

Band structure of quantum wells under crossed electric and magnetic fields

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We investigate the band structure in GaAs quantum wells in the presence of an electric field applied along the growth direction (z) and a magnetic field perpendicular to it. The strong coupling between heavy and light holes gives rise to a nonquadratic behavior of the hole states as a function of the magnetic field. The presence of the electric field introduces new transitions by breaking the z symmetry and by coupling with the magnetic field. The Kramers degeneracy is also lifted by the external fields. The results are discussed in terms of band-to-band transitions.

I. INTRODUCTION

Optical spectroscopy¹ in semiconductor quantum wells (QW) has been a powerful tool for exploring the physics of these new types of structures, particularly in the presence of external fields. Electric fields applied along the growth direction (defined as the z direction) have been extensively studied both experimentally^{2,3} and theoretically.^{3,4} Stark shift and luminescence quenching were observed and explained.² The QW confinement permits the observation of well-defined structures associated with excitons under strong electric fields.³ Also, the electric field can be used to tune the energy levels in the well so as to modify the heavy- and light-hole interaction. The effect of a magnetic field has been investigated in many heterostructures.^{5,6} For the magnetic field along the z direction, the in-plane motion is confined to cyclotron orbits with the formation of Landau levels. When the magnetic field is applied parallel to the interfaces, the situation becomes rather complex. For weak fields the barrier confinement is predominant; the carriers cannot complete the entire cyclotron orbits, and the energy levels are then the QW levels perturbed by the magnetic field. At high fields the magnetic confinement is predominant, and for carriers localized near the center of the QW, the magnetic orbits may be completed. However, when the centers of the orbits are close to the interface, the orbits are skipped at the barriers.⁷ Although some insight into this behavior has been obtained from the comparatively simple electron subbands,⁸ the valence band has to be considered in all its complexity to get a correct understanding of the transitions observed in this configuration.⁹

Maan⁷ studied the effect of the in-plane magnetic field on interband absorption in superlattices. Also, diamagnetic shifts in GaAs-(Ga,Al)As were observed under strong magnetic fields applied in the well planes.¹⁰ Recently, the situation with the simultaneous application of electric and magnetic fields has been considered.¹¹ When crossed electric and magnetic fields are applied, crossed field effects, namely the Hall drift, exist in addition to the possibility of tuning the levels. This effect has been studied in bulk semiconductors. The optical-absorption coefficient exhibits an oscillatory behavior as a function of the electric field for a fixed magnetic field.¹² In un-

doped heterostructures, optical spectra are generally dominated by the excitonic transitions. Indeed, the high quality of the GaAs-(Ga,Al)As samples permits the observation of some excited excitonic states besides the ground state. A detailed study of their behavior in the presence of external fields has then been made possible. Although the electric-magnetic behavior has been considered in electronlike subbands,¹³ it is essential to include the coupling between the heavy- and light-hole subbands if we want to analyze the detailed structure of the optical transitions.⁹

We consider in this work the energy levels and subband structures in GaAs-(Ga,Al)As QW's in the presence of crossed electric and magnetic fields. While such considerations are of interest in their own right, they are further motivated by recent experiments under those conditions where fine structures in photoluminescence and photoexcitation spectra have been observed.¹¹ A quantitative comparison with the experiments, however, must await the inclusion of excitonic effects which usually dominate the experimental spectra. Here we present calculations of the conduction- and valence-subband structures and discuss the band-to-band transition energies and their oscillator strengths. The focus is on the central effect of band mixing under crossed electric and magnetic fields. We will consider a magnetic field parallel and an electric field perpendicular to the interfaces limiting ourselves to the situation of predominant QW confinement so that we can describe the states in terms of the QW levels perturbed by the external fields. In Sec. II we discuss the details of our calculations, and in Sec. III we show some illustrative results and discuss their significance. In Sec. IV we summarize our conclusions.

II. THEORY

In our calculations we use the envelope-function approximation to describe the electrons and holes in the quantum well. The electric field \mathbf{F} is applied along the z direction. The magnetic field \mathbf{H} applied parallel to the interfaces is described by the vector potential $\mathbf{A} = (0, -zH, 0)$.

