Intradonor absorption spectra under external fields in quantum wells

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The effects of magnetic and electric fields on the infrared-absorption properties associated to transitions between the $1s$-like and $2p_{\pm}$-, $3p_{\pm}$-, and $4p_{\pm}$-like excited states of hydrogenic donors in GaAs-Ga$_{1-x}$Al$_x$As quantum wells are studied. The magnetic and electric fields are applied along the growth direction of the heterostructure, and donor envelope wave functions and energies are obtained within a variational procedure in the effective-mass approximation. Calculations for the intradonor transition strengths for x-polarized radiation and absorption coefficients are performed for finite-barrier potentials and as functions of applied magnetic and electric fields and quantum-well thicknesses. A discussion of a sum rule associated to donor transitions in quantum wells is presented. Theoretical results for the absorption spectra are in good agreement with available infrared-magnetospectroscopy measurements on doped quantums wells.

I. INTRODUCTION

Theoretical and experimental work on optical transitions between electronic states has been used as a basic tool for the determination of energy levels in semiconductor heterostructures and serve as a guide for technological applications in optoelectronics. Electronic and optical properties of impurities in semiconductor nanostructures have been largely studied[1–4] in the past two decades due to the important role impurities play in these systems. Suitable doping provides interesting changes in the semiconductor physics when one is interesting in tailor-made quantum structures. Magnetospectroscopy experiments have been carried out on shallow-donor impurities doped in the central region of a GaAs quantum well (QW) in GaAs-Ga$_{1-x}$Al$_x$As multiple QW's by Jarosik *et al.*[5] who found increased values for the $1s\rightarrow 2p_{\pm}$ transition energies with respect to bulk values. Helm *et al.*[6] have performed a detailed investigation of the far-infrared absorption spectra of GaAs-Ga$_{0.7}$Al$_{0.3}$As superlattices and have investigated intersubband and $1s\rightarrow 2p_z$ donor transitions. Far-infrared measurements performed by Yoo *et al.*[7] have allowed the observation of electric-field effects on the electronic states of shallow impurities in selectively donor-doped GaAs-Ga$_{1-x}$Al$_x$As QW's. The intensity of an intradonor transition is determined by the dipole matrix element between the initial and final donor states, and one may therefore obtain the intradonor absorption coefficient: the experimental energy transition is then associated to the position of the corresponding peak in the absorption spectra. The effects 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 in GaAs-Ga$_{1-x}$Al$_x$As QW's were recently studied[8] following a variational calculation within the effective-mass approximation. The theoretical infrared-absorption spectra associated to $1s\rightarrow 2p_{\pm}$ donor transitions in GaAs-Ga$_{1-x}$Al$_x$As 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 $1s\rightarrow 2p_{\pm}$ experimental measurements.

In this work we present a detailed study of the intradonor infrared-absorption spectra related to impurity transitions ($1s\rightarrow 2p_{\pm}$, $1s\rightarrow 3p_{\pm}$, and $1s\rightarrow 4p_{\pm}$) in donor-doped GaAs-Ga$_{1-x}$Al$_x$As QW's under the presence of electric and magnetic fields, both applied along the growth direction of the QW. In Sec. II we discuss the variational procedure followed within the effective-mass approximation to calculate the effects of these fields on the ground and excited states of donors in GaAs-Ga$_{1-x}$Al$_x$As QW's, present the expression for the absorption line shape, and derive a sum rule associated to donor transitions in QW's. Our results and discussion are in Sec. III and conclusions in Sec. IV.

