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Quenching of asymmetry-induced spontaneous spin splitting in *p*-type quantum wells by an applied magnetic field

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The spin splitting in the valence band in an $In_xGa_{1-x}As/In_xGa_{1-x}As_yP_{1-y}$ quantum well is investigated theoretically using a 6×6 Luttinger-Kohn Hamiltonian. We compare the Landau levels in a perpendicular magnetic field with the corresponding results for the subband dispersions. It is shown that the asymmetry of the quantum well has a very small impact on the Landau level splitting except for quite small magnetic fields. This is in sharp contrast to the subbands in the absence of a magnetic field. It is suggested that the standard interpretation of Shubnikov–de Haas experiments in terms of hole spin subband populations requires a closer analysis. [S0163-1829(99)52436-3]

A common way to investigate semiconductors experimentally is to study their properties under the influence of a magnetic field. The application of a magnetic field in a sense changes the electronic structure qualitatively: the bands (or subbands in low-dimensional structures) are split up into an infinite number of Landau levels. For simple parabolic bands the problem with a magnetic field becomes analogous to the harmonic oscillator problem with the cyclotron frequency $\omega_c = eB/m^*$ playing the role of the angular frequency of the oscillator. During the last few decades numerous studies of two-dimensional semiconductor heterostructures have been performed utilizing a magnetic field.

Effective masses are often determined with the use of cyclotron resonance experiments, in which optical transitions between Landau levels are detected. The classical Hall effect and the quantum Hall effect can be used to determine the sheet carrier density N_s. In similar experiments one can also measure the resistivity in the direction of the current ρ_{xx} which shows characteristic Shubnikov–de Haas oscillations. From their periodicities the population of individual subbands are often deduced.

These experiments in principle mirror the Landau level structure rather than the subband structure. It is worth investigating to which extent it is appropriate to interpret experiments in a magnetic field in terms of subband structures. In a semiclassical picture the carriers move in k space on surfaces (or contours in two dimensions) with constant energy and from the derivative of the area within a contour with respect to energy the semiclassical cyclotron mass can be determined theoretically. It was shown that the agreement between such semiclassical masses[1–4] and early cyclotron resonance experiments[5] was poor for a two-dimensional hole gas. The asymmetry of the potential at the modulation-doped interface gives rise to a spin splitting of the hole subbands with two different cyclotron masses. The calculated cyclotron masses had a clear dependence on the magnetic field and were found to change from $0.2m_0$ and $0.9m_0$ at $B=0$ (Refs. 1,4) to about $0.4m_0$ and $0.6m_0$, respectively,[1] at $B = 3-8$T, where the experiments[5] were carried out. For the latter values the agreement with experiment was very good.

Shubnikov–de Haas (SdH) experiments were also performed for samples with 2D hole gases[5,6] and the populations of the two subbands were determined with the use of a standard two-carrier expression. It has been subject to some debate if the periodicity of the oscillations at high magnetic fields reflects the population of the more highly populated subband or the sum of the subband populations, i.e., the total population[7]. With the former interpretation there was agreement between theory[1,4] and the experiments in Ref. 5 and with the latter interpretation the agreement between Refs. 1 and 6 was good. More recently the effect of in-plane stress on the spin splitting was investigated.[8] In this case the sum of the spin subband populations deduced from SdH experiments agreed with the total density according to Hall measurements. It is worth stressing that the analysis in Ref. 7 did not pertain to spin-split hole subbands but to Si inversion layers with states of two valleys filled.

Quite recently experiments have been carried out in which a gated structure was used to tune the asymmetry and thereby the spin splitting.[9–11] This method has the disadvantage that the applied electric field influences total carrier concentration as well as the asymmetry. An alternative way to vary the spin splitting of hole subbands by an order of magnitude is to apply stress.[12] In Ref. 11 the spin splitting was calculated and deduced experimentally from SdH experiments for different hole densities. The experimental values were clearly smaller than the calculated subband splittings but the trends were similar.

One important issue, which is the subject of this paper, is if the spin splitting at $B=0$ of a hole subband in an asymmetric potential remains intact when a magnetic field is applied or if the magnetic field not only gives an additional contribution to the spin splitting through the direct Zeeman coupling but also influences the "spontaneous" spin splitting. In particular it is worth investigating how strong a magnetic field can be without substantially modifying the deduced subband properties in different kinds of experiments.

