Spin splitting of conduction energies in GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunctions at $B=0$ and $B\neq 0$ due to inversion asymmetry

P. Pfeffer
Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, 02-668 Warsaw, Poland
(Received 17 September 1996)

Anisotropic spin splitting of the conduction energy in GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunctions at $B=0$ is calculated, taking into account bulk and structure inversion asymmetry of the system. It is shown that both asymmetries are of importance. The theory accounts well for the recent Raman data. The effect of an external magnetic field on the spin splitting is also calculated. It is predicted that the splitting does not change sign as a function of the field. [S0163-1829(97)50812-5]

Spin splitting of electric subbands in GaAs-$Ga_{1-x}Al_xAs$ heterojunctions has in recent years attracted considerable theoretical and experimental interest. The problem goes back to the well-known property of bulk semiconductors: in a material with bulk inversion asymmetry (BIA), the energy bands are spin split for a given direction of the wave vector **k**. In asymmetric quantum wells the spin splitting may also occur as a result of the structure inversion asymmetry (SIA), which was first pointed out by Bychkov and Rashba.[1] The history of the subject is quite controversial (cf. Ref. 2 and the references therein). An often-quoted theory of Malcher, Lommer, and Roessler[3] underestimated the influence of SIA in GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunctions, and concluded that the spin splitting is completely dominated by the BIA mechanism. However, the recent description of Pfeffer and Zawadzki,[2] as well as the Raman experiments of Jusserand and co-workers,[4,5] firmly established the importance of the SIA mechanism for the GaAs-$Ga_{1-x}Al_xAs$ system. This conclusion has been corroborated by the transport (antilocalization) experiments of Knap *et al.*[6] The effect of an external magnetic field **B** (parallel to the growth direction [100]) on the spin splitting was described theoretically by Lommer and co-workers.[7] Taking into account only the BIA mechanism at $B=0$, these authors concluded that the splitting changes sign as a function of the field.

The existing theory[2] calculated isotropic spin splitting averaging over $\mathbf{k}_F$ directions. However, the most recent anisotropic Raman data can discriminate between different directions of $\mathbf{k}_F$ by using specific photon polarizations. In this work we first calculate the anisotropy of the spin splitting in GaAs-$Ga_{1-x}Al_xAs$ heterostructures at $B=0$, and compare it with the existing Raman data. Second, we reexamine the magnetic-field dependence of the splitting, taking into account both BIA and SIA mechanisms. In contrast to the results of Lommer and co-workers,[7] we find that the splitting does not change sign as a function of the field.

We consider a GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunction at $B=0$, selectively doped in the $Ga_{1-x}Al_xAs$ barrier. For the usual electron densities N_s, only the ground electric subband is populated. On the far GaAs side, the potential is determined by the depletion charge N_d. We include the exchange-correlation potential energy $V_{xc}(z)$ using the simple analytic parametrization proposed by Hedin and Lundqvist[8] (cf. Stern and Das Sarma, Ref. 9). The self-consistent potential and the subband wave function are illustrated in Fig. 1. The spin splitting due to inversion asymmetry is calculated using a five-level $\mathbf{k}\cdot\mathbf{p}$ model, as derived by Pfeffer and Zawadzki.[10] The resulting 14×14 matrix for the bulk material is completed by the heterojunction potential $V(z)$ on the diagonal. This potential, as well as all band parameters, have different values on both sides of the interface (see below). Using the perturbation theory up to the third order, one obtains the following eigenvalue problem for the two spin states of the Γ_6^c conduction band:

$$\begin{pmatrix} \hat{A}+\hat{B}-\lambda & \hat{K} \\ \hat{K}^{\dagger} & \hat{A}-\hat{B}-\lambda \end{pmatrix}\begin{pmatrix} \Phi_1(z) \\ \Phi_2(z) \end{pmatrix}=0, \tag{1}$$

where λ is the eigenvalue, and all operators have been defined in Ref. 2. They involve contributions related to the bulk and the structure inversion asymmetry. To solve set (1), one can use general methods applicable to 2×2 eigenvalue matrices. After some manipulations we obtain