II. THEORY

The Hamiltonian of a hydrogenic donor in a GaAs-Ga$_{1-x}$Al$_x$As QW in the presence of both electric and magnetic fields (applied perpendicular to the interfaces) may be written as

$$H=\frac{1}{2m^*}(P_x^2+P_y^2+P_z^2)-\frac{e^2}{\varepsilon r}+eEz+V(z), \qquad (2.1)$$

where $V(z)$ is the barrier potential of the QW of width L, $r=[\rho^2+(z-z_i)^2]^{1/2}$ is the electron position with respect to the donor at z_i, E is the electric-field intensity, $-e$ is the electron charge, and m^* and ϵ are the GaAs conduction-band effective mass and dielectric constant, respectively, which we assume to be the same throughout the heterostructure. The components of the momentum operator are given by

$$P_i = p_i + \frac{e}{c} A_i \quad (i = x,y,z), \tag{2.2}$$

where **A** is the vector potential. If one chooses the gauge $\mathbf{A} = (B/2)(-y,x,o)$, where B is the magnetic field, it is straightforward to show that the momentum P_x and P_y, angular momentum L_z, and position x satisfy the following commutation relations:

$$[P_x,P_y] = -i\hbar m^* \omega_c, \quad [P_x,L_z] = -i\hbar P_y,$$

$$[P_y,L_z] = -i\hbar P_x, \quad [x,H] = i\hbar P_x/m^*, \tag{2.3}$$

with $\omega_c = eB/m^*c$ being the cyclotron frequency. Due to the rotational symmetry around the z axis, the eigenfunctions of the Hamiltonian (2.1) may be chosen as the same as for the L_z operator. These functions are denoted by $|nm\rangle$, where m is the magnetic quantum number and n represents the remaining quantum numbers. The variational $|nm\rangle$ donor envelope wave functions are taken as products of the exact solution of the square well in the presence of the electric field (a combination of Airy functions) and hydrogeniclike functions,[9] such as

$$\Gamma_{1s} = \exp(-\lambda_{1s} r), \tag{2.4a}$$

$$\Gamma_{2p_\pm} = \rho^{|m|} \exp(\pm i\varphi) \exp(-\lambda_{2p_\pm} r), \tag{2.4b}$$

$$\Gamma_{3p_\pm} = \rho^{|m|} (2 - \beta_{3p_\pm} r) \exp(\pm i\varphi) \exp(-\lambda_{3p_\pm} r), \tag{2.4c}$$

$$\Gamma_{4p_\pm} = \rho^{|m|} (5 - 5\beta_{4p_\pm} r + \alpha_{4p_\pm} r^2) \times \exp(\pm i\varphi) \exp(-\lambda_{4p_\pm} r), \tag{2.4d}$$

and the donor energies are minimized with respect to the variational parameters as detailed in previous work.[9]

By using (2.3), one may show that the matrix elements of x (for x-polarization light) satisfy the following sum rule:

$$\sum_n T_{n_o m_o, n} = 1, \tag{2.5}$$

where

$$T_{n_o m_o, n} = \sum_{m=m_o-1}^{m=m_o+1} \frac{(m-m_o) E^2_{nm,n_o m_o}}{(\hbar\omega_c)(\hbar^2/2m^*)} |\langle n_o m_o | x | nm \rangle|^2, \tag{2.6}$$

and $E_{nm,n_o m_o} = E_{nm} - E_{n_o m_o}$ is the transition energy between states with quantum numbers nm and $n_o m_o$, respectively. Notice that $T_{n_o m_o, n}$ corresponds to the oscillator strength for transitions between states $|n_o m_o\rangle$ and $|nm\rangle$, with $m = m_o \pm 1$.

The intradonor absorption coefficient is proportional to the square of the dipole matrix element between initial and final donor states and to the $P(z_i)$ distribution of impurities in the QW. For the case of $1s \to np_\pm$ ($n = 2$, 3, and 4) transitions, and for x-polarized radiation, the absorption coefficient is

