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Conduction-subband anisotropic spin splitting in III-V semiconductor heterojunctions

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The electrostatic potential experienced by a conduction electron at a III-V semiconductor heterojunction is a sum of the macroscopic confining and the microscopic bulk potentials. Both of them lack inversion symmetry. Two origins for the spin-orbit spin splitting can be assigned. We point out that, in first order in the in-plane wave vector $k_\parallel$, the $\mathbf{k}_\parallel$-dependent total spin splitting is highly anisotropic. The anisotropy increases as the ratio of the two contributions approaches unit and results from their interference. The relative size of the two spin splitting mechanisms, as a function of the electric field at the interface, is estimated for heterojunctions based on different III-V semiconductor compounds. Observable effects of the anisotropy in the spin splitting are predicted.

Most of the electronic-structure fine details of simple semiconductor heterostructures are well known these days. More recently, there has been an increasing interest in hyperfine details like spin splittings, i.e., the energy difference between states of opposite spins. Preservation of the spin degeneracy, after the spin-orbit interaction is turned on, is only assured when the system has spatial inversion symmetry.[1] A so-called zero-field spin splitting in III-V semiconductor compounds, due to inversion asymmetry in the zinc-blende structure, was predicted long ago[2] and has been observed experimentally.[3]

When the conducting electrons are confined by an asymmetric potential in a III-V semiconductor heterojunction, another contribution to the total spin splitting is introduced. Much effort has been directed to the problem of determining which contribution is the dominant one and when. Recently, Luo *et al.*[4] and Das *et al.*[5] investigated the spin splitting in InAs/GaSb asymmetric quantum wells and in $In_xGa_{1-x}As/In_yAl_{1-y}As$ heterostructures, respectively. In both experiments, the zero-field spin splitting was detected as a beating in the Shubnikov–de Haas oscillations. However, the problem of the origin of the spin splitting is not settled yet. Nevertheless, it is known that the bulk k^3 term dominates in large gap materials while, that from the asymmetric confining potential does in small gap materials.[6]

A demand for a better knowledge of the spin splitting in these heterostructures arises nowadays also connected with measurements of the luminescence polarization, which probe the spin dynamics in these systems.[7] An important spin relaxation mechanism proposed by D'yakonov and Perel[8] is related to the spin precession around the effective field responsible for the spin splitting. Very recently, Dresselhaus *et al.*[9] were able to observe such precession in GaAs inversion layers.

In this work we consider the total spin splitting in the conduction subband of a III-V semiconductor heterojunction. It is pointed out that its leading term, in the expansion in powers of the in-plane wave vector $k_\parallel$, presents a remarkable dependence on the direction of $\mathbf{k}_\parallel$ relative to the crystallographic cubic axis. Such anisotropy depends on the relative size of the two contributions, which we estimate using a 6×6 Kane Hamiltonian and treating the bulk k^3 term perturbationally. The anisotropy is shown to be relatively strong over an experimentally important and large group of structures.

A simple and convenient way to describe the zero-field spin splitting is by defining an effective magnetic field so that the spin Hamiltonian is written as

$$H=\tfrac{1}{2}\hbar\sigma\cdot\mathbf{B}_{\rm eff}(\mathbf{k}_\parallel)\,, \tag{1}$$

where σ is the Pauli matrices vector. The magnitude and direction of $\mathbf{B}_{\rm eff}$ will depend on the magnitude and direction of $\mathbf{k}_\parallel$. The effective field will also depend on the subband indice, but we will restrict ourselves to the first subband. The $\mathbf{k}_\parallel$-dependent spin splitting is then simply given by

$$\Delta(\mathbf{k}_\parallel)=\hbar|\mathbf{B}_{\rm eff}|\,. \tag{2}$$

As pointed out by Bychkov and Rashba,[10] the asymmetry in the macroscopic confining potential leads, in first order, to a term $H=\alpha_{\rm so}(\sigma\times\mathbf{k})\cdot\hat{\mathbf{z}}$ in the Hamiltonian, which corresponds to the following effective field:

$$\mathbf{B}_{\rm so}=(2/\hbar)\alpha_{\rm so}\mathbf{k}\times\hat{\mathbf{z}}\,, \tag{3}$$

where $\hat{\mathbf{z}}$ is the unit vector along the growth direction and $\alpha_{\rm so}$ is a structure-dependent parameter known as the spin-orbit coupling constant. Such effective field produces a spin splitting $\Delta_{\rm so}=2\alpha_{\rm so}k_\parallel$, which is isotropic and linear with $k_\parallel$.

