Donor $1s$-$2p_{\pm}$ transitions in doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells: Effects of electric and magnetic fields

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(Received 2 August 1994)

The effects of both electric and magnetic fields on the transition energies between the $1s$-like ground state and $2p_{\pm}$ excited states of hydrogenic donors in a GaAs-$Ga_{1-x}Al_xAs$ quantum well are studied. The effective-mass approximation within a variational scheme is adopted with electric and magnetic fields considered in the growth direction of the heterostructure, and treated directly in the variational calculation. Results for the finite-barrier potential are obtained as functions of both applied fields and for different GaAs-$Ga_{1-x}Al_xAs$ quantum-well thicknesses, and compared with available infrared magnetospectroscopy measurements on donor-doped quantum wells. Theoretical results indicate that a detailed study of the intradonor absorption spectra together with a proper consideration of the impurity-doping profile are necessary for a qualitative understanding of the experimental results.

I. INTRODUCTION

In the last two decades, much attention has been given to the understanding of the physical properties of impurities in semiconducting heterostructures.[1-13] From the theoretical point of view, Bastard[1] studied the binding energies and density of impurity states of shallow impurities in infinite-barrier quantum wells (QW's). Greene and Bajaj[2] calculated the ground state and first excited states of donors in finite-barrier GaAs-$Ga_{1-x}Al_xAs$ QW's, and Mailhiot, Chang, and McGill[3] and Fraizzoli, Bassani, and Buczko[3] included the effects of the discontinuity of the carrier effective masses across the interfaces and of the image potential on the impurity properties. The influence of the nonparabolicity of the GaAs conduction band on the donor properties was investigated by Chaudhuri and Bajaj,[4] whereas the mixing of the valence states was taken into account by Masselink, Chang, and Morkoç[5] in the case of acceptor impurities in GaAs-$Ga_{1-x}Al_xAs$ QW's. A more realistic screening of the impurity potential was considered by Oliveira and Falicov.[6] Various experimental measurements of the properties of impurities in GaAs-$Ga_{1-x}Al_xAs$ QW's have been reported,[7-13] and contain a detailed list of theoretical and experimental work on the properties of hydrogenic impurities in low-dimensional semiconducting systems.

Experimental and theoretical work on the effects of electric and magnetic fields in GaAs-$Ga_{1-x}Al_xAs$ QW's have also been the subject of interest in recent years.[10-16] In particular, electric- and magnetic-field effects on confined donor impurities in GaAs-$Ga_{1-x}Al_xAs$ QW's have recently been reported by Yoo *et al.*[12] In this work we present a variational calculation of the transition energies between the ground and excited states for a donor in a GaAs-$Ga_{1-x}Al_xAs$ QW, which explicitly takes magnetic- and electric-field effects into account. We work within the effective-mass approximation and adopt a variational envelope-wave function for the donor electron. In Sec. II we present the theoretical framework of the problem. Results for the transition energies are presented and discussed in Sec. III. Our conclusions are in Sec. IV.

II. THEORY

In the effective-mass approximation, the Hamiltonian of a hydrogenic donor in a GaAs-$Ga_{1-x}Al_xAs$ QW in the presence of a magnetic field B and an electric field F, may be written as

$$H=(1/2m^*)(\mathbf{p}-e\,\mathbf{A}/c)^2-e^2/\varepsilon r+|e|Fz+V_B(z)\ , \tag{2.1}$$

where $V_B(z)$ is the barrier potential, taken as a square well of height V_0 (an Al concentration of 0.3 would correspond to a potential barrier equal to 224 meV) and width L, $r=[\rho^2+(z-z_i)^2]^{1/2}$ 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. We assume m^* and ε to be constant along the heterostructure[2,6,14,16] ($m^*=0.0665m_0$, where m_0 is the free-electron mass). The electric field applied perpendicularly to the interfaces is denoted by F, and we ignore differences between external and internal screened electric fields, and neglect tunneling effects due to the presence of the electric field. The vector potential is

$\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2$, with the magnetic field applied along the growth direction.