The valence band structure was calculated in the multiband envelope-function approximation[13] using a 6×6 Hamiltonian, which incorporates the heavy-hole (HH), light-hole (LH), and spin-orbit split-off (SO) band. The potential, which is calculated self-consistently for $B=0$, is added along the diagonal. The Hamiltonian in a magnetic field along the z axis is found by replacing $\mathbf{k}$ with $\mathbf{k}+e\mathbf{A}/\hbar$ and introducing the ladder operators

$$a=\left(\frac{\hbar}{eB}\right)^{1/2}(k_x-ik_y),$$

$$a^\dagger=\left(\frac{\hbar}{eB}\right)^{1/2}(k_x+ik_y) \tag{1}$$

with the commutation relation $[a,a^\dagger]=1$. One also has to add terms proportional to $\kappa J_z B$ which correspond to the direct Zeeman coupling between the spin of the hole and the magnetic field. The Hamiltonian can be written $H=H_0+\delta H_{\epsilon k}+\delta H_k$, where H_0 is the Luttinger-Kohn Hamiltonian[14] with inclusion of strain terms, which is strictly valid only for the diamond crystal structure. The two latter terms result from microscopic inversion asymmetry and appear in crystals with the zinc-blende structure.

These additional terms are linear in k. The matrix δH_k is independent of strain and can usually be neglected. However, there is also the matrix $\delta H_{\epsilon k}$ which is proportional also to the strain and which is important in particular in quantum wells under biaxial tension when the uppermost hole subband is a light-hole subband.[12,15] The expressions for these matrices were derived in Ref. 16 and are explicitly given in Ref. 17 for the representation we have used. The Landau level calculations become simpler and the results more transparent if we make the axial approximation.[1] In the axial approximation it is clear by inspection of H_0 that the envelope function vector for the Landau level n must be in the form

$$\Psi_n=\begin{pmatrix}\phi_{n-1}(\boldsymbol{\rho})f_1(z)\\ \phi_n(\boldsymbol{\rho})f_2(z)\\ \phi_{n+1}(\boldsymbol{\rho})f_3(z)\\ \phi_{n+2}(\boldsymbol{\rho})f_4(z)\\ \phi_n(\boldsymbol{\rho})f_5(z)\\ \phi_{n+1}(\boldsymbol{\rho})f_6(z)\end{pmatrix}, \tag{2}$$

where $\boldsymbol{\rho}=(x,y)$ and ϕ_ν is the harmonic oscillator function: $a^\dagger a\phi_\nu=\nu\phi_\nu$. For small values of B the Hamiltonian H_0 becomes diagonal except for the strain-induced SO-LH coupling. For the highest subbands, that we consider here, this coupling is negligible, which means that every eigenstate, Ψ_n, will only contain one component. As B increases the off-diagonal elements will increase and the eigenstate becomes mixed, however, n is still a good quantum number. As soon as one leaves the axial approximation or takes δH_k or $\delta H_{\epsilon k}$ into account n is no longer a good quantum number. In many cases the solution is dominated by one value of n, though.

When $n=-2$, only the fourth component, i.e., heavy holes with $m_J=-3/2$, enters Ψ_n, Eq. (2) and H_0 becomes a scalar operator. For $n=-1$ also light holes and holes in the split-off band with $m_J=-1/2$ enter the solution and when $n=0$ holes with $m_J=+1/2$ are included. Only when $n\geqslant 1$ all hole components enter the solution.

There are several contributions to the spin splitting of hole subbands in a magnetic field. One is the direct coupling between the magnetic field and the spin of the hole which is proportional to κ, which can be considered as a ''bare'' g factor. This Zeeman coupling is quite strong for holes compared to electrons and it is three times stronger for heavy holes than for light holes. There is one important contribution from the asymmetry of the quantum well (called structure inversion asymmetry in Ref. 18) combined with spin-orbit coupling. This is commonly called the Rashba term for electron systems.[18–21] The corresponding effect is much stronger for holes and can give rise to spin splittings of the order meV. The origin of this effect is less transparent in hole systems. We have found that it almost vanishes if the Luttinger parameter γ_3 is set to zero. It is also strongly correlated to the degree of mixing between heavy-hole and light-hole character of the subband.[12] We have also included the effect of the bulk inversion asymmetry, especially the matrix $\delta H_{\epsilon k}$. This breaks the fourfold rotation symmetry and leads to an optical anisotropy.[22] We have found that the effect of bulk inversion asymmetry largely persists when a magnetic field is applied. In the present paper we only present results for the unstrained case, where this effect is small. Results for the strained case will be presented elsewhere. Finally, there is a contribution from the interface layer,[23] which is not considered in the present article.

The QW structure studied in this paper is an $In_{0.25}Ga_{0.75}As$ well with lattice-matched $In_{0.38}Ga_{0.62}As_{0.73}P_{0.27}$ barriers. The barrier height is 100 meV. By varying the composition of the $In_xGa_{1-x}As_yP_{1-y}$ substrate through the values of x and y the strain in the well can be changed without changing the barrier height. In this way a variation of the composition of the substrate is essentially equivalent to applying external stress but we can easily obtain both biaxial tension and biaxial compression.

