Effects of applied electric fields on the infrared transitions between hydrogenic states in GaAs low-dimensional systems

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(Received 15 October 1996)

Using a variational procedure within the effective-mass approximation we calculate the binding and transition energies of shallow-donor impurities in cylindrical pills of 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 binding and transition energies as a function of the system geometry, the applied electric field, and the donor-impurity position. We have found that the presence of the electric field breaks the axial symmetry for the binding energy of the ground and excited states of the impurity and together with the impurity position, the geometric confinement is determinant for the existence of bounded excited states in these structures. In the two-dimensional limit and with low electric fields we obtained the expected four effective Rydbergs for the binding energy of the $1s$-like state. In addition, and only for high electric fields, we obtained the reverse transitions $2p_z$-like$\rightarrow 3s$-like and $3p_z$-like$\rightarrow 2s$-like. [S0163-1829(97)02716-1]

I. INTRODUCTION

With the development of experimental techniques such as molecular-beam epitaxy, metal-organic chemical-vapor deposition, and electron-beam lithography combined with reverse-mesa etching, there has been much work devoted to the study of the states of hydrogenic impurities in low-dimensional semiconductor heterostructures such as quantum wells (QW's), quantum-well wires (QWW's), and quantum dots (QD's). 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.

Theoretical studies for the binding energy of the ground state in GaAs QW's,[1] infinite QWW's,[2,3] and QD's (Refs. 4–6) have shown that for an infinite confinement potential the binding energy increases monotonically as the finite dimension (length or radius) is reduced, whereas for finite confinement potential the binding energy increases up to a maximum and then begins to decrease. Studies for donor-doped QW's (Ref. 1) and infinite QWW's (Ref. 2) have shown that the binding energy present a maximum when the impurity is located at the center of the structure and decreases for positions close to the edges. In an experimental work Méndez, Chang, and Esaki[7] 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 QW's have been studied by some authors,[8–13] 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. Theoretical calculations by Fraizzoli and Pasquarello[14] were in excellent agreement with photoluminescence and resonant Raman scattering measurements by Holtz *et al.*,[15] which provided an accurate determination of the difference in energy of the $1s$ and $2s$ acceptor states in GaAs-(Ga,Al)As QW's. Greene and Bajaj[16] and Chaudhuri and Bajaj[17] 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. Also, they found that inclusion of nonparabolic effects on the energy levels leads to more binding for all values of L. In addition, they found that for finite values of the potential barriers the variation of the binding energies of $1s$, $2s$, and $2p_{\pm}$ states as a function of L is essentially very similar: namely, the values of the binding energies increase as L is reduced until they reach their respective maximum values and then begin to decrease. For infinite barriers, the binding energies increase monotonically as L is reduced, approaching their two-dimensional values at $L=0$. Latgé, Porras-Montenegro, and Oliveira[18] have calculated infrared transitions between hydrogenic states in cylindrical infinite 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 GaAs low-dimensional systems (LDS).[19] We found that the binding energy depends on the structure geometry and on the impurity position and increases noticeably

