Effects of Electric and Magnetic Fields on the $1s \rightarrow 2p_+$ Donor Transitions in Quantum Wells

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We calculate the effects of both electric and magnetic fields on the donor transition energies on a GaAs-$Ga_{1-x}Al_xAs$ quantum well by following a variational calculation within the effective-mass approximation which takes into account the anisotropy effects of the applied electric field. A detailed analysis of the absorption spectra considering the impurity-doping profile was performed and the results are compared with experimental data by Yoo *et al.* [Phys. Rev. **44**, 13152 (1991)]. The theoretical results for the donor transition energies for GaAs-$Ga_{1-x}Al_xAs$ quantum well are in good agreement with the reported measurements.

I. Introduction

The important role played by impurities on bulk semiconductor systems has achieved its natural counterpart into the physics of low-dimensional heterostructures as it is the case of selectively-doped quantum wells (QW's). Spectroscopic measurements of various kinds have been used over the past few years to determine the effects of confinement on shallow impurities in QW's structures. In particular, Parihar *et al.*[1] have recently shown how impurity transitions can be used to avoid the rapid nonradiative intersubband relaxation of carriers and could naturally find applications as infrared detectors and emitters. Jarosik *et al.*[2] have reported $1s \rightarrow 2p_\pm$ transitions in GaAs-$Ga_{1-x}Al_xAs$ quantum wells by analysing the transmission spectra of far-infrared magnetospectroscopic measurements on shallow impurities in these QW's. The effects of magnetic and electric fields on the confined impurities in selectively-donor-doped quantum wells have been studied by Yoo *et al.*[3]. By investigations on the far-infrared magnetospectroscopy measurements they observed that the impurity distribution is strongly reflected in the absorption line shape.

In a recent theoretical work[4], we have calculated the $1s \rightarrow 2p_\pm$ transition energies of hydrogenic donors in a GaAs-$Ga_{1-x}Al_xAs$ QW under electric and magnetic fields by adopting a simple variational calculation. The results evidenciated a strong dependence on the impurity position along the well and also show that the theoretical results for the transition energies deviate from the experirnental data for large range of electric field values. In that case the donor hydrogen-like part of the envelope-wave function deviate from the simple form considered in that work since it does not take into account the strong anisotropy introduced by the electric field and therefore a more realistic description would be necessary. Comparisons with experimental data also indicated that a detailed study of the intradonor absorption spectra together with a proper consideration of the impurity-doping profile were necessary for a quantitative understanding of the experimental results[5].

In this work we present a variational calculation of the $1s \rightarrow 2p_+$ transition energies for a donor in a GaAs-$Ga_{1-x}Al_xAs$ QW which explicitly takes magnetic- and electric-field effects into account. We adopt a more realistic trial envelope-wave function for the donor electron which considers the anisotropy introduced by the electric field. The theoretical results clearly evidenciate good agreement with the experimental data by Yoo *et al.*[3].

II. Theory

In the effective-mass approximation, the Hamiltonian for a hydrogenic impurity in a GaAs-$Ga_{1-x}Al_xAs$ QW, in the presence of a magnetic field B and an electric field F, both applied perpendicularly to the interfaces, can be written as

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

where V_B is the barrier potential, $r = [\rho^2 + (z - z_i)^2]^{1/2}$ is the electron position with respect to the donor at z_i and m^* and ϵ are the GaAs conduction-band effective-mass and dieletric constant, respectively. Using a cylindrical gauge, the vector potential is defined as $\mathbf{A} = \frac{(\mathbf{B}x\mathbf{r})}{2}$. The variational donor-envelope-wave functions are taken as product of the exact solution of the square well with applied electric field[6] (a linear combination of Airy functions) and variational hydrogen-like functions[7] for the $1s - (m = 0)$ and $2p_+(m = +1)-$like states

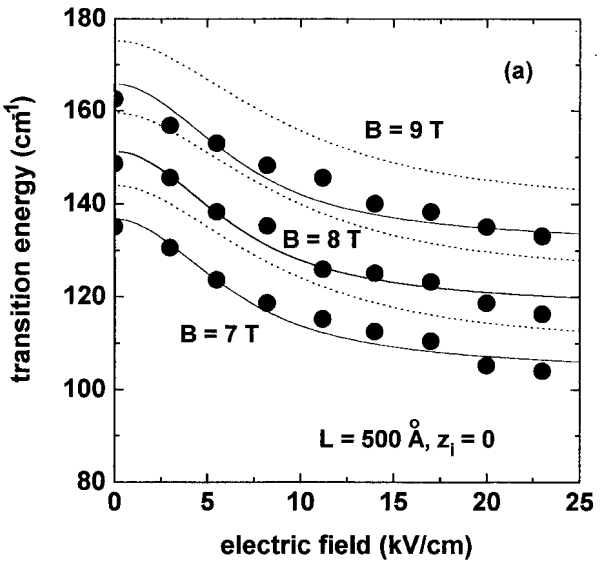
$$\Gamma_{n,l,m} = \rho^{|m|}e^{im\phi}e^{-(\alpha r + \beta\rho^2 + \gamma(z-z_i)^2)}, \quad (2)$$

