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Spin splitting of conduction subbands in III-V heterostructures due to inversion asymmetry

P. Pfeffer and W. Zawadzki

Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, 02-668 Warsaw, Poland

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A formula for the spin splitting of conduction subbands in III-V heterostructures due to inversion asymmetry is derived and it is explicitly shown that the splitting is not proportional to the average electric field in the system. Calculated magnetic-field dependence of the splitting successfully describes the available experimental data for the $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ heterostructure. The theory of splitting for a magnetic field parallel to the interfaces is discussed in relation to the metal-insulator transition in two-dimensional systems. [S0163-1829(99)50108-2]

Spin splitting of electric subbands in III-V semiconductor heterostructures has attracted in recent years considerable and continuously growing theoretical and experimental interest. In a crystal with a bulk inversion asymmetry (BIA), the energy bands are spin split for a given direction of the wave vector **k**. In heterostructures, the spin splitting may also occur as a result of structure inversion asymmetry (SIA) (Bychkov and Rashba[1]). The history of the subject is very controversial. In the first theory, Ohkawa and Uemura[2] concluded that in a system with an asymmetric potential $V(z)$ the spin splitting is proportional to $-\partial V/\partial z = qE$. However, as remarked by Darr, Kotthaus, and Ando,[3] in a bound state the average value of electric field E vanishes. Malcher, Lommer, and Roessler[4] pointed out that a difference of effective masses in various parts of a heterostructure results in an additional force. Still, as shown by Pfeffer and Zawadzki,[5] the result of Ref. 4 underestimated the SIA mechanism of spin splitting in $GaAs/Ga_{1-x}Al_xAs$ heterostructures. Sobkowicz[6] (cf. also Ref. 7) emphasized the role of spin-dependent boundary conditions for the SIA mechanism. Lommer, Malcher, and Roessler[8] calculated the effect of an external magnetic field B on the spin splitting in $GaAs/Ga_{1-x}Al_xAs$ heterostructures and, taking into account only the BIA mechanism, concluded that the splitting changes sign as a function of B. Pfeffer and Zawadzki,[9,10] considering both BIA and SIA mechanisms, showed that the spin splitting does not change sign. In spite of the explicit statements that in a bound state the average electric field is exactly or nearly zero (cf. Refs. 3,5,9–12), it is still often claimed that the spin splitting due to SIA (Bychkov-Rashba) mechanism is proportional to the average field (cf. Refs. 13–18). This is frequently accompanied by an erroneous omission of the potential discontinuities at the interfaces.

In this paper we show explicitly that the average electric field contributes only a very small portion of the total spin splitting. Next we describe the effect of a magnetic field transverse to the interfaces and compare it to the experiments of Das *et al.*[19] on $In_xGa_{1-x}As/In_{0.52}Al_{0.48}As$ heterostructures. Finally, we calculate the effect of a magnetic field parallel to the interfaces and discuss it in connection with the current debate on the metal-insulator transition in two-dimensional (2D) systems.

We first consider the case of $B=0$, beginning with the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian written in the three-level model of Γ_6^c, Γ_8^v, and Γ_7^v levels.[20] The resulting 8×8 differential matrix is completed by the external potential $V(z)$, characterized by jumps at the interfaces at $z=0$ and $z=a$. In addition, the 8×8 Hamiltonian is completed by the F terms resulting from BIA, as derived by Kane.[20] The initial set is reduced by substitution to the eigenvalue problem for the two spin states of the Γ_6 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

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

$$\hat{B} = i(k_x^2 - k_y^2)\left(\frac{1}{2}\frac{\partial \gamma}{\partial z} + \gamma\frac{\partial}{\partial z}\right). \tag{3}$$

The off-diagonal term consists of two parts: $\hat{K} = \hat{K}_{SIA} + \hat{K}_{BIA}$, in which

$$\hat{K}_{SIA} = \frac{-ik_-}{\sqrt{2}}\frac{\partial \eta}{\partial z}, \tag{4}$$

$$\hat{K}_{BIA} = -i\sqrt{2}k_x k_y k_- \gamma - \sqrt{2}k_+ \frac{\partial}{\partial z}\gamma\frac{\partial}{\partial z}. \tag{5}$$