Close to the fundamental gap, in the GaAs system, we have one conduction band (Γ_6), two valence bands (Γ_8)

degenerate at $\mathbf{k}=0$, and one split-off valence band Γ_7 . The spin-orbit coupling between Γ_8 and Γ_7 bands will be taken as infinite. In that way we can restrict our system to a 6×6 Hamiltonian (where we have considered the spin degeneracy). We shall also neglect the conduction-band nonparabolicity since we are interested in the transitions among the first QW subbands, which are typically separated by several tens of meV, while the GaAs bandgap is 1.519 eV. The conduction-band Hamiltonian which we have to handle is then a scalar,

$$\begin{aligned} \mathcal{H}_c = & \frac{-\hbar^2}{2m_e} \frac{d^2}{dz_e^2} + V_c Y(z_e^2 - L^2/4) \\ & + eFz_e + \frac{\hbar^2}{2m_e} [k_x^2 + (k_y - z_e/\lambda_M^2)^2] \\ & + \frac{\hbar^2}{2m_0} \frac{g^* s_z}{\lambda_M^2}, \end{aligned} \quad (1)$$

where $Y(x)$ is the unit step function [$Y(x)=1$ if $x > 0$ and $Y(x)=0$ if $x < 0$], V_c is the electron barrier, $\lambda_M (= \sqrt{\hbar c/He})$ is the magnetic length, s_z is the electron spin, and g^* is the effective Landé factor. We take into consideration the continuities of the wave functions and the current density at the interfaces following the work of Ben Daniel and Duke.¹⁴

For the valence band the problem is more complex. Besides the coupling between Γ_6 and Γ_8 , which we are considering in second order in \mathbf{k} , as described above, we have to include the coupling of Γ_8 with the higher bands to obtain the correct heavy-hole dispersion. This coupling is taken into account as a perturbation, keeping the second-order term in \mathbf{k} . This results in off-diagonal terms in the Γ_8 Hamiltonian, coupling the heavy- and light-hole bands and leading to strong nonparabolicity in the hole-subband dispersion in quasi-two-dimensional heterostructures. We neglect here the splitting due to the inversion asymmetry in the III-V system. Following the work developed by Luttinger,¹⁵ the valence Hamiltonian can be written as

$$\underline{\mathcal{H}}_v = \underline{H}_v(H) + [V_v Y(z_h^2 - L^2/4) - eFz_h] \underline{1} + \frac{\hbar^2}{m_0} \frac{\kappa \underline{J}_x}{\lambda_M^2} \quad (2)$$

where $\underline{1}$ is a unit matrix and

$$\underline{H}_v(H) = \begin{pmatrix} a_+ & c & b & 0 \\ c^* & a_- & 0 & -b \\ b^* & 0 & a_- & c \\ 0 & -b^* & c^* & a_+ \end{pmatrix} \begin{matrix} + \frac{3}{2} \\ -\frac{1}{2} \\ +\frac{1}{2} \\ -\frac{3}{2} \end{matrix} \quad (3)$$

with

$$\begin{aligned} a_{\pm} = & -\frac{\hbar^2}{2m_0} (\gamma_1 \mp 2\gamma_2) \frac{d^2}{dz_h^2} \\ & + \frac{\hbar^2}{2m_0} (\gamma_1 \pm \gamma_2) \left[k_x^2 + \left[k_y + \frac{z_h}{\lambda_M^2} \right]^2 \right], \end{aligned} \quad (4a)$$

$$c = -\sqrt{3/2} \frac{\hbar^2}{m_0} \gamma [(k_- - iz_h/\lambda_M^2)^2], \quad (4b)$$

$$b = -\sqrt{3} \frac{\hbar^2}{m_0} \gamma_3 (k_- - iz_h/\lambda_M^2) k_z, \quad (4c)$$

and

$$\underline{J}_x = \begin{pmatrix} 0 & 0 & \sqrt{3/2} & 0 \\ 0 & 0 & 1 & \sqrt{3/2} \\ \sqrt{3/2} & 1 & 0 & 0 \\ 0 & \sqrt{3/2} & 0 & 0 \end{pmatrix}, \quad (5)$$

where γ_i 's are the Luttinger parameters¹⁵ and $k_- = k_x - ik_y$. Here we have used the axial approximation,⁵ $\gamma = \gamma_2 = \gamma_3 = (\gamma_2 + \gamma_3)/2$. The origin of the coordinates is taken at the center of the well.