where n, l, and m are integers which correspond to the principal, orbital and azimuthal quantum numbers of the hydrogen-like functions, respectively, and α, β and γ are variational parameters. The energies of the $1s$ and $2p_+$-like states are calculated from the minimization of the energy with respect to the variational parameters (α, β, and γ) as functions of the electric and magnetic fields.

The absorption spectra for x-polarized radiation between donor states $1s$ and excited states $2p_+$ can be obtained by[8]

$$\alpha(\omega) \approx \omega \int_{-L/2}^{L/2} |< 1s|x|2p_+ >|^2 P(z_i)\delta(E_{1s-2p_+} - \hbar\omega)dz_i\ , \quad (3)$$

where $P(z_i)$ is the donor density distribution in the QW, $E_{1s\rightarrow 2p_+}$, are the transition energies between the $1s$-like and $2p_+$-like states, and a sum over donor positions has been approximated by the integral on z_i.



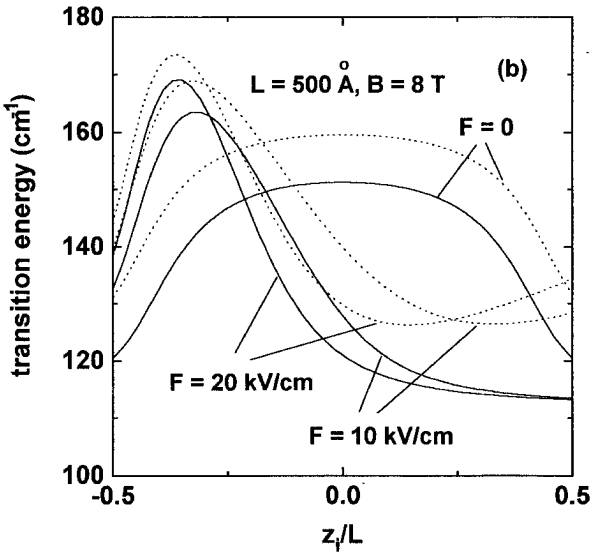


Figure 1. Intradonor $1s \rightarrow 2p_+$ transition energies for an L = 500Å GaAl-$Ga_{1-x}Al_xAs$ QW and for (a) B = 7, 8 and 9T as a function of the applied electric field and for (b) B = 8T as a function of the donor position within the well for three values of the electric field. Full curve corresponds to the present calculation whereas the dotted curves are concerned with a simple one parameter envelope wave-function. The full dots in (a) correspond to experimental data by Yoo *et al.* [see Ref.3].

III. Results

Theoretical results and experimental data[3] for $1s \rightarrow 2p_+$ intradonor transition energies for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW under diferent values of magnetic fields as a function of the applied electric field are shown in Fig. (1a). Experimental data are concerned to a central 1/3 doped GaAl-$Ga_{1-x}Al_xAs$ QW whereas the theoretical results are for on-center donors. A comparison between the present calculation and one related to a simple one parameter envelope wave-function (dotted curves) is also shown in the figure evidenciating a reduction on the $1s \rightarrow 2p_+$ intradonor transition energies. The dependence of the donor $1s \rightarrow 2p_+$ transitions energies on the donor position within the quantum well is detailed in Fig. (1b) for three values of the electric field. An enhancement on the transition energies for donors at the left well edge ($z_i = -L/2$) is clearly noted as the electric field increases due to the larger concentration of the electronic charge around the impurity caused by distortion of the QW in the presence of the applied electric field.

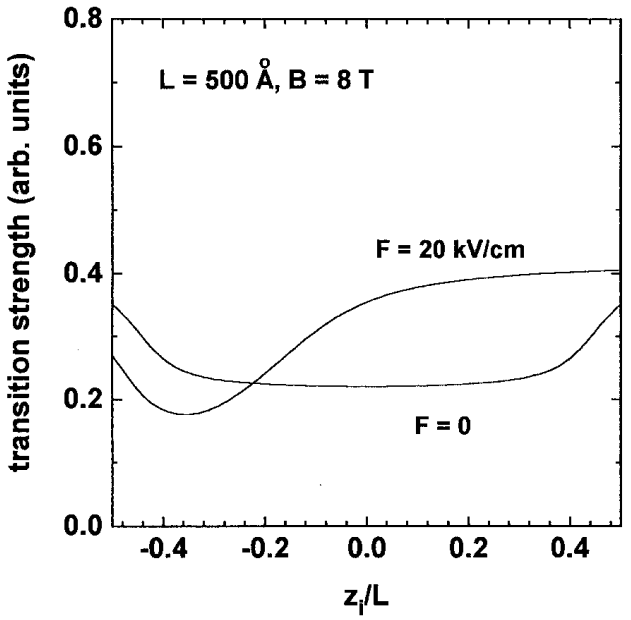


Figure 2. $| < 1s|x|2p_+ > |^2$ transition strength for L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW under a magnetic field of 8T applied along the growth direction for zero and 20 kV/cm electric field.

