Infrared transitions between hydrogenic states in cylindrical GaAs quantum-well wires under applied magnetic fields

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Using the effective-mass approximation within the variational approach, we have calculated the binding and the allowed transition energies between the $1s$-, $2s$-, $2p_{\pm}$-, $2p_z$-, $3s$-, $3p_{\pm}$-, and $3p_z$-like states of a hydrogenic on-center donor impurity in a cylindrical GaAs quantum-well wire, under the action of a magnetic field applied in the axial direction. Our results are obtained for several wire radii and as a function of the applied magnetic field. We have found that some excited states are not bounded for some values of the radius of the wire and of the applied magnetic field, and that the geometric confinement and the applied magnetic field split the degeneracy of some excited states. [S0163-1829(99)06503-0]

Much attention has been focused during recent years on the optical properties of low-dimensional systems. Magneto-spectroscopy experiments have been carried out on shallow donor impurities doped in the central region of the wells in a GaAs-$Ga_{1-x}Al_xAs$ multiple QW's by Jarosik *et al.*,[1] who found increased values for the $1s$-$2p_{\pm}$ transition energies with respect to the bulk values. Far infrared measurements performed by Yoo *et al.*[2] have allowed the observation of electric-field effects on the electronic states of shallow impurities in selectively donor-doped GaAs-$Ga_{1-x}Al_xAs$ QW's. The effect of electric and magnetic fields on the intradonor transition energies between the $1s$-like ground state and $2p_{\pm}$-like excited states of hydrogenic donors were recently studied by Latgé *et al.*[3] following a variational calculation within the effective-mass approximation. The theoretical infrared-absorption spectra associated to $1s$-$2p_{\pm}$ donor transitions in GaAs-$Ga_{1-x}Al_xAs$ QW's under electric and magnetic fields, and for x-polarized radiation, were calculated taking into account the appropriate doping profile and have provided an adequate understanding of the available $1s$-$2p_{\pm}$ experimental measurements. Many authors have worked on the calculation of the binding energies, density of impurity states, transition energies, and photoluminescence spectra associated with shallow impurities in GaAs-$Ga_{1-x}Al_xAs$ quantum-well wires (QWW's). However, there are no theoretical studies considering the effects of applied magnetic fields on the infrared transitions between excited states of donor impurities in cylindrical GaAs QWW's.

In this work, using the effective-mass approximation within the variational approach we calculate the binding energy and some transition energies associated with the ground and some excited states of a hydrogenic on-center donor in a cylindrical GaAs QWW's under the action of a magnetic field applied in the axial direction. The Hamiltonian of a donor impurity, located at the axis of a cylindrical GaAs QWW in the presence of an applied magnetic field $\mathbf{B}=B\mathbf{z}$ can be written as

$$H=-\nabla^2-i\gamma\left(\frac{\partial}{\partial\varphi}\right)+\frac{\gamma^2\rho^2}{4}-\frac{2}{r}+V(\rho), \qquad (2.1)$$

where we have used the atomic units of length $a^*=\varepsilon\hbar^2/m^*e^2$ and energy $R^*=e^2/2\varepsilon a^*$. Here $r=(\rho^2+z^2)^{1/2}$, z is the relative coordinate of the separation between the electron and the ion of the impurity in the axial direction of the wire, ε is the dielectric constant of the GaAs, and m^* is the electron effective mass. The components of the vector potential in cylindrical coordinates are $A_\rho=A_z=0$, $A_\varphi=\frac{1}{2}(B\rho)$. In Eq. (2.1) $\gamma=e\hbar B/2m^*cR^*$ is the measure of the electron energy in the first Landau level $(n=0)$, due to the action of the magnetic field. For GaAs (Refs. 4–7) $m^*=0.065$, $\varepsilon=12.58$; for donor impurities $a^*\cong 100$ Å and $R^*=5.83$ meV. We assume that the carriers are free to move in the z direction and the confinement potential is $V(\rho)=0$ for $0\leqslant\rho\leqslant R$ and $V(\rho)=\infty$ for $\rho>R$.