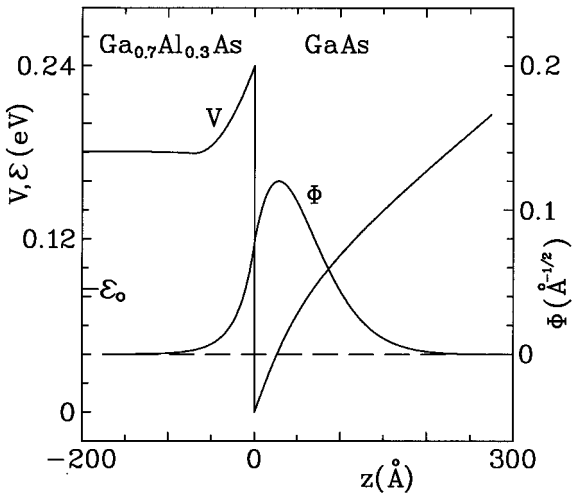

FIG. 1. Potential profile in the conduction band of a GaAs/$Ga_{0.7}Al_{0.3}As$ heterojunction, as calculated self-consistently for $N_s=1\times 10^{12}$ cm^{-2} and $N_d=3.5\times 10^{11}$ cm^{-2}. The exchange and correlation effects are included. The subband edge of the lowest electric subband and its wave function are also shown.

$$K^2(\hat{A}+\hat{B}-\lambda)\Phi_1+C(\hat{G}_R-i\hat{G}_I)\Phi_2=0, \tag{2a}$$

$$|K|(\hat{G}_R+i\hat{G}_I)\Phi_1+|K|C(\hat{A}-\hat{B}-\lambda)\Phi_2=0, \tag{2b}$$

where $K\hat{K}^\dagger=\hat{G}_R+i\hat{G}_I$ and $K^\dagger\hat{K}=\hat{G}_R-i\hat{G}_I$, while $K^2=\langle\Psi_1|\hat{K}|\Psi_2\rangle\langle\Psi_2|\hat{K}^\dagger|\Psi_1\rangle$ and $C=(\epsilon_{12}^2+K^2)^{1/2}-\epsilon_{12}$, in which $\epsilon_{12}=\epsilon_1^0-\epsilon_2^0$. Energies ϵ_1^0 and ϵ_2^0 are eigenvalues of the equations $(\hat{A}+\hat{B})\Psi_1=\epsilon_1^0\Psi_1$ and $(\hat{A}-\hat{B})\Psi_2=\epsilon_2^0\Psi_2$. In general, set (2) is equivalent to four coupled differential equations for real and imaginary parts of Φ_1 and Φ_2. The inspection of the final results shows that the $\hat{B}$ terms in Eq. (1) have a negligible influence on the spin splitting. Hence we omit them in the following considerations. In this approximation $\epsilon_1^0=\epsilon_2^0$, $\Psi_1=\Psi_2=\Psi_0$, and $C=|K|$.

For $\mathbf{k}\|[110]$ and $\mathbf{k}\|[1\bar{1}0]$ crystal directions, the situation is simpler, since the imaginary part $\hat{G}_I$ vanishes. One can then add and subtract Eqs. (2a) and (2b), which gives

$$\left(\hat{A}-\lambda+\frac{\hat{G}_R}{|K|}\right)F_1=0, \tag{3a}$$

$$\left(\hat{A}-\lambda-\frac{\hat{G}_R}{|K|}\right)F_2=0, \tag{3b}$$

where $F_1=|K|\Phi_1+C\Phi_2$, and $F_2=|K|\Phi_1-C\Phi_2$, while $\hat{G}_R/|K|=k_\perp T$, and

$$T=\left(\frac{\pm M}{2}+\frac{k_\perp^2}{2}\gamma+\gamma\frac{\partial^2}{\partial z^2}\right). \tag{4}$$