First, we have to find a solution for the electronlike Hamiltonian. We restrict the field range to values where the barrier confinement is predominant over the magnetic confinement. We are thus considering either low values of magnetic fields or QW's which are not very wide. In both cases, the eigenstates are QW-like states perturbed by the external fields. We approximate the solution of the electronlike subband by projecting the full Hamiltonian in the basis formed by the eigenstates of the single QW at $H=0$ and $F=0$. The effects of the external fields are described by the interaction among these eigenstates. The eigenvalues are obtained by diagonalizing the Hamiltonian. We have also numerically solved Eq. (1). No significant difference in the eigenvalues was observed when compared to the method described above in the regime of electric and magnetic fields considered here.

To solve the valence-band problem we extend the method used to calculate the in-plane hole dispersion¹⁶ and the Landau levels.⁶ Essentially, we project the 4×4 hole Hamiltonian in the basis formed by the diagonal solutions in the absence of external fields

$$\Psi_v(H) = \begin{pmatrix} \sum_i \alpha_i^+(k_y, k_x) \chi_i(z) \\ \sum_j \beta_j^-(k_y, k_x) \xi_j(z) \\ \sum_j \beta_j^+(k_y, k_x) \xi_j(z) \\ \sum_i \alpha_i^-(k_y, k_x) \chi_i(z) \end{pmatrix} \exp(\mathbf{k}_\perp \cdot \rho_\perp) \quad (6)$$

where $\rho_\perp = (x, y)$, $k_\perp = (k_x, k_y)$, χ_i and ξ_j are the i th and j th heavy- and light-hole levels, respectively. This method was applied successfully to describe the in-plane hole dispersion in the presence of an electric field.¹⁷ The off-diagonal terms in the Luttinger Hamiltonian and the spin-field term couple the heavy- and light-hole subbands in the presence of the magnetic field even at $k_\perp = 0$. The holes display a free motion along the direction of the applied magnetic field (x direction) but exhibit a complex k_x dispersion pattern because of the couplings due to the magnetic field as well as higher-band interactions. The magnetic field couples the z and y directions, and k_y determines the position of the center of orbit in which the carriers will move if there were no QW.

The method we use to find the valence eigenstates involves two basic approximations. First, we limit the basis in which we are projecting the Hamiltonian to the bound eigenstates of the QW in the absence of external fields, neglecting the QW continuum. The continuum states should be included for a complete description of the problem. However, for the first few subbands, the approximation is well justified as will be seen later. The second approximation is that, although we ensure the current density conservation when we calculate our basis, such conservation is not always preserved when we write the hole eigenfunctions in the form of Eq. (5). The off-diagonal terms of Eq. (2) introduce some discontinuity in the current density which comes from the differences in the effective parameters (γ_i 's) and the values of the wave functions at the interfaces. However, for systems like GaAs-(Ga,Al)As, these parameters do not change significantly from one material to the other (unless the Al concentration is very high), and the wave functions associated with the first subbands have a small value at the interfaces. The deviation from strict current density conservation is then not very important.

In the absence of external fields, when the off-diagonal terms of the valence Hamiltonian are neglected, the optical transitions in QW obey a general rule $\Delta n = \text{even}$ (where the strongest transitions are $\Delta n = 0$). The interaction between the heavy and light holes induced by the higher-band interaction breaks this simple rule. Some of the so-called "forbidden" transitions are now allowed and many new transitions may become observable. Besides, in the optical transitions, k_y is not necessarily conserved because of the crossed effects of the external fields and $V(z)$. We will not discuss here the complete spectra of the band-to-band transitions but, as a first step, we will restrict ourselves to the transitions where $k_y^e = k_y^h = 0$. This simple picture permits us the analysis of the behavior of the higher subbands mixing as a function of the external fields to gain insight of the expected transitions. A more detailed description, including the excitonic effects, will be considered in a future work.

