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Reduced g factor of subband Landau levels in AlGaAs/GaAs heterostructures

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The reduction of the g factor of subband Landau levels in the n-inversion channel of AlGaAs/GaAs heterostructures, which has been observed in electron-spin-resonance experiments by Stein, von Klitzing, and Weimann [Phys. Rev. Lett. **51**, 130 (1983)], can be explained quantitatively by the taking into account of the nonparabolicity of the bulk band structure in the subband calculation.

Electron-spin-resonance experiments on subband Landau levels in AlGaAs/GaAs heterostructures[1] yielded the unexpected result of a g factor, which is strongly reduced with respect to the bulk value. Moreover, a linear extrapolation of the experimental data obtained in a small magnetic-field window (see Fig. 1) led to speculations about a zero-field spin splitting. These results cannot be understood in the standard model of subbands in a heterostructure[2] according to which the spacing of Landau levels in a subband is determined by the bulk effective mass m^*, and the spin splitting is given by $g^*\mu_B H$, where g^* is the bulk g factor. A deviation of the subband parameters from the bulk values is possible because of the fact that the conduction-band discontinuity, which for $Al_{0.3}Ga_{0.7}As/GaAs$ is about 300 meV, allows the subband wave function of the n-inversion channel to penetrate into the large gap region of AlGaAs. Thus the subband electron is subject not only to the bulk band parameters of GaAs but also to some extent to those of AlGaAs. Subband calculations[3–5] show, however, that the probability of finding the subband electron on the AlGaAs side is so small that it cannot cause the observed reduction of the g factor by about 30% of the bulk value. In a very recent paper Lassnig ascribes the reduction of the g factor to band-mixing effects but fails to describe the observed values quantitatively.[6] We present here a calculation of Landau-level energies in the lowest subband of AlGaAs/GaAs heterostructures, which includes the nonparabolicity of the bulk band structure and yields quantitative agreement with the observed spin splittings.

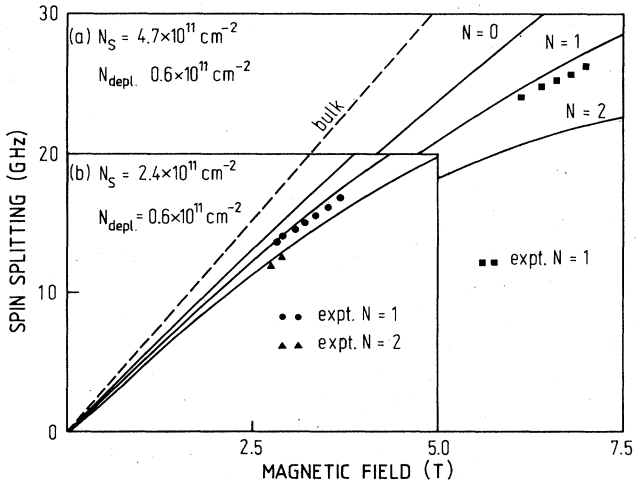

FIG. 1. Spin splitting of Landau levels in the lowest subband of $Al_{0.3}Ga_{0.7}As/GaAs$ heterostructures with (a) $N_s = 4.7\times10^{11}$ cm^{-2}, $N_{depl} = 0.6\times10^{11}$ cm^{-2}; (b) $N_s = 2.4\times10^{11}$ cm^{-2}, $N_{depl} = 0.6\times10^{11}$ cm^{-2}. Comparison of calculated values of $N = 0, 1, 2$ with the bulk value ($g^* = -0.44$) and with experimental data of Ref. 1. (The experimental data for $N = 2$ are obtained with a tilted magnetic field.)

It is known that the bulk conduction band not only of small-gap semiconductors but also of materials with a larger band gap (like GaAs) deviates from the isotropic parabolic shape. These deviations, which can be properly described in an extended version of the Kane model (including besides the lowest conduction band also the p-antibonding conduction band), are an isotropic, an anisotropic (warping) nonparabolicity, and a lifting of the spin degeneracy (except for the high symmetric $\langle 100\rangle$ and $\langle 111\rangle$ direction in k space).[7] In an effective conduction-band Hamiltonian they can be described by third-, fourth-, and higher-order terms in the components of the electron wave vector $\mathbf{k}$, and corresponding terms in a magnetic field $\mathbf{H}$ when $\mathbf{k}$ becomes an operator with $\mathbf{k}\times\mathbf{k} = (e/i\hbar c)\mathbf{H}$. The weighting factors of these terms can be expressed by momentum matrix elements and energy gaps[8] and are thus well defined material parameters as the bulk effective mass and the g value. As the Fermi energy in a n-inversion channel is well above the conduction-band edge, these higher-order terms become important in the subband problem and are considered in our calculation. Our subband Hamiltonian,

$$H = H_0 + H_1 , \tag{1}$$

acts in the twofold space of the spin-degenerate conduction band. It contains the standard model Hamiltonian,[2,4,5]

$$H_0 = \left[-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz} + U(z) + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2) \right] \mathbb{1}_2 , \tag{2}$$

where $m^*(z)$ is the bulk mass of GaAs ($Al_xGa_{1-x}As$) for $z > 0$ ($z < 0$) and has a discontinuity at $z = 0$.