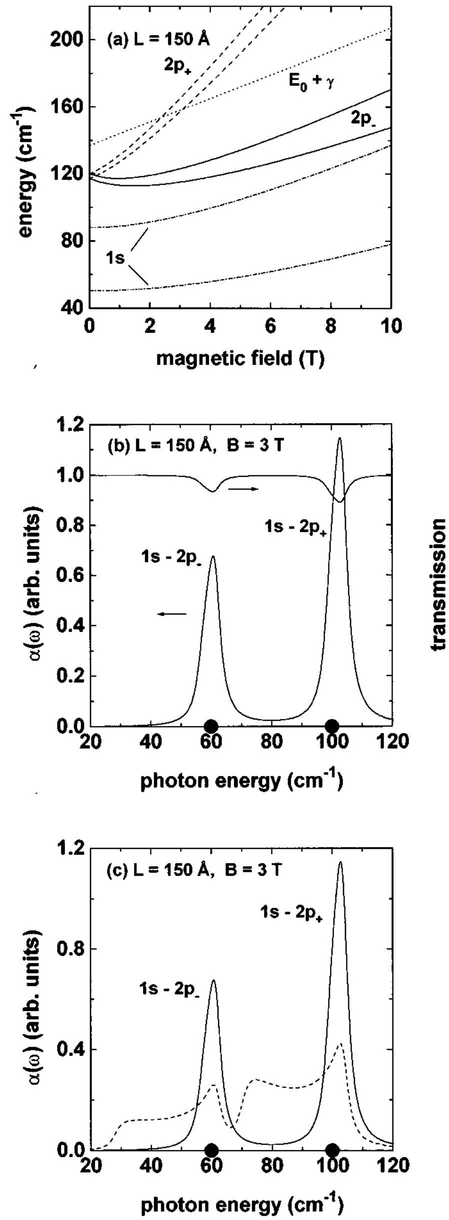

FIG. 1. (a) Magnetic-field dependence of the donor energies for the $1s$- (dashed-dotted lines), $2p_+$- (dashed lines), and $2p_-$- (full curves) like states for an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW. For each donor state, the lower (upper) curve corresponds to on-center (on-edge) results. The lowest Landau level $E_0 + \gamma$ of the QW in the absence of impurity is also shown (dotted line). (b) $1s$-$2p_\pm$ intradonor absorption coefficient (for x-polarized radiation) and the corresponding transmission spectra as a function of the photon energy for an $L = 150$ Å donor-doped (in the central $\frac{1}{3}$) QW under a magnetic field of 3 T. (c) $1s$-$2p_\pm$ intradonor absorption coefficient (for x-polarized radiation): comparison of the central $\frac{1}{3}$ doping results (full curve) with the case of an homogeneous donor distribution (dashed line). Full dots on the energy axis correspond to the experimental results by McCombe *et al.* (Ref. 11).

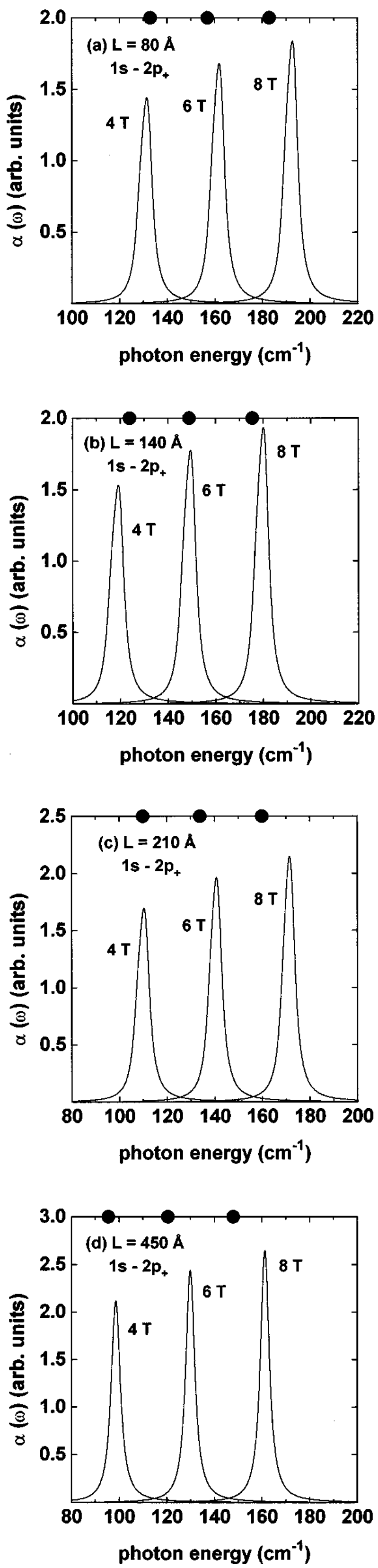

FIG. 2. Intradonor absorption coefficient (for x-polarized radiation) for $1s \rightarrow 2p_+$ transitions in GaAs-$Ga_{0.7}Al_{0.3}$As QW's of different widths and donor doped in the central $\frac{1}{3}$, under different values of the magnetic field. Full dots on the upper energy axis correspond to the experimental results by Jarosik *et al.* (Ref. 5).

