$1s$-$2p_{\pm}$ infrared-absorption spectra of donor-doped quantum wells under electric and magnetic fields

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We present a theoretical study of the intradonor infrared-absorption properties associated with transitions between the $1s$-like ground state and $2p_{\pm}$-like excited states of hydrogenic donors in a GaAs-$Ga_{1-x}Al_xAs$ quantum well under electric and magnetic fields, both applied along the growth direction of the heterostructure. Donor energies and envelope wave functions of $1s$-like and $2p_{\pm}$-like states are obtained within a variational procedure in the effective-mass approximation, and the line strengths for intradonor $1s$-$2p_{\pm}$ transitions are obtained for x-polarized radiation and for donor positions along the quantum well. The $1s$-$2p_{\pm}$ absorption spectra are calculated and theoretical results compare rather well with experimental data by Jarosik *et al.* [Phys. Rev. Lett. **54**, 1283 (1985)] and Yoo *et al.* [Phys. Rev. B **44**, 13 152 (1991)]. Also, the present work unambiguously shows that a calculation of the absorption spectra with the appropriate doping profile is needed if one aims to a full understanding of experimental measurements.

Selective doping in semiconductor heterostructures plays quite an important role in their electronic and optical properties and has been largely studied in the last few years.[1–8] A great number of studies concern the understanding of the nature of impurity states in low-dimensional semiconducting systems. Experimental progress through spectroscopic techniques made possible a detailed analysis of the effects of confinement on shallow impurities in quantum wells (QW's). Far-infrared magnetospectroscopic measurements on shallow donor impurities in GaAs-$Ga_{1-x}Al_xAs$ multiple-quantum-well (MQW) structures were performed by Jarosik *et al.*[5] who assigned structures in the transmission spectra to intraimpurity $1s$-$p_{\pm}$ transitions. Work on magnetic-field effects on shallow impurities in GaAs-$Ga_{1-x}Al_xAs$ MQW structures was also recently reported by Barmby *et al.*[7] The effects of electric and magnetic fields on the confined impurities in selectively-donor-doped QW's have been studied in some detail by Yoo, McCombe, and Schaff.[6] They observed that the sensitivity of the absorption-line profile to the impurity distribution increases as the electric-field strength increases, and the impurity distribution is strongly reflected in the absorption-line shape; their theoretical discussion and interpretation of the experimental data was, however, too simple minded. In a recent theoretical work,[8] it was shown that a detailed study of the intradonor absorption spectra with a proper consideration of the impurity-doping profile is necessary for a quantitative understanding of the experimental data. Such a detailed work is therefore the purpose of the present investigation, in which we study the effects of electric and magnetic fields, both applied perpendicular to the interfaces of the GaAs-$Ga_{1-x}Al_xAs$ QW, on the intradonor infrared-absorption spectra associated with transitions between the $1s$-like donor-hydrogenic ground state and $2p_{\pm}$-like excited states of donors selectively doped in the QW. The Hamiltonian, in the effective-mass approximation, for a shallow donor in a single GaAs-$Ga_{1-x}Al_xAs$ QW in the presence of electric and magnetic fields is written as

$$H=(1/2m^*)(\mathbf{p}-e\,\mathbf{A}/c)^2-e^2/\varepsilon r+|e|Fz+V_B(z)\ , \quad (1)$$

where we have used the standard notation for each term.[8] In the above, we ignore differences between the external F and internal screened electric field and neglect tunneling effects due to the presence of the electric field. We choose the vector potential as $\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2$ with the magnetic field along the growth direction. We follow a variational procedure and take the variational $1s$- and $2p_{\pm}$-like donor wave functions as products of the exact solution $\phi_0(z)$ of the square well with electric field and hydrogeniclike functions $1s$ and $2p_{\pm}$ given as

$$\varphi_{nlm}(\mathbf{r})=\rho^{|m|}e^{im\phi}\exp\{-(1/\lambda)[\rho^2+(z-z_i)^2]^{1/2}\}\ ,$$

where λ is a variational parameter. Energies and wave functions of the donor ground and excited states are obtained variationally as functions of the electric and magnetic fields, which are explicitly included in the calculation through Eq. (1). Details of the calculation for the