$$U(z) = V_0\theta(-z) + V_H(z) \tag{3}$$

is the one-dimensional potential, which consists of the conduction-band discontinuity ($V_0 = 300$ meV for $x = 0.3$) at $z = 0$ and the Hartree potential. The 2×2 unit matrix $\mathbb{1}_2$ indicates that H_0 is diagonal in the twofold spin space of the lowest conduction band. The eigenvalue problem with H_0 is solved self-consistently either by a variational calculation[3,4] or by a numerical procedure, under the assumption that only the lowest subband is occupied. The matching conditions at $z = 0$ are those used in the literature: continuous wave function but discontinuous derivative (due to the

mass discontinuity).

The additional terms can be represented by an invariant expansion

$$H_1 = \sum_{\kappa,\lambda} a_{\kappa\lambda} \sum_L X_L^{(\kappa,\lambda)} \mathcal{K}_L^{(\kappa,\lambda)*} , \tag{4}$$

and are described in detail in Ref. 8. They are products of 2×2 matrices $X_L^{(\kappa,\lambda)}$ (1_2 and the Pauli spin matrices $\sigma_\pm$ and σ_z) and irreducible tensor components $\mathcal{K}_L^{(\kappa,\lambda)*}$ which are constructed from components of $\mathbf{k}$ (up to fourth order) and transform according to the irreducible representations Γ_κ of the zinc-blende point group T_d. In the presence of a magnetic field we have to consider the commutation relation of $\mathbf{k}$ and introduce the operators $a^\dagger$ and a for the Landau oscillator. Table I, which is obtained from Table I of Ref. 8 by specializing to the magnetic field direction $\mathbf{H}\parallel(001)$, contains all the terms considered in H_1. In the vein of effective-mass theory we replace the wave vector parallel to the magnetic field (normal to the interface) by $(1/i)d/dz$. $\mathcal{K}_1^{(1,3)*}$ and $\mathcal{K}_1^{(1,4)*}$ derive from the isotropic and anisotropic k^4 nonparabolicity and are responsible for unequal spacing of the Landau levels. The remaining terms of Table I contribute to a spin splitting. The numerical values of the material specific prefactors $a_{\kappa\lambda}$ can be calculated by using the expressions of Table 3 in Ref. 8; they represent the bulk g^* factor (a_{41}), the inversion-asymmetry spin splitting (a_{42}), the isotropic (a_{43}), and anisotropic (a_{44} and a_{45}) k-dependent contribution to the g factor. In addition to those terms discussed in Ref. 8, we have to take into account also the spin-orbit coupling,[9] which is proportional to $\boldsymbol{\sigma}\cdot(\mathbf{k}\times\mathbf{E})$, where $\mathbf{E}$ is the electric field in the interface. It results as the cross term in a second-order perturbation treatment of the $\mathbf{k}\cdot\mathbf{p}$ and $e\mathbf{E}\cdot\mathbf{r}$ couplings and has the weighting factor

$$a_{64} = \frac{2i}{3}\left[PR\left(\frac{1}{E_0} - \frac{1}{E_0+\Delta_0}\right) - P'R'\left(\frac{1}{E_0'+\Delta_0'-E_0} - \frac{1}{E_0'-E_0}\right)\right] , \tag{5}$$

TABLE I. Irreducible tensor components $\mathcal{K}_L^{(\kappa,\lambda)*}$ for $\mathbf{H}$ and $\mathbf{E}\parallel(001)$; $a^\dagger$ and a are the creation and annihilation operators of a Landau oscillator and $\zeta=\lambda_c(1/i)d/dz$.

$\mathcal{K}_1^{(1,3)*}$:		$4(a^\dagger a+\frac{1}{2}+\frac{1}{2}\zeta^2)^2$
$\mathcal{K}_1^{(1,4)*}$:		$\frac{1}{4}(a^{\dagger 4}+a^4)+2(a^\dagger a+\frac{1}{2})\zeta^2+\frac{1}{2}[(a^\dagger a)^2+a^\dagger a+1]$
$\mathcal{K}_L^{(4,1)*}$:	$L=-1$	0
	$L=z$	1
$\mathcal{K}_L^{(4,2)*}$:	$L=-1$	$\frac{1}{2}i(a^3+a^\dagger a a^\dagger-2a^\dagger\zeta^2)$
	$L=z$	$i(a^{\dagger 2}-a^2)\zeta$
$\mathcal{K}_L^{(4,3)*}$:	$L=-1$	0
	$L=z$	$2(a^\dagger a+\frac{1}{2}+\frac{1}{2}\zeta^2)$
$\mathcal{K}_L^{(4,4)*}$:	$L=-1$	ζ
	$L=z$ 0	0
$\mathcal{K}_L^{(4,5)*}$:	$L=-1$	0
	$L=z$	ζ^2
$\mathcal{K}_L^{(4,6)*}$:	$L=-1$	$-(i/\lambda_c)a^\dagger E_z$
	$L=z$ 0	0

where E_0, $E_0+\Delta_0$, and $E_0'+\Delta_0'-E_0$, $E_0'-E_0$ are the energy separations of the conduction-band minimum from the spin-orbit split valence and p-antibonding conduction band, respectively. P,R, and P',R' are the corresponding matrix elements of the operators $\mathbf{p}$ and $\mathbf{r}$. The latter can be expressed via the quantum-mechanical equation of motion by the momentum matrix elements P and P'.