As a reference, we consider a symmetric 100 Å well with p-type doped barriers ($N_A=3\times10^{18}$ cm^{-3}) and equal spacer layers in the barriers. The carrier concentration N_s in the well is 3×10^{11} cm^{-2} in all the cases.

We introduce asymmetry of the quantum well by having the same doping as above on one side only. The other side is n-type due to background doping and the result is a built-in electric field over the well.

The fan diagrams for the symmetric and asymmetric wells are presented in Fig. 1. It is remarkable that without a magnetic field there is a significant difference between the subband structures,[12] whereas the Landau levels are very similar and one expects the results of Shubnikov–de Haas experiments to be similar.

To analyze this effect more closely, especially for smaller magnetic fields, we would like to examine the measurable spin splittings in more detail. However, the Landau level splitting for holes is much more difficult to analyze than the subband splitting. If we want to compare with the subband splitting at a given value of $\mathbf{k}_\parallel$, it is at first sight not obvious which pair of Landau levels we should compare to each other. For $n=-2$ the eigenstate is a simple product:

$$\Psi_{-2}(\mathbf{r})=\phi_0(\boldsymbol{\rho})f_4(z)\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle. \tag{3}$$

There is no eigenstate with $n<1$ that contains the $\left|\tfrac{3}{2},\tfrac{3}{2}\right\rangle$ component. It is therefore natural to calculate the Landau level splitting using an eigenstate with the same in-plane wave function, in this case ϕ_0, and with $m_J=\tfrac{3}{2}$. This means that we wish to find another simple product function

$$\Psi_n(\mathbf{r})=\phi_0(\boldsymbol{\rho})f_1(z)\left|\tfrac{3}{2},\tfrac{3}{2}\right\rangle \tag{4}$$

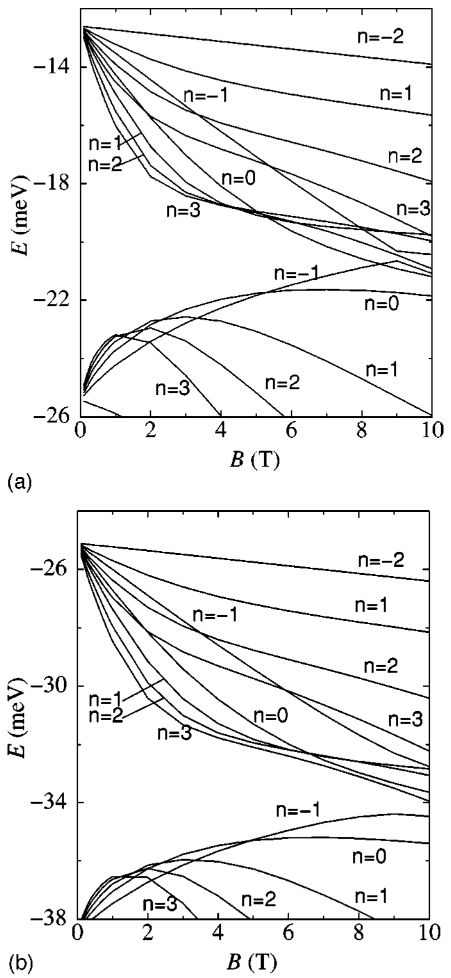

FIG. 1. Fan diagrams with Landau levels for the reference well (a) and the asymmetric well (b). The strain is taken to be zero. Note the similarity between the two diagrams.

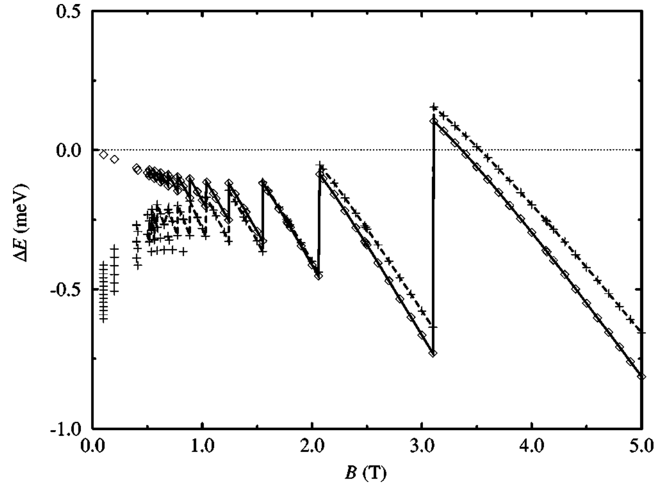

FIG. 2. Landau level splitting between the corresponding levels (see text) in the different wells as a function of B. The lines refer to the most intense transitions and the symbols to all possible transitions. The transitions in the symmetric reference well are shown with diamonds and a solid line and the transitions of the asymmetrically doped well are shown with plus signs and a dashed line.