Here

$$\frac{m_0}{m^*(z)} = 1 + C - \frac{E_P}{3}\left(\frac{2}{\tilde{\epsilon}_i} + \frac{1}{\tilde{f}_i}\right), \tag{6}$$

$$\gamma(z) = \frac{2P_0 F}{3}\left(\frac{1}{\tilde{\epsilon}_i} - \frac{1}{\tilde{f}_i}\right), \tag{7}$$

$$\eta(z) = \frac{2P_0^2}{3}\left(\frac{1}{\tilde{\epsilon}_i} - \frac{1}{\tilde{f}_i}\right), \tag{8}$$

where $\tilde{\epsilon}_i(z) = \epsilon_i + V(z) - \lambda$ and $\tilde{f}_i(z) = \epsilon_i + \Delta_i + V(z) - \lambda$, $k_\pm = (k_x \pm ik_y)/\sqrt{2}$, $E_p = 2m_0P_0^2/\hbar^2$, C represents far-band

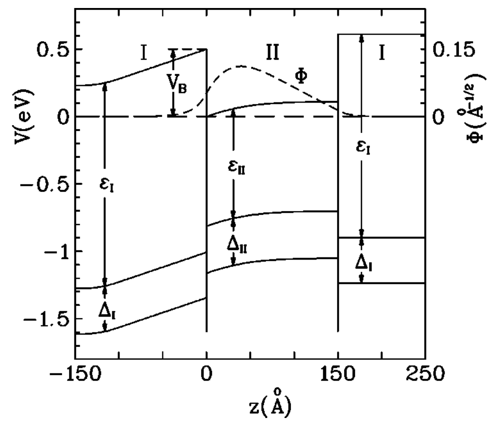

FIG. 1. Potential profiles of the conduction and the valence bands in the modulation-doped $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ quantum well (left scale), and the wave function of the ground conduction subband (right scale) versus distance along the growth direction.

contribution to the effective mass, F is the BIA parameter (denoted B by Kane[20]), and P_0 is the interband matrix element of momentum. The functions $\tilde{\epsilon}_i(z)$ and $\tilde{f}_i(z)$ depend on z not only via $V(z)$, but also due to the jumps of ϵ_i and Δ_i at the interfaces (cf. Fig. 1). The inspection of the final results shows that the $\hat{B}$ terms in Eq. (1) give a negligible contribution to the spin splitting, so they are omitted in the following.

First, the solutions for the diagonal terms are found. Since $\hat{B}$ is neglected, there is $\Phi_1(z)=\Phi_2(z)=\Phi(z)$. Calculating the average value of the nondiagonal $\hat{K}$ part, taken over $\Phi(z)$, we take into account the offsets in $\tilde{\epsilon}_i(z)$ and $\tilde{f}_i(z)$ energies, which result in the Dirac δ functions at $z=0$ and $z=a$. After some manipulation, the average of $\hat{K}_{SIA}$, caused by the structure inversion asymmetry, is brought to the form

$$\langle\Phi|\hat{K}_{SIA}|\Phi\rangle=\frac{-ik_-\sqrt{2}P_0^2}{3}\left[\left\langle\Phi\left|\frac{-\partial V}{\partial z}D_i\right|\Phi\right\rangle+\Phi^2(0)C_0-\Phi^2(a)C_a\right], \tag{9}$$