Following Green and Bajaj[4] we calculate the binding energy of a given state Ψ_{nlm} by means of

$$E_{b,nlm}(R,B)=E_{10}+\gamma-\langle\Psi_{nlm}|H|\Psi_{nlm}\rangle, \qquad (2.2)$$

where E_{10} is the lowest subband energy of the well potential and $\langle\Psi_{nlm}|H|\Psi_{nlm}\rangle$ is the expected value of the Hamiltonian (2.1) for the impurity state under consideration. n, l, and m are the principal, orbital and magnetic quantum numbers, respectively. The value of E_{10} is $E_{10}=[2.4048\,a^*/R^2]^2$.

When the impurity is present, we use the trial wave functions proposed by Latgé *et al.*[5] These wave functions are expressed as the product of electronic wave functions in the well of the wire without impurity and without magnetic field, multiplied by the hydrogenic wave function corresponding to the excited state under consideration, that is,

$$\Psi_{nlm}(r)=\begin{cases}N_{nlm}\Phi_{10}(\rho)\Gamma_{nlm}(r,\{\lambda_{nl},\beta_{nl},\alpha_{nl}\}), & \rho\leqslant R,\\ 0, & \rho>R,\end{cases} \qquad (2.3)$$

where the N_{nlm} are the normalization constants and the Γ_{nlm} are the hydrogenic wave functions that correspond to nlm states. $\Phi_{10}(\rho)$ is the eigenfunctions of the Hamiltonian (2.1) without impurity and without magnetic field, which is given by

