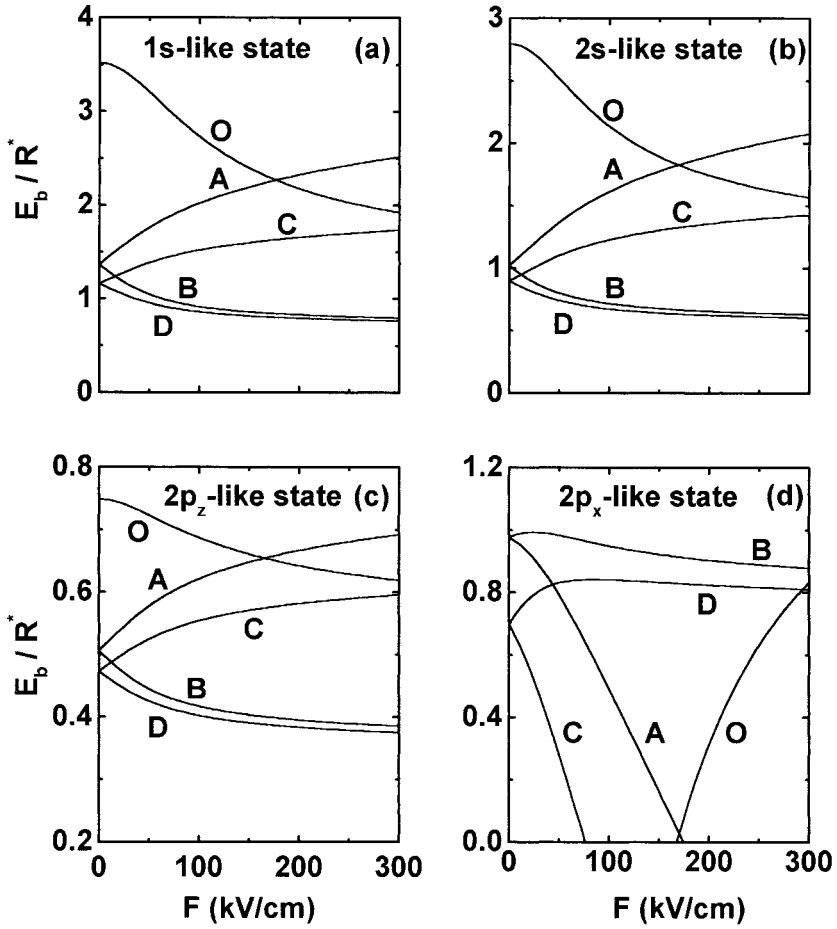

Fig. 2. Binding energies of the 1s, 2s, $2p_x$, and $2p_z$-like states of a donor impurity in a rectangular cross-sectional area GaAs QWW, with $L_x = 2L_y = 2a^*$, as a function of the applied electric field and for different impurity positions (see Fig. 1)

direction of the applied electric field are shown. The reference frame axis is taken at the center of the transversal section of the wire.

In Fig. 2 we present the binding energy for the ground and some few excited states in a rectangular cross-sectional area GaAs QWW, with $L_x = 2L_y = 2a^*$, as a function of the applied electric field and for different impurity positions (see Fig. 1). It is observed that for zero electric field the binding energy is degenerate for impurity states corresponding to symmetrical positions of the impurity. Notice that when the electric field is not zero the degeneracy is removed and the difference in energies increases with the applied electric field. In Figs. 2a, b, and c the breaking of the degeneracy, for symmetrical positions of the impurity (A and B or C and D), is well understood considering the fact that the probability density increases (decreases) close to the impurity position due to the action of the applied electric field. One observes in Figs. 2a, b, and c that for increasing values of electric field, the impurity binding energy for the special point B tends rapidly to the same value at the on-edge D and in both cases goes to a constant value, due to the fact that the electronic probability density is displaced further to the left of the impurity. Fig. 2d shows that for the impurity positions labeled B and D, when their degeneracies are broken with increasing field, the binding energies increase until a certain field strength and beyond this value they start to decrease smoothly. This is due to the fact that the wave function expands with increasing field strength, resulting in a lower kinetic energy. At the beginning of this process the kinetic term is the dominant one and the binding energy increases; but as the probability amplitude of the carrier becomes expanded a competitive situation arises between the kinetic and electrostatic terms until the last term becomes predominant. Eventually, this term also decreases as a consequence of the separation between the electron and the impurity which in turn results in a slow decrease of the binding energy. Note that in Fig. 2d we obtain unbound states beyond field strengths of 174 and 72 kV/cm for impurity positions A and