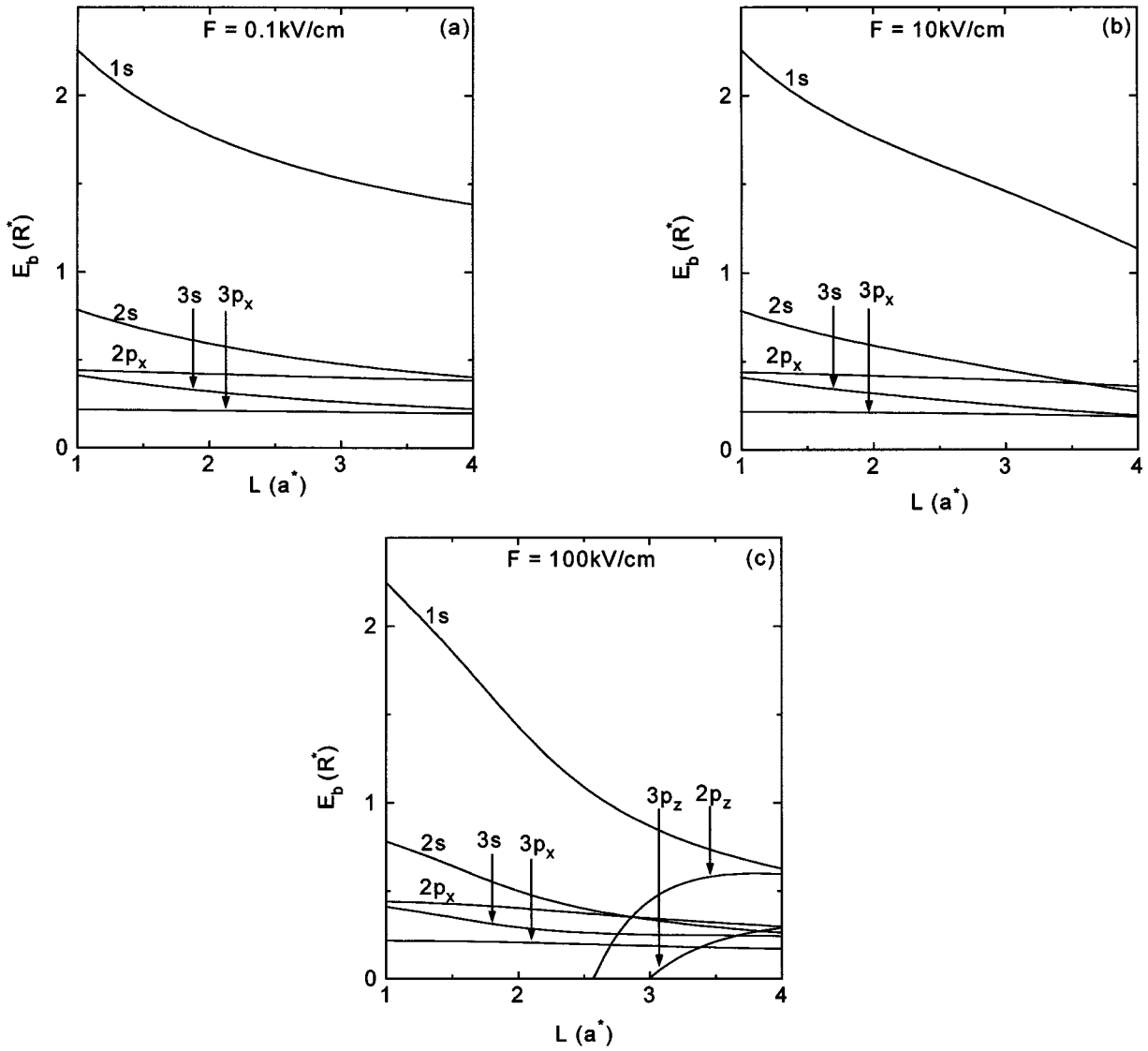

FIG. 1. Binding energy for ground and first few excited states of a donor impurity located at the center of a cylindrical GaAs LDS, as a function of the axial length, with $R=30a^*$, and for different values of the applied electric field.

when its location is shifted in a direction contrary to that of the applied electric field. Salib *et al.*[20] in a recent work have reported the observation of internal transitions of confined excitons in GaAs $Ga_{1-x}Al_xAs$ QW's, and studied them as a function of applied magnetic fields, with the $1s \rightarrow 2p_+$ as the dominant transition.

At the moment, to our knowledge, there have been no reported results about the effects of applied electric fields on the binding and infrared transition energies for excited states of shallow impurities in GaAs-(Ga,Al)As QWW's and QD's. It is for this reason that in this work we calculate the binding and transition energies for the first few excited states of hydrogenic impurities in cylindrical 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. Due to the fact that for the usual Al concentrations the height of the potential barrier is high enough in comparison with the energy level of the $1s$-like state and first few excited states and because of computing simplifications, in our calculations we use the infinite-model approximation for the confinement potential. 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 GaAs quantum pill 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 pill.

