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Donor transition energies and their line strengths in GaAs/$Al_xGa_{1-x}As$ quantum-well structures in the presence of a magnetic field applied parallel to the interfaces

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We have calculated the transition energies between the ground state (1*s*-like) and three excited states (2*s*-, $2p_y$-, and $2p_z$-like) of a hydrogenic donor associated with the first subband in a GaAs quantum well sandwiched between two semi-infinite layers of $Al_xGa_{1-x}As$ in the presence of a magnetic field applied parallel to the interfaces. In addition, we have also calculated the line strengths of these transitions in various polarizations. Results have been obtained both as a function of the applied magnetic field and the position of the donor ion along the direction of growth. We have followed a variational approach in which the trial wave functions are expanded in terms of appropriate Gaussian basis sets.

INTRODUCTION

There has been a great deal of interest in both the theoretical[1–24] and experimental[25–31] investigations of the behavior of shallow hydrogenic donors in GaAs-$Al_xGa_{1-x}As$ quantum-well structures in recent years. Bastard[1] was the first to calculate the binding energy of the ground state of a hydrogenic donor as a function of the well size and the position of the impurity ion, assuming an infinite potential at the interfaces. This work was followed by several calculations[2,4–7,9,14,24] in which the authors calculated the binding energies of the ground state and of several low-lying excited states of a donor assuming finite values of the potential at the interfaces. The effect of a space-dependent dielectric constant on the energy levels was investigated by Czavinszky and Elabsy[17] and by Oliveira and Falicov.[22] Brum, Bastard, and Guillemot,[8] Guillemot,[13] and Hawrylak and Quinn[20] studied the effect of electron-electron interaction on the ground state energy of a donor in a quantum well. The effect of an electron–optical-phonon interaction on the properties of donors in quantum wells was investigated by several groups.[15,16,19,21] Bastard *et al.*[3] and Greene and Bajaj[22] have calculated the absorption profiles of shallow donor transitions in quantum wells. Recently, Bajaj and co-workers[10,11,22] have calculated the binding energies of the ground state and of a few low-lying excited states of a donor in a quantum well in the presence of a magnetic field applied perpendicular to the interfaces. The transition energies thus calculated agree very well with their measured values.[31]

In this paper we report a first calculation of the transition energies between the ground state (1*s*-like) and three excited states (2*s*-, $2p_y$-, and $2p_z$-like), referred to from hereon as 1*s*, 2*s*, $2p_y$, and $2p_z$, respectively, of a hydrogenic donor associated with the first subband in a GaAs quantum well sandwiched between two semi-infinite (> 100 Å, in practice) layers of $Al_xGa_{1-x}As$ in the presence of a magnetic field applied parallel to the interfaces. In addition, we also present the line strengths of these transitions in various polarizations. Our results are given both as a function of the applied magnetic field and the position of the donor ion along the direction of growth. We follow a variational approach in which the trial wave functions are expressed in terms of appropriate Gaussian basis sets.

THEORY

Within the framework of an effective-mass approximation, the Hamiltonian of a hydrogenic donor in a GaAs quantum well can be written as

$$H=\frac{1}{2m_e^*}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]^2-\frac{e^2}{\epsilon_0 r}+V_B(x)\ , \qquad (1)$$

where the barrier potential $V_B(x)$ is assumed to be a square well of height V_0 and width L,

$$V_B(x)=\begin{cases}0, & |x|<L/2\\ V_0, & |x|>L/2\ .\end{cases} \qquad (2)$$

We take the origin of the coordinate system to be at the center of the well. The position of the electron is denoted by $\mathbf{r}$, where $r=[(x-x_i)^2+y^2+z^2]^{1/2}$, x_i being the x coordinate of the impurity ion. The quantity m_e^* is the electron effective mass, which is taken to be different in the two semiconductors. The values of the static dielectric constant ϵ_0 are assumed to be the same in GaAs and $Al_xGa_{1-x}As$.

