Impurity Excited States in GaAs Low Dimensional Systems Under Applied Electric Fields

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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 low dimensional systems with finite length cylindrical geometry, 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 in the quantum well, quantum-well wire and quantum dot limits of the finite length cylinder our results are in good agreement with previous reports in those structures. Also, we found that the presence of the electric field breaks down the degeneracy of positioned symmetrical impurity ground and excited states in these kind of structures.

I. Introduction

The understanding of the properties of impurity energy levels in low-dimensional semiconductors structures, such as quantum wells (QW's), quantum-well wires (QWW's), and quantum dots (QD's)[1-4], is a subject of interest due to possible technological applications in electronic devices associated with these systems. In these nanostructures, besides Coulombic interactions, the impurities are affected by confining potentials which are more important as the dimension of the system is reduced.

In an experimental work Méndez et al.[5] have found that the application of an electric field may induce semiconductor-semimetal transition in multiple heterostructures. The effects of electric and magnetic fields on the confined impurities in QWs have been studied by some authors[6-11], 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. Extensive theoretical studies about the effects of an applied electric field on energy levels in a surface quantum wire and on the transmission properties of electrons in Fibonacci semiconductor superlattices have been made[12, 13]. Greene and Bajaj[14] and Chaudhuri and Bajaj[15] have calculated the binding energies of the ground and first few excited impurity states for QW heterostructures without applied electric fields. They found that for certain well widths (L) some impurity excited states are not bounded, particularly those for which the wave function is oriented in the growth direction of the structure. Latgé et al.[16] have calculated infrared transitions between hydrogenic states in cylindrical infinite length GaAs-(Ga,Al)As QWW's without applied electric field. They have also found that the states $2p_x(2p_y)$ and $3p_x$ $(3p_y)$ are not bounded when the radius of the wire is sufficiently small. Additionally they showed that with the increase of the wire radius it is possible to find reversed transitions between some states. Recently, we have studied the effects of an applied electric field on the binding energy of the ground state of donor shallow impurities in cylindrical finite length GaAs low-dimensional systems (LDS)[18]. We found that the binding energy depends on the structure geometry and on the impurity position and increases noticeable when its location is shifted in a direction contrary to that of the applied electric field.

In this work we calculate the binding and transition energies for the ground and first few excited states of hydrogenic impurities in cylindrical finite length GaAs LDS under the action of an electric field, applied in the axial direction, which is an excellent probe to study and modify the electric response of optoelectronic devices. In this calculation we work within the effective-mass

approximation and adopt a variational envelope-wave function for the donor electron. In Sec. II we present the theory of the problem. Our results are presented and discussed in Sec. III, and our conclusions are given in Sec. IV.

II. 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 center and the z axis is defined to be the growth direction of the quantum structure coincident with the axis of the cylinder.

In the effective mass-approximation, the Hamiltonian of a hydrogenic donor impurity in a GaAs-(Ga,Al)As LDS, such as the described above, and in the presence of an electric field, F, applied in the z direction may be written as:

$$H = \frac{p^2}{2m^*} + |e|Fz + V(\rho, z) - \frac{e^2}{\epsilon r}, \qquad (1)$$

where r is the distance between the carrier and the impurity site, m^* is the donor-impurity effective mass, ϵ is the static dielectric constant, e is the electron charge, and $V(\rho, z)$ is the barrier potential, which is taken as zero inside the heterostructure (with radius R and length L) and infinite otherwise.

In our calculations we use for the donor effective mass $m^* = 0.0665m_0$, where m_0 is the free electron mass. Additionally our results, for donor impurities, are given in reduced atomic units[2].

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

$$\Psi_{nl}(\mathbf{r}) = N_{nl}\Phi(\rho, z)\Gamma_{nl}(\mathbf{r}, \{\lambda_n\beta_{nl}, \alpha_{nl}\}), \qquad (2)$$

where $\Phi(\rho, z)$ is the eigenfunction of Hamiltonian in Eq. (1) without the impurity-potential term at the right and Γ_{nl} are the hydrogenic wave functions[16, 17]. n and l are the principal and orbital angular momentum quantum numbers, respectively. In this work we consider $n = 1, 2, 3$ with $l = 0, \pm 1$ (which correspond to the hydrogenic states s, pz, and $p_{x,y}$). Here the λ_{nl} are variational parameters. We determine the parameters β_{nl} and α_{nl} by requiring that the form a set of orthogonal functions in all space[15-17]. The function $\Phi(\rho, z)$ is given by ,

$$\Phi(\rho, z) = \begin{cases} J_0(\beta)[B_i(+)A_i(\zeta) - A_i(+)B_i(\zeta)]; & \rho < R, |z| < L/2 \\ 0; & \rho \geq R, |z| \geq L/2, \end{cases} \qquad (3)$$

where $J_0(\beta)$ is the ordinary Bessel function of order zero, and $A_i(B_i)$ are the Airy functions.