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

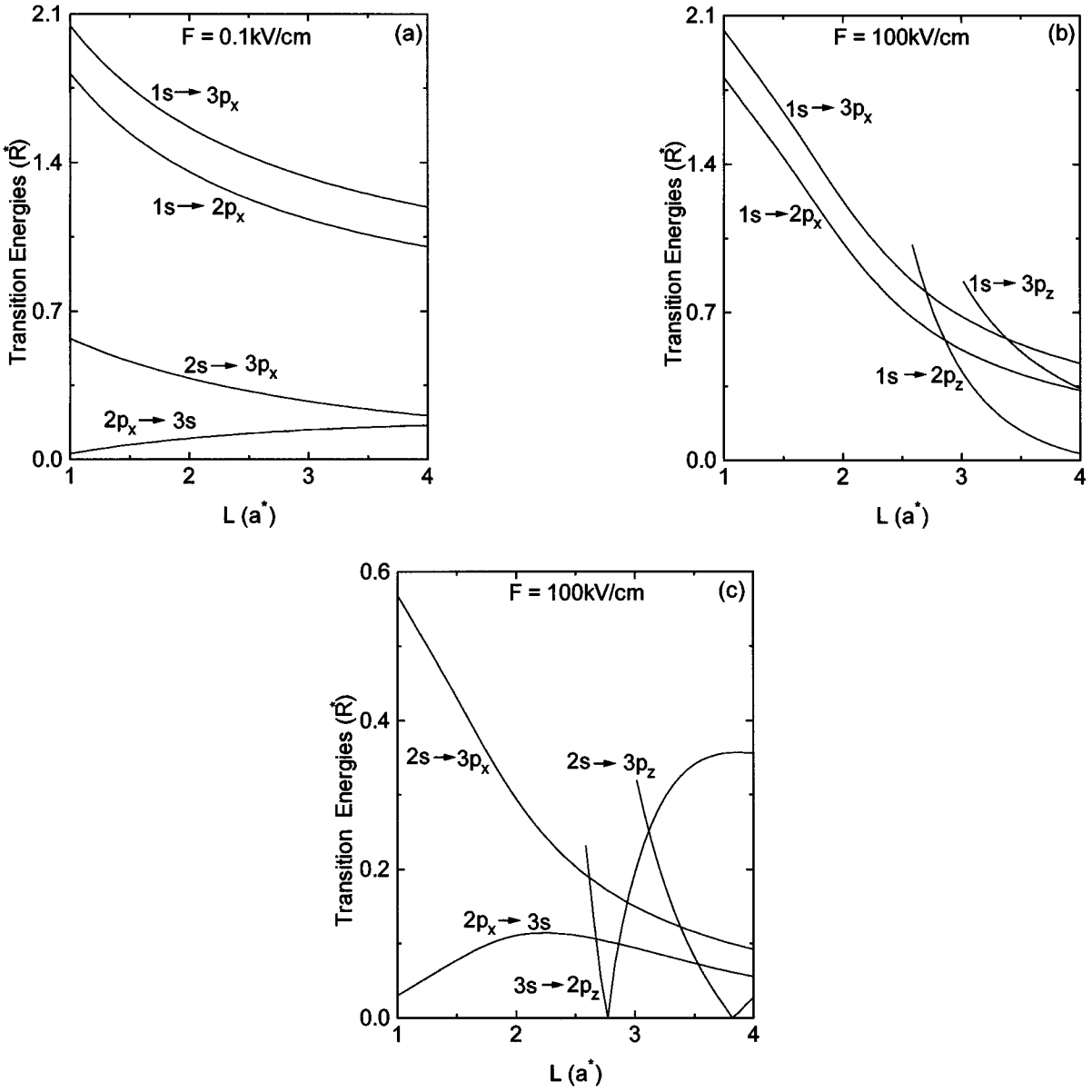

FIG. 2. Infrared transition energies as a function of the axial length of a cylindrical GaAs LDS for a donor located at the center of the system with $R=30a^*$, and with different values of applied electric field.

$$H=H_0-\frac{e^2}{\varepsilon_0 r}, \tag{1}$$

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 between the carrier and the impurity site, m^* is the donor-impurity effective mass, ε_0 is the static dielectric constant, and $V(\rho,z)$ is the well potential, defined as

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

where R and L are the LDS 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 results, for donor impurities, are given in reduced atomic units that correspond to a length unit of one effective Bohr radius, $a^*=h^2\varepsilon_0/4\pi^2m^*e^2\cong 100$ Å, and an energy unit of one effective Rydberg, $R^*=2\pi^2m^*e^4/h^2\varepsilon_0^2\cong 5.72$ meV.

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

$$\Psi_{nl}(\mathbf{r})=N_{nl}\Phi(\rho,z)\Gamma_{nl}(\mathbf{r},\{\lambda_{nl},\beta_{nl},\alpha_{nl}\}), \tag{4}$$

where $\Phi(\rho,z)$ is the eigenfunction of the Hamiltonian in Eq. (2) and Γ_{nl} are the hydrogenic wave functions.[18] The numbers n and l are principal and orbital angular momentum quantum numbers. In this work we consider $n=1,2,3$ with $l=0,\pm 1$ (which corresponds to the hydrogenic states s,