The vector potential $\mathbf{A}$ is defined as

$$\mathbf{A}=\tfrac{1}{2}(\mathbf{B}\times\mathbf{r})\ . \qquad (3)$$

Assuming that the magnetic field is applied parallel to the interfaces (taken to be the z direction), the Hamiltonian of our system can be expressed as

$$H=-\frac{m^*}{m_e^*}\nabla^2-\frac{2}{r}+\gamma L_z+\tfrac{1}{4}\gamma^2(x^2+y^2)+V_B(x)\ . \tag{4}$$

Here we have used the effective Bohr radius in GaAs, $a_0=\epsilon_0\hbar^2/m^*e^2$, as our unit of length and the effective Rydberg $R=e^2/2\epsilon_0 a_0$ as our unit of energy. For GaAs ($m^*=0.067m_e$, $\epsilon_0=12.5$) these quantities are 98.7 Å and 5.83 meV, respectively. In Eq. (4), L_z is the z component of the angular-momentum operator (in units of $\hbar$), and γ is a dimensionless measure of the strength of the magnetic field, defined as

$$\gamma=\frac{e\hbar B}{2m^*cR}\ . \tag{5}$$

In Ref. 11, where the magnetic field was perpendicular to the interfaces, the Hamiltonian was cylindrically symmetric, and therefore L_z was conserved. In the present case, however, we do not have such a symmetry, and therefore the wave functions will not be eigenfunctions of L_z. The conduction-band discontinuity or the barrier height V_0 in Eq. (2) is taken to be 60% of the band-gap difference between GaAs and $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$. We obtain the band-gap difference from the empirical relationship given by Lee *et al.*,[32]

$$\Delta E_g=1.155x+0.37x^2\ \mathrm{eV}\ . \tag{6}$$

We have calculated the eigenvalues of the Hamiltonian described by Eq. (4) using a variational approach very similar to that used in Ref. 11. We write the variational wave function as a product of $f(x)$, the wave function of the ground state of the electron in the one-dimensional potential V_0, and a function $G(x-x_i,y,z)$ which depends on the relative impurity coordinates,

$$\psi=f(x)G(x-x_i,y,z)\ . \tag{7}$$

The solution to the square-well problem $f(x)$ is given as[33]

$$f(x)=\begin{cases}\cos(kx), & |x|<L/2\\ Ae^{-\kappa x}, & |x|>L/2\ .\end{cases} \tag{8}$$

The parameter k is determined from the energy of the first subband and quantities κ and A are obtained from the matching conditions at the interface. We require that $f(x)$ and $(m^*/m_e^*)(\partial f/\partial x)$ be continuous across the interfaces.

We write $G(x,y,z)$ as a series of terms of three distinct symmetries, as given below:

$$G(x,y,z)=\sum_{i=1}^{5}(A_i+B_iy+C_iz)e^{-\alpha_ir^2}e^{-\beta(x^2+y^2)}\ , \tag{9}$$

where β is a variational parameter which is determined from the minimization of the energy and is affected most strongly by the size of the magnetic field. As in Ref. 11, the quantities α_i (13.4, 2.01, 0.454, 0.123, 0.0267) are taken from the results of Huzinaga,[34] who performed a detailed study of the use of Gaussian basis functions in the calculations of the energy levels of a hydrogen atom. The donor-off-center case is obtained by replacing x by $x-x_i$.

For convenience, we will refer to the terms proportional to y and z as p_y and p_z terms, respectively, and the other set of terms as s terms keeping in mind, though, that the angular momentum is not a good quantum number in the present case. The Hamiltonian [Eq. (4)] does not couple the p_z terms with either the s or p_y terms, so that our solutions will be either even or odd functions of z, which reduces the size of our eigenvalue problem accordingly. The s and p_y terms are coupled by the L_z part of the Hamiltonian (except when the donor is located at the center of the well). This is because the function $f(x)$ is symmetric about the center of the well and not about the location of the donor ion.

If the donor is located at the center of the well a wave function proportional to $x(p_x)$ is associated with the second conduction subband.[14] For the well sizes we consider the energy separation between the subbands sufficiently large that there should be negligible mixing between them as long as the magnetic field parameter γ is not much greater than 1. If the donor is located away from the center, the $f(x)$ function introduces terms that have p_x symmetry. Consequently, we have not included a