The splitting due exclusively to the inversion asymmetry in the zinc-blende structure is well known to be given in the bulk, for small values of $\mathbf{k}$, by an effective field whose x component reads

$$\mathbf{B}_{\rm bulk}\cdot\hat{\mathbf{x}}=(2\gamma/\hbar)k_x(k_y^2-k_z^2)\,, \tag{4}$$

and the other components are obtained by cyclic permutation of the indices.[11] The constant γ is a material-dependent parameter. It should be emphasized that the components are relative to the crystallographic cubic axis, i.e., x, y, and z correspond here to the [100], [010], and [001] directions, respectively. We consider heterojunctions grown in the [001] direction.

This k^3 splitting is in general much smaller than the quantized energies of the confined electrons and its effects,

in the case of a heterojunction, can be treated within first-order perturbation theory.[12] In this case, we replace k_z and k_z^2 by the expected values of $-id/dz$ and $-d^2/dz^2$ in the first unperturbed conduction subband, respectively. The first one is zero and the second we call q^2. Assuming $k_\parallel^2 \ll q^2$ we further simplify and use

$$\mathbf{B}_{\text{bulk}} = (2\gamma/\hbar) q^2 (-k_x \hat{\mathbf{x}} + k_y \hat{\mathbf{y}}) . \tag{5}$$

The resulting splitting we call Δ_{bulk}. As one can see, it turns out to be linear with $k_\parallel$ and isotropic as well.

When Δ_{bulk} and Δ_{so} are of the same order, one must look at the total spin splitting, which is not equal to $\Delta_{\text{bulk}} + \Delta_{\text{so}}$ but is given by $\hbar |\mathbf{B}_{\text{so}} + \mathbf{B}_{\text{bulk}}|$. The latter can be written as

$$\Delta_{\text{tot}} = [\Delta_{\text{so}}^2 + \Delta_{\text{bulk}}^2 - 2\Delta_{\text{so}}\Delta_{\text{bulk}} \sin(2\theta)]^{1/2} , \tag{6}$$

where θ is the angle between $\mathbf{k}_\parallel$ and [100].[13] The surprising result is that the total spin splitting, in first order in $k_\parallel$, depends on $\mathbf{k}_\parallel$'s direction. As shown in Fig. 1, Δ_{tot} can be much bigger for electrons moving in one direction than in another. The degree of anisotropy depends only on the ratio $\Delta_{\text{so}}/\Delta_{\text{bulk}}$ and is independent of $k_\parallel$. It is also found that whenever one contribution, Δ_{so} or Δ_{bulk}, is much bigger than the other (100 times or more), the splitting turns isotropic. The anisotropy is maximum when $\Delta_{\text{so}}/\Delta_{\text{bulk}} = 1$ and can be seen to be a result of the interference between the two mechanisms. As $\mathbf{k}_\parallel$ goes around a circle, the two effective fields, $\mathbf{B}_{\text{so}}$ and $\mathbf{B}_{\text{bulk}}$, move with opposite angular velocities. The largest spin splitting corresponds to the situation when they are parallel and the smallest when they are antiparallel, leading to a spectrum with twofold symmetry (Fig. 1).

Eppenga and Schuurmans[12] obtained for symmetric III-V quantum wells a fourfold-symmetric spin splitting. In their case the symmetry of mirror reflection at the center of the well preserves the cubic symmetry of the crystal. In our case the lack of mirror plane in the growth direction reduces the symmetry by a factor of 2. By looking at the zinc-blende structure along the [001] direction, one can see that the system's rotation symmetry around it is, in fact, twofold. We want to stress, however, that the anisotropy in the total spin splitting obtained here occurs in lower order in $k_\parallel$ than that of Ref. 11, which is in pure Δ_{bulk}.