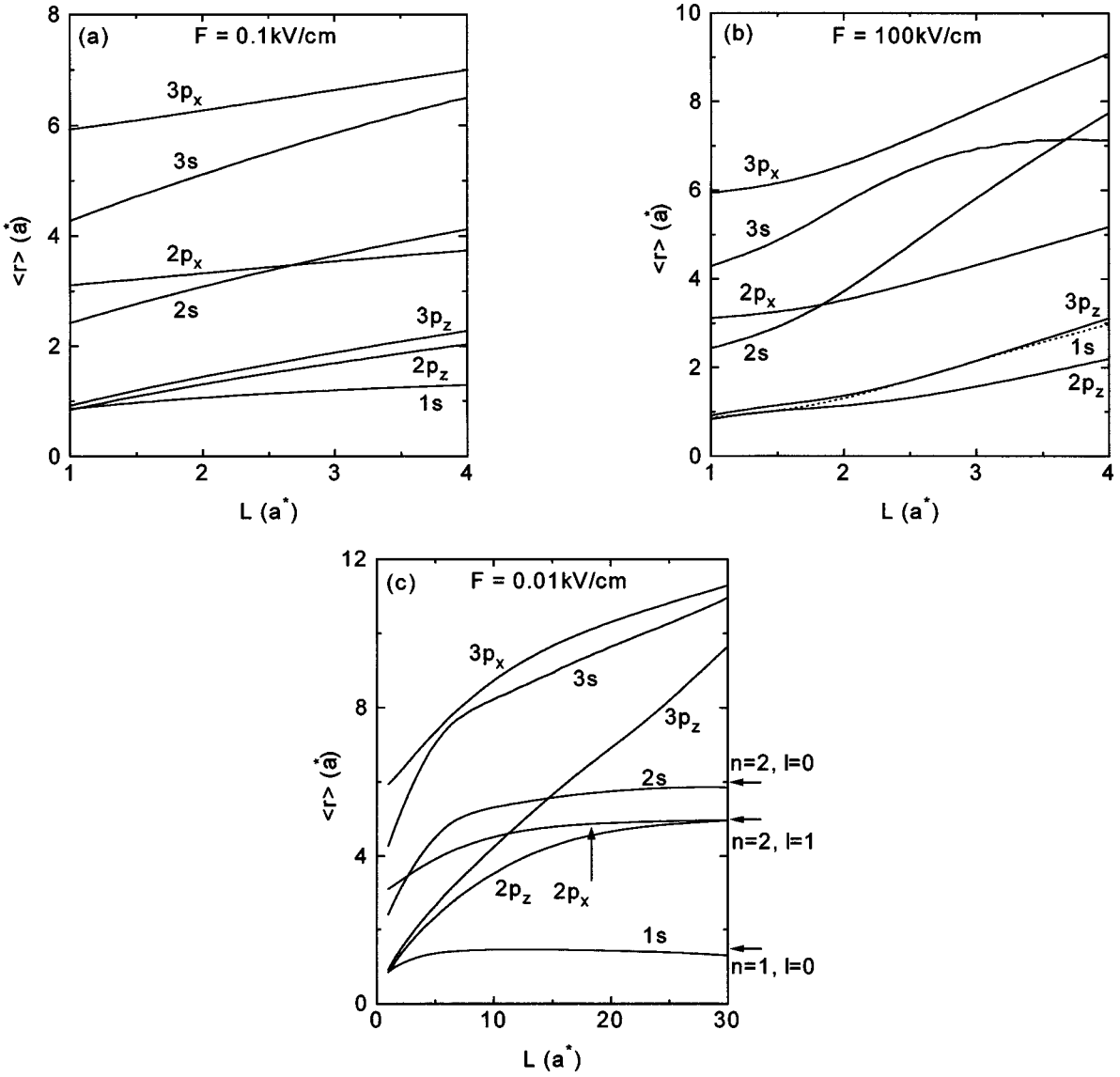

FIG. 3. Expectation value of the electron separation from the impurity in the ground and various excited donor-impurity states in a cylindrical GaAs LDS, of radius $30a^*$, with the donor impurity located at the center of the system, as a function of the axial length, and for different applied electric fields.

p_z, and $p_{x,y}$). Here the λ_{nl} are variational parameters; we follow the work by Chaudhuri and Bajaj[17] in GaAs-(Ga,Al)As QW's and Latgé, Porras-Montenegro, and Oliveira[18] in GaAs-(Ga,Al)As infinite QWW's and determine the β_{nl} and α_{nl} by requiring that the Γ_{nl} form a set of orthogonal functions in all space. The function $\Phi(\rho,z)$ is given by

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

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

$$Z(\zeta)=B_i(+)A_i(\zeta)-A_i(+)B_i(\zeta). \tag{6}$$

The arguments of the Bessel and Airy functions are

$$\beta=B_{10}\rho/R \tag{7}$$

and

$$\zeta=a_c\frac{z}{L}-\frac{E_0-(B_{10}a^*/R)^2}{w_c}, \tag{8}$$

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 Eq. (6)

$$A_i(\pm)[B_i(\pm)]=\mathrm{Ai[Bi]}\left(\pm a_c/2-\frac{E_0-(B_{10}a^*/R)^2}{w_c}\right), \tag{9}$$