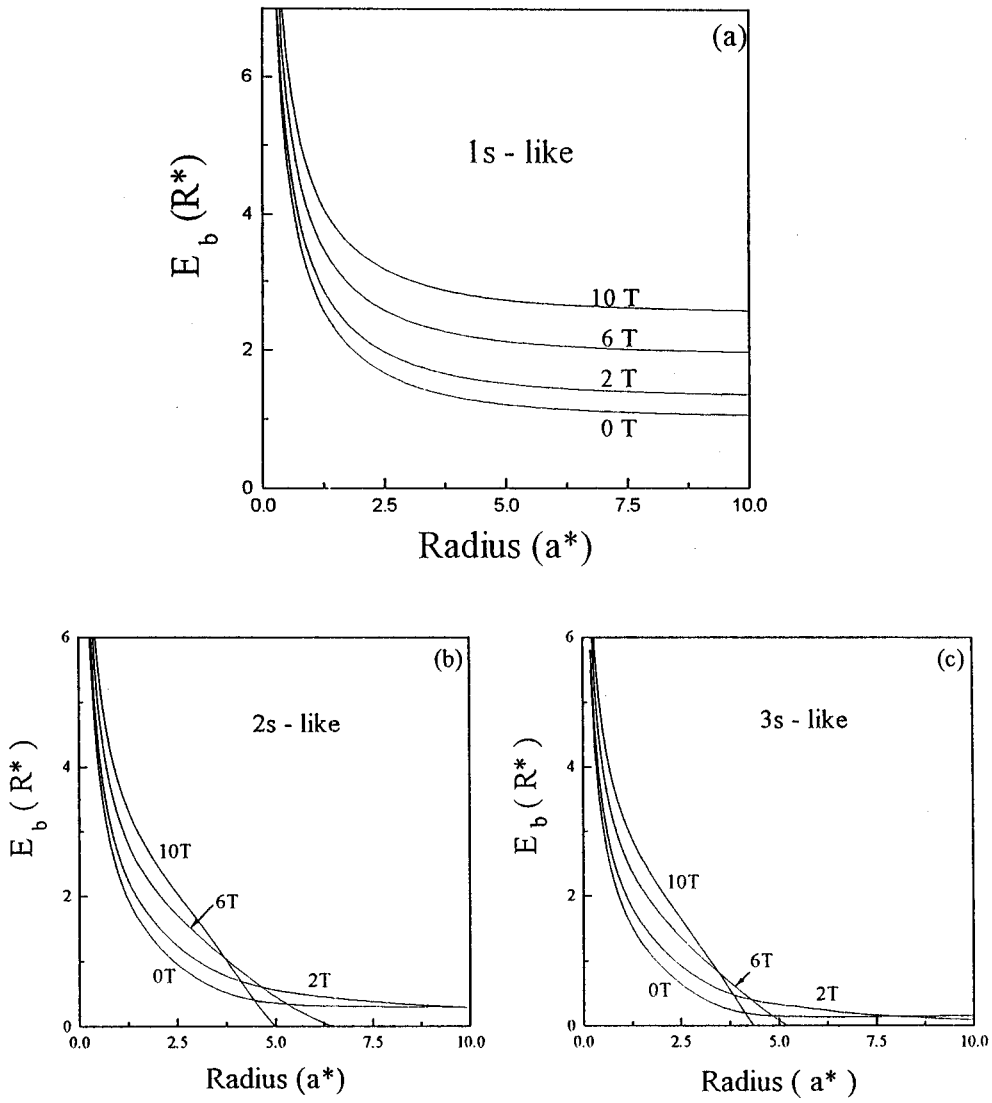

FIG. 1. Binding energy of some excited states of a donor impurity located at the center of a cylindrical GaAs QWW, as a function of the wire radius and for different values of the magnetic field.

$$\Phi_{10}(\rho)=\begin{cases} J_0(k_{10}\rho), & \rho \leqslant R, \\ 0, & \rho > R. \end{cases} \tag{2.4}$$

Here J_0 is an ordinary Bessel function of zero order, and $k_{10}R$ is the first zero of $J_0(k_{10}R)$. The λ_{nl}, β_{nl}, and α_{nl} are variational parameters used by Chaudhuri and Bajaj[6] that vary according to λ_{nl} in such a way that the orthogonalization is preserved.

The allowed transition energies are given by

$$E_T(nlm \rightarrow n'l'm') = |E_{b,nlm}(R,B) - E_{b,n'l'm'}(R,B)|, \tag{2.5}$$

and the selection rules used for the allowed transitions are

$$\Delta l = l - l' = \pm 1, \qquad \Delta m = m - m' = 0, \pm 1. \tag{2.6}$$

The competition between the magnetic and the geometric confinements can be visualized by means of the relation between the cyclotronic radius $r_c=(1/\gamma)^{1/2}$ and the radius of the wire R, $r_c/R=[R^2\gamma]^{-1/2}$. For $r_c=R$ we have the limit for the transition from the geometric to the magnetic confinement regime. If $\gamma > 1/R^2$ the magnetic confinement governs over the geometric one and vice versa.

In Fig. 1 we show the binding energy of the $1s$-, $2s$-, and $3s$-like states as a function of the QWW radius for different values of the applied magnetic field. For all states we observe that the binding energies increase significantly for small values of the radius independently of the applied magnetic field; that is, for small values of the QWW radius the geometric confinement governs the behavior of the binding energy over the magnetic one. For large values of the radius R the magnetic field determines the behavior of the binding energy for all of the ns-like states. For the $1s$-like state the corresponding binding energy increases with the applied magnetic field in the intermediate and weak geometrical confinement regimes. For the $2s$- and $3s$-like states it is seen that there is a critical radius $R_c(B)$ such that for $R > R_c$ there are not bounded states. This is due to the fact that for $R > R_c(B)$ the changes undergone by the kinetic and dia-