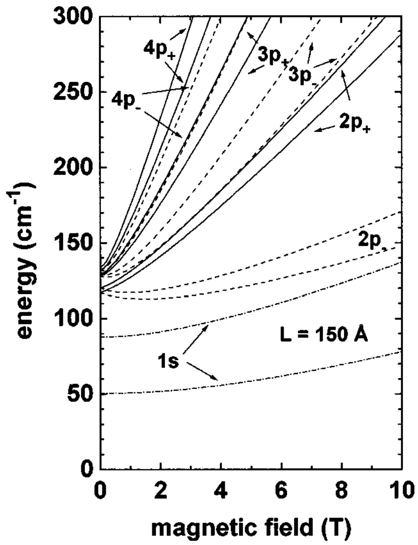

FIG. 3. Donor energies for the $1s$-, $2p_{\pm}$-, $3p_{\pm}$-, and $4p_{\pm}$-like states of an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}$As QW as a function of the magnetic field. For each donor state, the lower (upper) curve corresponds to on-center (on-edge) results.

$$\alpha(\omega) \approx \omega \sum_{n,m=\pm 1} \int_{-L/2}^{L/2} dz_i |\langle 1s|x|nm\rangle|^2 P(z_i) \times \delta(E_{nm,1s} - \hbar\omega). \tag{2.7}$$

In evaluating the above intraband absorption coefficient, we follow Yoo *et al.*,[7] and replace the δ function in Eq. (2.7) by a Lorentzian with a width equal to 4 cm^{-1} ($\approx$0.50 meV). This may be understood as a numerical artifact to simulate broadening processes that have not been included in the theoretical derivation of Eq. (2.7).

III. RESULTS AND DISCUSSION

The magnetic-field dependence of the on-center and on-edge donor energies for $1s$-, $2p_+$-, and $2p_-$-like states for an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}$As QW are shown in Fig. 1(a). The lowest Landau level $E_0 + \gamma$, where E_0 is the ground-state energy of the QW in the absence of impurity and magnetic field and γ is a dimensionless measure of the magnetic field,[10] is also shown (dotted line). The infrared $1s$-$2p_{\pm}$ intradonor absorption coefficient (for x-polarized radiation) and the corresponding transmission spectra (for an arbitrary sample width) are shown in Fig. 1(b) as a function of the photon energy for an $L = 150$ Å donor-doped (in the central $\frac{1}{3}$) QW under a magnetic field of 3 T. This result for the absorption coefficient is compared with the absorption for a homogeneously doped QW and with the experimental results by McCombe *et al.*[11] (full dots on the energy axis) in Fig. 1(c). One should note that the widths of the computed absorption line shapes depend both on the phenomenological width (4 cm^{-1}) of the Lorentzian[7] used to simulate the δ function of Eq. (2.7), and on the spatial donor distribution. The agreement between the peaks in the experimental data (with central $\frac{1}{3}$ doped samples) and the theoretical line shapes incorporating the correct central $\frac{1}{3}$ doping profile is quite good. Also, the line shape of the experimental spectra[7] un-