The variational donor envelope-wave functions are taken as products of the exact solution of the square well with electric field, $\phi_0(z)$, and hydrogeniclike functions $\varphi_{nlm}(\mathbf{r})$, i.e.,

$$\Psi_{nlm}(\mathbf{r})=N_{nlm}\phi_0(z)\varphi_{nlm}(\mathbf{r}) , \tag{2.2}$$

where n, l, and m are integers corresponding to the principal, orbital, and azimuthal quantum numbers of the hydrogeniclike functions, respectively, and N_{nlm} is the normalization factor. $\phi_0(z)$ is the envelope function of the well with applied electric field, which is written as[16]

$$\phi_0(z)=\begin{cases} C_1\exp[k_1(z+L/2)] , & z\le -L/2 \\ \alpha\text{Ai}(\xi)+\beta\text{Bi}(\xi) , & -L/2\le z\le L/2 \\ C_2\exp[-k_2(z-L/2)] , & z\ge L/2 , \end{cases} \tag{2.3}$$

with Ai (Bi) being the Airy functions, $k_{2,1}=[(V_0\pm|e|FL/2-E_0)2m^*/\hbar^2]^{1/2}$, and E_0 the ground-state energy of the QW with the applied field.[16] All the constants and parameters appearing in Eq. (2.3) are the same as in Ref. 16. The $1s$- and $2p_\pm$-like variational envelope-wave functions are taken as hydrogenic functions, i.e.,

$$\varphi_{nlm}(\mathbf{r})=\rho^{|m|}e^{im\phi}\exp\{-(1/\lambda)[\rho^2+(z-z_i)^2]^{1/2}\} , \tag{2.4}$$

where λ is a variational parameter. Finally, the energies of the $1s$-, $2p_+$-, and $2p_-$-like states, i.e., $\varepsilon_{nlm}=\langle\varphi_{nlm}|H|\varphi_{nlm}\rangle$, are obtained variationally as functions of the electric and magnetic fields which are explicitly included in the calculation via Eq. (2.1). We would like to emphasize that this variational procedure in the effective-mass approximation proved to be very successful in explaining experimental data on impurity-doped low-dimensional semiconducting heterostructures.[17,18]

III. RESULTS AND DISCUSSION

Intradonor theoretical results for $1s$-$2p_-$ and $1s$-$2p_+$ on-center transitions as functions of the magnetic field and for zero electric field are shown in Fig. 1 for different GaAs-$\text{Ga}_{1-x}\text{Al}_x$As QW's and compared with experimental results of Jarosik *et al.*,[10] McCombe *et al.*[11] [Fig. 1(a)], and of Barmby *et al.*[13] [Fig. 1(b)]. Note that experimental results are for wells donor doped over the central $\frac{1}{3}$. Agreement between theory and experiment is quite reasonable for low magnetic field, whereas for large values of B, one may find deviations from experimental data. Of course, an appropriate comparison with experiment would involve a calculation of the donor absorption line shape, which would depend on the impurity distribution along the GaAs-$\text{Ga}_{1-x}\text{Al}_x$As QW. It is important to notice that a more realistic (with three variational parameters[14]) description of the hydrogeniclike part of the donor-electron envelope-wave function [cf. Eq. (2.2)] would probably be needed for large values of the applied magnetic field, together with a $\phi_0(z)$ which would correspond to the exact solution of the square well taking into account the effect of the magnetic field.[19,20] Intradonor

