Spin Splitting in Semiconductor Heterostructures for $B \rightarrow 0$

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Spin splitting of subband states in semiconductor heterostructures at $B=0$ is ascribed to the inversion-asymmetry-induced *bulk* k^3 term, which dominates in large-gap materials, and to the *interface* spin-orbit or Rashba term, which becomes important in narrow-gap systems. We show for AlGaAs/GaAs heterostructures how this finite spin splitting at $B=0$ evolves from the Zeeman splitting for $B\neq 0$, and predict a *vanishing spin splitting at a finite magnetic field,* which depends on the electron concentration in the inversion layer.

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The spin splitting of conduction-band states in bulk semiconductors as well as in inversion layers of semiconductor heterostructures has attracted considerable interest recently. Spin polarization of photoemitted electrons from a GaAs(110) surface has been ascribed[1] and quantitatively explained[2] as being due to the inversion-asymmetry-induced k^3 term of the zinc-blende structure. This term, which lifts the spin degeneracy of the bulk conduction band for $B=0$ except for $\mathbf{k}\parallel\langle 001\rangle$ and $\langle 111\rangle$,[3] is considered also to be responsible for the spin relaxation of electrons[4] and holes.[5] Electron-spin-resonance data from AlGaAs/GaAs heterostructures[6] gave rise to speculations about a zero-field spin splitting because of a linear extrapolation of results measured at finite magnetic field for Landau levels with Landau quantum numbers $N=1$ and $N=2$. An attempt has been made to explain this zero-field splitting by the spin-orbit or Rashba term.[7] Calculations, however, have ruled out this linear extrapolation by showing that the spin splitting of Landau levels depends nonlinearly on the magnetic field as a result of the nonparabolicity of the conduction band.[8] This nonlinear dependence has been ascribed mainly to a k^4 term, identified as the isotropic k-dependent contribution to the g factor. Spin splitting of electrons states in inversion layers on narrow-gap semiconductors like InSb[9,10] and $Hg_xCd_{1-x}Te$[11-13] is not yet really understood, except that for zero magnetic field it seems to be dominated by the spin-orbit coupling in the presence of the interface electric field. Until now, a comprehensive theoretical study of spin splitting in semiconductor heterostructures for $B\rightarrow 0$, i.e., the connection between spin splitting at finite and at zero magnetic field, was missing.

In this Letter we present detailed calculations for Landau-level spin splittings in the degenerate electron system of AlGaAs/GaAs heterostructures for $B\rightarrow 0$ at the Fermi energy, i.e., for increasing Landau-level quantum numbers N. These calculations demonstrate how the spin splitting for small N at finite magnetic field, which is dominated by the bulk g factor and a k^4 nonparabolicity term, evolves into the zero-field spin splitting caused by the k^3 nonparabolicity. We predict a vanishing spin splitting at a finite magnetic field, which depends on the concentration N_S of the electron system. Moreover, we discuss the material-specific aspects of terms contributing to spin-splitting and find that the spin-orbit term, which is negligibly small in AlGaAs/GaAs heterostructures, becomes important in inversion layers on narrow-gap semiconductors.

The energy of Landau levels of electrons in inversion layers of AlGaAs/GaAs has been calculated before[14] in order to explain the observed reduction of the g factor[8,14] and the increase and oscillation of cyclotron masses.[15] These calculations start from a 2×2 conduction-band Hamiltonian,

$$H_{2\times 2}=H_0+H_1, \tag{1}$$

which contains, besides the subband Hamiltonian in parabolic approximation,

$$H_0=-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz}+\frac{\hbar^2 k_\parallel^2}{2m^*(z)}+U(z) \tag{2}$$

terms of higher order in the electron momentum and the spin-orbit term, which can be formulated as

$$H_1(\mathbf{k},\mathbf{E})=\sum_{\kappa,\lambda}a_{\kappa\lambda}\sum_L H_L^{(\kappa,\lambda)}\mathcal{H}_L^{(\kappa,\lambda)*}(\mathbf{k},\mathbf{E}) \tag{3}$$