The important question at this point is whether $\Delta_{\text{so}}/\Delta_{\text{bulk}}$ ever gets close to one in real systems. If it does, one should look for the effects of such anisotropy. Lommer, Malcher, and Rössler[6] performed complete calculations of Δ_{tot} including both contributions from the beginning. Their method however does not give $\Delta_{\text{so}}/\Delta_{\text{bulk}}$ explicitly. We use here a general model to estimate $\Delta_{\text{so}}/\Delta_{\text{bulk}}$ as a function of the electric field at the interface of a heterojunction.

The model consists in an electron in a III-V semiconductor compound under a triangular confining potential formed by the sum of a constant electric field ϵ along the growth direction and an infinite barrier at the interface.

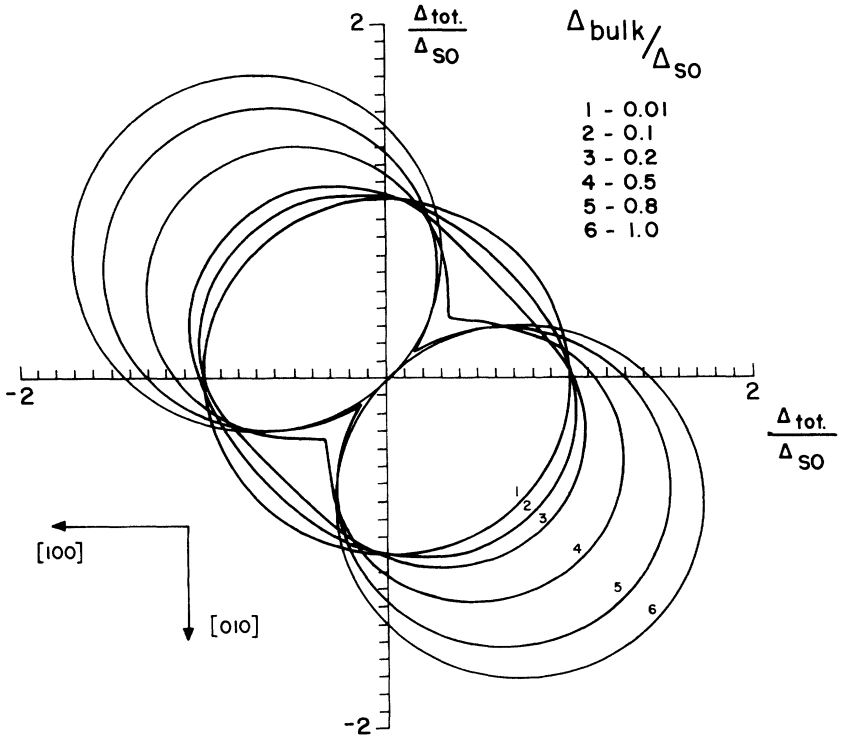

FIG. 1. Spin splitting of the first conduction subband as a function of $\mathbf{k}_\parallel$'s direction for varying $\Delta_{\text{so}}/\Delta_{\text{bulk}}$. The splitting, for each direction, is given by the distance from the origin to the curve. The spin splitting is almost isotropic for $\Delta_{\text{so}}/\Delta_{\text{bulk}} = 100$ and its anisotropy is maximum when the same ratio is equal to 1. In this case, the splitting is zero for $\mathbf{k}_\parallel \| [110]$. Note that time-reversal symmetry is satisfied, i.e., $\Delta_{\text{tot}}(\mathbf{k}_\parallel) = \Delta_{\text{tot}}(-\mathbf{k}_\parallel)$.

We work within the multiband effective-mass approximation and describe the compound by a 6×6 $\mathbf{k}\cdot\mathbf{p}$ Kane Hamiltonian including the conduction Γ_6 and the valence Γ_8 bands *only*.[14] The model is particularly transparent in the spin splitting calculation, besides being quite accurate for low-lying conducting levels. With a decoupling similar to that in Ref. 15, we find, in a good approximation for the first conducting subband and a not too high electric field ($\epsilon < 10^7$ V/m for GaAs, for example),

$$\Delta_{so} = \hbar^2 e\epsilon k_{\parallel}/2m^* E_g , \tag{7}$$

where e is the electron's charge, m^* is the effective mass at the bottom of the conduction band, and E_g is the width of the gap.[16] The spin-orbit coupling constant, in this model, is then found to be given by $\alpha_{so} = \hbar^2 e\epsilon/4m^* E_g$. Equation (7) represents a simple limit of the more complicated expressions obtained before by Ohkawa and Uemura[17] and by Lassnig.[18]