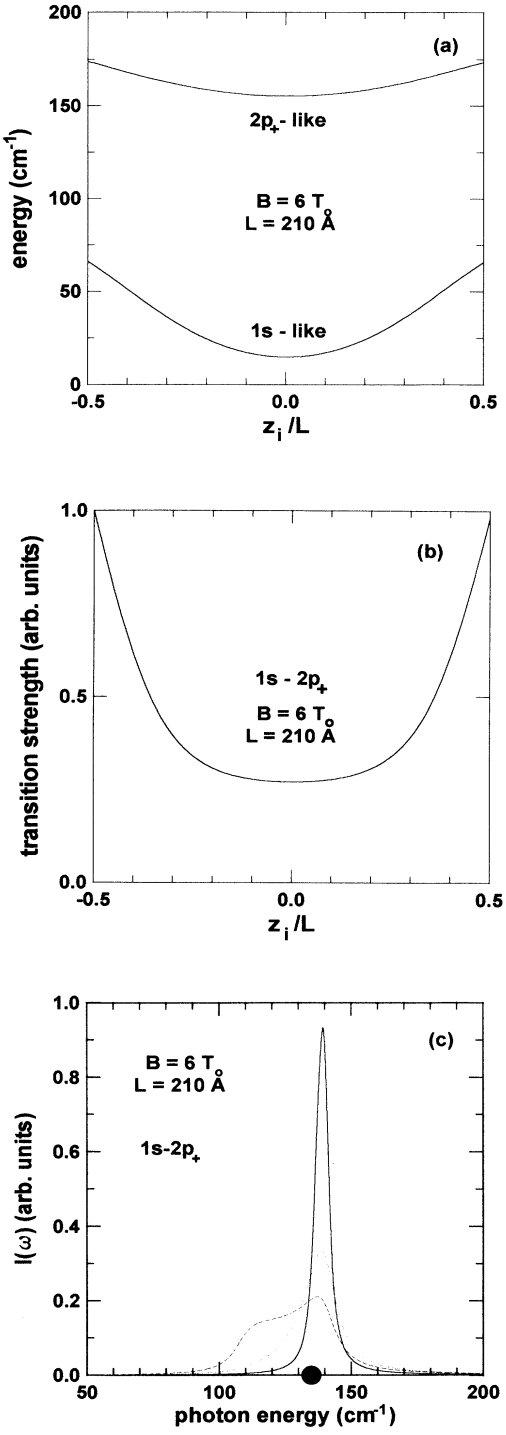


FIG. 1. (a) Energies of the 1s- and $2p_+$-like states of donor impurities at the z_i position, (b) $|\langle 1s|x|2p_+\rangle|^2$ transition strength, and (c) $1s$-$2p_+$ intradonor absorption coefficients $I(\omega)$ for an $L=210$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under a magnetic field of 6 T applied along the growth direction, and for a homogeneous distribution (dashed line), an on-center Gaussian distribution (dotted curve) of half-width equal to $L/3$, and for a distribution over the QW central $\frac{1}{3}$ (full line) of donor impurities. The full dot on the horizontal axis corresponds to the experimental result by Jarosik *et al.* (Ref. 5).