to compare with. Normally such a state is not an eigenstate due to band mixing but we here only consider states with $n=1$ which are dominated by the $|\frac{3}{2},\frac{3}{2}\rangle$ component. As a consequence we choose to compare the eigenenergies of the two HH- or LH-like states with the same in-plane part $\phi_\nu(\boldsymbol{\rho})$ of the wave function at a given value of B. In a previous article[17] the Landau level splitting at the highest level ($\nu=0$), which should be relevant for large B values, was compared for the symmetric and asymmetric wells and it was shown that the Landau level splittings differed by no more than 0.1 meV.

In this paper we choose to calculate the spin splitting near the Fermi energy. This choice of levels is more appropriate in order to compare with the subband splitting and it is also better related to what can be measured experimentally. For a transition to be possible between the two Landau levels compared, they should not both be above or below the Fermi energy. In general several pairs of Landau levels fulfill these conditions.

In Fig. 2 we display the spin splitting as a function of magnetic field for the symmetric and the asymmetric wells. For relatively large magnetic fields one first notes the strong oscillations of the spin splitting. The (negative) spin splitting between a given pair of Landau levels increases with B but there are jumps at integral filling factors when transitions between new Landau level pairs become possible.

It is also verified that for large B there is virtually no difference between the symmetric and the asymmetric well. For magnetic fields below 1 T a significant difference becomes visible. For the symmetric well the spin splitting approaches zero when $B\to 0$ while it tends to a finite value in the asymmetric well. It was pointed out for electrons in Ref. 21 that as $B\to 0$ the Fermi level goes to higher and higher Landau levels and therefore the spin splitting at the Fermi level does not necessarily go to zero for small B.

The small impact of the asymmetric potential on the Landau level splitting even at comparatively small magnetic fields (1–3 T), where one could expect the magnetic field to be a small perturbation to the subband structure, is important to note. In several experiments where several spin subbands were filled the number of carriers in each spin subband were deduced from the periodicities of the Shubnikov–de Haas oscillations[5,6,9–11] and in some cases conclusions about the spin splitting at zero field were drawn. However, our findings that the Landau fans are quite insensitive to structure inversion asymmetry, which is the main contribution to the subband splitting, cast some doubts on the common interpretation in terms of subband populations in the case of spin-split hole subbands. A closer analysis will be the subject of future work.

To give a tentative semiclassical explanation to the remarkable result that the clear effect of structure inversion asymmetry on the subband splitting almost disappears when a magnetic field is applied perpendicular to the interfaces we consider the expression

$$\mathbf{B}'=\mathbf{B}\cdot\hat{\mathbf{e}}_{\mathbf{v}}+\gamma\left(\mathbf{B}-\mathbf{B}\cdot\hat{\mathbf{e}}_{\mathbf{v}}-\frac{\mathbf{v}}{c^2}\times\mathbf{E}\right). \qquad (5)$$

Here $\mathbf{B}$ and $\mathbf{E}$ are the magnetic and electric fields, respectively, in the laboratory frame and $\mathbf{B}'$ is the magnetic field in the frame of a hole moving with the velocity $\mathbf{v}$. In our case $\mathbf{E}$

is in the z direction. With a strong magnetic field in the z direction the hole is forced to move in the xy plane. If $\mathbf{v}$ at one moment is in the y direction, $\mathbf{v}\times\mathbf{E}$ is in the x direction. As the hole moves along an orbit in the xy plane, the contribution of this term should average to zero. For $B\leqslant 1$ T the applied magnetic field is apparently not dominating so strongly over the induced magnetic field.

This argument indicates that the spin splitting in tilted magnetic fields[24] should also be considered in future experimental and theoretical work.

Similar calculations have previously been performed for the spin splitting of electron subbands, where it is easier to distinguish between the different contributions of the spin splitting (see Refs. 18 and 21 and references therein). For sufficiently strong magnetic fields it was found that the spin splitting is dominated by the Zeeman term. The Landau fans for symmetric and asymmetric potentials were recently calculated for the more complex $InAs/Al_xGa_{1-x}Sb$ structures in Ref. 25 and the difference was fairly small also in that case.

In conclusion it has been shown that spatial asymmetry has a small influence on the spin splitting in an unstrained p-type quantum well in a magnetic field. This Landau level splitting differs considerably from subband splitting. At high magnetic fields the Landau level splittings show strong oscillations, which are related to the change with filling factor of the pair of Landau levels between which transitions are possible. Only for magnetic fields smaller than about 1 T there is a significant effect of the structure inversion asymmetry. A tentative explanation of the origin of this difference is presented but the issue deserves further investigation.

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