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

$$B_i(+)A_i(-)-A_i(+)B_i(-)=0. \tag{10}$$

The ground and first excited states energy E_n of a hydrogenic impurity in a GaAs-(Ga,Al)As LDS with an applied electric field F is given by

$$E_{nl}=E_0-N_{nl}^2\int_0^{2\pi}\int_0^R\int_{-L/2}^{L/2}|\Phi(\rho,z)|^2\Gamma_{nl}\times\left[(a^*)^2(\nabla^2\Gamma_{nl})+2a^*\frac{\Gamma_{nl}}{r}\right]d\nu-2a^*N_{nl}^2\int_0^{2\pi}\int_0^R\int_{-L/2}^{L/2}|\Phi(\rho,z)|\Gamma_{nl}\times[(\nabla\Phi)\cdot(\nabla\Gamma_{nl})]d\nu, \quad (11)$$

where

$$1/N_{nl}^2=\int_0^{2\pi}\int_0^R\int_{-L/2}^{L/2}(\Phi\Gamma_{nl})^2d\nu. \quad (12)$$

The binding energy is calculated from the definition

$$E_b(n,l)=E_0-E_{nl}|_{\{(\lambda_0,\beta_0,\alpha_0\}}, \quad (13)$$

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

With the above equations we calculate the binding energy for the ground and first excited states of a donor impurity in a cylindrical GaAs-(Ga,Al)As LDS, as a function of the pill geometry, applied electric field, and impurity position.

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 for the ground and some few excited states in a LDS with $30a^*$ in radius, as a function of the length with hydrogenic impurity located at the center of the pill and for different values of the applied electric field. In Fig. 1(a) where the electric field is small it is observed that for high lengths of the pill the binding energy of the impurity states with equal n approximates to the same hydrogenic bulk limit. We have also found, in this limit of the electric field, that the states $2p_z$-like and $3p_z$-like are not bounded when L is less than $6.6a^*$ and $7.5a^*$, respectively. This is due to the rather large increase in the kinetic energy as the wave function of the p_z-like state is compressed along the z direction. Contrary to the results reported by Greene and Bajaj,[16] for QW's where they found that the $2p_x$-like state is more bounded than the $2s$-like state, we found that for small values of the electric field, Fig. 1(a), the $2s$-like state is more bounded than the $2p_x$-like state for the length range that we have considered in this figure. A similar situation occurs for $3s$-like and $3p_x$-like states, independent of the intensity of the applied electric field and in the whole range of the length that we have considered in our calculations, as is shown in Figs. 1(a), 1(b), and 1(c). It is observed in Figs. 1(b) and 1(c) that as the electric field is increased the $2p_x$-like state begins to be more bounded than the $2s$-like state for a wider range of the length of the structure. We observed the crossover between $3p_x$-like state and $3s$-like state for an applied electric field of 0.01 kV/cm and for length values higher than $6.0a^*$. In Fig. 1(c) we observe that for high values of the electric field the $2p_z$-like and $3p_z$-like states are bounded only for length values greater than $2.6a^*$ and $3.0a^*$, respectively. In comparing Figs. 1(a) and 1(c) we observe that the effect of the electric field is more apparent for high values of the pill length due to the wider spatial extension of the wave function. Notice that for higher values of the electric field the binding energy diminishes, except for $2p_z$-like and $3p_z$-like states, due to the displacement of the maximum of the probability density to negative values in the axial direction, an effect that is stronger for the ground state.

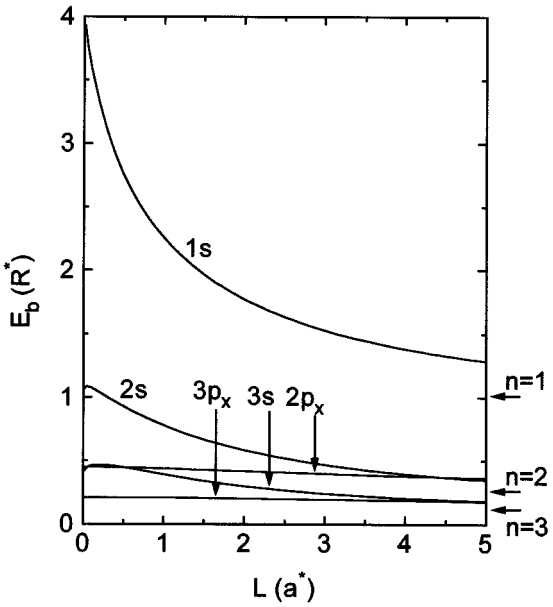

FIG. 4. Binding energy for the ground and first few excited states of a donor impurity located at the center of a cylindrical GaAs LDS, with $R=40a^*$, as a function of the axial length, for an applied electric field of 0.01 kV/cm.