in terms of invariants expressed by Pauli spin matrices $X_\pm^{(4)}=\sigma_x\pm i\sigma_y$, $X_3^{(4)}=\sigma_z$ and the 2×2 unit matrix $X^{(1)}=I_{2\times 2}$, and irreducible tensor components of the electron wave vector $\mathbf{k}$ and the interface electric field $\mathbf{E}=-e^{-1}\nabla U(z)$, which transform according to the irreducible representation Γ_κ of the zinc-blende point group T_d. The material-specific coefficients $a_{\kappa\lambda}$ can be expressed by momentum matrix elements and energy gaps,[16] which are well known for most semiconductors.[17] The eigenvalue problem of H_0 is solved self-consistently together with the Poisson equation for the Hartree potential $V_H(z)$, determined by the charge distribution of the modulation-doped heterostructure. The total interface potential $U(z)$ in Eq. (2) consists of the band offset V_0 ($=0.65\Delta Eg$ for AlGaAs/GaAs), $V_H(z)$, and a pa-

rametrized exchange-correlation potential.[18] With use of the wave function $\xi_0(z)$ of the lowest subband (the only one which is occupied in AlGaAs/GaAs heterostructures with usual electron concentrations), the Landau-level energies for $B\|\langle 001\rangle$ are obtained by our replacing $\hbar^2 k_\parallel^2/2m^*(z)$ by $\hbar\omega_c^*(N+\frac{1}{2})\pm\frac{1}{2}g^*\mu_B B$ and treating H_1 by perturbation theory.[8,14] Taking all terms of H_1 (see Table I of Ref. 8) into account leads us to a secular problem whose order is twice (because of spin) the number of Landau levels considered.

Electron-spin resonance in a Landau level of quantum number N, i.e., the transition $|N\uparrow\rangle \rightarrow |N\downarrow\rangle$, can be observed only if the lower level is occupied and the upper level is empty, which is possible only in a limited magnetic field range.[6] As with decreasing magnetic field the Fermi energy shifts to Landau levels with higher N, the spin-flip transition becomes observable in Landau levels with increasing N; i.e., for $B\rightarrow 0$ we have to look at the spin splitting for $N\rightarrow\infty$.

Figure 1 contains calculated results of the spin-splitting energy $E_{N\downarrow}-E_{N\uparrow}$ in an AlGaAs/GaAs heterostructure with electron concentration $N_S=10^{11}$ cm^{-2} and a background charge density $N_D=0.5\times10^{11}$ cm^{-2}. In Fig. 1(a) the total spin splitting shown for a wide magnetic field range demonstrates the evolution of the spin splitting at $B=0$ from the spin splitting at finite magnetic field and low Landau level N. Because the Fermi energy is located in the Nth Landau level only for a limited magnetic field range,

$$\frac{h}{2e}\frac{N_S}{N+1} < B < \frac{h}{2e}\frac{N_S}{N}, \tag{4}$$

we obtain a piecewise continuous curve for the spin splitting. The different mechanisms which determine the splitting at finite and at zero magnetic field are resolved for $B<1$ T in Fig. 1(b) (the discontinuities being suppressed). For magnetic fields $B>0.5$ T, the total spin splitting (full line) is dominated by the Zeeman term, $\langle\xi_0|g^*(z)|\xi_0\rangle\mu_B B\sigma_z$, and a contribution from the k^4 nonparabolicity,[14] $\langle\xi_0|a_{43}(z)(2N+1+\zeta^2)|\xi_0\rangle$, where $\zeta=-i\lambda_c\partial_z$ [see dashed line of Fig. 1(b)]. For decreasing magnetic field, the contribution of the bulk k^3 term becomes increasingly important (dotted line) and determines the total spin splitting for $B\rightarrow 0$, which con-