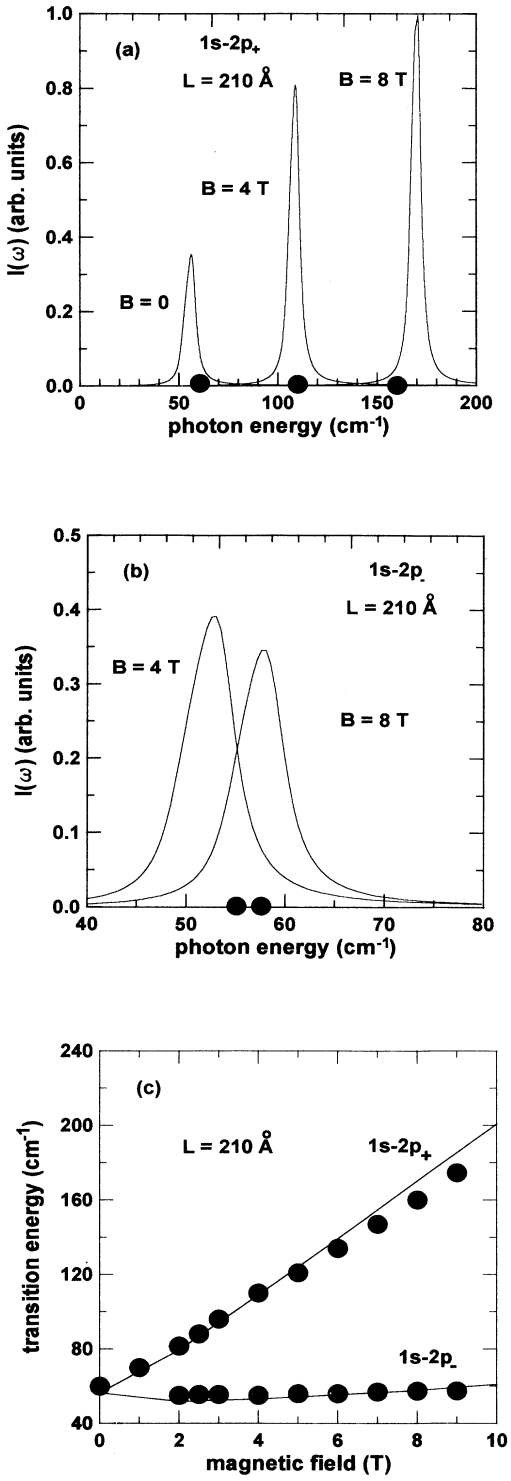


FIG. 2. Intradonor absorption spectra for $1s$-$2p_+$ (a) and $1s$-$2p_-$ (b) transitions (with x-polarized radiation), and theoretical [peaks of absorption spectra $I(\omega)$—full curves in (c)] $1s$-$2p_+$ and $1s$-$2p_-$ transition energies (c) for an $L=210$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under magnetic fields applied along the growth direction, and for a donor distribution over the central $\frac{1}{3}$ of the QW. Full dots correspond to the experimental result by Jarosik *et al.* (Ref. 5).

impurity states may be found elsewhere.[8,9]

The line strength for transitions from the donor $1s$ ground state to $2p_{\pm}$ excited states is proportional to the square of the momentum matrix elements between the initial and final states, which may alternatively be obtained by calculating the corresponding effective-mass position matrix elements,[10] which for absorption of light polarized in the x direction may be expressed as

$$|\langle 1s|x|2p_{\pm}\rangle|^2=(\hbar^2/m^*E_{1s\text{-}2p_{\pm}})^2 \times\left|\left\langle 1s\left|\frac{\partial}{\partial x}+\frac{eA_x}{i\hbar c}\right|2p_{\pm}\right\rangle\right|^2, \quad (2)$$

where x is the carrier position with respect to the donor impurity and $E_{1s\text{-}2p_{\pm}}$ is the difference in energy between the initial and final states involved in the intradonor transition. One should note that energies are measured from the bottom of the first GaAs conduction subband. Finally, the absorption spectra between donor states $1s$ and excited final states $2p_{\pm}$ can be obtained by

$$I(\omega)\approx\omega\int_{-L/2}^{L/2}dz_i|\langle 1s|x|2p_{\pm}\rangle|^2P(z_i)\delta(E_{1s\text{-}2p_{\pm}}/\hbar-\omega), \quad (3)$$

where $P(z_i)$ is the donor density in the QW.

Figure 1(a) shows the energies of the $1s$- and $2p_{\pm}$-like states of donor impurities at the z_i position, for an $L=210$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under a magnetic field of 6 T applied along the growth direction, whereas the $1s$-$2p_{\pm}$ transition strength $|\langle 1s|x|2p_+\rangle|^2$ as a function of the z_i donor position is shown in Fig. 1(b). We have calculated the related intradonor $1s$-$2p_+$ absorption spectra [Fig. 1(c)] by taking into account different donor distributions inside the GaAs well, i.e., a homogeneous distribution (dashed line), an on-center Gaussian distribution (dotted curve) of half-width equal to $L/3$, and a distribution over the QW central $\frac{1}{3}$ (full line). The full dot