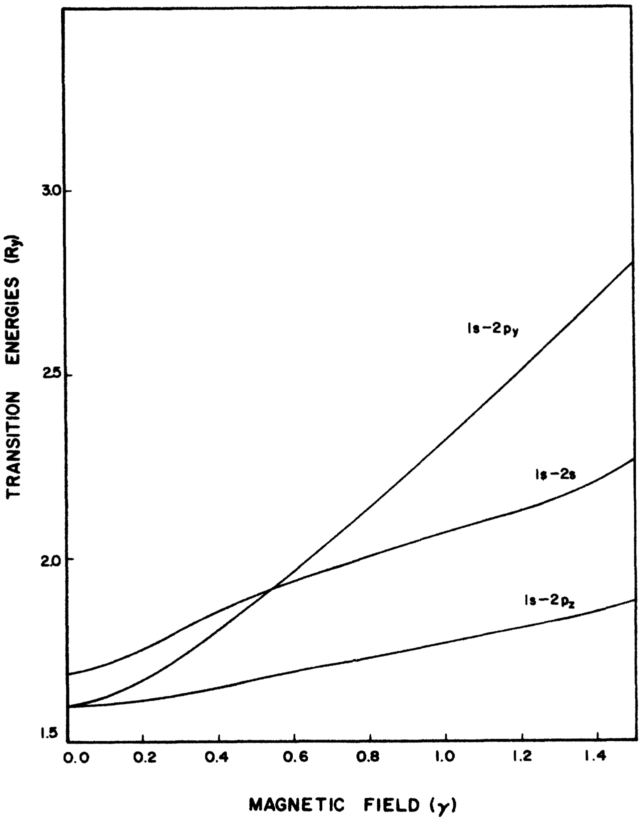

FIG. 1. Variation of the 1s-2s, 1s-2p_y, and 1s-2p_z transition energies as a function of the magnetic field parameter γ (defined in the text) for a donor located at the center of the well of size $L=1.0a_0$. All energies are expressed in terms of an effective Rydberg R ($=5.83$ meV). Al concentration in the barriers is $x=0.3$.

group of terms proportional to x in the expansion of $G(x,y,z)$.

Since we use five distinct α_i values (given earlier), our even-z variational function contains ten terms, while our odd-z function has five terms. For a given value of γ we solve the standard matrix eigenvalue equation for each z symmetry. We minimize the energy of the lowest odd-z state with respect to β. For even-z states, it is not feasible for us to minimize the energy of each state separately with respect to β. For this case we minimize the sum of the ground and the two lowest excited states. We believe that this procedure yields good values of these energies because the ground state is relatively insensitive to the value of β, and the two excited states have roughly comparable energies. Our eigenvalues are upper bounds to the correct values since the states are mutually orthogonal.

The binding energy of a given state, say the 1s state, E_{1s}, is then given by

$$E_{1s}=E_1+\gamma-E \ , \tag{10}$$

where E_1 is the lowest subband energy of the square-well potential, γ is the energy of the first Landau level, and E is the eigenvalue of the Hamiltonian [Eq. (4)] corresponding to the 1s level, which has been determined variationally. The value of E_1 is determined numerically by solving the following transcendental equation,[33]

$$\left[\frac{E_1}{V_0}\right]^{1/2}=\cos\left[(E_1)^{1/2}\frac{L}{2}\right] . \tag{11}$$

The binding energies of the excited states are obtained in a similar fashion.

RESULTS AND DISCUSSION

We first consider the effect of the magnetic field upon the transition energy from the ground state (which for convenience we will call the 1s state) to the first three excited states. We will refer to the excited states as 2s, $2p_y$, and $2p_z$ in keeping with the symmetry type of the dominant basis functions for each wave function when the donor is at the center of the well. Note that these states should not be identified with hydrogenic states of the same names. In general, the wave functions of these states are highly distorted by the barriers and by the magnetic field. The Al concentration in the barriers is taken to be 0.3, and the conduction-electron mass in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ is given as[2] $m_e^*/m_e=0.067+0.083x$.