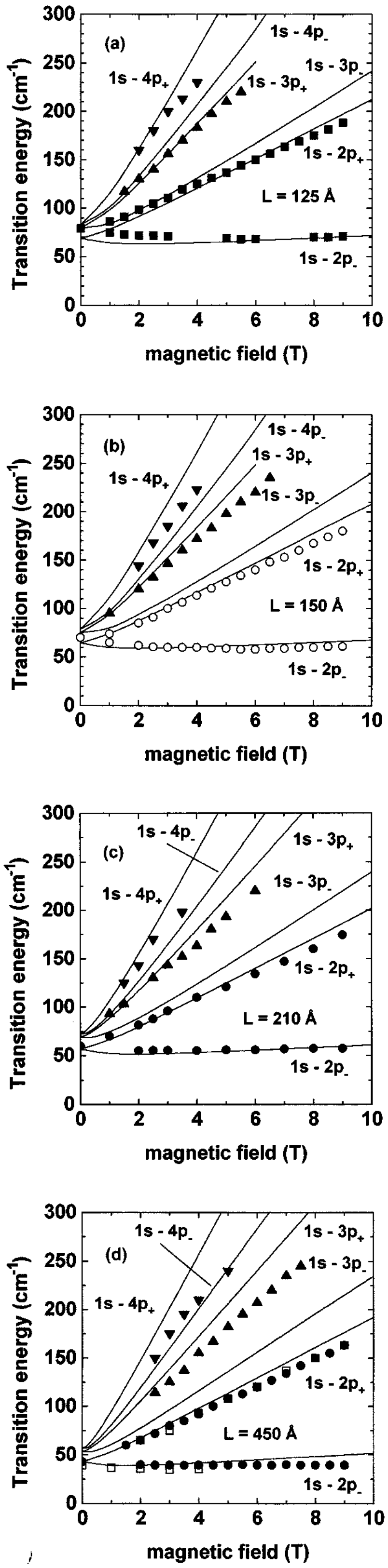

FIG. 4. Intradonor transition energies for GaAs-$Ga_{0.7}Al_{0.3}$As QW's for (a) $L=125$ Å, (b) $L=150$ Å, (c) $L=210$ Å, and (d) 450 Å, as functions of the magnetic field. Theoretical results are obtained from the peaks of the absorption coefficient for QW's doped on the central $\frac{1}{3}$, and are compared with experimental data by Jarosik *et al.* (Ref. 5), McCombe *et al.* (Ref. 11) and Chen *et al.* (Ref. 12). Experimental data (dots, squares, triangles, etc.) correspond, in increasing energy, to $1s$-$2p_-$, $1s$-$2p_+$, $1s$-$3p_+$, and $1s$-$4p_+$ transitions, respectively.

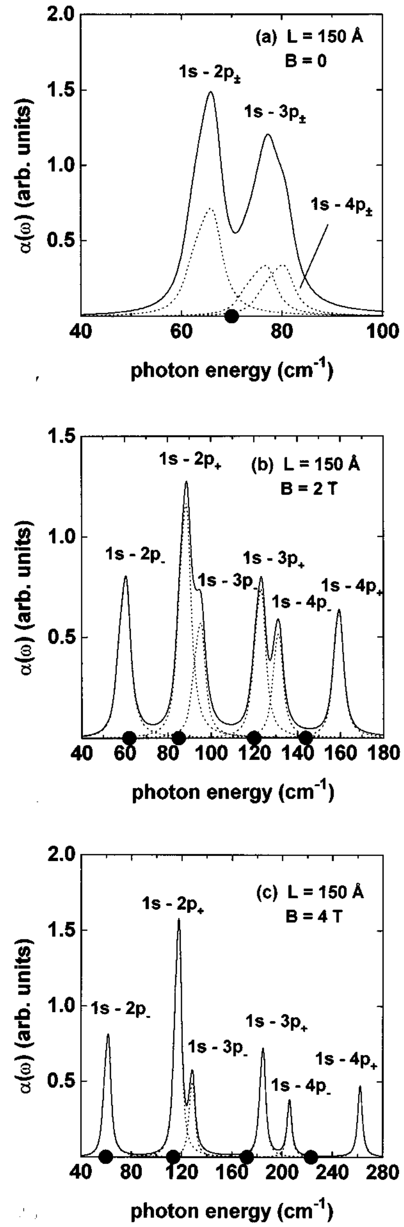

FIG. 5. Intradonor absorption coefficient (for x-polarized radiation) for a donor distribution over the central $\frac{1}{3}$ of an $L=150$ Å GaAs-$Ga_{0.7}Al_{0.3}$As QW, and for different magnetic fields. The contributions associated to the various intradonor transitions are given by dotted lines whereas full lines correspond to the total absorption coefficient. Full dots on the energy axis correspond to the experimental results by McCombe *et al.* (Ref. 11).