The upper signs correspond to $\mathbf{k}\|[110]$, and the lower ones to $\mathbf{k}\|[1\bar{1}0]$, respectively. Generally speaking, the terms involving γ are related to BIA, while those involving $M=\partial\eta/\partial z$ are related to SIA (cf. Ref. 2). In set (3) the functions F_1 and F_2 are decoupled, and the eigenvalue problems can be solved separately for the two states and energies of interest (for each direction of $\mathbf{k}$). The boundary conditions are found by integrating Eqs. (3) across the interface at $z=0$. For F_1 we obtain

$$F_1|_{+0}=F_1|_{-0}, \tag{5}$$

$$\left.\frac{\partial F_1}{\partial z}\right|_{+0}=\left(\frac{\hbar^2}{2m_l^*}\left.\frac{\partial F_1}{\partial z}\right|_{-0}+R\right)\left(\frac{\hbar^2}{2m_r^*}-S\right)^{-1}, \tag{6}$$

where

$$R=\frac{Tk_\perp}{|T|}\left[\frac{\pm(\eta_r-\eta_l)}{2}F_1\Big|_{-0}-\gamma_l\left.\frac{\partial F_1}{\partial z}\right|_{-0}\right], \tag{7}$$

$$S=\frac{Tk_\perp}{|T|}\gamma_r. \tag{8}$$

The upper signs are for $\mathbf{k}\|[110]$, and the lower for $\mathbf{k}\|[1\bar{1}0]$.

For $\mathbf{k}\|[100]$ the imaginary part $\hat{G}_I$ does not vanish, but it is very small, so that to a very good approximation one can again reduce the problem to separate equations of the type (3), where

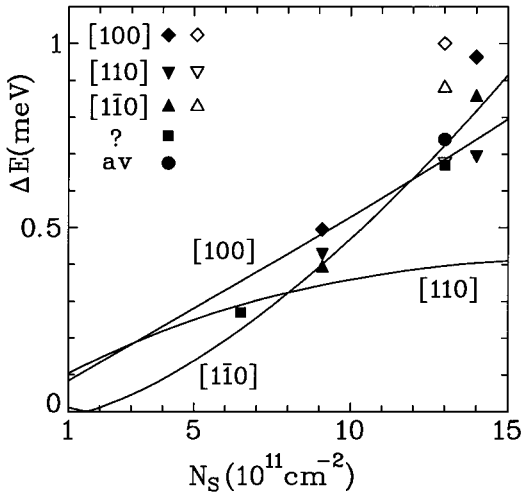

FIG. 2. Spin splitting of the lowest subband in a $GaAs/Ga_{0.7}Al_{0.3}As$ heterojunction versus electron density. Theoretical curves are calculated for $\mathbf{k}_F\|[110]$, $\mathbf{k}_F\|[1\bar{1}0]$, and $\mathbf{k}_F\|[100]$ taking $N_d=1.5\times10^{11}$ cm^{-2}. Experimental values are as follows. Jusserand *et al.* (Ref. 13): ● (averaged over $\mathbf{k}_F$ directions). Jusserand *et al.* (Ref. 4): ◇, $\mathbf{k}_F\|[100]$; △, $\mathbf{k}_F\|[1\bar{1}0]$; and ▽, $\mathbf{k}_F\|[110]$. Richards *et al.* (Ref. 5): ◆, $\mathbf{k}_F\|[100]$; ▲, $\mathbf{k}_F\|[1\bar{1}0]$; ▼, $\mathbf{k}_F\|[110]$; and ■, $\mathbf{k}_F$ direction unknown.

$$\hat{G}_R=k_\perp^2\left(\frac{M\langle M\rangle}{4}+\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle\gamma\frac{\partial^2}{\partial z^2}\right) \tag{9}$$

and

$$|K|=k_\perp\left(\frac{\langle M\rangle^2}{4}+\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle^2\right)^{1/2}. \tag{10}$$

The symbol $\langle I\rangle$ means $\langle\Psi_0|I|\Psi_0\rangle$. The boundary conditions are again given by Eqs. (5) and (6), in which

$$R=\frac{k_\perp^2}{|K|}\left[\frac{\langle M\rangle(\eta_r-\eta_l)}{4}F_1\Big|_{-0}-\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle\gamma_l\left.\frac{\partial F_1}{\partial z}\right|_{-0}\right], \tag{11}$$

$$S=\frac{\gamma_r k_\perp^2}{|K|}\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle. \tag{12}$$

The boundary conditions for F_2 have opposite signs in front of R and S. We emphasize that the spin determines also the boundary conditions (cf. Refs. 11 and 12).