where $D_i=1/\tilde{\epsilon}_i^2-1/\tilde{f}_i^2$ and the averaging in the first term excludes the points $z=0$ and $z=a$. Further $C_0=\Delta_{II}/\tilde{\epsilon}_{II0}\tilde{f}_{II0}-\Delta_I/\tilde{\epsilon}_{I0}\tilde{f}_{I0}$ and $C_a=\Delta_{II}/\tilde{\epsilon}_{IIa}\tilde{f}_{IIa}-\Delta_I/\tilde{\epsilon}_{Ia}\tilde{f}_{Ia}$, in which $\tilde{\epsilon}_{I0}=\epsilon_I+V_B-\lambda$, $\tilde{f}_{I0}=\epsilon_I+\Delta_I+V_B-\lambda$, $\tilde{\epsilon}_{II0}=\epsilon_{II}-\lambda$, $\tilde{f}_{II0}=\epsilon_{II}+\Delta_{II}-\lambda$, $\tilde{\epsilon}_{Ia}=\epsilon_I+V(a)+V_B-\lambda$, $\tilde{f}_{Ia}=\epsilon_I+\Delta_I+V(a)+V_B-\lambda$, $\tilde{\epsilon}_{IIa}=\epsilon_{II}+V(a)-\lambda$, $\tilde{f}_{IIa}=\epsilon_{II}+\Delta_{II}+V(a)-\lambda$, and $\Phi(0)$ and $\Phi(a)$ are the values of the envelope function $\Phi(z)$ taken at $z=0$ and $z=a$, respectively. It can be seen that the spin splitting of the conduction band due to SIA mechanism is proportional to the spin-orbit energies in the valence bands.

To make connection with the claims that the SIA spin splitting is proportional to the average electric field, we transform the above expression observing that the electric field in the conduction band is $Eq=-\partial V/\partial z+V_B\delta(z)-V_B\delta(z-a)$, where the first term excludes the points $z=0$ and $z=a$. Since the envelope function $\Phi(z)$ is nonzero mostly in the well (region II), we add and subtract $V_B\Phi^2(0)D_0$ and $V_B\Phi^2(a)D_a$ from the right-hand side of Eq. (9), and obtain

$$\begin{aligned}\langle\Phi|\hat{K}_{SIA}|\Phi\rangle=&\frac{-ik_-\sqrt{2}P_0^2}{3}\left[\left\langle\Phi\left|\frac{-\partial V}{\partial z}D_i\right|\Phi\right\rangle\right.\\&\left.+V_B\Phi^2(0)D_0-V_B\Phi^2(a)D_a\right]\\&+\frac{-ik_-\sqrt{2}P_0^2}{3}[\Phi^2(0)(C_0-V_BD_0)\\&-\Phi^2(a)(C_a-V_BD_a)],\end{aligned} \tag{10}$$

where $D_0=1/\tilde{\epsilon}_{II0}^2-1/\tilde{f}_{II0}^2$ and $D_a=1/\tilde{\epsilon}_{IIa}^2-1/\tilde{f}_{IIa}^2$. The expression in the first square bracket is approximately proportional to the average electric field E (i.e., the field averaged with the square of the wave function including the potential jumps at the interfaces). However, the average field is near zero and, as we show below, this term contributes only few percent to the total SIA spin splitting. Thus, we are left with the dominant second term in Eq. (10), which requires only the knowledge of the band parameters on both sides of the interfaces and of the envelope function at the interfaces.

If one averages over the directions in (k_x,k_y) plane, the mixed term $\langle\Phi|\hat{K}_{SIA}|\Phi\rangle\langle\Phi|\hat{K}_{BIA}|\Phi\rangle$ vanishes, and the total spin splitting is

$$\Delta\epsilon=2(|\langle\Phi|\hat{K}_{SIA}|\Phi\rangle|^2+|\langle\Phi|\hat{K}_{BIA}|\Phi\rangle|^2)^{1/2}, \tag{11}$$

where $\hat{K}_{BIA}$ is given in Eq. (5). One should bear in mind that the two resulting levels do not represent spin-up and spin-down states, but the mixed-spin states (cf. Ref. 14).