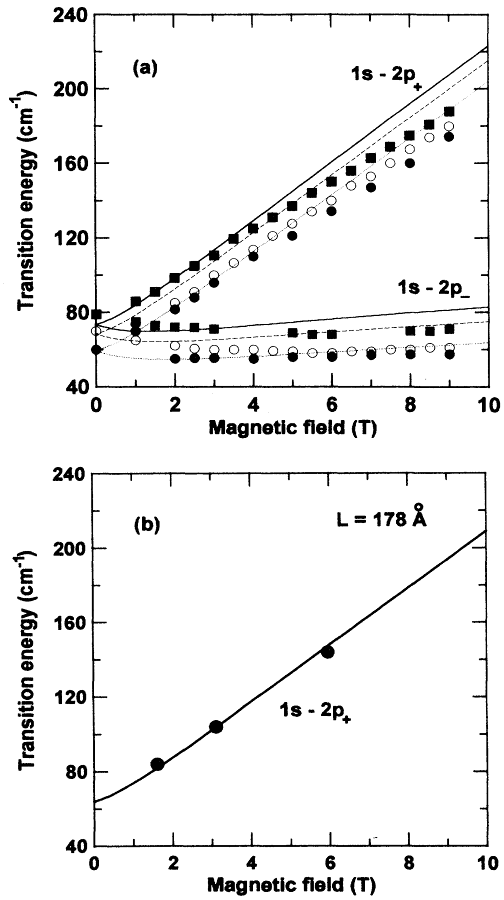

FIG. 1. On-center intradonor (a) $1s$-$2p_-$ and $1s$-$2p_+$ transition energies for GaAs-$\text{Ga}_{0.7}\text{Al}_{0.3}$As QW's of different widths as functions of the magnetic fields: $L=125$ Å [full curve: theory, ■: expt. (Ref. 11)]; $L=150$ Å [dashed curve: theory, ○: expt. (Ref. 11)]; $L=210$ Å [dotted curve: theory, ●: expt. (Ref. 10)]; (b) $1s$-$2p_+$ transition energies for an $L=178$ Å GaAs-$\text{Ga}_{0.67}\text{Al}_{0.33}$As QW as a function of the magnetic field [full curve: theory, ●: expt. (Ref. 13)].

$1s$-$2p_+$ transition energies for GaAs-$\text{Ga}_{0.7}\text{Al}_{0.3}$As QW's versus well widths at various magnetic fields are shown in Fig. 2 for on-center and on-edge donors together with the experimental data (well-center-doped samples) by Jarosik *et al.*[10] Note that all experimental results fall in between the two theoretical curves for on-center and on-edge intradonor transitions, indicating that a calculation of the infrared absorption line shape should be performed for a proper quantitative explanation of the experimental data.

The effects of simultaneous application of electric and magnetic fields on the donor $1s$-$2p_+$ transition energies were studied by Yoo *et al.*[12] Their results on confined shallow donors in GaAs-$\text{Ga}_{1-x}\text{Al}_x$As QW's under electric and magnetic fields (both along the growth direction) were tentatively explained via a variational calculation for the donors inside an infinite-barrier QW. In their theory, they did not include magnetic-field effects in the variational calculation and shifted the theoretical results on-center transitions in order to fit experiment at zero

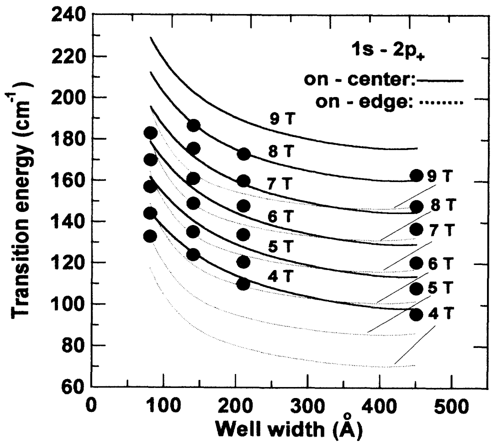

FIG. 2. Intradonor $1s$-$2p_+$ transition energies for GaAs-$Ga_{0.7}Al_{0.3}As$ QW's vs well widths at various magnetic fields. Full circles correspond to experimental data from Jarosik *et al.* (Ref. 10); solid (dotted) curves are the theoretical results for on-center (on-edge) donors. All results for the transition energies decrease in values with decreasing magnetic fields.

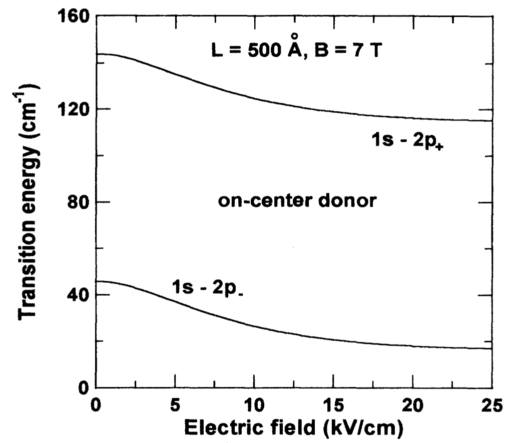

FIG. 4. Intradonor on-center $1s$-$2p_-$ and $1s$-$2p_+$ transition energies for an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, $B=7$ T, vs applied electric fields.

electric field. Figure 3 shows our calculated results (using the same parameter as Yoo *et al.*[12]) at zero magnetic field, infinite-barrier QW, and the same trial wave function as in Ref. 12, for the $1s$-like ground state of on-center donors, as well as the corresponding theoretical results obtained by Yoo *et al.*[12] and by using Bastard's theory[1] (which corresponds to the exact limit of both model calculations for zero applied fields). The agreement between our results and Bastard's[1] for zero electric field is clearly shown in Fig. 3.