We take the following band parameters for GaAs (cf. Ref. 10): $m^*=0.0660m_0$, $\eta=-9.131$ eV Å^2, $\gamma=24.12$ eV Å^3, $E_0=-1.519$ eV, $G_0=-1.86$ eV, $E_1=2.969$ eV, $G_1=3.14$ eV, $\Delta=-0.061$ eV, $E_{P_0}=2m_0P_0^2/\hbar^2=27.86$ eV, $E_{P_1}=2.36$ eV, and $E_Q=15.56$ eV. For $Ga_{0.7}Al_{0.3}As$ we take $m^*=0.0880m_0$, $\eta=-7.31$ eV Å^2, $\gamma=18.03$ eV Å^3, $E_0=-1.921$ eV, $G_0=-2.242\,86$ eV, $E_1=2.671$ eV, and $G_1=2.842$ eV (the values of matrix elements and Δ are taken to be the same as for GaAs). The offset value is $V_b=0.240$ eV. The value of η above for $Ga_{0.7}Al_{0.3}As$ differs somewhat from that used in Ref. 2, since in η_l (for the left side of interface) the conduction-band gaps E_i and G_i have been replaced by E_i+V_b and G_i+V_b.

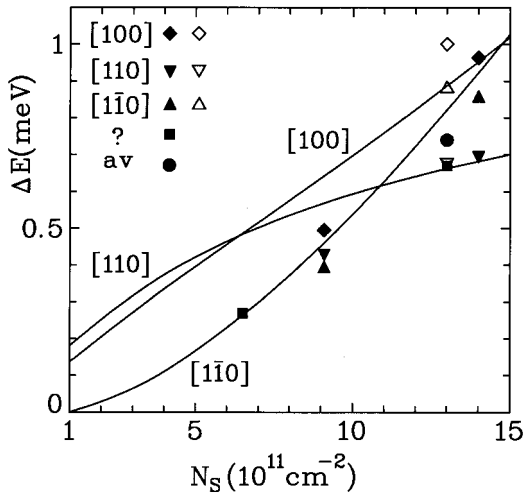

FIG. 3. The same as in Fig. 2, but with the theoretical curves calculated taking $N_d=3.5\times10^{11}$ cm^{-2}.

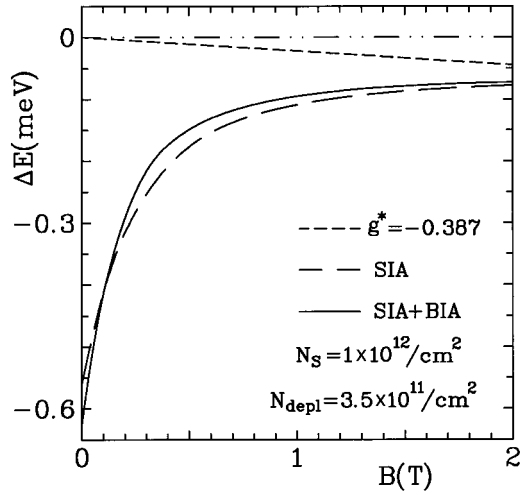

FIG. 4. Spin splitting of the ground subband, calculated as a function of magnetic field $\mathbf{B}\|[001]$, for $N_s=10^{12}$ cm^{-2} and $N_d=3.5\times10^{11}$ cm^{-2}. In the dashed curve, only structure inversion asymmetry is included. At higher magnetic fields the splitting is dominated by the free-electron g value.

In Figs. 2 and 3 we show the theoretical spin splitting for $\mathbf{k}_F\|[110]$, $\mathbf{k}_F\|[1\bar{1}0]$, and $\mathbf{k}_F\|[100]$ crystal directions, calculated for two values of N_d (1.5×10^{11} and 3.5×10^{11} cm^{-2}), which is the only unknown parameter for the heterojunctions in question. The value of N_d influences the penetration of the subband wave function into the $Ga_{1-x}Al_xAs$ region (cf. Fig. 1) which, in turn, affects the splitting. We find (cf. Figs. 2 and 3) that the value of N_d affects the splitting differently for various directions of $\mathbf{k}_F$.

Our results are compared with the Raman data of Richards *et al.*[5] and Jusserand and co-workers.[4,13] The theory accounts quite well for the absolute values of the experimental splitting and its dependence on N_s, as well as its anisotropy. The calculation for $N_d=3.5\times10^{11}$ cm^{-2} gives the best overall fit to the data. The values of N_d taken for the calculations are reasonable.[14] The fact that the splittings for [110] and $[1\bar{1}0]$ directions are not the same is by itself a proof that both SIA and BIA mechanisms contribute to the effect, since BIA alone gives the same values for these two $\mathbf{k}_F$ directions. Thus both theory and experiment confirm the conclusions of Ref. 2 that the structural inversion anisotropy is an important mechanism for the spin splitting in GaAs-$Ga_{0.7}Al_{0.3}As$ heterostructures.