To describe the experimental data, as obtained by Das *et al.*[19] on the $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ quantum well, we take the following band parameters. For $In_{0.53}Ga_{0.47}As$: $m^*=0.041m_0$, $\epsilon_g=-0.813$ eV, $\Delta=0.349$ eV, $E_p=24$ eV, $C=-3.175$, $2C'=-0.589$, $g^*=-4.5$, $\gamma=55$ eV Å^3, $F=-24.21$ eV Å^2; for $In_{0.52}Al_{0.48}As$: $m^*=0.0754m_0$, $\epsilon_g=-1.508$ eV, $\Delta=0.336$ eV, $E_p=24$ eV, $C=-2.6859$, $2C'=-0.589$, $g^*=-0.5225$, $\gamma=33$ eV Å^3, $F=-44.41$ eV Å^2. The modulation doped well was 150-Å wide and had the electron density $N_S=1.46\times10^{12}$ cm^{-2}. The conduction-band offset is $V_B=0.5$ eV. The above values of γ are taken by scaling from the known value for GaAs (Ref. 21) according to the respective energy gaps. We first calculate self-consistently $V(z)$ and $\Phi(z)$ without the spin splitting (cf. Fig. 1). The calculated mass at the Fermi energy is $m^*=0.0446m_0$, which agrees with measured value $m^*_{exp}=0.046m_0$. Then the spin splitting is calculated to give $\Delta E_{SIA}=1.37$ meV and $\Delta E_{BIA}=0.74$ meV (cf. Fig. 2 for $B=0$). Thus in the considered system SIA is the dominant mechanism. The first term in Eq. (10) contributes only 3.1% to the complete ΔE_{SIA}, which explicitly disproves the claim that the SIA spin splitting is proportional to the average electric field.

It has been recently possible to influence the spin splitting in III-V heterostructures by an external electric field.[17,18,22] External field affects the splitting neither by changing the average value of the field in the well (the latter must remain

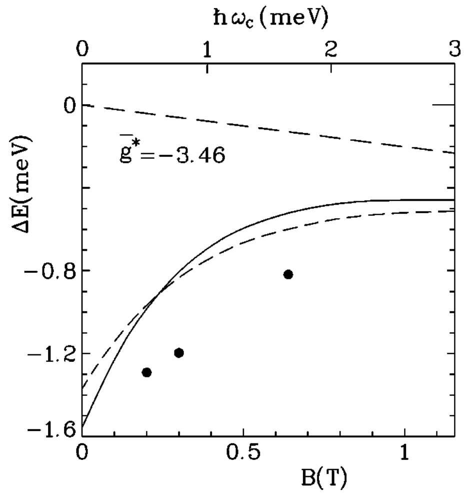

FIG. 2. Spin splitting of the conduction subband energy for the quantum well shown in Fig. 1 versus the magnetic field transverse to the interfaces. Dashed line: the theory for a structure inversion asymmetry alone; full line: the theory for both structure and bulk inversion asymmetries. The straight dashed line indicates the Pauli spin splitting. The full points show experimental values as measured by Das *et al.* (Ref. 19).

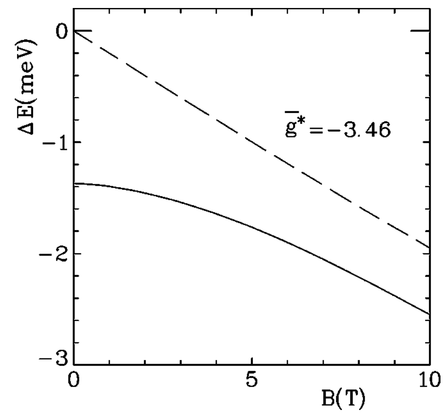

FIG. 3. Spin splitting of the conduction subband energy for the quantum well shown in Fig. 1 versus the magnetic field parallel to the interfaces. The solid line is theoretical for the structure inversion asymmetry. The straight dashed line indicates the Pauli spin splitting.

near zero in a bound state), nor by controlling the spin-orbit interaction (since the applied fields of about 10^2 V/cm are much lower than the atomic fields), but by changing the Fermi wave vector and the asymmetry of the well [cf. Eq. (10)]. The main difficulty in describing such data is an unknown distribution of the field in the structure.

In order to include the effect of an external magnetic field transverse to the interfaces, $\mathbf{B}\|[001]$, we use the three-level $\mathbf{P}\cdot\mathbf{p}$ model,[23] where $\mathbf{P}=\mathbf{p}+(e/c)\mathbf{A}$, in which $\mathbf{A}$ is the vector potential of magnetic field. The initial set is again reduced by substitution to the eigenvalue problem (1), where one should account for the noncommutation of P_i components. The term $\hat{B}$ contains now the Pauli spin splitting $\mu_B Bg^*/2$, where

$$g^*(z)=2+2C'+\frac{2E_P}{3}\left(\frac{1}{\tilde{\epsilon}_i}-\frac{1}{\tilde{f}_i}\right), \qquad (12)$$

is the Landé g^* factor. Here C' represents the far-band contributions. Set (1) is in general not soluble in terms of two harmonic oscillator functions and one has to resort to the method of Evtuhov,[24] expanding the solutions in series of such functions. Our procedure has been restricted to the first terms of this expansion, we deal then with two sets of four coupled differential equations. If BIA is neglected, one can obtain the energies for the SIA mechanism analytically (cf. Refs. 1 and 14). For high Landau numbers n one gets to a good approximation.