Intradonor on-center $1s$-$2p_-$ and $1s$-$2p_+$ transition energies for an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW, $B=7$ T are shown in Fig. 4 as functions of the applied electric fields. Far-infrared magnetospectroscopy data reported by Yoo *et al.*[12] are only available in the 80–220-cm^{-1} frequency range which corresponds to the region of the $1s$-$2p_+$ transition energies, and therefore in what follows we restrict ourselves to an analysis of the $1s$-$2p_+$ transition. Theoretical results in the case of different magnetic fields [explicitly included in the calculation via the Hamiltonian in Eq. (2.1)] and an $L=500$ Å GaAs-$Ga_{1-x}Al_xAs$ QW are shown in Fig. 5 as functions of the electric field for intradonor $1s$-$2p_+$ transition energies and for various donor positions in the well. It is apparent from Fig. 5 that, except for large values of the electric field, the experimental data fall within the donor-position-dependent theoretical transition curves. It is important to notice that, for large values of the electric field, the donor hydrogeniclike part of the envelope-wave function would deviate from the simple form considered in Eq. (2.4), and therefore a more realistic description of the hydrogenic part of the donor-electron variational envelope wave function (taking into account the strong anisotropy introduced by the large electric field) would certainly be necessary. Figure 6 details the dependence of the intradonor $1s$-$2p_+$ transition energies with the donor position within the QW, for three values of the electric field. Comparison between our calculations and experimental results[12] (full dots) clearly indicates that a proper interpretation of the magnetospectroscopy experimental data should involve an adequate consideration of the impurity doping profile in a theoretical calculation of the intradonor absorption line shape in the infrared region. Notice that Figs. 5 and 6 show unambiguously that the theoretical interpretation by Yoo *et al.*[12] of their experimental data is too simplistic.

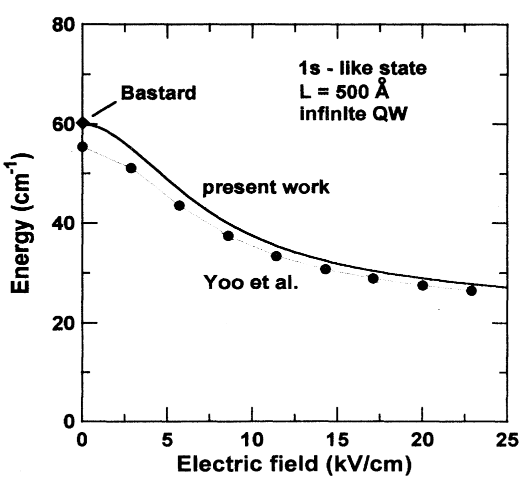

FIG. 3. Binding energy of the $1s$-like ground state for a donor on-center impurity in a GaAs-$Ga_{1-x}Al_xAs$ infinite-barrier QW. Results of the present work are compared with those of Yoo *et al.* (Ref. 12) and Bastard (Ref. 1).

IV. CONCLUSIONS

In this work, we have considered the effects of both electric and magnetic fields in the calculation of the transition energies from the $1s$-like ground state to $2p_+$ excited states of shallow donors in GaAs-$Ga_{1-x}Al_xAs$ QW's. We used the effective-mass approximation within a variational scheme and, for the first time, the electric and magnetic fields applied along the growth direction of the system were directly taken into account in the variational calculation of the shallow-donor energy levels. Theoretical transition energies were compared with available experimental data, and results indicate that a detailed study of the intradonor absorption spectra together with a proper consideration of the impurity-doping profile are necessary for a quantitative understanding of the experimental results.