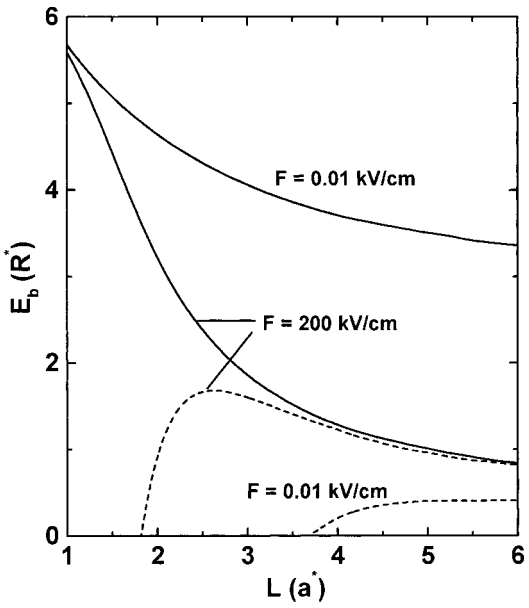

Fig. 3. Binding energy of the ground and some donor impurity excited states, for impurities at the center of the system, as a function of the length of a cylindrical GaAs low-dimensional system of radius $1a^*$ and considering two situations for an external electric field. Solid lines are for 1s, 2s, and 3s-like states. Dashed lines are for $2p_z$ and $3p_z$-like states

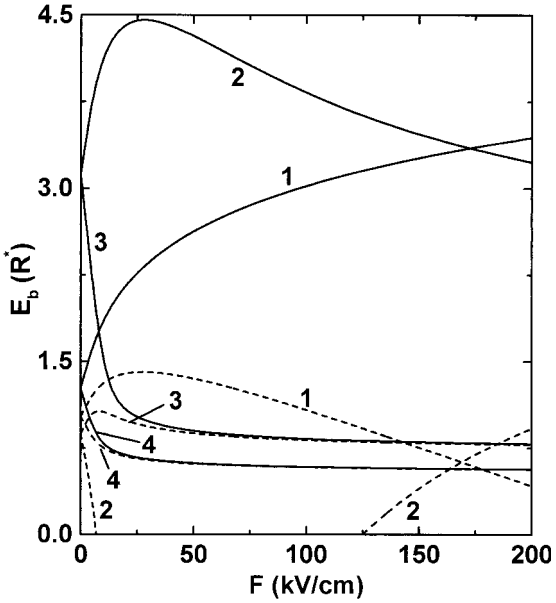

Fig. 4. Binding energy for the ground and some donor impurity excited states as a function of applied electric field for impurities implanted at four different positions along the z-axis (1) $z_i = -L/2$, (2) $-L/4$, (3) $+L/4$, and (4) $= +L/2$ in a cylindrical GaAs low-dimensional system of radius $1a^*$ and length $4a^*$. Solid lines are for 1s, 2s, and 3s-like states. Dashed lines are for $2p_z$ and $3p_z$-like states

C, respectively. In the case in which the position of the impurity is at the center (curve O), the kinetic energy decreases as the field increases until the bound state appears for electric fields greater than 168 kV/cm, approximately.