Fig. 2 show the transition strengths, $| <1s|x|2p_+> |^2$, for an x-polarized radiation, for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW under a magnetic field of 8 T for two values of the electric field as a function of the donor position within the QW. One should notice that since the experimental data are concerned to 1/3 central-doped samples, the actual region which deserves a detailed study goes from -L/6 to L/6. As expected, in the case of zero electric field, the transition strength exhibits perfect symmetry around the center of the well. In the presence of an electric field, the square shape of quantum well changes to a triangular one concentrating the electronic charge on one of the sides of the QW; this effect is also reflected on the transition strengths. As expected, the transition strength is very sensitive to the value of the electric field and to the impurity position within the well indicating unanbiguously that absorption spectra calculations are fundamental for a correct theoretical treatment of the experimental data. Absorption coefficients for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW as functions of the photon energy for some values of the applied fields are presented in Fig. 3. It is interesting to notice that for the case of zero electric field [see Fig. 3(a)] the intradonor absorption spectra exhibits a well-defined peak at the energy corresponding to the intradonor $1s \rightarrow 2p_+$ transition whereas for F = 5.5 kV/cm a broad feature is found in the structure of the absorption spectra. This indicates that a crude analysis of the absorption spectra, taking into account the impurity profile, must be viewed with caution for a large range of electric field since it does not always exhibit a well defined peak which characterize the transition energy of interest. The strong evolution on the shape of the absorption spectra as the electric field changes from zero to 23 kV/cm is shown in Fig. 3(b). Also shown in Fig. 3(a) are the results for a calculation considering a simple donor envelope-wave function with only one variational parameter (dotted curves). It is apparent from a comparison between both theoretical results that when absorption coefficient does not exhibit a well defined peak [see the case for F = 5.5kV/cm] the intradonor transition energy can not be simply associated with its larger value since it does not always correspond to the actual transition energy; for an electric field of 5.5kV/cm the intensity of the absorption coefficient is almost constant for a large range of photon energy in both calculations.