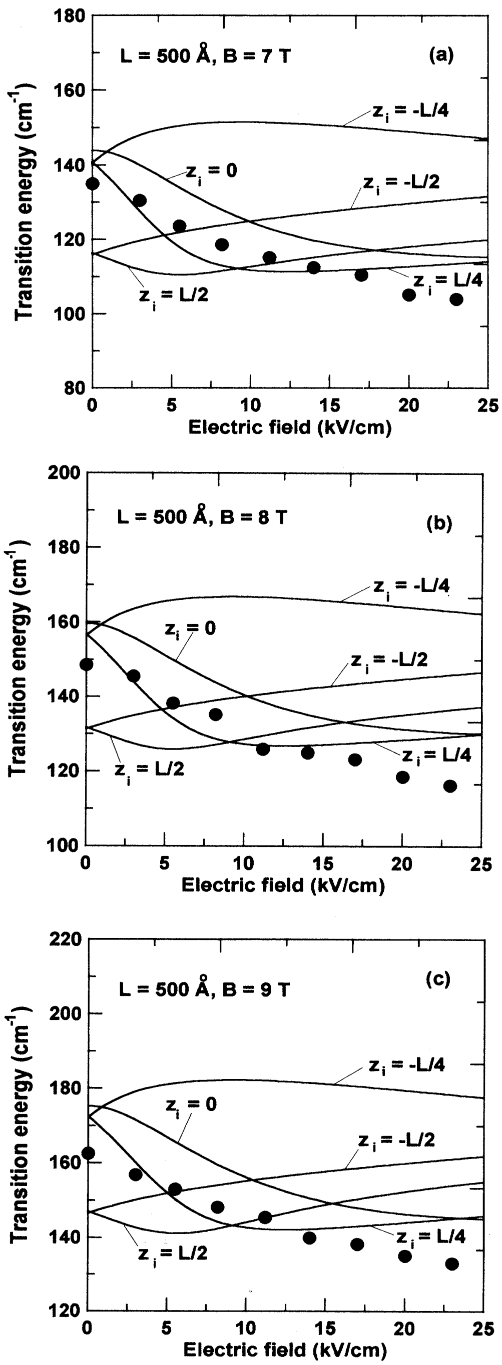

FIG. 5. Intradonor $1s$-$2p_+$ transition energies for (a) $B=7$ T, (b) $B=8$ T, and (c) $B=9$ T magnetic fields and an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW. Theoretical results (solid curves) are given as functions of the electric field at various z_i donor positions in the well, whereas full dots correspond to the far-infrared magnetospectroscopy experimental results (Ref. 12).

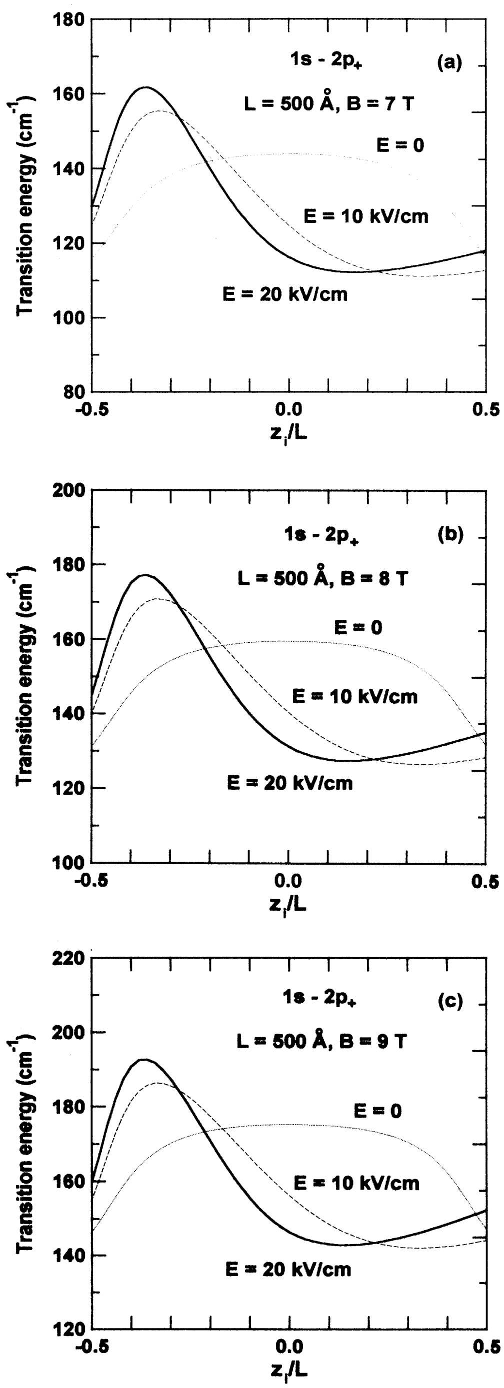

FIG. 6. Intradonor $1s$-$2p_+$ transition energies for (a) $B=7$ T, (b) $B=8$ T, and (c) $B=9$ T magnetic fields and an $L=500$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW. Theoretical results for three electric fields are given as functions of the donor position within the well.

ACKNOWLEDGMENTS

This work was partially financed by Colciencias-Colombia and Brazilian Agencies FAEP-UNICAMP, FAPESP, and CNPq.

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