ambiguously supports the interpretation that the central $\frac{1}{3}$ doping is the correct model for the donor distribution in the QW. The $1s$-$2p_+$ intradonor absorption coefficient (for x-polarized radiation) in GaAs-$Ga_{0.7}Al_{0.3}$As QW's donor doped in the central $\frac{1}{3}$, under different values of the magnetic field ($B=4$, 6, and 8 T), are shown in Fig. 2 for different well widths. The peaks on the theoretical results for the absorption coefficients compare well with the experimental data by Jarosik *et al.*[5] for low values of the applied magnetic field. We believe that a better description of the experimental measurements for high magnetic fields would require more realistic (with more variational parameters) hydrogeniclike variational wave functions in order to better allow distortions caused by the applied magnetic field.

The effect of the magnetic field on the theoretical donor energies for the $1s$-, $2p_\pm$-, $3p_\pm$-, and $4p_\pm$-like states of an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW is shown in Fig. 3 for the case of on-center and on-edge donors. It is worth noticing that the energies corresponding to the higher levels ($2p_+$-, $3p_\pm$-, and $4p_\pm$-like states) are more sensitive to the intensity of the magnetic field than the lower states. Our results in Fig. 3 for *on-center* donors qualitatively agree with the theoretical results presented in Fig. 1 of Chen *et al.*[12] It is clear from the theoretical results in Fig. 3 that the intradonor transition energies would very much depend on the impurity *position* in the QW, and therefore that a proper understanding of experimental data on doped QW's must in principle involve a donor-profile-dependent calculation of the full absorption coefficient.

Theoretical results for donor transitions between the $1s$-like and $2p_\pm$-, $3p_\pm$-, and $4p_\pm$-like excited states, obtained from the peaks of the absorption coefficients for GaAs-$Ga_{0.7}Al_{0.3}As$ QW's, doped on the central $\frac{1}{3}$, are compared with experimental data by Jarosik *et al.*,[5] McCombe *et al.*,[11] and Chen *et al.*[12] in Fig. 4. One should note that the two highest experimental transitions (up and down triangles in Fig. 4) were assigned by McCombe *et al.*[11] and Chen *et al.*[12] to $1s$-$3p_+$ and $1s$-$4p_+$ transitions. The intradonor absorption coefficients (for x-polarized radiation and for a donor distribution over the central $\frac{1}{3}$ of the QW) of an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, and for different magnetic fields, are shown in Fig. 5. It is apparent, therefore, that a proper understanding of the experimental data should involve a careful analysis of the infrared-absorption spectra. For zero magnetic fields, the absorption spectra clearly exhibit structures corresponding to an admixture of different donor transitions [see the case of $1s \rightarrow 3p_\pm$ and $1s \rightarrow 4p_\pm$ transitions in Fig. 5(a)]. Of course, an additional broadening mechanism could produce a large homogeneous linewidth that might result in a *single* inhomogeneously broadened resonance at the experimentally measured position [cf. Fig. 5(a)]. For increasing magnetic field, one may notice that the agreement between theory and experimental data for $1s$-$2p_\pm$ transitions is in general good for all QW widths. For $1s \rightarrow 3p_\pm$ and $1s \rightarrow 4p_\pm$ transitions, theoretical results deviate considerably from the experimental measurements for increasing values of the magnetic field, due to the absence of electron-phonon interactions in our theoretical calculation. As shown by Cheng *et al.*,[13] phonon effects may be quite important for donor transitions in the region near the energies corresponding to the TO and LO phonons.