Some of the infrared transition energies are presented in Fig. 2 as a function of the length of the cylindrical GaAs LDS for a donor impurity located at the center of the system and for different values of the applied electric field. In Fig. 2(a) as the LDS length increases, these transition energies approach the correct energy values corresponding to the difference between the energies in the bulk limit. Note that for $L\cong 2.75a^*$ there is a crossing in the energy levels of the $3s$-like and $2p_z$-like states [cf. Fig. 1(c)] which explains the behavior of the curve labeled $3s\rightarrow 2p_z$ in Fig. 2(c). For $L>2.75a^*$, the transition is reversed,[18] and occurs from a $2p_z$-like state to a $3s$-like state. The same behavior occurs for the transitions $2s\rightarrow 3p_z$. Also, in comparing Figs. 2(a) and 2(b) we observe that the variation of the energy for the $1s\rightarrow 3p_x$ and $1s\rightarrow 2p_x$ transitions diminishes more considerably for higher than for low electric fields as the length of the structure is increased.

We consider it important, for clarity reasons, to estimate the expectation value of the electron separation from the impurity $\langle r\rangle$ as a function of the length of the LDS for different values of the applied electric field when the impurity is lo-

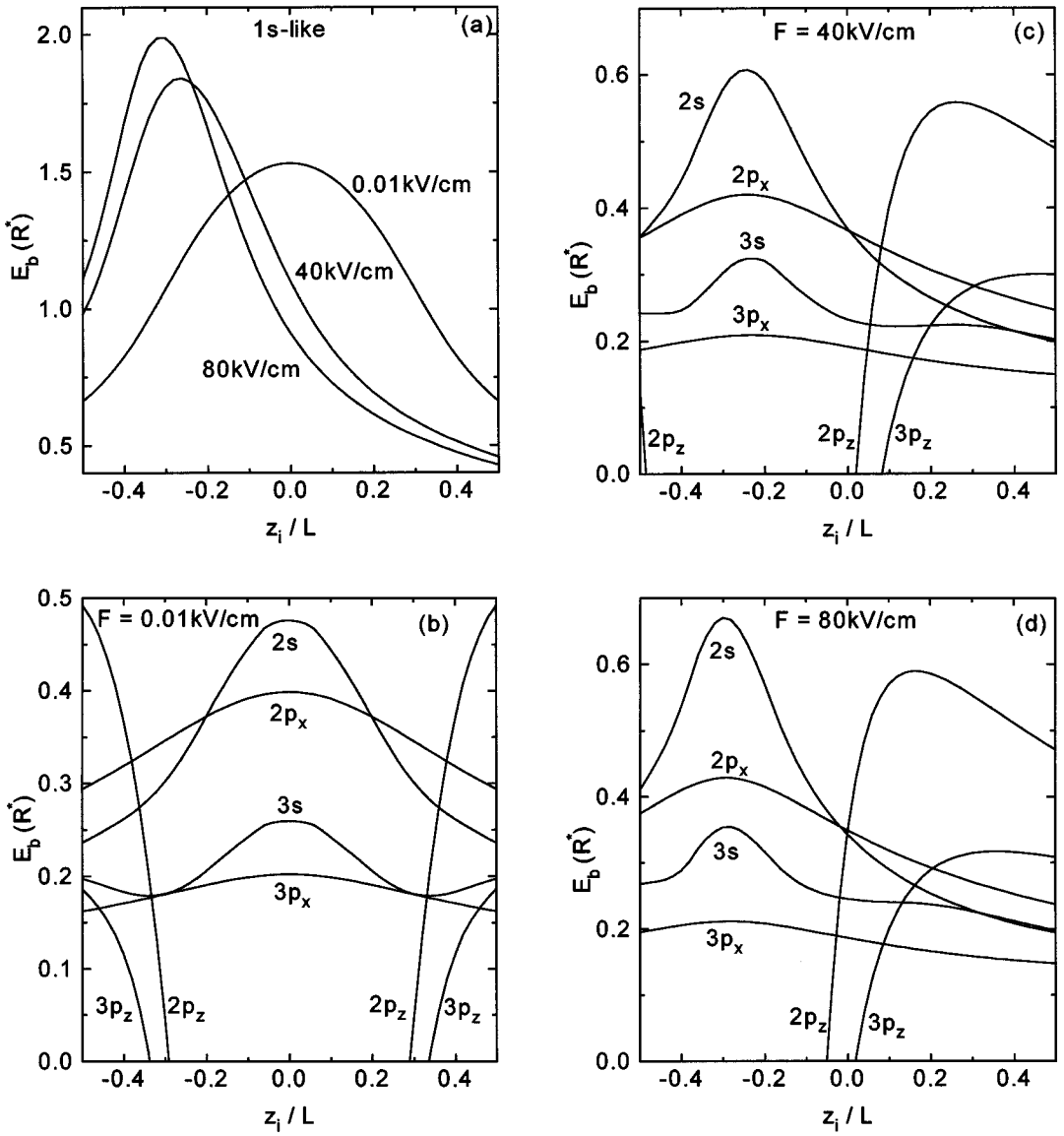

FIG. 5. Binding energy for the ground and some few excited states of a donor impurity in a cylindrical GaAs LDS with $R=30a^*$ and $L=3a^*$ as a function of the impurity position in the axial direction and for different values of the electric field.

cated at the center of the structure. In Fig. 3 we display these results for some excited states and for three values of the electric field. This results were obtained by means of the expression $\langle\Psi|r|\Psi\rangle$, where Ψ is the total wave function of the state under consideration. In comparing Figs. 3(a), 3(b), and 3(c) we observe that, independent of the applied electric field and for small pill lengths, $\langle r\rangle$ approaches the same value for a given excited state, due to the strong