The oscillator strength is proportional to

$$|\langle \Psi_c | \hat{\epsilon} \cdot (\mathbf{p} + e \mathbf{A}/c) | \Psi_v \rangle|^2.$$

The only significant terms in this expression are of the type

$$\langle \psi_e(\mathbf{r}_e) | \psi_h(\mathbf{r}_h) \rangle \langle u_\mu | \hat{\epsilon} \cdot \mathbf{p} | u_\nu \rangle \quad (7)$$

while the other terms can be neglected. Here ψ_e and ψ_h are the electron and hole envelope functions, and u_μ and u_ν are their respective Bloch functions.^{18,16} Essentially, the oscillator strength is proportional to the overlap between the electron and hole envelope functions and their mixing induced by the external fields and the off-diagonal terms of Eq. (4).

III. RESULTS AND DISCUSSION

The parameters used in our calculations are $m_e(\text{GaAs}) = 0.067m_0$ and $m_e(\text{AlAs}) = 0.124m_0$ (where m_0 is the free-electron mass), $\gamma_1 = 6.85$, $\gamma_2 = 2.10$, and

$\gamma_3 = 2.90$ for GaAs and $\gamma_1 = 3.45$, $\gamma_2 = 0.68$, and $\gamma_3 = 1.29$ for AlAs. The values for the (Ga,Al)As are taken as linear interpolations of these values. The energy gap of GaAs is taken as 1.519 eV and of $\text{Ga}_x\text{Al}_{1-x}\text{As}$ as $E_g(\text{GaAs}) + 1.247x$ eV. The ratio between conduction- and valence-band discontinuities is assumed to be $\frac{7}{3}$. The Landé g^* factor is taken to be zero throughout. The top of the GaAs valence band is defined as zero in energy.

In Fig. 1 we show the hole levels as a function of the magnetic field with the center of orbit at the center of the QW ($k_y = 0$) for a QW with 175 Å width and 35% of Al in the barrier. The dotted curves represent the case with $N = 2$, where N is the number of heavy- and light-hole states included in our basis. The dashed lines are the $N = 3$ approximation and the full lines include all the bound QW levels in the basis (seven heavy and four light holes). We can see clearly the strong nonquadratic behavior arising from the coupling between the heavy- and light-hole subbands. The light-hole ground state exhibits a stronger nonparabolic behavior due to the proximity of the first-excited heavy-hole state which pushes upward the light-hole state. We can also see the lifting of the spin degeneracy by the magnetic field. This lifting of degeneracy is more significant for the light-hole subband. We also observe that for $N = 3$ the first two subbands have already saturated. Clearly, the higher subbands play an insignificant role and may be neglected. For states close to the top of the QW, the continuum would have to be included, of course, to get a correct description.

In Fig. 2 we plot the energy levels as a function of k_y for a QW width of 175 Å and 35% Al in the barrier for a magnetic field of 10 T. The cyclotron radius for this magnetic field is 81 Å and the orbits are close to the QW width. In this case we expect a strong dependence of the energy levels on the position of the center of the orbits, as can be observed in Fig. 2. The relation $\lambda_M^2 k_y = L/2$ cor-

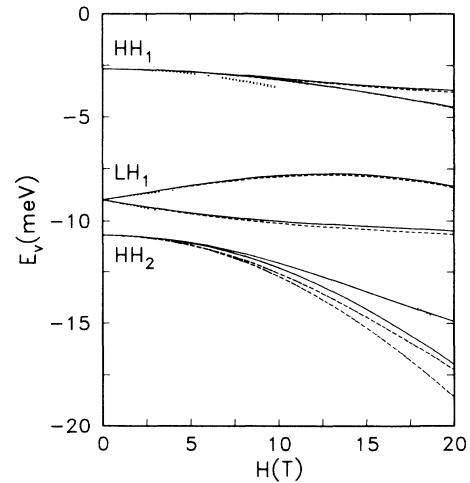


FIG. 1. Hole subbands as a function of magnetic field for a single GaAs-(Ga,Al)As quantum well with a width of 175 Å and an Al fraction of 0.35 in the barriers. The dotted, dashed, and solid lines represent the results obtained using 2, 3, and all the bound heavy- and light-hole subbands in the basis, respectively.