Figures 1 and 2 illustrate the dependence of the transition energies on magnetic field. In Fig. 1 the donor impurity is located at the center and in Fig. 2 at the edge of an isolated quantum well of width $L=1.0a_0$. In each

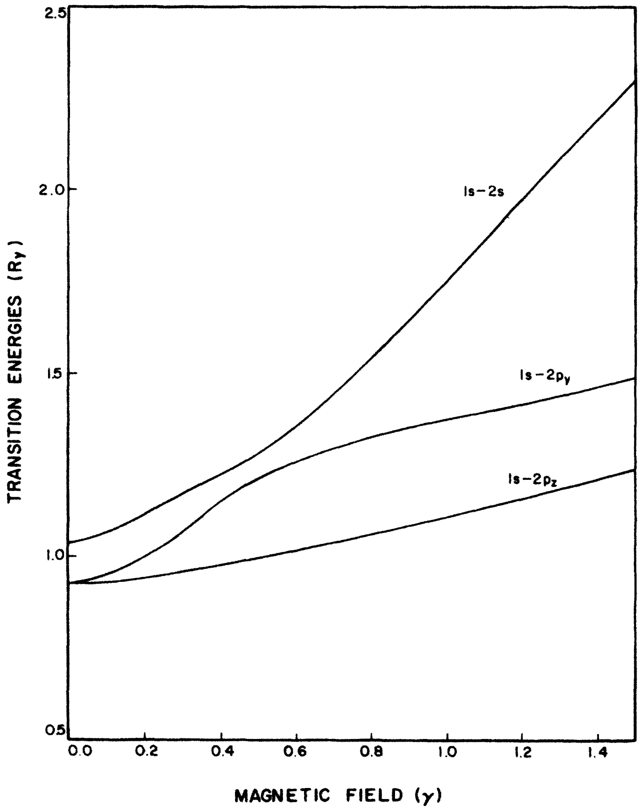

FIG. 2. Variation of 1s-2s, 1s-$2p_y$, and 1s-$2p_z$ transition energies as a function of the magnetic field parameter γ (defined in the text) for a donor located at the edge of the well of size $L=1.0a_0$. All energies are expressed in terms of an effective Rydberg R ($=5.83$ meV). Al concentration in the barriers is $x=0.3$.

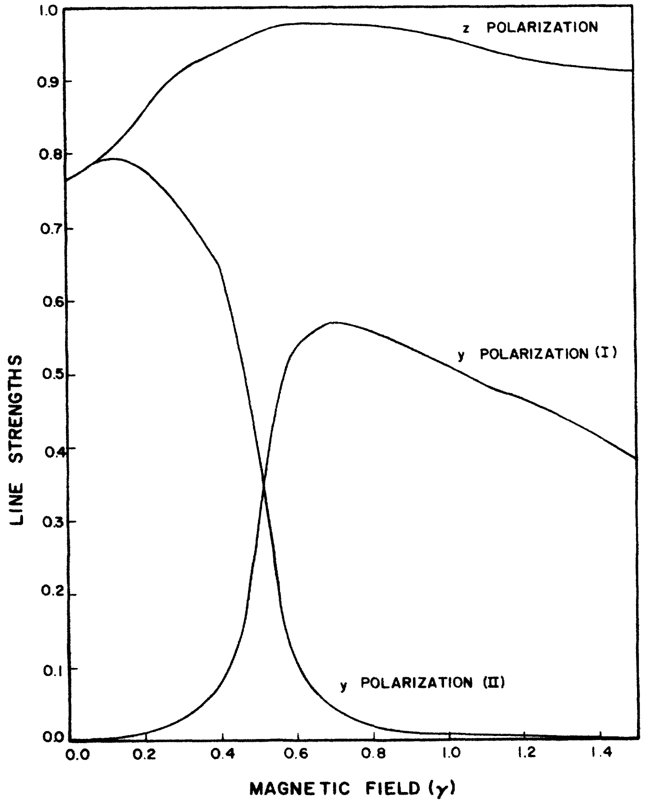

FIG. 3. Variation of the line strengths (expressed in terms of a_0^2) of y polarization (I), y polarization (II), and z polarization as a function of the magnetic field parameter γ (defined in the text) for a donor located at the edge of the well of size $L=1.0a_0$. Al concentration in the barriers is $x=0.3$.