axial confinement of the wave function. Also, in Fig. 3(b), we notice that as the length is increased $\langle r\rangle$ takes higher values than in Fig. 3(a) for each state because the electric field extends the probability density in a wider range in the axial direction. As expected, it is clear that as $\langle r\rangle$ increases (decreases) the binding energy decreases (increases), except for $2p_z$-like and $3p_z$-like states, which is in excellent agreement with results presented in Fig. 1. In Fig. 3(c) we observe that for small values of the electric field (0.01 kV/cm) and large values of length, $\langle r\rangle$ tends to the hydrogenic bulk limit, that is to $n^2a^*\{1+1/2[1-l(l+1)/n^2]\}$ (see, for example, Bransden and Joachain[21]). In Fig. 3(c) these limits are indicated by the arrows at the right. For the size of our system ($R=30a^*$, $L=30a^*$) the states with $n=3$ are strongly compressed and for this reason we do not observe the bulk limit for these cases.

In Fig. 4 we present the binding energy for the $1s$ like and some excited impurity states as a function of the length in a LDS of $40a^*$ in radius with the impurity located at the center of the pill and for an electric field of 0.01 kV/cm applied in the axial direction. The largest effect of the quantum confinement is observed on the $1s$-like state, while the weak influence is on the $2p_x$-like and $3p_x$-like states as the length of the pill is diminished. States $2p_z$-like and $3p_z$-like states are not observed because they are not bounded in the range of lengths we have considered. It is clear that states labeled by x and y are geometrically equivalent in this system. As the length of the LDS is increased, the limiting behavior of the binding energies, for all states hereby considered, corresponds to the exact bulk value $(1/n^2)R^*$. The arrows at the

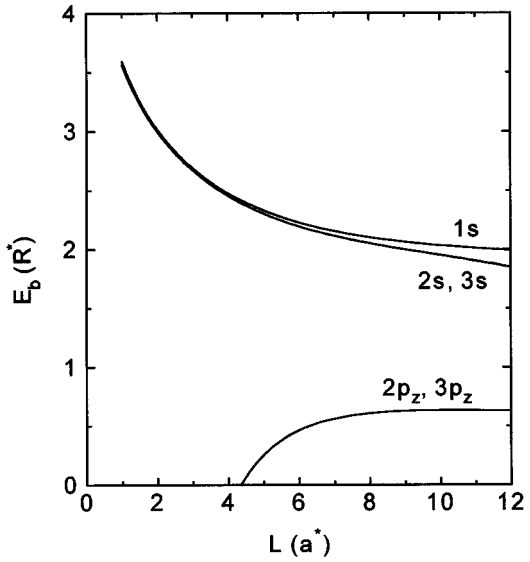

FIG. 6. Binding energy of the ground and some excited states of a donor impurity in a GaAs LDS of radius $2a^*$ and for an applied electric field of 0.01 kV/cm, as a function of the length of the structure.