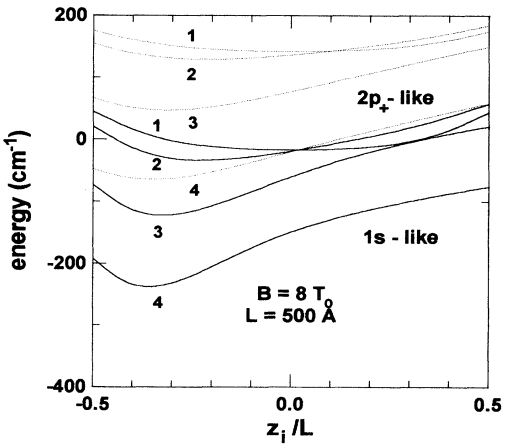
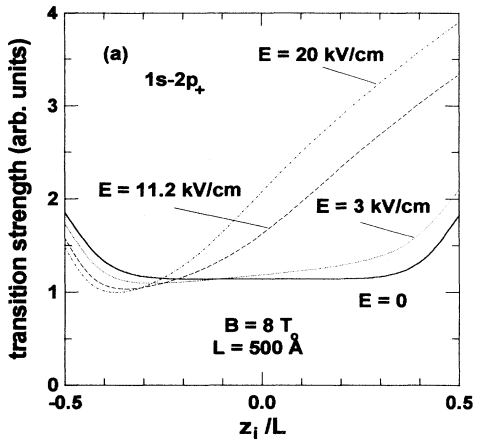
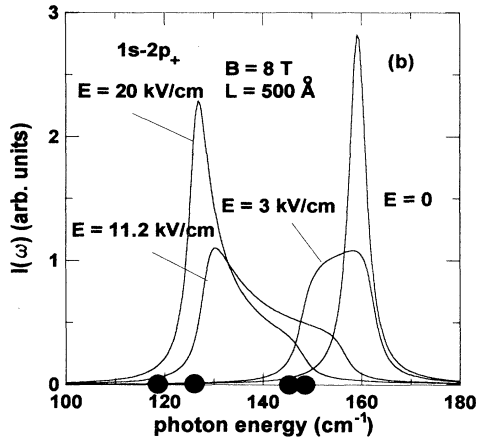


FIG. 3. Energies of $1s$- (full lines) and $2p_+$-like (dotted curves) states as functions of z_i donor positions for an $L=500$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under $B=8$ T and different electric fields, with both fields applied along the growth direction. Curves 1, 2, 3, and 4 correspond to electric fields of 0,3, 11.2, and 20 kV/cm, respectively.





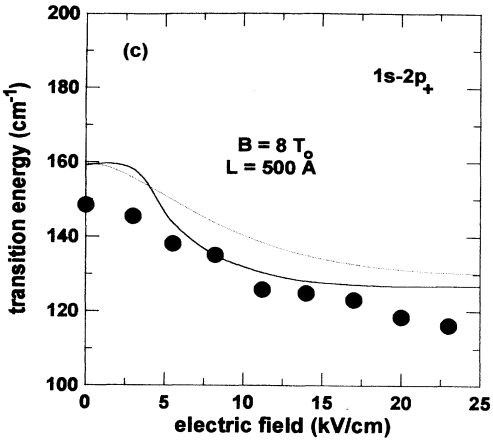


FIG. 4. (a) Intradonor $|\langle 1s|x|2p_+\rangle|^2$ transition strengths as functions of z_i donor positions, (b) $1s$-$2p_+$ absorption spectra $I(\omega)$ for a donor distribution over the central $\frac{1}{3}$ of the QW, and (c) theoretical [peaks of absorption spectra—full curve in (c); donor on-center transition energies—dotted line in (c)] for an $L=500$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under a $B=8$ T and different applied electric fields. Full dots correspond to the experimental results by Yoo, McCombe, and Schaff (Ref. 6).