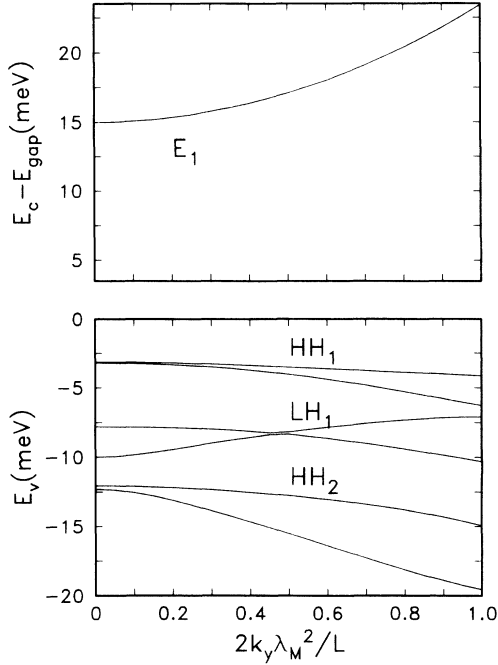


FIG. 2. Energy subbands as a function of the center of orbit for the GaAs-(Ga,Al)As quantum well under a magnetic field of 10 T and zero electric field.

responds to the situation where the carriers have the center of the magnetic orbit at the interface. The electron subband shows a quadratic behavior as expected. However, the hole subbands show a more complex behavior. In particular, the light-hole ground state presents strong nonparabolic behavior. The removal of the spin degeneracy is stronger for holes with center of orbit close to the interface. Besides the spin-magnetic coupling, for holes with orbits not centered in the center of the well, the z potential is no longer symmetric under inversion, enhancing the breaking of the Kramers degeneracy. We have also calculated the energy levels as a function of the center of the orbit for narrower QW's. In particular, for a 100-Å QW, the levels exhibit a very weak shift. In this case the QW confinement is much more important than the magnetic effects and the electron motion is strongly dominated by the barrier confinement. Following our approximation, we do not expect the carriers to be able to traverse the entire orbits. For this narrow QW, irrespective of the position of the center of orbit, the carriers would see the QW barrier since their possible orbits are larger than the QW width. That explains why their dependence on k_y is very weak. We have compared our method with a more sophisticated calculation performed for infinite QW's.⁹ We conclude that our approximation gives the correct behavior for the width range described here. The results are practically the same for a 160-Å QW, but some discrepancies begin to occur only for rather large QW ($L = 350$ Å).⁹

In Fig. 3 we plot the hole levels as a function of k_y for the same case as before but under the presence of an elec-

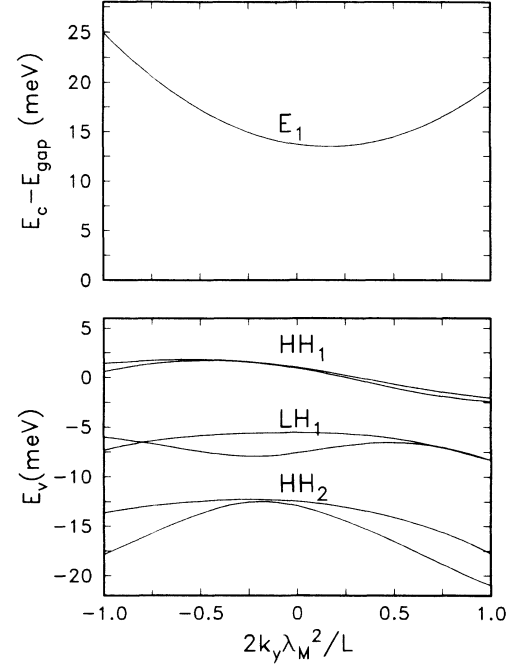


FIG. 3. Energy subbands as a function of the center of orbit for the GaAs-(Ga,Al)As quantum well under a magnetic field of 10 T and an electric field of 20 kV/cm.

tric field of 20 kV/cm. Rigorously, in the absence of the magnetic field we have no true bound states but resonant states. However, in the presence of the magnetic field we recover again the bound-state picture. Here, we consider weak values for the electric field so that the possibility of the carriers being swept out of the well is of no concern.