right show the bulk limit that we have obtained when $L=30a^*$. As expected, states with the same quantum number n become degenerate in the bulk limit ($L\rightarrow\infty$, $R\rightarrow\infty$). The inversion between the binding energies of the $2s$-like and $2p_x$-like states ($3s$-like and $3p_x$-like states), for $L>4.5a^*$ ($L>6.0a^*$), is due to the presence of the small applied electric field. It is important to note that in the two-dimensional limit, that is for the pill length closed to zero, we obtained the $4R^*$ value for the binding energy of the $1s$-like state. In the two-dimensional limit it is not possible to reach the bulk value for the binding energy due to the infinite confinement potential that we are using, which prohibits the penetration of the wave function outside the potential well. For this reason in this limit our results differ from those found by Greene and Bajaj,[16] who used a finite-potential well. Anyway, independent of the confinement potential and for small values of the length, the binding energy of the $2s$-like and $3s$-like states must be greater than those of $2p_x$-like and $3p_x$-like states, respectively, due to the spatial distribution of the probability density of these states in contradiction with the results by Greene and Bajaj.[16]

In Fig. 5 we display the binding energy for the ground and some excited state as a function of the impurity position along the axial direction of a cylindrical GaAs LDS, and for different values of the applied electric field. We observe that our results for this kind of LDS structure ($R=30a^*$ and $L=3a^*$) are in good agreement with those reported by Weber[22] for donor impurities in a QW under the action of an applied electric field. In Figs. 5(a) and 5(b), which are for $F=0.01$ kV/cm, we observe, as expected, that the binding energy is symmetrical along the axial direction, while in Figs. 5(a), 5(c), and 5(d) for higher values of the electric field this symmetry is broken due to the fact that the electric field moves the electronic-probability density to the left region of the pill. For high electric fields in all cases 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. It is interesting to notice that for high electric fields the appearance of the $2p_z$-like and $3p_z$-like bounded states is allowed for a wider range of impurity positions along the z direction, as is shown in Figs. 5(c) and 5(d). This is an effect in which besides the impurity position, the quantum confinement and the applied electric field compete for the existence of these excited states.

In Fig. 6 we present the binding energy of the ground and some excited states of a donor impurity in a GaAs LDS of radius $2a^*$ and for an applied electric field of 0.01 kV/cm, as a function of the length of the structure in order to simulate QD-like and QWW-like structures as the length is varied. For the sizes of the structure allowed by the variation of the length, the $2s$-like and the $3s$-like states are degenerate, and for QD-like geometries this degeneracy is extended to the $1s$-like state. This is due to the high compression of the wave function of the $2s$-like and $3s$-like states which converge to the $1s$-like wave function. Our results are in perfect agreement with those obtained by Ribeiro and Latgé[6] who calculated the binding energy of a donor impurity in a cubic GaAs quantum box of side L. Effectively, we obtained $3.01R^*$ for the binding energy of a donor impurity in a cylindrical GaAs quantum box of length $L=2a^*$, coincident with the value reported by Ribeiro and Latgé[6] for a quantum box of the same volume, that is, of side $L=2.93a^*$. Also, in the limit of a QWW-like geometry our results coincide quite well with those reported by Latgé, Porras-Montenegro, and Oliveira[18] for the ground and the excited states depicted in Fig. 6. Our results for the binding energies for each state are a little greater than those reported by Latgé, Porras-Montenegro, and Oliveira[18] because our model is of infinite-confinement potential and our geometry is of finite length.

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 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 the determinant for the existence of bound donor impurity excited states in LDS where the quantum confinement plays a fundamental role. Also, we found reverse transitions for the cases $3s$-like$\rightarrow$ $2p_z$-like and $2s$-like$\rightarrow 3p_z$-like. As in previous works we found that the binding energy of the ground and some excited states of a donor-shallow impurity in a LDS in the limit of low-electric field and large size of the potential well approximates quite well to the bulk-limit values with the ap-

propriate degeneracy for states with the same n number. In the two-dimensional limit and with low-electric field we obtained approximately $4R^*$ for the binding energy of the $1s$-like state. It is important to stress that irrespective of the confinement potential and for low-electric field the binding energy of the $2s$-like and $3s$-like states must be greater than those of $2p_x$-like and $3p_x$-like states, respectively, in contradiction with the results of Greene and Bajaj.[16] 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

This work was partially financed by Colombian Scientific Agency COLCIENCIAS. C.A.D. is grateful for the hospitality at the Department of Physics of the Universidad del Valle where part of this work was done. N.P.-M. thanks Dr. M. Virasoro for his hospitality at the I.C.T.P. in Trieste, where part of this work was done. The authors want to thank Dr. L. E. Oliveira for suggestions and a critical reading of this manuscript.

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