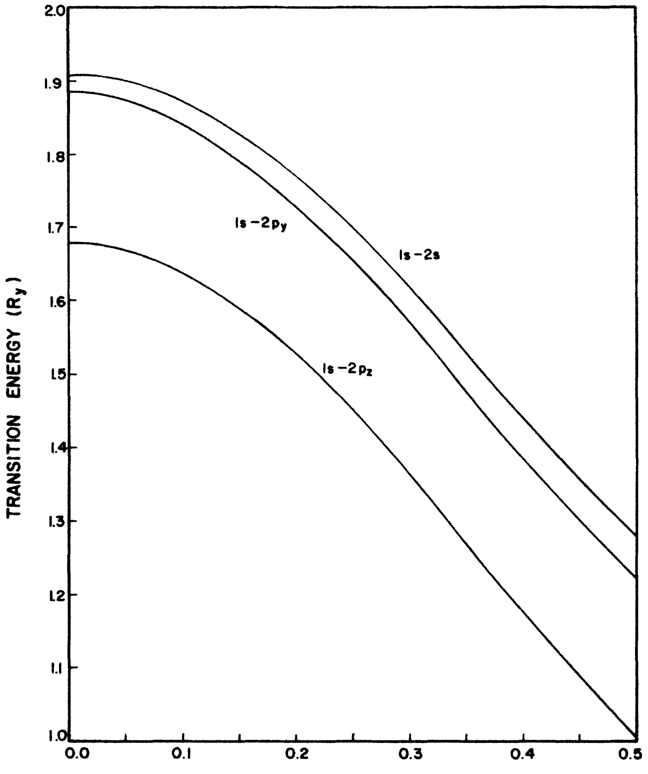

FIG. 4. Variation of the $1s$-$2s$, $1s$-$2p_y$, and $1s$-$2p_z$ transition energies as a function of the position of the donor in a GaAs well of size $L = 1.0a_0$ for a magnetic field parameter γ (defined in the test) of 0.5. All energies are expressed in terms of an effective Rydberg R ($=5.83$ meV). Al concentration in the barriers is $x = 0.3$.

case, the $2p_y$ and $2p_z$ states are degenerate at $\gamma = 0.0$, while the $2s$ state is split off due to the barrier potential. With the donor at the center of the well, the $1s$-$2p_y$ transition energy increases more rapidly than that of the other two states, crossing the $1s$-$2s$ transition energy at about $\gamma = 0.55$. This crossing is allowed because, as noted earlier, the Hamiltonian does not mix the two symmetries in the on-center case. When the donor is at an interface, the results are somewhat different. Again the $1s$-$2p_y$ energy begins to rise rapidly with increasing γ. However, strong mixing occurs between the $2s$ and $2p_y$ symmetries in the region $0.4 < \gamma < 0.6$. Beyond $\gamma = 0.6$ the state responsible for the curve that we have labeled $1s$-$2s$ is actually dominated by $G(x - x_i, y, z)$ basis functions with p_y symmetry.

A better understanding of these effects can be obtained by examining the line strengths for these transitions, which are proportional to the square of the momentum matrix elements between the initial and the final states. Within the framework of the effective-mass approximation, the momentum matrix elements can be expressed as[35]

$$|\langle i | p_x | f \rangle|^2 = \frac{m_e^* E_{if}}{\hbar^2} |\langle i | x | f \rangle|^2 ,$$

where E_{if} is the difference in energy between the initial and the final states. We have, therefore, examined the matrix elements

$$|\langle 1s | y | 2s \rangle|^2, \quad y \text{ polarization (I)}$$

$$|\langle 1s | y | 2p_y \rangle|^2, \quad y \text{ polarization (II)}$$

and

$$|\langle 1s | z | 2p_z \rangle|^2, \quad z \text{ polarization}$$

for the three excited states discussed above. Because of the symmetry of the Hamiltonian, the strength of the z polarization is nonzero only for the $1s$-$2p_z$ transition, while that of the y polarization can be nonzero for both $1s$-$2s$ and $1s$-$2p_y$ transitions, depending on the s-p_y mixing. For the case of the donor at the center of the well, there is no s-p_y mixing, so that the line strength for the $1s$-$2s$ transition vanishes for all γ. The strengths for the other two transitions are nonzero, but they are roughly the same size and relatively insensitive to magnetic field in the range $0.0 < \gamma < 1.5$ (~ 0.3 for $1s$-$2p_y$ and ~ 0.4 for $1s$-$2p_z$, in units of a_0^2), so that we do not illustrate this case with a figure.