Next we consider the effect of an external magnetic field $\mathbf{B}\|[001]$ on the spin splitting. This is done by using the five-level $\mathbf{P}\cdot\mathbf{p}$ model of the band structure in the presence of magnetic field, as developed in Ref. 10. The perturbation theory up to the third order leads again to Eqs. (1a) and (1b), in which

$$\hat{A}=-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z}+\frac{1}{m^*}(P_+P_-+P_-P_+)+V(z), \tag{13}$$

$$\hat{B}=\frac{\mu_B B}{2}g^*+\frac{i}{\hbar^2}(P_+^2+P_-^2)\gamma\frac{\partial}{\partial z}, \tag{14}$$

$$\hat{K}=-\frac{iM}{\sqrt{2}\hbar}P_--\frac{\sqrt{2}\gamma}{\hbar}\left[P_+\frac{\partial^2}{\partial z^2}+\frac{1}{4\hbar^2}(P_-P_+^2+P_+^2P_-)\right]+\frac{\gamma}{\sqrt{2}\hbar^3}P_-^3, \tag{15}$$

where $P_\pm$ are proportional to the raising and lowering operator for the harmonic-oscillator functions $|n\rangle$. The second term in Eq. (14) makes a negligible contribution to the splitting, and it is omitted.

The term M alone (i.e., assuming vanishing BIA) couples states $\uparrow|n\rangle$ with $\downarrow|n+1\rangle$ (set a), and the state $\downarrow|n\rangle$ with $\uparrow|n-1\rangle$ (set b). Forming appropriate combinations of the wave functions, one can find two differential equations for set a and two for set b. For set a we obtain

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z}+\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\mu_B B}{2}g^*+V(z)-\lambda\right]F_1+\left[\frac{1}{L}\left(\frac{n+1}{2}\right)^{1/2}\frac{CM}{K}\right]F_2=0, \tag{16}$$

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z}+\hbar\omega_c\left(n+\frac{3}{2}\right)-\frac{\mu_B B}{2}g^*+V(z)-\lambda\right]F_2-\left[\frac{1}{L}\left(\frac{n+1}{2}\right)^{1/2}\frac{CM}{K}\right]F_1=0, \tag{17}$$

where C and K are defined in Eq. (2), and L is the magnetic radius. The boundary conditions are

$$F_1|_{+0}=F_1|_{-0}, \tag{18}$$

$$F_2|_{+0}=F_2|_{-0}, \tag{19}$$

$$\left.\frac{\partial F_1}{\partial z}\right|_{+0}=\frac{m_r^*}{m_l^*}\left.\frac{\partial F_1}{\partial z}\right|_{-0}+\left.\frac{2m_r^*}{\hbar^2}\frac{C(\eta_r-\eta_l)}{\langle M\rangle}F_2\right|_{-0}, \tag{20}$$

$$\left.\frac{\partial F_2}{\partial z}\right|_{+0} = \frac{m_r^*}{m_l^*}\left.\frac{\partial F_2}{\partial z}\right|_{-0} - \frac{2m_r^*}{\hbar^2}\frac{C(\eta_r-\eta_l)}{\langle M\rangle}F_1\Big|_{-0}. \quad (21)$$

We obtain similar equations for set b. In order to make connection with $B=0$ results, we replace the Fermi energy $E_F=(\hbar^2k_F^2)/(2m^*)$ by $(\hbar eB/m^*)(n+\frac{1}{2})$, which averages over the two spin energies. Thus for a fixed E_F value, and B approaching zero, one has to take correspondingly high values of the Landau number n.