The arguments of the Bessel and Airy functions are $\beta = B_{10}\rho/R$ and $\zeta = a_c\frac{z}{L} - \frac{(E_0-(B_{10}a^*/R)^2)}{w_c}$, where B_{10} is the first zero of the Bessel function, $w_c = (|e|Fa^*/R^*)^{2/3}$ and $a_c = (w_c)^{1/2}L/a^*$. E_0 is the eigenvalue for the Hamiltonian (1) without the impurity-potential term at the right, and which is obtained as the first root of one transcendental equation [6]. $A_i(+)[B_i(+)]$ correspond to evaluate the argument ζ in $z = +L/2$.

The binding energy, E_b, is calculated from the definition:

$$E_b(n, l) = E_0 - \langle\Psi_{nl}|H|\Psi_{nl}\rangle|_{\{\lambda_0,\beta_0,\alpha_0\}}, \qquad (4)$$

where $\{\lambda_0, \beta_0, \alpha_0\}$ is the set of variational parameters that minimizes E_b.

The possible infrared transitions are conditioned by $\Delta l = \pm 1$ and the respective energies are obtained from $|E_b(n, l) - E_b(n', l')|$, where the bars correspond to the absolute value.

III. Results

In Fig. 1. we present the binding energy as a function of the axial length for the ground and some few excited states in a cylindrical finite length GaAs LDS with hydrogenic impurity located at the center of the cylinder and for an applied electric field of 100 kV/cm. In (a), where the radius of the system is 30 a^* and the applied electric field is 100 kV/cm, we observe that the $2p_z$-like and $3p_z$-like states are bounded only for length values greater than 2.6 a^* and 3.0 a^*, respectively. Additionally it is noticed that the binding energy diminishes, except for the $2p_z$-like and $3p_z$-like states, due to the displacement of the maximum of the probability density to negative values in the axial direction. In (b), where the radius of the cylinder is 1 a^*, we consider two situations for the applied electric field: the zero physical limit ($F \sim 0.01$ kV/cm) and 200 kV/cm. In this

case, 1 (b), 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 $l = 1$ the binding energy increases. For states with $l = 0$ the situation is due to a reduction on the electrostatic interaction, whereas for states with $l = 1$ the situation occurs due to a reduction on the kinetic energy of the electron.

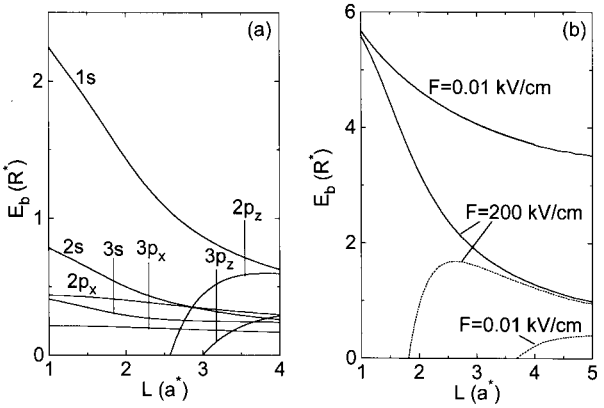

Figure 1. Binding energy as a function of the axial length of the system for the ground and first few excited states of a donor impurity located at the center of a cylindrical finite length GaAs low-dimensional system. In (a) the radius of the system is 30 a^* and the applied electric field is 100 kV/cm. In (b) the radius 1 a^* and two values of the applied electric field are considered. In (b) solid lines are for states 1s, 2s, and 3s-like whereas dotted lines are for states $2p_z$ and $3p_z$-like.

Some of the infrared transition energies are presented in Fig. 2 as a function of the length of the cylindrical finite length GaAs LDS for a donor impurity located at the center of the system and for an applied electric field of 100 kV/cm. Note that for $L = 2.75a^*$ there is a crossing in the energy levels of the $3s$-like and $2p_z$-like states [cf. Fig. 1] which explains the behavior of the curve labeled $3s \rightarrow 2p_z$ in Fig. 2. For $L > 2.75a^*$, the transition is reversed[16], and occurs from $2p_z$-like state to $3s$-like state. The same behavior occurs for the transitions $2s \rightarrow 3p_z$. The reverse transitions are observed for values of the radius (the length) of the structure for which the energy of the second state becomes greater than the binding energy of the first one. In this situation the probability amplitude of the second state is greater than the probability amplitude for the first one. Thought in terms of the uncertainty principle it means that the binding energy of the second state must be greater than that of the one leading to the reverse transition.