The sum rule[14] defined by Eqs. (2.5) and (2.6) was analyzed in Fig. 6, which presents the intradonor oscillator strengths for an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW as a function of the magnetic field for on-center and on-edge donors. Also shown in Fig. 6 is the dependence of the oscillator strength with the QW width for a magnetic field of 2 T in the case of on-center donors. Of course, the exact result predicted by Eq. (2.5) for the total oscillator strength was not achieved in our theoretical calculation since it involves a variational procedure and therefore the envelope wave functions and related matrix elements are not exact as commented by the authors[15] in a previous work. It is worthwhile

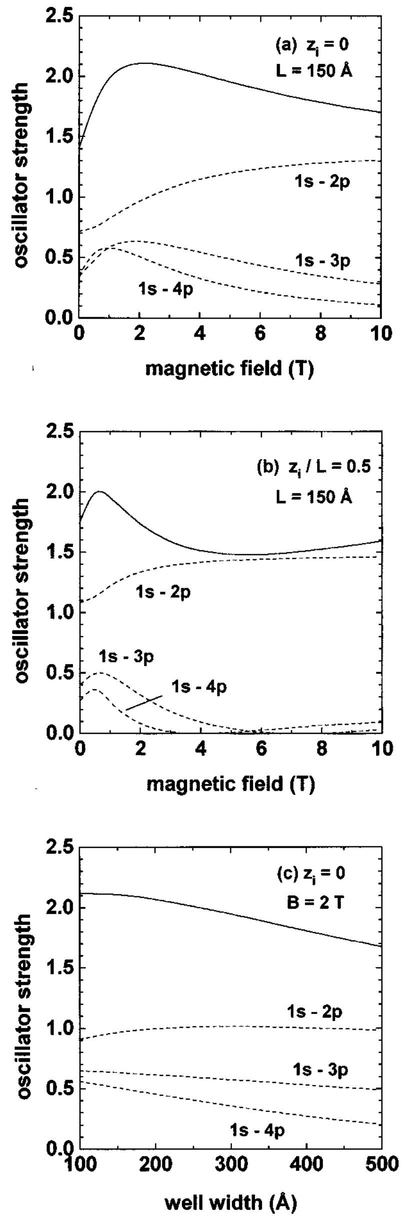

FIG. 6. Intradonor oscillator strengths for an $L = 150$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW as a function of the magnetic field for on-center (a) and on-edge (b) donors; also shown is the oscillator strength vs well width for a magnetic field of 2 T in the case of on-center donors. Dashed curves represent contributions associated to $1s \rightarrow np$ ($n = 2$, 3, and 4) transitions whereas full curves correspond to the sum of these contributions.

to notice that as the magnetic field increases the contribution to the total oscillator strength coming from transitions related to $1s$- to $3p_\pm$-, and $4p_\pm$-like states is reduced.

The effects of an externally applied electric field on the intradonor $1s$-$2p_\pm$ transition energies are shown in Fig. 7 for an $L = 500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW under different values of the magnetic field. Theoretical results obtained from the peak of the absorption coefficient (donor distribution over the central $\frac{1}{3}$ of the QW) are shown in the full curves whereas the dashed curves correspond to intradonor on-center transitions. Notice that the peaks of the absorption spectra and on-center transitions are essentially identical if no electric