We have considered H_1 in a perturbation calculation by replacing the operator $(1/i)d/dz$ (and powers of this operator) by expectation values with the self-consistent eigenfunction of H_0. With use of the Landau states $|N\rangle$ as a basis set, the matrix of H_0+H_1 has nondiagonal terms due to the coupling between different N by the terms of Table I. In order to calculate the spin splitting of the lowest Landau levels ($N=0,1,2$) as a function of the magnetic field it was sufficient to diagonalize a 12×12 matrix. Figure 1(a) shows the results for a heterostructure with an electron concentration $N_s=4.7\times10^{11}$ cm^{-2} and a depletion charge density of $N_{\text{depl}}=0.6\times10^{11}$ cm^{-2} in comparison with the spin splitting obtained from the bulk g factor of GaAs ($g^*=-0.44$) and with the experimental data of Ref. 1 for the second subband Landau level ($N=1$). The results obtained with the variational and numerical eigenfunctions of H_0 are almost identical and are in good quantitative agreement with the experimental data. Calculations for a heterostructure with lower electron concentration ($N_s=2.4\times10^{11}$ cm^{-2}) reproduce the experimental data for $N=1$ and $N=2$ [Fig. 1(b)].

It is interesting to note that the reduction of the spin splitting is mainly due to the term $\mathcal{K}_L^{(4,3)*}$, which is diagonal in N and corresponds in the bulk to an isotropic k-dependent contribution to the g factor. Thus the spin splitting of the subband Landau levels can be described approximately by

$$\Delta\nu = |\langle g^*\rangle + 4\langle a_{43}\zeta^2\rangle + 8\langle a_{43}\rangle(N+\tfrac{1}{2})|\mu_B H/h , \tag{6}$$

where the bracket refers to the mean values of the corresponding z-dependent material parameters, which are

$$g^* = \begin{cases} -0.44, & z>0 \text{(GaAs)} \\ +0.45, & z<0 \text{(Al}_{0.3}\text{Ga}_{0.7}\text{As)} \end{cases}$$

and

$$a_{43} = \begin{cases} 9.8\times10^{-4}H/(1\text{ T}), & z>0 \\ 4.2\times10^{-4}H/(1\text{ T}), & z<0 \end{cases} .$$

The contribution of the GaAs (AlGaAs) side to the norm of the subband wave function and to $\langle a_{43}\zeta^2\rangle$ for $N_s=4.7\times10^{11}$ cm^{-2} is 0.984 (0.016) and 0.0158 (−0.0095), respectively.

As can be seen from Fig. 1 and Eq. (6) the spin splitting vanishes for zero magnetic field. The zero-field spin splitting reported in Ref. 1 turns out to be an artifact of the linear extrapolation from experimental data observed in a small magnetic field window for which the Fermi energy is between the spin-split Landau levels. Nevertheless, the spin degeneracy of the subband is lifted without the magnetic field but only at finite values of the wave vector parallel to the interface. Calculations for this case will be published separately.

The calculations of Lassnig[6] start from a multiband Hamiltonian for the subband problem, which in an extended Kane model considers the influence of the interface potential. This problem is not solved, however, but reduced to

the 2×2 conduction-band problem by eliminating the off-diagonal $\mathbf{k}\cdot\mathbf{p}$ terms in lowest order. The conduction-band Hamiltonian then consists of H_0 and two additional terms, a diagonal and a nondiagonal one. The nondiagonal one turns out to be the spin-orbit term ($\mathcal{H}_L^{(4,6)*}$ of Table I), which in our calculations has only minor influence on the spin splitting. Lassnig calculated this term by assuming that the mean value of the electric field vanishes for the bound subband state. This assumption is not corrected, however, since also the mass discontinuity results in a force. The correct statement is that the mean value of the *force* on a bound state vanishes. The diagonal correction in Lassnig's conduction band Hamiltonian reduces to $\langle g^*\rangle$ of Eq. (6) if the denominators in his N and M are replaced by the energy gaps E_0 and $E_0+\Delta_0$, respectively. Thus it is not clear to what extent his calculation considers the effect of nonparabolicity, as represented by H_1 of Eq. (4).

In conclusion, we have calculated the spin splitting of subband Landau levels in AlGaAs/GaAs heterostructures by taking into account the nonparabolic corrections known for the bulk conduction band. Our results are in quantitative agreement with the experimental data and demonstrate the importance of the nonparabolicity of the bulk band structure for the subband problem.

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