We next calculate q^2 variationally using Fang-Howard trial functions and obtain

$$\frac{\Delta_{so}}{\Delta_{bulk}} = 0.61 \left(\frac{\hbar^2}{2m^*} \right)^{5/3} \frac{(e\epsilon)^{1/3}}{\gamma E_g} . \tag{8}$$

In Fig. 2 we plot $\Delta_{so}/\Delta_{bulk}$ as a function of ϵ for heterojunctions based on different III-V semiconductor compounds. Effective masses and gap energies used are the low-temperature figures in the Landolt-Börnstein tables and the values of γ we use are the theoretical values quoted in Ref. 3. The first and most important thing to note is that, for all these different compound-based heterojunctions, the ratio never deviates much from unit, which indicates an anisotropic spin splitting in this range of the interface electric field. To have a feeling of the magnitude of the field, note that a superficial carrier concentration $n_s = 10^{12}$ cm^{-2} corresponds to an electric field $\epsilon = en_s/k_{sc}$ of the order of 10^7 V/m. We also see that, for small gap materials, Δ_{so} dominates, according to what is observed experimentally.[4,19] In this range of field, Δ_{so} is always important even for large gap materials like GaAs and InP. Finally, it is interesting to note that even though GaSb has a relatively small gap, its Δ_{so} contribution is the smallest one, which is due to a large γ.

Now, if the anisotropy is there, how can one detect it? In principle, it could be done by measuring the polarization of *laterally* photoemitted electrons. One could either excite electrons with linearly polarized light and detect spontaneous spin polarization of the photoelectrons[20] or use circularly polarized light and measure the precession of the spin polarization.[21] Different results for electrons emitted along the [110] and [1$\bar{1}$0] directions would be a signature of the anisotropy in the spin splitting of the confined electrons since the bulk background should be the same in both directions.

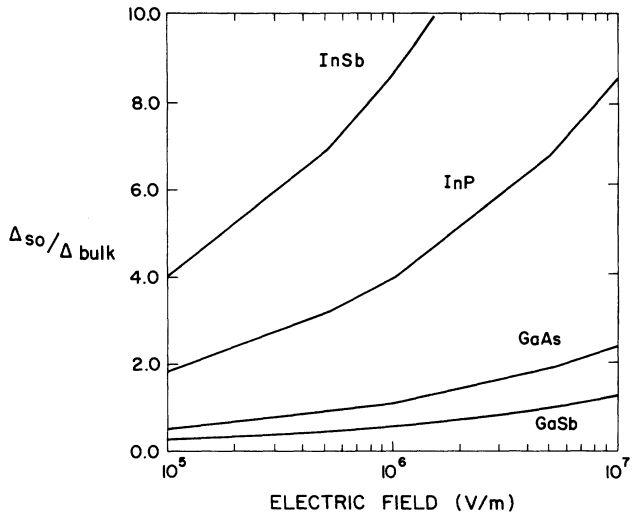

FIG. 2. Relative size $\Delta_{so}/\Delta_{bulk}$ for the first conduction subband of a III-V semiconductor heterojunction, as a function of the electric field at the interface and for different III-V semiconductor compounds, as given by the constant electric field and infinite barrier model for a heterojunction.

In spite of the approximations made, we believe that we have given here enough ground to conclude that there exists a dominant anisotropy in the spin splitting of the conduction subband of most III-V semiconductor heterojunctions of interest, which can be observed experimentally. The relative contribution of the two zero-field spin splitting mechanisms was estimated as a function of the interface electric field, for different III-V semiconductor-based heterojunctions. It was found that the contribution from the asymmetry in the confining potential is in most of the cases the dominant one. And finally, as spin-off, we obtained simple analytical expressions for both Δ_{so} and Δ_{bulk} in the infinite barrier and constant electric field model for a heterojunction.

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