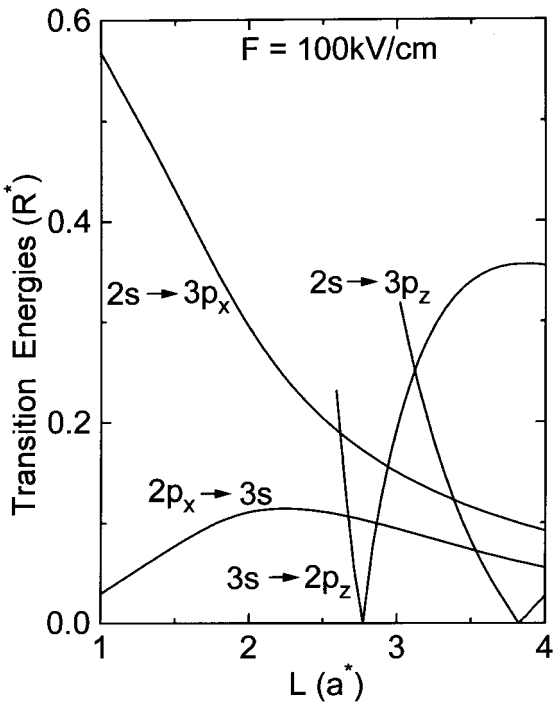

Figure 2. Infrared transition energies as a function of the axial length of a cylindrical finite length GaAs low-dimensional system for a donor impurity located at the center of the system (30 a^* in radius), and for an applied electric field of 100 kV/cm.

In Fig. 3 we display the binding energy for the ground and some donor impurity excited states as a function of the impurity position along the axial direction of a cylindrical finite length GaAs LDS, and for an applied electric field of 80 kV/cm. Our results for this LDS ($R = 30a^*$ and $L = 3a^*$) are in good agreement with those reported by Weber[19] in a QW. In all impurity states, the binding energy decreases for impurity positions close to the edges of the structure, due to the increasing of the carrier kinetic energy as a result of the compressing of the wave function for impurity positions close to the left edge of the well, while for impurity positions close to the right edge this reduction of the binding energy is due to decompressing of the wave function by the action of the applied electric field. In the physical limit of zero field (in our case $F \sim 0.01$ kV/cm due to the argument of Airy functions where it is impossible to put $F = 0$) the states $2p_z$-like and $3p_z$-like are symmetrically bounded for impurities implanted close to the two axial borders of the system. The presence of an external field breaks this symmetry and for this reason the states p_z-like are bounded for impurities implanted close to the center of the structure.

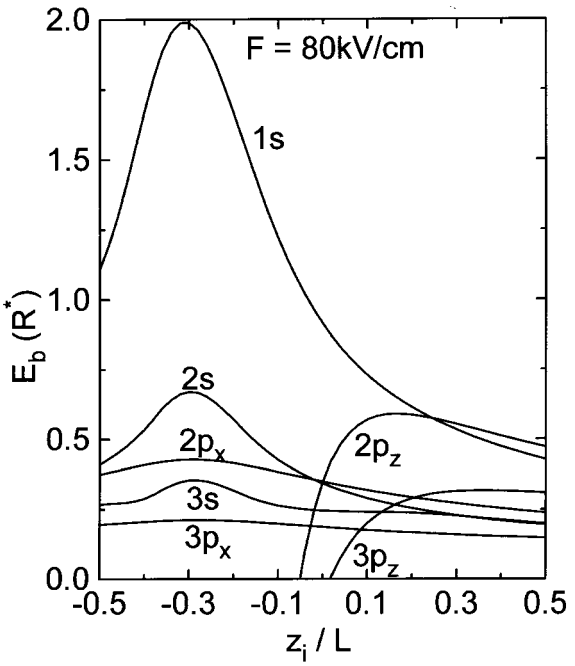

Figure 3. Binding energy for the ground and some few excited states of a donor impurity in a cylindrical finite length GaAs low-dimensional system with radius 30 a^* and length 3 a^* as a function of the impurity position in the axial direction and for an applied electric field of 80 kV/cm.