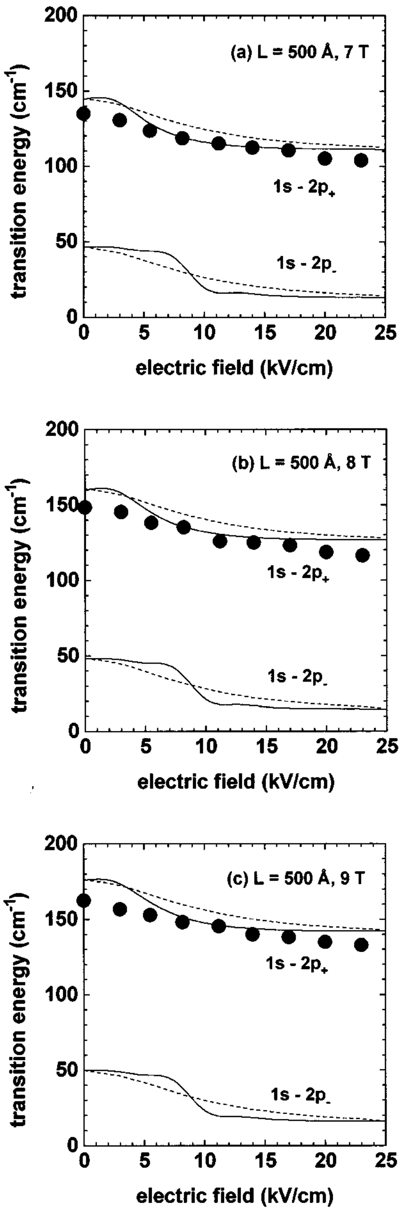

FIG. 7. Intradonor $1s$-$2p_{\pm}$ transition energies for an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW under (a) $B=7$ T, (b) $B=8$ T, and (c) $B=9$ T magnetic fields, and as functions of applied electric field. Full curves correspond to theoretical results obtained from the peak of the absorption coefficient (donor distribution over the central $\frac{1}{3}$ of the QW) whereas dashed lines are associated to on-center donor transitions; experimental data (full dots) are from Yoo *et al.* (Ref. 7).

field is applied; if an electric field is applied, the symmetry of the QW along the growth direction is broken and a proper consideration of the doping profile is needed. The overall agreement between the theoretical calculations and the experimental data[7] is apparent provided the absorption spectra and doping profile are properly taken into account in the theoretical description of the problem. This is clearly seen in Fig. 8, which presents the absorption spectra for $B=8$ T and $E=5$ kV/cm. One may notice from Fig. 8 a half-width of the order of 25 cm^{-1} for the $1s \rightarrow 2p_-$ and $1s \rightarrow 2p_+$ transitions, and very small intensities for the $1s \rightarrow 3p_{\pm}$ transitions.

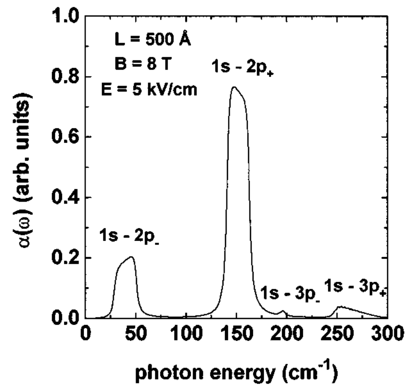

FIG. 8. Intradonor absorption coefficient (for x-polarized radiation) for a donor distribution over the central $\frac{1}{3}$ of an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW for a magnetic field of 8 T and electric field of 5 kV/cm.

Also, although the experimental work did not report the $1s$-$2p_-$ transition energies, our theoretical results (see Figs. 7 and 8) unambiguously indicate that they have enough strength to be observable in a far-infrared-magnetospectroscopy experiment.

IV. CONCLUSIONS

In this work we have presented a study of the effects of magnetic and electric fields on the infrared-absorption properties associated to transitions between the $1s$-like and $2p_{\pm}$-, $3p_{\pm}$-, and $4p_{\pm}$-like excited states of hydrogenic donors in GaAs-$Ga_{1-x}Al_xAs$ QW's. Donor envelope wave functions and energies are obtained within a variational procedure in the effective-mass approximation. A discussion of the sum rule associated to donor transitions in QW's was presented, and the absorption spectra corresponding to intradonor transitions were calculated and related to available infrared-magnetospectroscopy experimental work. We have unambiguously shown that a quantitative understanding of the experimental data must involve a detailed analysis of the intradonor absorption coefficient together with a proper consideration of the profile of the donor distribution in the QW. Our results for transition from $1s$- to $2p_{\pm}$-like donor states were in overall agreement with available experimental measurements whereas theoretical results for transitions involving $3p_{\pm}$- and $4p_{\pm}$-like donor excited states should probably take into account the electron-phonon interaction together with a better description of the donor-hydrogenic part of the trial envelope wave function for a better understanding of the experimental data.

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