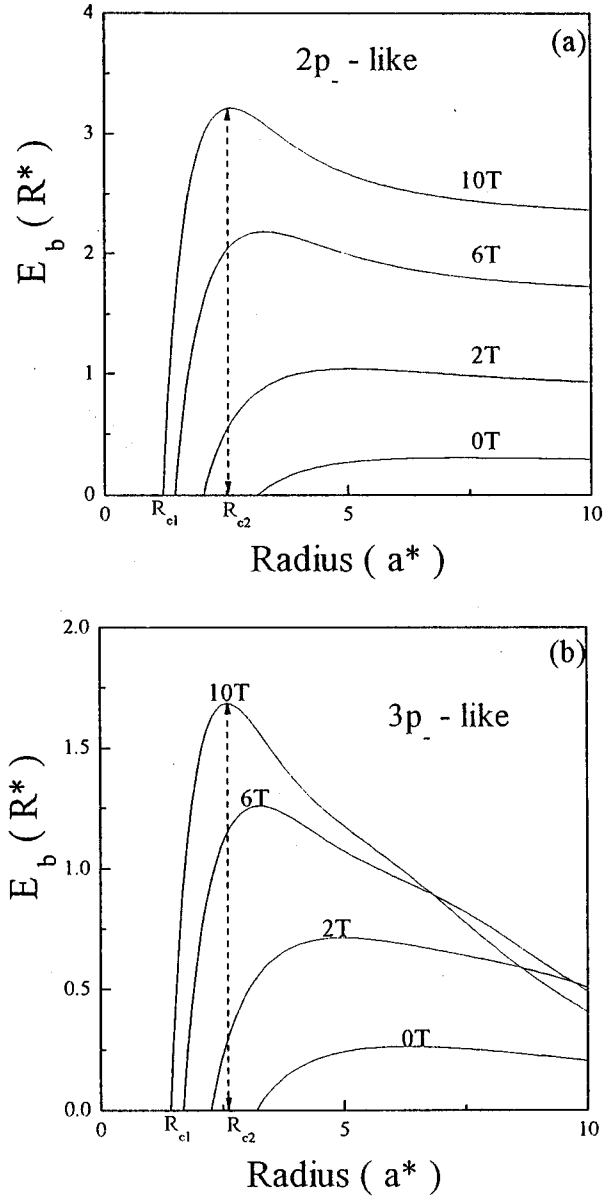

FIG. 2. Binding energy of some excited states of a donor impurity located at the center of a cylindrical GaAs QWW, as a function of the wire radius and for different values of the magnetic field.

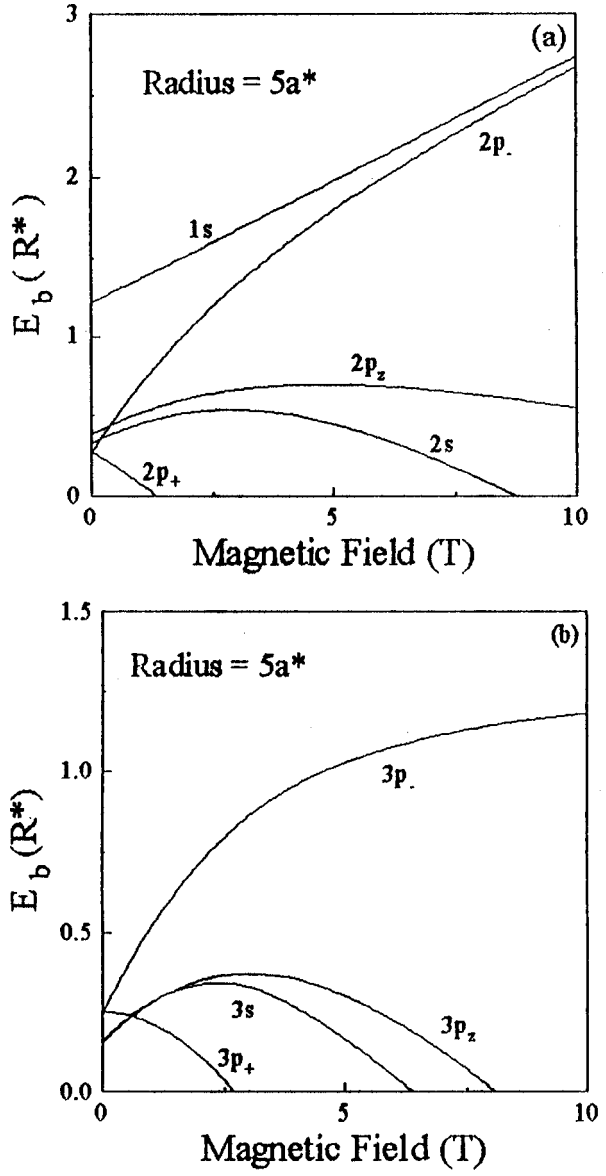

FIG. 3. Binding energy of some excited states of a donor impurity located at the center of a cylindrical GaAs QWW, as a function of the magnetic field and for a wire of $5a^*$ in radius.