If BIA is also included [γ terms in Eq. (15)], set (1) with the full $\hat{K}$ operators (15) is not soluble in terms of just two harmonic-oscillator functions, and one has to recourse to the method of Evtuhov,[15] expanding the solutions in series of harmonic-oscillator functions. Our procedure is restricted to the first terms of this expansion, which couple state $\uparrow|n\rangle$ with $\downarrow|n+1\rangle$, $\downarrow|n-1\rangle$, and $\downarrow|n+3\rangle$, and state $\downarrow|n\rangle$ with $\uparrow|n-1\rangle$, $\uparrow|n+1\rangle$, and $\uparrow|n-3\rangle$. We deal then with sets of four coupled differential equations for the spin-up and spin-down states, respectively. One finds the corresponding boundary conditions, and solves for the energies.

The results are shown in Fig. 4. First, it can be seen that for $B=0$ the total splitting is to a considerable degree dominated by SIA. This agrees with the conclusion of antilocation experiments for higher N_s values.[6] Second, as the magnetic field increases from zero, the spin splitting quickly drops, going smoothly over to the free-electron splitting with the corresponding g factor: $\Delta E=g^*\mu_B B$. A simple interpretation of the initial drop is that the circular motion in $\mathbf{k}$ space (caused by magnetic field) averages over opposite directions of the $\mathbf{k}_F$ vector. Since the energies at $B=0$ satisfy the relation $E_{\mathbf{k}\uparrow}=E_{-\mathbf{k}\downarrow}$, this averaging process leads to low values of the splitting until the Pauli term takes over. Thus, in contrast to the prediction of Lommer and co-workers,[7] who neglected the SIA mechanism, we find that the spin splitting in the GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunction does not change sign as a function of magnetic field.[16] There exist spin resonance data from Stein, von Klitzing, and Weimann,[17] but they do not go to sufficiently low magnetic fields to detect the inversion asymmetry anomalies.

I am grateful to Professor W. Zawadzki for elucidating discussions. I thank Dr. B. Jusserand for useful correspondence, and the permission to use the data of Ref. 5 prior to publication. This work was supported in part by the Polish Committee for Scientific Research under Grant No. 2P03B13911.

[1] Y. A. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984).
[2] P. Pfeffer and W. Zawadzki, Phys. Rev. B **52**, R14 332 (1995).
[3] F. Malcher, G. Lommer, and U. Roessler, Superlatt. Microstruct. **2**, 267 (1986).
[4] B. Jusserand, D. Richards, G. Allan, C. Priester, and B. Etienne, Phys. Rev. B **51**, 4707 (1995).
[5] D. Richards, B. Jusserand, G. Allan, C. Priester, and B. Etienne, Proceedings of MSS7, Madrid, edited by C. Tejedor and L Vina [Solid State Electron. **40**, 127 (1996)].
[6] W. Knap *et al.*, Phys. Rev. B **53**, 3912 (1996).
[7] G. Lommer, F. Malcher, and U. Roessler, Phys. Rev. Lett. **60**, 728 (1988); U. Roessler, F. Malcher, and G. Lommer, in *Proceedings of the International Conference on High Magnetic Fields in Semiconductor Physics II, Wuerzburg, 1988*, edited by G. Landwehr (Springer-Verlag, Berlin, 1988), p. 376.
[8] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).
[9] F. Stern and S. Das Sarma, Phys. Rev. B **30**, 840 (1984).
[10] P. Pfeffer and W. Zawadzki, Phys. Rev. B **41**, 1561 (1990); **53**, 12 813 (1996).
[11] P. Sobkowicz, Semicond. Sci. Technol. **5**, 183 (1990).
[12] G. Bastard, J. A. Brum, and R. Ferreira, in *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1991), Vol. 44, p. 229.
[13] B. Jusserand, D. Richards, H. Peric, and B. Etienne, Phys. Rev. Lett. **69**, 848 (1992).
[14] B. Etienne (private communication).
[15] V. Evtuhov, Phys. Rev. **125**, 1869 (1962).
[16] As mentioned in Ref. 2, Lommer, Malcher, and Roessler (Ref. 7) underestimated the influence of the SIA mechanism by assuming that spin splitting is proportional to the average electric field in the conduction band of the heterostructure, which is nonzero only due to the difference of electron effective masses in GaAs and $Ga_{0.7}Al_{0.3}As$. In reality the splitting is strongly related to the electric fields in the Γ_8 and Γ_7 valence bands, which are far from zero because of the different values of the offsets, including their signs.
[17] D. Stein, K. v. Klitzing, and G. Weimann, Phys. Rev. Lett. **51**, 130 (1983).