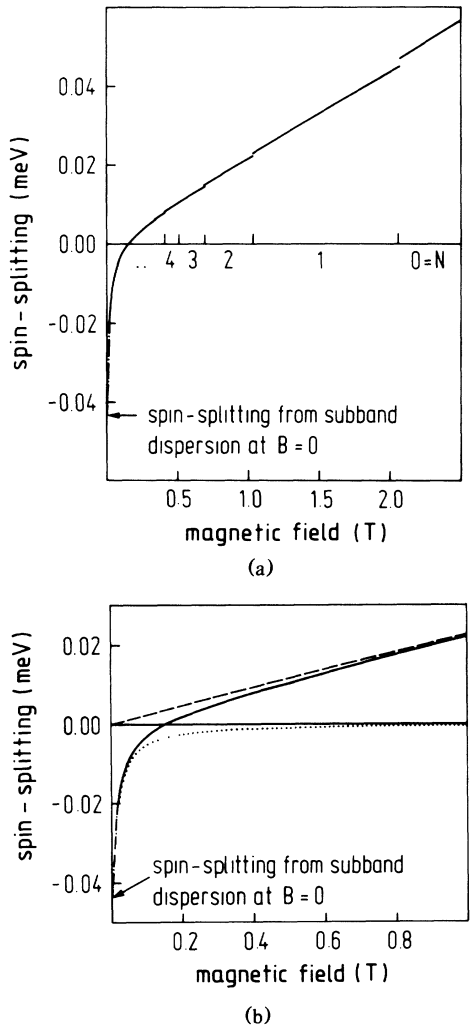

FIG. 1. Spin splitting of subband Landau levels vs magnetic field and spin splitting of the subband dispersion at $B=0$, both calculated at the Fermi energy, i.e., for corresponding Landau levels N [see Eq. (4)] for $B\neq 0$ and at $k_\parallel=k_F$ for $B=0$, respectively. Calculations were done for an $Al_{0.3}Ga_{0.7}As/GaAs$ heterostructure with an electron concentration $N_S=10^{11}$ cm^{-2} and an assumed background charge density $N_D=0.5\times10^{11}$ cm^{-2}. (a) Spin splitting calculated in a magnetic field range $0\leq B\leq 2.5$ T for Landau levels $0\leq N\leq 120$ and at $k_\parallel=k_F$. (b) Spin splitting calculated in a magnetic field range $0\leq B\leq 1$ T (full line) for Landau levels up to 120 compared with spin splitting due to the modified Zeeman term (dashed line) and due to the k^3 term (dotted line).

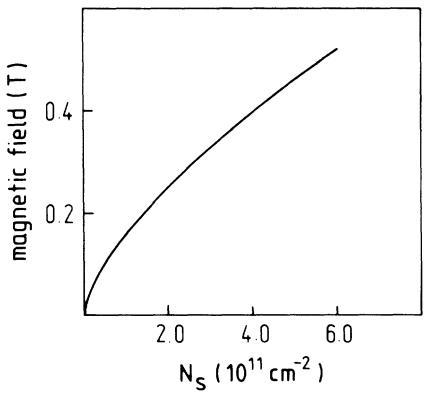

FIG. 2. Magnetic field positions B_0 for vanishing spin splitting vs electron concentration N_S for $Al_{0.3}Ga_{0.7}As/GaAs$ heterostructures with an assumed background charge density $N_D=0.5\times10^{11}$ cm^{-2}.

verges towards a value obtained for $B=0$ from the subband dispersion at $k_{\parallel}=k_F$.[18] It turns out that the k^3 term, whose essential contribution,[14] $\langle\xi_0|-a_{42}a^{\dagger}\zeta^2\sigma_-+\text{H.c.}|\xi_0\rangle$ ($a^{\dagger}$ being the Landau creation operator), is off diagonal in the basis of Landau states, compensates the Zeeman splitting. Thus we find a zero spin splitting at a finite magnetic field B_0. As the spin splitting depends on the expectation values of ζ and ζ^2 taken with the subband wave function $\xi_0(z)$, B_0 varies with the electron concentration N_S as shown in Fig. 2. Note that at B_0, the Landau levels, which can be classified by the dominant eigenvector component as $|N\uparrow\rangle$ and $|N\downarrow\rangle$, interchange. As a consequence, we expect a change in the dipole-selection rule[19] for the spin-resonance transition from left circular polarization for $B>B_0$ to right circular polarization for $B<B_0$.