on the horizontal axis of Fig. 1(c) corresponds to the experimental result by Jarosik *et al.*[5] of a sample doped with silicon donors at the central third of the QW. The good agreement between our theoretical results for the central-$\frac{1}{3}$-doped QW and the experimental measurement by Jarosik *et al.*[5] is apparent. Also, our results for the homogeneously doped QW show a low-energy peak which is clearly associated with $1s$-$2p_+$ intradonor transitions at the edge of the QW [cf. Fig. 1(a)], due to the rather large $1s$-$2p_+$ transition strength for on-edge donors. Theoretical results for the $1s$-$2p_{\pm}$ intradonor absorption spectra for x-polarized radiation are shown in Figs. 2(a) and 2(b), for an $L=210$ Å GaAs-$Ga_{1-x}Al_xAs$ QW, considering different values of the magnetic field, i.e., $B=0$, 4, and 8 T. The peaks of the absorption spectra corresponding to the $1s$-$2p_{\pm}$ transition energies are compared with the experimental data by Jarosik *et al.*[5] It is worthwhile to note that the appropriate way to compare theoretical and experimental results is through an analysis of the infrared-absorption line shape, which depends on the impurity distribution along the GaAs QW [see, e.g., Fig. 1(c)]. It is also evident that the agreement between our theoretical results and experimental data[5] is quite good for low values of the magnetic-field strength. We believe that a better agreement with the experimental results for higher values of the magnetic field might be achieved with a more realistic description[3] of the $\varphi_{nlm}(\mathbf{r})$ hydrogenic part of the donor-electron envelope wave function.

The effects of both electric and magnetic fields on the energies of the $1s$- and $2p_+$-like states as functions of the z_i donor positions for an $L=500$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under $B=8$ T are shown in Fig. 3. It is apparent that the effect of the electric field on the energies of the donor states is to lower the energy for donors at the left side of the QW, due to the higher confinement caused by the triangular-shaped potential. Intradonor $|\langle 1s|x|2p_+\rangle|^2$ transition strengths as functions of z_i donor positions are shown in Fig. 4(a) for an $L=500$ Å GaAs-$Ga_{1-x}Al_xAs$ QW under the effect of a magnetic field of 8 T and for different intensities of electrical field. As the electrical field increases, the $1s$-$2p_+$ transition strength increases (decreases) for donors on the right (left) side of the QW, due to the increasing (decreasing) overlap between the $1s$ and $2p_+$ wave functions caused by the electric-field potential distortion; notice that, for donors at the left side of the QW, the higher confinement of the $1s$ wave function around the impurity position corresponds to a decrease in the overlap with the $2p_+$ wave function, as the latter is zero at the donor position. The $1s$-$2p_+$ absorption spectrum is shown in Fig. 4(b) for $B=8$ T and different values of the electric-field strengths. For the $E=3$ kV/cm absorption spectrum, the theoretical results indicate a clear contribution from donors at the right side of the QW due to their high values of the $1s$-$2p_+$ transition strength [see Fig. 4(a)]. In Fig. 4(c) we display the theoretical peaks of the absorption spectra for varying electric fields as well as the theoretical results for the donor on-center transition energies. One should note that the error bars associated with the experimental data[6] are quite large for high values of electric-field strength. A comparison with the experimental data by Yoo, McCombe, and Schaff[6] clearly indicates that a proper consideration (as done in this work) of the theoretical absorption spectra is essential for a quantitative understanding of the experiment. Moreover, it is apparent from Fig. 4(c) that a better description of the experimental measurements for high values of the electric-field strength (and for $B\approx 8$ T) would require more realistic hydrogenic variational wave functions (with more variational parameters in order to better allow distortions caused by the applied fields[3]).

In conclusion, we have presented a theoretical study of the intradonor infrared-absorption spectra associated with transitions between the $1s$-like ground state and $2p_{\pm}$-like excited states of hydrogenic donors in GaAs-$Ga_{1-x}Al_xAs$ QW's under electric and magnetic fields. Donor energies and envelope wave functions are obtained within a variational procedure in the effective-mass approximation. The $1s$-$2p_{\pm}$ absorption spectra are calculated for x-polarized radiation and theoretical results compare well with available experimental data. Moreover, the present work unambiguously shows that a calculation of the absorption spectra with the appropriate doping profile is needed if one aims to a full understanding of experimental measurement.

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