$$\Delta(B)\approx\hbar\omega_c-[(\hbar\omega_c-g^*\mu_B B)^2+\Delta_{SIA}^2]^{1/2}, \qquad (13)$$

where $\omega_c=eB/m^*c$ and Δ_{SIA} is the splitting at $B=0$. Thus, for small fields the splitting decreases linearly with B.

The calculated magnetic-field dependence of the spin splitting is shown in Fig. 2. As the magnetic field increases from zero, the splitting quickly drops, going smoothly over to the Pauli splitting with the corresponding g value: $\Delta E=g^*\mu_B B$. The quoted experimental data of Das *et al.*,[19] measured by beatings of Shubnikov–de Haas oscillations at low fields, confirm the characteristic decrease of the spin splitting as the field increases. To our knowledge, these are the only available data in the intermediate fields between the Bychkov-Rashba and the Pauli regimes. Considering that the theory does not contain any adjustable parameters, the agreement with the data should be considered very satisfactory.

Next we consider the spin splitting in a magnetic field $\mathbf{B}\|[100]$, parallel to the interfaces. For the gauge $\mathbf{A}=[0,-Bz,0]$, the wave-vector components k_x and k_y are still good quantum numbers. The resulting eigenvalue problem has the form (1), in which $\hat{B}$ contains the Pauli contribution $\mu_B Bg^*/2$ [cf. Eq. (12)], the terms k_x remain unchanged, while the terms k_y are replaced by $k_y-zeB/\hbar$. This adds a quadratic term in z to the potential $V(z)$. As a result, a magnetic field parallel to interfaces causes small diamagnetic shifts of the electric subbands, but strongly affects their spin splittings (cf. Ref. 23). We calculated the splitting for the dominant mechanism SIA alone, taking $k_x=2.65\times10^6\,\mathrm{cm}^{-1}$ and $k_y=0$, which corresponds to $N_S=1.12\times10^{12}\,\mathrm{cm}^{-2}$. The results are shown in Fig. 3. The splitting reaches the Pauli regime at much higher magnetic fields than those for the transverse case. (The dependence of spin splitting on k_y is more complicated, in particular its values for k_y and $-k_y$ are not the same.)

The above result is in connection with a recent discovery of the metallic phase in two-dimensional systems.[25] A magnetic field of about 2 T parallel to the interface destroys the metallic phase in silicon metal-oxide-semiconductor (MOS) structures.[26] This indicates that the metal-insulator transition is governed by the spin properties of 2D gas. Pudalov[27] suggested that the metallic phase is related to the existence of spin gap. Extrapolating ShdH-type oscillations of the Fermi energy to $B=0$, the spin splitting was estimated to be $\Delta E=0.3$ meV.[28] The spin g factor in Si is known to have almost exactly the free-electron value of $+2$. If the spin splitting at $B=0$ in Si-MOS had the same sign as that shown in Fig. 3, the positive g factor would lead to the closing of the spin gap for increasing field and, according to Ref. 27, to the resulting destruction of the metallic phase. However, there exist two major objections to such an interpretation. First, the value of

$g^* = +2$ indicates that the spin-orbit interaction in Si is very small, so that the spin splitting of 0.3 meV at $B=0$ is certainly overestimated. Second, as follows from Ref. 28, for an increasing magnetic field the measured spin splitting does not go through zero, but increases. Thus, our theory indicates that at $B=0$ the spin splitting in Si-MOS structures should be very close to zero, so that the experimentally observed destruction of the metallic phase by a parallel magnetic field is rather caused by an *appearance* of the Pauli spin gap.

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