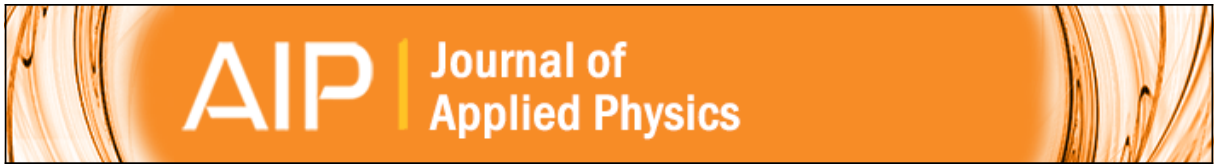

Effects of external fields on the far-infrared 1s→2p + intradonor absorption spectra in quantum wells

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Citation: Journal of Applied Physics **80**, 2536 (1996); doi: 10.1063/1.363041

View online: http://dx.doi.org/10.1063/1.363041

View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/80/4?ver=pdfcov

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Effects of external fields on the far-infrared $1s \rightarrow 2p_+$ intradonor absorption spectra in quantum wells

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(Received 8 February 1996; accepted for publication 14 May 1996)

The effects of both electric and magnetic fields (applied perpendicular to the interfaces) on the donor transition energies on a GaAs-$Ga_{1-x}Al_xAs$ quantum well are studied by following a variational calculation within the effective-mass approximation with two-parameter variational envelope hydrogenic wave functions for the $1s$- and $2p_+$-like donor states. A detailed analysis of the far-infrared intradonor absorption spectra, taking into account a proper consideration of the impurity-doping profile, is performed and results are compared with recent experimental data. The agreement between the reported magnetospectroscopic data and the average photon energy at the width at half-maximum of the calculated infrared-absorption spectra is quite apparent. It is unambiguously shown that the absorption spectra must be evaluated with an adequate choice of the variational envelope wave function for a correct quantitative understanding of the experimental measurements. © *1996 American Institute of Physics.* [S0021-8979(96)04116-3]

The important role played by impurities on bulk semiconductor systems has achieved its natural counterpart into the physics of low-dimensional heterostructures as is the case of selectively doped quantum wells (QWs). Spectroscopic measurements of various kinds have been used over the past few years to determine the effects of confinement on shallow impurities in QW structures. In particular, Parihar and Lyon[1] have recently shown how impurity transitions can be used to avoid the rapid nonradiative intersubband relaxation of carriers and would naturally find applications as infrared detectors and emitters. Jarosik *et al.*[2] have reported $1s \rightarrow 2p_+$ transitions in donor-doped GaAs–$Ga_{1-x}Al_xAs$ quantum wells by analyzing the transmission spectra via far-infrared magnetospectroscopic techniques. This work was followed by a number of theoretical and experimental investigations.[3–6] The effects of magnetic and electric fields on the confined impurities in selectively donor-doped QWs have been studied by Yoo, McCombe, and Schaff.[7] By performing far-infrared magnetospectroscopy measurements, they argue that the impurity distribution is strongly reflected in the absorption line shape for a QW under electric fields.

In a recent theoretical work, Latgé *et al.*[5] have calculated the $1s \rightarrow 2p_+$ transition energies of hydrogenic donors in GaAs–$Ga_{1-x}Al_xAs$ QWs under electric and magnetic fields by adopting a simple one-parameter variational wave function for the $1s$- and $2p_+$-like states. Results show a strong dependence on the impurity distribution within the well and good agreement with experimental data. Also, Latgé *et al.*[5,6] conclude that a better description of the experimental data would require more realistic hydrogenic variational wave functions in order to better allow for distortions caused by the electric and magnetic applied fields.

In this work, therefore, we present a variational calculation of the $1s \rightarrow 2p_+$ transition energies for a neutral donor in a GaAs–$Ga_{1-x}Al_xAs$ QW which explicitly takes magnetic- and electric-field effects into account in the variational scheme, and consider a more realistic two-parameter trial envelope wave function for the donor $1s$ and $2p_+$ states.

In the effective-mass approximation, the Hamiltonian for a neutral-donor 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 perpendicular to the interfaces, may be written as

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

where V_B is the barrier potential, e is the electron charge, $r=[\rho^2+(z-z_i)^2]^{1/2}$ is the electron position with respect to the donor at z_i, and m^* and ϵ are the GaAs conduction-band effective mass and dielectric constant, respectively, which we take as constants throughout the heterostructure. Using a cylindrical gauge, the vector potential is taken as $\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2$. The variational donor-envelope wave functions are written as products of the exact solution of the square well with applied electric field[5,6,8] (a linear combination of Airy functions) and two-parameter[9,10] variational hydrogeniclike functions for the $1s$ $(m=0)$ and $2p_+$ $(m=+1)$ -like states,

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

where n, l, and m are integers corresponding to the principal, orbital, and azimuthal quantum numbers of the hydrogeniclike functions, respectively, and α and β are variational parameters. For the case of applied external fields, the use of a single-parameter trial envelope wave function is certainly not adequate since it preserves the spherical symmetry of the hydrogeniclike wave function and does not take into account the anisotropy effects introduced by the external fields, i.e., a