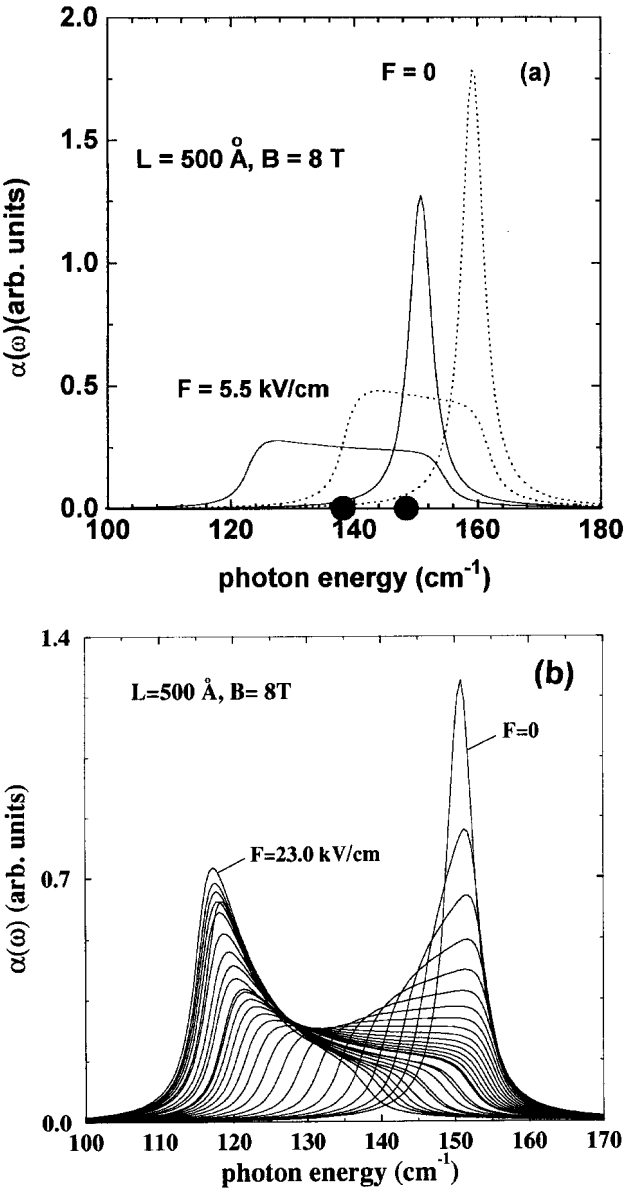


Figure 3. $1s \rightarrow 2p_+$ intradonor absorption coefficient, $\alpha(\omega)$, for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW under a magnetic field of 8T and for a distribution over the central 1/3 of donor impurities for (a) 0 kV/cm and 5.5 kV/cm, and (b) for a large range of electric field (from 0 to 23 kV/cm). The full dots on the horizontal axis of Figure (a) correspond to experimental data by Yoo *et al.* [Ref. 3].

Results for the intradonor $1s \rightarrow 2p_+$ transitions energies as functions of the electric field for B = 8T for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW are presented in Fig. 4. We compare both theoretical results obtained via the "peaks" of the absorption coefficient (full curves) with the on-center donor results (dotted curves). The experimental data which are for wells donor doped over the central 1/3, are denoted by full dots. The remarkable differences found between the theoretical results obtained via the "peaks" of the absorption coefficient for a large range of electric field value for both calculations, and experimental data, can mainly be understood from inspections of Fig. 3 by analysing the shape of the absorption spectra for different values of the applied electric field.

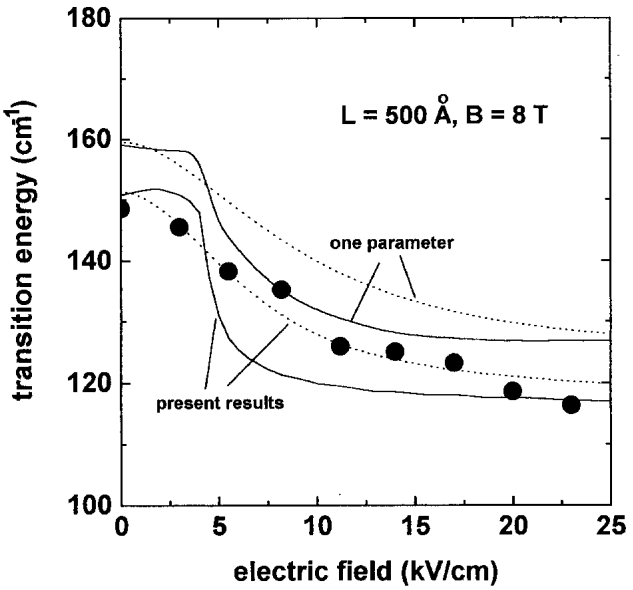


Figure 4. Intradonor $1s \rightarrow 2p_\pm$ transition energies for an L = 500 Å GaAl-$Ga_{1-x}Al_xAs$ QW and for B = 8T for theoretical donor on-center calculations (dotted curves) and transition energies obtained via the peaks of the absorption spectra (solid curves) as functions of the applied electric field. Full dots correspond to experimental results by Yoo *et al.* [Ref 3].

In summary we have presented a theoretical study of the effects of electric and magnetic fields on the intradonor infrared-absorption spectra associated with $1s \rightarrow 2p_+$ transitions of donors in GaAs-GaAlAs quantum wells following a variational treatment within the effective-mass approximation. The choice of a more adjustable trial wave-function for the hydrogenic part of the envelope wave-function which includes the effects of the applied fields together with an appropriate calculation of the absorption coefficients (which takes into account the profile of the impurity distribution) provides a quantitative understanding of the magnetospectroscopic measurements.

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References

1. S. R. Parihar and S. A. Lyon, Aply. Phys. Lett. **62,** 2396 (1993).
2. N. C. Jarosik, B. D. McCombe, B. V. Shallabrook, J. Comsa, J. Ralston and G. Wicks, Phys. Rev. Lett. **54**, 1283 (1985).
3. B. S. Yoo, B. D. McCombe and W. Schaff, Phys. Rev. **B 44,** 13152 (1991).
4. A. Latgé, N. Porras-Montenegro and L. E. Oliveira, Phys. Rev. **B 51**, 2259 (1995).
5. A. Latgé, N. Porras-Montenegro and L. E. Oliveira, Phys. Rev. **B 51**, 13344 (1995).
6. J López-Gondar, J. d'Albuquerque e Castro and L. E. Oliveira, Phys. Rev. **B 42**, 7069 (1990).
7. S. Chaudhuri and K. K. Bajaj, Sol. St. Commun. **52**, 967 (1984).
8. R. L. Greene and K. K. Bajaj, Phys. Rev. **B 34,** 951 (1986).