The presence of the electric field induces a Stark shift.² This Stark shift is more important for large QW's, where the carriers are more apt to move and so be displaced to the interfaces. The removal of the mirror symmetry with respect to the center of the well by the electric field is clearly reflected from the asymmetry of the energy levels as a function of k_y . In particular, the minimum for the electron ground state is now achieved for values of k_y different from zero. This is expected since the electric field displaces the center of the orbit. For electronlike carriers, this center is given by

$$y_0 = k_y \lambda_M^2 - eFm^* \lambda_M^4 / \hbar^2. \quad (8)$$

In general, for the holes this picture is more complex because of the heavy- and light-hole coupling. Still, for the heavy-hole ground state which retains some of the parabolicity, we see clearly the minimum in energy being displaced by the electric field.

The crossed electric and magnetic fields effects and the interactions between heavy and light holes are expected to strongly affect the optical transitions. The carrier distribution in the different orbits may broaden these transitions. However, the tendency of the carriers to relax to lower-energy states and the Coulombic interaction would

have the opposite effect. A complete description of the optical transitions should also include the excitonic structures. However, some insight may be obtained by analyzing the band-to-band transitions as they provide the background and shape the general trend. We do not intend to analyze the entire problem but rather limit ourselves to transitions occurring between carriers with $k_y=0$. This will provide us a first clue as to the influence of the coupling of the electric and magnetic fields and the off-diagonal terms. In Fig. 4 we plot the transitions for on-center orbit carriers as a function of the magnetic field for a QW with 175 Å width and 35% Al in the barrier with 4(a) $F=0$ and 4(b) $F=20$ kV/cm. In the absence of an electric field the fundamental transition shows a blue shift of 7.3 meV from 0 to 20 T. The spin splitting is very weak for this transition (typically 0.8 meV). The transition between the ground electron (E) subband and the ground light-hole (LH) subband ($E_1 \rightarrow LH_1$) shows a relatively large Zeeman effect, which may reach 2 meV. However, this value is probably still too small to be observed. When we apply the electric field, besides the Stark shift, the fundamental transition shows a larger shift with the magnetic field, reach 9.1 meV at 20 kV/cm. The $E_1 \rightarrow LH_1$ transition shows a weaker dependence on the electric field.

Narrower QW's present a weaker dependence on the magnetoelectric fields. In particular, for a 100 Å width QW (not shown here), the fundamental transition shows a blue shift of 3.8 meV from 0 to 20 T, in the absence of the electric field, and of 4.2 meV for an electric field of 40 kV/cm in the same range of magnetic field.

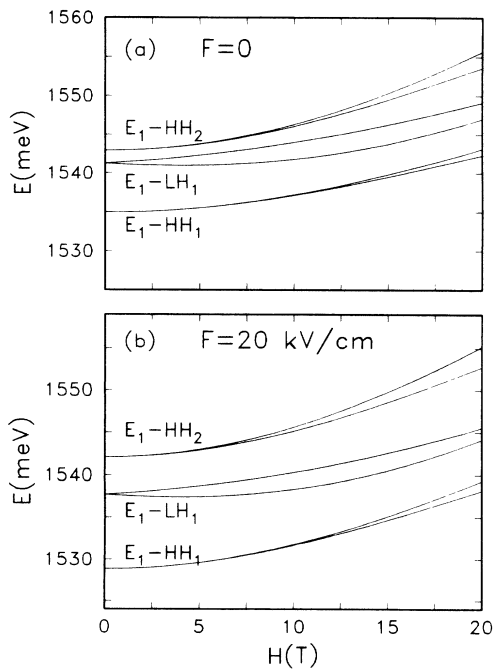


FIG. 4. Energy transitions as a function of the magnetic field for the GaAs-(Ga,Al)As quantum well for (a) zero electric field and for (b) an electric field of 20 kV/cm.