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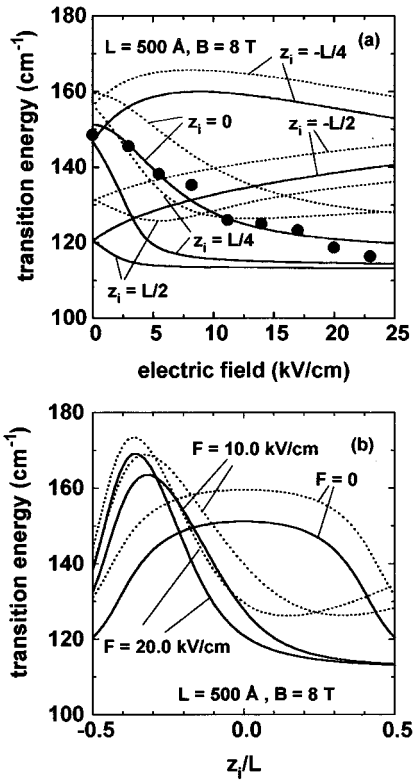

FIG. 1. Intradonor $1s\rightarrow 2p_+$ transition energies for an $L=500$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ QW and $B=8$ T as functions (a) of the applied electric field for different positions of the donor inside the QW, and (b) of the donor position within the well for $F=0$, 10 and 20 kV/cm. Solid curves correspond to the present calculation whereas the dotted lines correspond to a calculation with a trial one-parameter envelope wave function (Ref. 5). Full dots in (a) correspond to experimental data by Yoo and co-workers (Ref. 7).

distortion on the z direction and an electronic confinement in the layers. One should note that these effects are somehow considered through the variational parameters α and β included in the choice for the trial wave function in the present calculation [Eq. (2)]. The energies of the $1s$- and $2p_+$-like states are calculated from the minimization of the energy with respect to the variational parameters as functions of the electric and magnetic fields.

The absorption spectra, for x-polarized radiation, between donor states $1s$ and excited states $2p_+$ may be obtained by[5,6,9]

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

where $P(z_i)$ is the donor distribution in the QW, and $E_{1s\rightarrow 2p_+}$ represents the transition energy between the $1s$- and $2p_+$-like states. In order to simulate broadening processes, we replace the above delta function by a Lorentzian with a width of 4 cm^{-1} ($\approx$0.50 meV).[7,11]

Theoretical results and experimental data for $1s\rightarrow 2p_+$ intradonor transition energies for an $L=500$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ QW under a magnetic field of 8 T as functions of the applied electric field are shown in Fig. 1(a) for different positions of the donor within the QW. Experimental data correspond to a central-1/3-doped QW. One

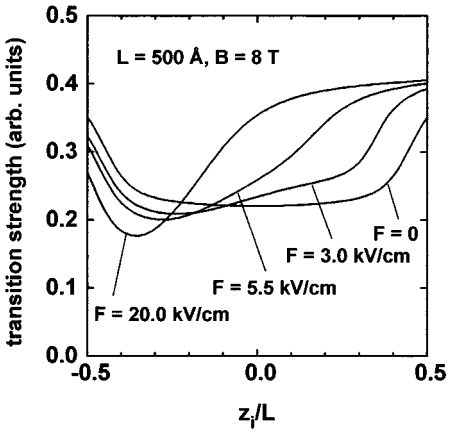

FIG. 2. $|\langle 1s|x|2p_+\rangle|^2$ transition strengths for an $L=500$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ QW under a magnetic field of 8 T, and for zero, 3.0, 5.5, and 20.0 kV/cm applied electric fields.

should notice that a comparison between the intradonor transition energies obtained by the present two-parameter variational calculation (solid lines) with results obtained with a trial one-parameter envelope wave function (dotted curves) shows a reduction in the intradonor $1s\rightarrow 2p_+$ transition energies. The dependence of the transition energies on the donor positions within the QW is depicted in Fig. 1(b) for three values of the electric field. An enhancement of the transition energies for donors at the left-hand-side well edge ($z_i=-L/2$) is clearly seen as the electric field increases due to the larger concentration of the electronic charge around the impurity caused by a distortion of the QW potential in the presence of the electric field.

The transition strengths, $|\langle 1s|x|2p_+\rangle|^2$, for x-polarized radiation, and for an $L=500$ Å QW under a magnetic field of 8 T are shown in Fig. 2 for different values of the electric field as functions of the donor position within the QW. One should notice that since the experimental data are related to 1/3-central-doped samples, the actual region which deserves a detailed theoretical study is associated with donor positions 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 the QW changes to a triangular one, which concentrates the electronic charge in one of the sides of the QW; this effect is also reflected in the transition strengths. Also, it is apparent from Fig. 2 that the transition strength is quite sensitive to the values of the applied electric fields and to the donor position within the QW, indicating unambiguously that absorption spectra calculations are fundamental in a correct theoretical treatment for a proper understanding of the experimental data.