It is interesting to look at the material-specific aspects of the terms which cause a spin splitting. For this purpose we refer to the representation of the $a_{\kappa\lambda}$ of Eq. (3) in terms of band-structure parameters. In a similar way as the g factor is expressed in terms of momentum matrix elements and energy gaps,[20] we find for the k^3 term[16]

$$a_{42}=\frac{C_kP^2}{\sqrt{3}E_g^2}-\frac{4i}{3}PQP'\left(\frac{1}{(E_g+\Delta_0)(E_g'+\Delta_0'-E_g)}-\frac{1}{E_g(E_g'-E_g)}\right) \tag{5}$$

and for the spin-orbit term[8]

$$a_{46}=\frac{2i}{3}\left[PR\left(\frac{1}{E_g}-\frac{1}{E_g+\Delta_0}\right)-P'R'\left(\frac{1}{E_g'+\Delta_0'-E_g}-\frac{1}{E_g'-E_g}\right)\right], \tag{6}$$

where E_g, $E_g+\Delta_0$ and $E_g'+\Delta_0'-E_g$, $E_g'-E_g$ are the energy separations of the conduction-band minimum from the spin-orbit-split valence band and p-antibonding conduction band, respectively. P,R and P',R' are the corresponding matrix elements of $(\hbar/m)\mathbf{p}$ and $\mathbf{r}$, while Q is the matrix element of $(\hbar/m)\mathbf{p}$ between the p-bonding valence and p-antibonding conduction band. Using the quantum-mechanical equation of motion, one finds $R=-ieP/(E_g+\Delta_0/3)$ and a corresponding expression for R'. C_k is the inversion-asymmetry induced k-linear term.[21] Because the momentum matrix elements do not vary rapidly with chemical composition,[22] the coefficients of Eqs. (5) and (6) depend mainly on the energy gaps. They increase with decreasing fundamental gap E_g and increasing spin-orbit splitting Δ_0. As a result of the additional dependence of R on E_g, a_{46} increases more rapidly than a_{43}, when going, e.g., from GaAs to InSb and to $Hg_{0.8}Cd_{0.2}Te$ ($E_g=60$ meV). Moreover, the expectation value of the interface electric field, which appears in the tensor components $\mathcal{H}_L^{(46)*}$ of the spin-orbit term, is usually larger in inversion layers on narrow-gap semiconductors than in AlGaAs/GaAs heterostructures. Therefore, in narrow-gap systems the spin-orbit term is expected to dominate the spin splitting for $B\rightarrow 0$ (see Table I).[23]

TABLE I. Values of weighting factors for the k^3 term and the spin-orbit term calculated by Eqs. (5) and (6) for GaAs, InSb, and $Hg_{0.8}Cd_{0.2}Te$.

	a_{42} (eV Å^3)	a_{46} (eV Å^2)
GaAs[a]	−27.6	5.5
InSb	−770	400
$Hg_{0.8}Cd_{0.2}Te$	−2485	1930

[a]Reference 18.

In conclusion, we have calculated the spin splitting of subband Landau levels in AlGaAs/GaAs heterostructures at the Fermi energy, where experimental observation is possible. The results are a nonvanishing spin splitting for $B\rightarrow 0$, which converges towards the value calculated from the subband dispersion at $B=0$. We predict a zero spin splitting at a finite magnetic field, which is due to compensation between different spin-splitting mechanisms, and a change of optical selection rules for the spin-flip transition. We also give a discussion of material-specific aspects of the spin splitting in different semiconductor systems.

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[23]One has to keep in mind that for symmetric quantum wells the expectation value of the electric field is zero and, therefore, the spin-orbit term does not contribute to a spin splitting. By studying symmetric and asymmetric structures of the same semiconductor materials it should be possible to discriminate between contributions to spin splitting from the k^3 and the spin-orbit terms.