magnetic energies under the action of the applied magnetic field overwhelm the corresponding change in the potential energy. With the increasing of the applied magnetic field, R_c (B) decreases and its value lies in the range of weak and intermediate confinement. For QWW radius $R<R_c(B)$ the binding energy is a decreasing function of R and the speed of its decrement increases with B.

The binding energies of $2p_-$- and $3p_-$-like states are represented in Fig. 2 as a function of the QWW radius and for different values of the applied magnetic field. It is seen that there are two characteristic radii R_{c1} (B) [at which the bounded states appear for $R \geqslant R_{c1}(B)$] and R_{c2} (B) (at which the binding energy reaches its maximum value). Both characteristic radii diminish with the increasing of B and their values lie in the range of strong and intermediate geometrical confinement. For QWW radii R_{c1} $(B)<R<R_{c2}$ (B) the binding energy increases with R and the slope of the curve becomes larger when the magnetic field is augmented. In the range $R>R_{c2}$ the binding energy decreases when R increases and the speed of such decreasing is substantially large for great magnetic fields. The existence of the critical radius R_{c1} is due to the strong confinement of the wave function in the radial direction and therefore the corresponding energy is higher than the first ionization level within the structure.

In Fig. 3, for a wire of $5a^*$ in radius, we represent the binding energy of some excited states as a function of the applied magnetic field. It is observed that the energy of the $1s$-like state increases approximately linearly with the applied magnetic field in agreement with the results by Branis *et al.*[7] Unfortunately for the other states considered by us, there are neither theoretical nor experimental results to compare ours with. It is observed that the separation between the binding energy of the excited states increases with the applied magnetic field. Also, it is important to note that for B

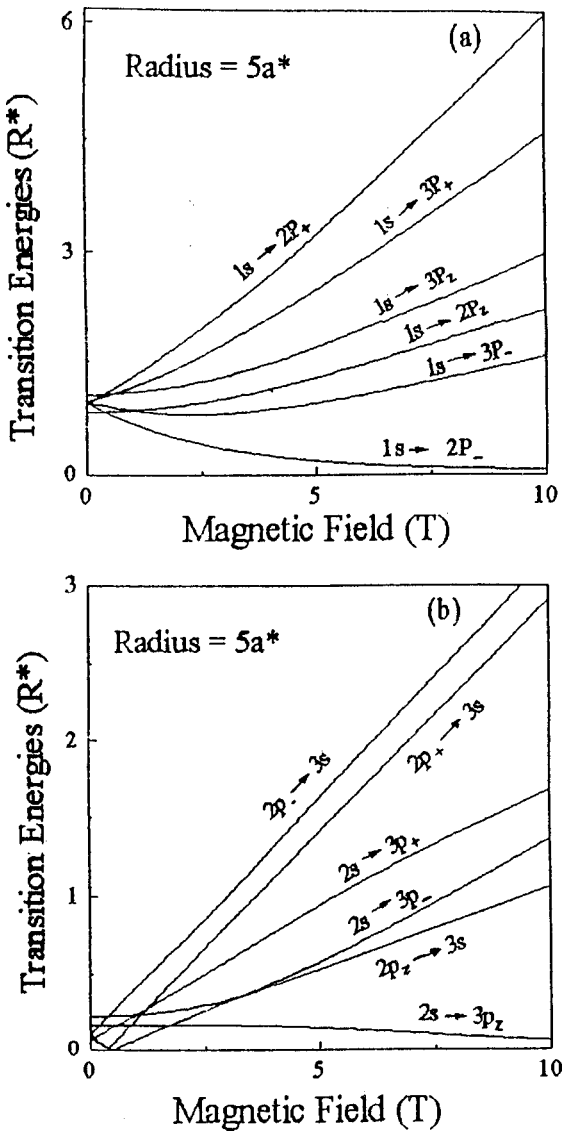

FIG. 4. Infrared transition energies of a donor impurity located at the center of a cylindrical GaAs QWW, as a function of the magnetic field and for a wire of $5a^*$ in radius.