In Fig. 3 we report the binding energy for the ground and some impurity excited states, for impurities on the center of the system, as a function of the length of the cylinder of radius $1a^*$ and considering two situations for the applied electric field. We observe that the states with same l and different n are degenerate due to the small values of the dimensions of the system. It is because we consider the orthogonality between the hydrogenic functions over all space and for this reason the zeros of the 2s and 3s-like functions fall out of the cylinder. The same situation occurs for $2p_z$-like and $3p_z$-like states. For a fixed value of the length we observe that the binding energy for states with $l = 0$ diminishes with the presence of an external electric field, whereas for states with $l = 1$ on the contrary the binding energy increases. For states with $l = 0$ the situation is due to a reduction in the electrostatic interaction, whereas for states with $l = 1$ the situation occurs due to a reduction in the kinetic energy of the electron.

In Fig. 4 we present the binding energy for the ground and some impurity excited states for donor impurities implanted at four different positions along the z-axis in a cylindrical finite length GaAs LDS of radius $1a^*$ and length $4a^*$. In accordance with the results in Fig. 1, we observe that the states with same n and different l are degenerate. The increase or decrease in the binding energy is due to the fact that the electric field produces a variation of the expected value of the electron distance with respect to the impurity and for this reason the electrostatic interaction changes.

Conclusions. Using the effective-mass approximation within a variational scheme, we have studied the role of the electric field on the binding energy of the ground and first few excited states of a shallow donor impurity in rectangular cross-sectional area and

cylindrical finite length GaAs–(Ga,Al)As low-dimensional structures. We found that electric field breaks down the degeneracy of the ground and excited states corresponding to symmetrically positioned impurities along the axial direction, in the cylindrical structure, or in the transversal section for rectangular-cross sectional QWWs. Also, we observed that together with the geometry of the system and the impurity position, the applied electric field is determinant for the existence of bound donor impurity excited states in heterostructures where the quantum confinement plays a fundamental role (see p_x-like states in rectangular QWWs and p_z-like states in cylindrical systems). For the cylindrical case, we obtain that the states with same l and different n are degenerate. This behavior does not occur for rectangular QWWs due to the infinite length along the z-direction. 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 applied electric fields.

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References

[1] G. BASTARD, Phys. Rev. B **24**, 4714 (1981).
[2] J. W. BROWN and H. N. SPECTOR, J. Appl. Phys. **59**, 1179 (1986).
[3] F. J. RIBEIRO and A. LATGÉ, Phys. Rev. B **50**, 4913 (1994).
[4] R. B. SANTIAGO, L. E. OLIVEIRA, and J. ÁLBUQUERQUE E CASTRO, Phys. Rev. B **46**, 4041 (1992).
[5] B. YOO, B. D. MCCOMBE, and W. SCHAFF, Phys. Rev. B **44**, 13152 (1991).
[6] A. LATGÉ, N. PORRAS-MONTENEGRO, and L. E. OLIVEIRA, Phys. Rev. B **51**, 2259 (1995).
[7] R. L. GREENE and K. K. BAJAJ, Solid State Commun. **45**, 825 (1983).
[8] S. CHAUDHURI and K. K. BAJAJ, Phys. Rev. B **29**, 1803 (1984).
[9] A. LATGÉ, N. PORRAS-MONTENEGRO, and L. E. OLIVEIRA, Phys. Rev. B **45**, 9420 (1992).
[10] C. A. DUQUE, A. MONTES, A. L. MORALES, and N. PORRAS-MONTENEGRO, J. Phys.: Condensed Matter **9**, 5977 (1997).
[11] A. MONTES, C. A. DUQUE, and N. PORRAS-MONTENEGRO, J. Appl. Phys. **81**, 7890 (1997).
[12] A. LATGÉ, M. DE DIOS-LEYVA, and L. E. OLIVEIRA, Phys Rev. B **49**, 10450 (1994).