Things are more interesting in the case of the donor at the edge of the well, as shown in Fig. 3. The y-polarization curves clearly show the rapid exchange of

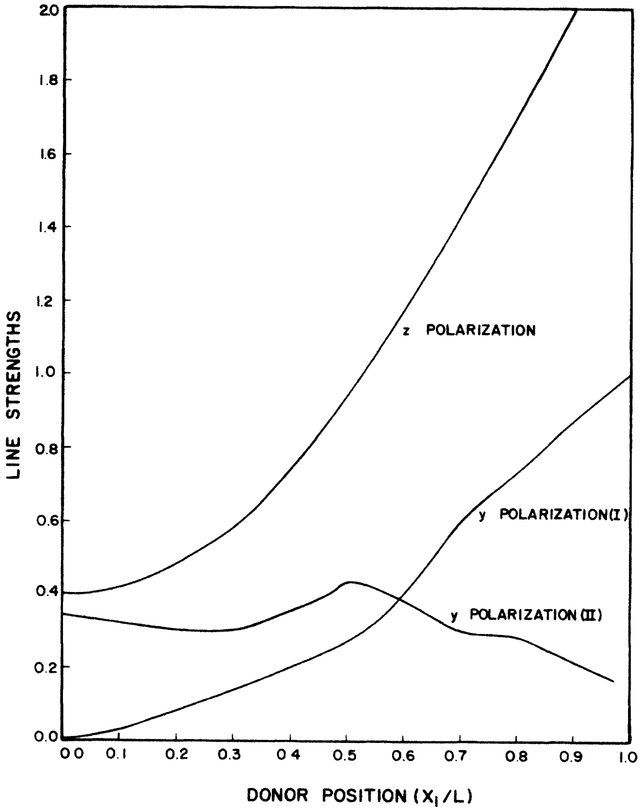

FIG. 5. Variation of the line strengths (expressed in terms of a_0^2) of y polarization (I), y polarization (II), and z polarization as a function of the position of the donor in a GaAs well of size $L = 1.0a_0$ for a magnetic field parameter γ (defined in the text) of 0.5. Al concentration in the barriers is $x = 0.3$.

dominant symmetry type between the $2s$ and $2p_y$ states in the region $0.4<\gamma<0.6$. By contrast, the $1s$-$2p_z$ strength changes relatively little over the entire range of γ shown.

The variation of these ground- to excited-state transition energies with donor position is shown in Fig. 4. A typical value of the field, $\gamma=0.5$, was chosen for this figure. As was seen for the case of the magnetic field along the growth direction,[11] the transition energies decrease monotonically as the donor impurity is moved from the center of the well to the edge. The zero slopes of these curves for the donor at the center of the well would normally suggest a peak in the absorption spectra, but remember that the line strength of the $1s$-$2s$ transition vanishes when the impurity is at the center. Values of the line strengths of the $1s$-$2p_z$ and $1s$-$2s$ transitions increase from 0.4 to near 1.0 ($1s$-$2p_z$) and from 0.0 to about 0.3 ($1s$-$2s$) as the donor impurity is moved from the center of the well to the edge (units of a_0^2). The strength of the $1s$-$2p_y$ transition is roughly constant (within 20% of 0.35) over the same range.

In Fig. 5 we display the variation of the line strengths of the various transitions as a function of the position of the donor ion for a quantum-well size $L=1.0a_0$ for $\gamma=0.5$. The strength of the y polarization of the $1s$-$2s$ transition increases rapidly as the donor ion is moved towards the interface and into the barrier layer. The same is true for the z polarization of the $1s$-$2p_z$ transition. The strength of the y polarization of the $1s$-$2p_y$ transition, however, shows very little variation as a function of the position of the donor ion.

It should be mentioned that it is not possible for us to compare the results of our calculations with experimental data as these data are not available at this time. Such data, however, will be very useful in further understanding the behavior of donors in quantum wells. Finally, for a given value of the magnetic field, the changes in the binding energies of the various states are larger in the case of the field applied perpendicular[11] than parallel to the interface, as it is easier to modify the wave functions in the former case.

CONCLUSIONS

We have calculated the transition energies between the ground state ($1s$-like) and three excited states ($2s$-, $2p_y$-, and $2p_z$-like) of a hydrogenic donor in a GaAs-$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ quantum-well system in the presence of a magnetic field applied parallel to the interfaces. In addition, we have calculated the line strengths of these transitions in various polarizations. We have presented results both as a function of the applied magnetic field and the position of the donor ion along the direction of growth. We have followed a variational approach in which the trial wave functions are expressed in terms of appropriate Gaussian basis sets.

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