$=0$ T there is a splitting in the binding energy of the excited states with equal n due to the geometric confinement. Here it is interesting to observe that one of the roles of the magnetic field is to increase the binding energy of the states $1s$ and $2p_-$ like. Otherwise the magnetic field augments the energy of the $2s$-, $2p_+$-, $2p_z$-, $3s$-, $3p_+$-, $3p_z$-like states over the energy of the first electron level in the well of the wire, in such a way that these states become unbounded for large values of the magnetic field. The splitting of the energy degeneracy between $2s$- and $2p_z$-like states and between the $3s$- and $3p_z$-like states presented in Figs. 3(a) and 3(b), respectively, is entirely due to the response of s- and p-type wave functions to the quantum geometrical (for $B=0$) and magnetic (for $B\neq 0$) confinements.

We represent some transition energies as a function of the applied magnetic field in Fig. 4. It is of importance to observe that for the geometry we are using and with the magnetic field applied parallel to the axis of the cylinder, the transition $1s\rightarrow 2p_+$ has a higher energy than $1s\rightarrow 3p_+$ for all the range of the applied magnetic field, opposite to the results obtained by Latgé *et al.*[8] in GaAs-(Ga, Al)As QW's. This is entirely due to the different geometric confinement in which the *np*-like states are now confined. In all of the ways, excepting $1s\rightarrow 2p_-$ and $2s\rightarrow 3p_z$, the other transitions increase in a wide range of the applied magnetic field. We expect that these transitions must be observed in photoluminescence spectra in GaAs QWW's when these structures can be fabricated and these measurements performed.

In this work, using the effective-mass approximation within the variational approach, we have calculated the binding and the allowed transition energies between the $1s$-, $2s$-, $2p_\pm$-, $2p_z$-, $3s$-, $3p_\pm$-, and $3p_z$-like states of a hydrogenic on-center donor impurity in a cylindrical GaAs QWW, under the action of a magnetic field applied in the axial direction. We have found that some excited states are not bounded for some values of the radius of the wire and of the applied magnetic field, and that the geometric confinement and the applied magnetic field raise the degeneracy of some excited states. We believe the present calculation will be of importance in the understanding of future experimental work in this subject. Even though this work has been performed for GaAs QWW's using the infinite potential model, its results could be used to discuss experimental results not only in GaAs, but in GaAs-$Ga_{1-x}Al_xAs$ QWW's under the action of applied magnetic fields, whenever $0.30<x<0.45$ in order to have high enough potential barriers.

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[1] N. C. Jarosik *et al.*, Phys. Rev. Lett. **54**, 1283 (1985).
[2] B. S. Yoo *et al.*, Superlattices Microstruct. **8**, 297 (1991); Phys. Rev. B **44**, 13 152 (1991).
[3] A. Latgé, N. Porras-Montenegro, and Luiz E. Oliveira, Phys. Rev. B **51**, 2259 (1995).
[4] R. Greene and K. Bajaj, Phys. Rev. B **37**, 4604 (1988).
[5] A. Latgé, N. Porras-Montenegro, and Luiz E. Oliveira, Phys. Rev. B **45**, 9420 (1992).
[6] S. Chaudhury and K. Bajaj, Phys. Rev. B **29**, 1803 (1984).
[7] S. V. Branis, Gang Li, and K. K. Bajaj, Phys. Rev. B **47**, 1316 (1993).
[8] A. Latgé, N. Porras-Montenegro, M. de Dios-Leyva, and Luiz E. Oliveira, Phys. Rev. B **53**, 10 160 (1996).