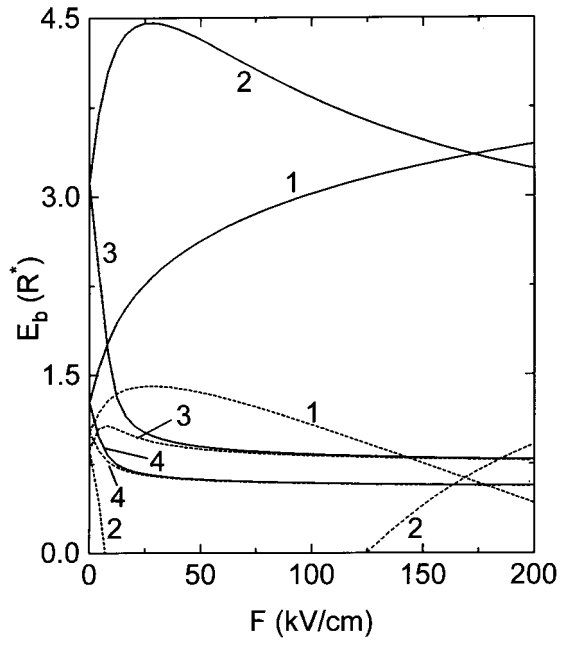

Figure 4. Binding energy for the ground and some donor impurity excited states as a function of an applied electric field for impurities implanted at four different positions along the z-axis ($zi = -L/2$(1), $z_i = -L/4$(2), $z_i = +L/4$ (3), and $z_i = +L/2$ (4)) in a cylindrical finite length GaAs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

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 1 a^* and length 4 a^*. We observe that the states with same n and different l are degenerate due to the small values of the dimensions of the system [see to Fig. 1 (b)]. It is because we consider the orthogonality between the hydrogenic functions over all space and for this reason the zeros of the functions $2s$-like and $3s$-like fall out of the system. The same situation occur between states $2p_z$-like and $3p_z$-like. Additionally, due to the small value of the radius the wave function for states p_x-like are strongly compressed and for this reason they are not bounded. The increases or decreases on 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.

IV. Conclusions

By means of the effective-mass approximation and within a variational procedure we have calculated the binding energy of the ground and some excited states of a donor impurity in cylindrical finite length GaAs-(Ga,Al)As low-dimensional structures, within the infinite confinement potential model and with an electric field applied parallel to the axial direction. We have found that the presence of the electric field resolves the degeneracy of the ground and excited impurity states corresponding to impurity positions symmetrically located with respect to the center of the structure. Also, we found that together with the system geometry and the impurity position, the applied electric field is determinant for the existence of bound donor impurity excited states in LDS where the quantum confinement plays a fundamental role. 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.

Acknowledgments

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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] N. Porras-Montenegro and S. T. Pérez-Merchancano, Phys. Rev. B**46**, 9780 (1992).

[4] F. J. Ribeiro and A. Latgé, Phys. Rev. B**50**, 4913 (1994).

[5] E. E. Méndez, L. L. Chang, and L. Esaki, Surf. Sci. **113**, 474 (1982).

[6] J. López-Gondar, J. d'Albuquerque e Castro and L. E. Oliveira, Phys. Rev. B**42**, 7069 (1990).

[7] R. B. Santiago, L. E. Oliveira, and J. d'Albuquerque e Castro, Phys. Rev. B**46**, 4041 (1992).

[8] B. Yoo, B. D. McCombe, and W. Schaff, Phys. Rev. B**44**, 13152 (1991).

[9] A. Latgé, N. Porras-Montenegro, and L. E. Oliveira, Phys. Rev. B**51**, 2259 (1995).

[10] A. Latgé, N. Porras-Montenegro, and L. E. Oliveira, Phys Rev. B**51**, 13344 (1995).

[11] A. Latgé, N. Porras-Montenegro, M. de Dios-Leyva, and L. E. Oliveira, Phys Rev. B**53**, 10160 (1996).

[12] H. T. Cao and D. B. Tran Thoai, Solid State Commun. **97**, 643 (1996).

[13] M. Castro and F. Domínguez-Adame, Phys. Lett. A**225**, 321 (1997).

[14] R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).

[15] S. Chaudhuri and K. K. Bajaj, Phys. Rev. B**29**, 1803 (1984).

[16] A. Latgé, N. Porras-Montenegro, and L. E. Oliveira, Phys Rev. B**45**, 9420 (1992).

[17] A. Latgé, M. de Dios-Leyva, and L. E. Oliveira, Phys Rev. B**49**, 10450 (1994).

[18] C. A. Duque, A. Montes, A. L. Morales and N. Porras-Montenegro, J. Phys.: Condens. Matter (in press).

[19] G. Weber, Phys. Rev. B**41**, 10043 (1990).