In the absence of the electric field, for carriers with on-center orbits, the z potential is symmetric. In this case, the coupling between heavy and light holes occurs among subbands of the same parity. The electric field breaks the z symmetry and any heavy-hole subband is coupled with all the light-hole subbands, enhancing the nonquadratic behavior with the magnetic field. However, the heavy-hole ground state shows a larger Stark shift than the light-hole ground state due to its heavier z -related effective mass. In contrast, the first-excited heavy-hole (HH) state shows a weaker shift with the electric field. The final result is that the relative separation between the positions of the ground heavy and light hole and the first-excited hole subbands, HH_1 , LH_1 and HH_2 , respectively, increases with the electric field, thus decreasing their coupling. Also, in this configuration, the electric and magnetic effect are coupled. In other words, both fields modify the z motion. In particular at $k_y=0$, the quadratic term in H in the conduction Hamiltonian (and also in the diagonal part of the valence Hamiltonian) tends to recover the z symmetry, modifying again the heavy- and light-hole interaction. This complex pattern can be observed in Fig. 5, where we plot the square of the overlap between the electron and hole wave functions, S . In the absence of the electric field only the $\Delta n = \text{even}$ transitions are allowed. When the electric field is applied, the $E_1 \rightarrow HH_2$ transition is allowed, decreasing its intensity on the magnetic field because of the quadratic diamagnetic term. In the same way the

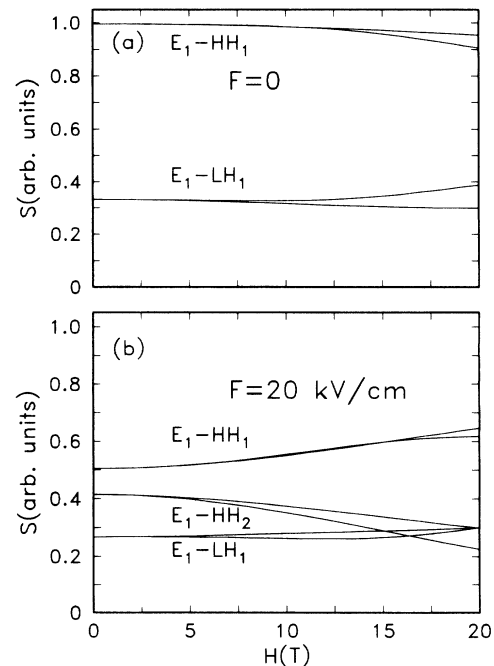


FIG. 5. Square of the overlap of the electron and hole wave function, S , as a function of the magnetic field for the transitions illustrated in Fig. 4. (a) $F=0$ and (b) $F=20$ kV/cm. (a) The overlap of $E_1 \rightarrow HH_2$ is equal zero and does not appear here.

$E_1 \rightarrow HH_1$ increases its intensity. However, the most nonparabolic transition $E_1 \rightarrow LH_1$ shows a weak dependence of its intensity on the magnetic field, as a result of the competition between the two mechanisms described above.

IV. CONCLUDING REMARKS

In conclusion, we have presented here the results of calculations of the QW subband structure in the presence of crossed electric and magnetic fields. The strong nonparabolic behavior induced by the interaction of the heavy- and light-hole states is described, together with the coupling between the electric and magnetic effects. Many of the features which may be optically observable were discussed in terms of band-to-band transitions although without including the k_y dispersion.

In real situations, the transition energies and the oscillator strengths are expected to be broadened by the dispersion of the carriers upon the position of the center of orbit and the crossed electric and magnetic effects which do not necessarily conserve k_y . Besides, they are folded in several excitonic lines by the Coulombic interaction between the electron-hole pair. A complete analysis of the optical transitions has to include these aspects of the problem.

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