Intradonor absorption coefficients for an $L=500$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ QW as functions of the photon energy are presented in Fig. 3, for $B=8$ T. For the case of zero electric field the intradonor absorption spectra exhibits a well-defined peak at the energy corresponding to the $1s\rightarrow 2p_+$ transition, whereas for $F=5.5$ kV cm, a broad feature is found in the corresponding structure of the absorption spectra. Figure 3 also shows the results of calculations con-

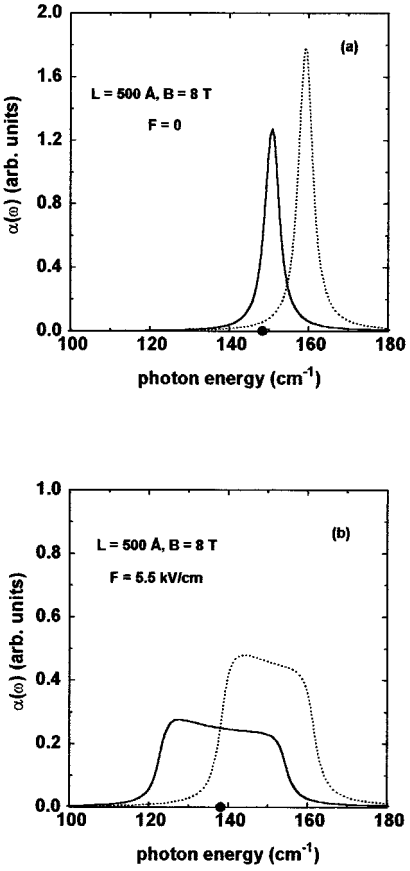

FIG. 3. $1s \rightarrow 2p_+$ infrared-absorption coefficient, for an $L = 500$ Å QW under a magnetic field of 8 T and for a donor distribution over the central 1/3 of the QW: (a) $F = 0$; (b) $F = 5.5$ kV/cm. Solid dots on the horizontal axis are the experimental data by Yoo and co-workers (Ref. 7). Solid curves correspond to the present calculation whereas the dotted lines correspond to a calculation with a trial one-parameter envelope wave function (Ref. 5).

sidering a simple donor envelope wave function with only one variational parameter[5] (dotted curves). It is clear from Fig. 3 that the two-parameter variational scheme, with the donor profile taken into account in the calculation of the absorption coefficient, is essential (as compared to the one-parameter results) for a proper understanding of the experimental data. In Fig. 4 we display, as functions of the applied electric field, the $1s \rightarrow 2p_+$ transition energies associated with the maximum and minimum photon energies at the width at half-maximum of the infrared-absorption spectra, whereas the dashed curve corresponds to the average photon energy at the width at half-maximum. The agreement between the calculated averaged photon energy with the experimental data by Yoo and co-workers[7] is apparent. One may conclude, from Figs. 3 and 4, that a correct understanding of the experimental data may only be obtained from a detailed analysis of the far-infrared–absorption spectra properly calculated with adequate envelope wave functions and

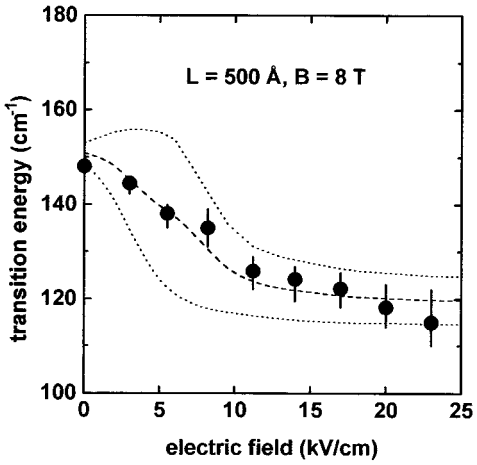

FIG. 4. Intradonor $1s \rightarrow 2p_+$ transition energies for an $L = 500$ Å $GaAs–Ga_{0.7}Al_{0.3}As$ QW under magnetic fields of 8 T, and for a donor distribution over the central 1/3 of the QW. The dotted curves are associated with the maximum and minimum photon energies at the width at half-maximum of the infrared-absorption spectra, whereas the dashed curve corresponds to the average photon energy at the width at half-maximum. Experimental data by Yoo and co-workers (Ref. 7) are represented as solid dots.

with the impurity profile taken into consideration.

In summary, we have presented a theoretical study of the effects of electric and magnetic fields (perpendicular to the QW interfaces) on the intradonor infrared-absorption spec tra associated with $1s \rightarrow 2p_+$ transitions of donors in $GaAs–Ga_{1-x}Al_xAs$ QWs following a variational treatment within the effective-mass approximation. Our results unambiguously show that an appropriate choice for the trial envelope wave function together with a full calculation of the intradonor absorption coefficients is essential for a proper quantitative understanding of the reported magnetospectroscopic measurements.

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