Rashba and Dresselhaus spin-orbit interaction strength in GaAs/GaAlAs heterojunctions

M. A. Toloza Sandoval¹, A. Ferreira da Silva¹, E. A. de Andrada e Silva² and G. C. La Rocca³
¹ Instituto de Física, Universidade Federal da Bahia 40210-340, Salvador, Bahia, Brazil
² Instituto Nacional de Pesquisas Espaciais, C.P. 515, 12201-970 São José dos Campos, São Paulo, Brazil
³ Scuola Normale Superiore and CNISM, Piazza dei Cavalieri 7, I-56126 Pisa, Italy

Abstract

Using a recently developed variational theory for the spin split subbands, we investigate the relative strength of the Rashba and Dresselhaus spin orbit terms in GaAs/GaAlAs heterojunctions. The envelope function formalism is employed using the 8-band $k \cdot p$ Kane model for the bulk, and the Rashba split subbands are obtained with spin-dependent trial functions. The total spin splitting is then calculated analytically by including also the bulk Dresselhaus contribution via quasi-degenerate first order perturbation theory. The total spin-orbit splitting at the Fermi energy of the two dimensional electron gas (2DEG) is calculated as a function of the direction of the Fermi wave-vector. The obtained total spin-orbit splittings along [11] and [1¯1] in-plane directions are shown to be in good agreement with recent experiments. The well known ratio $\alpha/\beta$ between the Rashba and Dresselhaus contributions is a fundamental parameter in different proposals for new semiconductor spintronic devices. Due to barrier penetration and the corresponding spin dependent boundary conditions, the total spin-orbit anisotropy calculated here is shown to be in general determined by more then one parameter, and thus the above ratio should not be estimated using the common $\alpha$ and $\beta = \langle \gamma k_z^2 \rangle$ expressions.

© 2012 Published by Elsevier B.V. Selection and/or peer-review under responsibility of Universidade Federal de Juiz de Fora, Brazil. Open access under CC BY-NC-ND license.
Keywords: semiconductor spintronics, two-dimensional electron gas, spin-orbit interaction, III-V heterojunctions, experiment-theory comparison

1. Introduction

Different electronic devices have been developed thanks to the detailed knowledge of the electronic structure of semiconductor nanostructures. For new spintronics devices, in particular, the anisotropy of the spin-orbit interaction is attracting a lot of interest. As first discussed in ref. [1], there is a special anisotropy in the spin-orbit splitting of two-dimensional electron gases (2DEGs) formed at III-V semiconductor heterojunctions, which is due to the interplay between the two main contributions, namely Rashba and Dresselhaus. Instead of the four-fold rotational symmetry of the splitting in symmetric quantum wells (pure Dresselhaus) [2], the splitting in heterojunction triangular wells present a reduced two-fold rotational symmetry with respect to the direction of the electron wave-vector in the plane $k_0$, as first observed by Jusserand et al. [3] with Raman spectroscopy.

It is a special anisotropy because it can be tuned with the gate voltage. In particular, there is the possibility to make the splitting very small or negligible for electrons moving along a given direction, with drastic consequences
for the spin relaxation and coherence times. In the linear (in $k_f$) and infinite barrier approximation, this corresponds to Rashba and Dresselhaus interaction terms with the same strength. The anisotropy in this case is determined by a single parameter $\alpha/\beta$, given by the ratio between the two contributions; $\alpha$ being the Rashba coupling parameter and $\beta = \gamma < k_z^2 >$, $\gamma$ being the bulk Dresselhaus or $k^3$ parameter and $< k_z^2 >$ the average momentum squared along the growth direction. However, as we show here, it is in general not possible to separate the two contributions, and such ratio becomes ill defined. Indeed different and recent attempts to measure $\alpha/\beta$ find very poor agreement with the theory [4]. Good agreement with recent experiments is obtained here using the total spin-orbit splittings along [11] and [11] in-plane directions, from which effective $\alpha^*$ and $\beta^*$ can be deduced. For this purpose, a variational solution of the effective Hamiltonian for the envelope function is used and the Dresselhaus spin-orbit term included via first-order quasi-degenerate perturbation theory [2]. The total spin-orbit splitting at the Fermi level is calculated as a function of the 2DEG carrier concentration and Fermi wave-vector direction, and its anisotropy studied with different approximations. We compare our results with recent experimental data for the total splitting along different directions in GaAs/AlGaAs heterojunctions obtained with spin-dependent photo current (SPC) [5] and electron spin resonance (ESR) [5] techniques.

2. Model

Our calculation is based on a recently proposed spin resolved variational solution for the Rashba split electronic subbands in III-V heterojunctions [6, 7]. In the envelope function approximation, the Rashba split subbands correspond to the eigen-states of

$$H_R|\Psi_{\uparrow\downarrow}\rangle = e^{R}_{\uparrow\downarrow}(k_f)|\Psi_{\uparrow\downarrow}\rangle,$$

(1)

where $H_R$ is the effective Hamiltonian (derived from the 8x8 Kane model) which includes barrier penetration effects, renormalized parameters and band nonparabolicity [6, 7]. We take these spin resolved envelope functions $\Psi_{\uparrow\downarrow}$, for polarized electrons in the first conduction subband, as our pair of quasi-degenerate unperturbed states. They are obtained variationally with the following trial functions:

$$\Psi_{\uparrow\downarrow}(z) = \begin{cases} A_{\uparrow\downarrow} e^{k_zz/2}, & z \leq 0 \\ B_{\uparrow\downarrow}(z + c_{\uparrow\downarrow}) e^{-k_zz/2}, & z \geq 0 \end{cases}$$

(2)

where $k_b = 2\sqrt{2m\hbar^2}/(\bar{m}$ being the renormalized effective mass in the barrier and $v_0$ the conduction band-offset) and $b$ is the variational parameter determined by minimizing the 2DEG total energy. The details of the calculations of $A_{\uparrow\downarrow}, B_{\uparrow\downarrow}, c_{\uparrow\downarrow}$ and $e^{R}_{\uparrow\downarrow}(k_f)$ are presented in Ref.[7]. With the resulting spin splitting $\Delta_R$, the Rashba parameter $\alpha$ is then determined from:

$$\Delta_R(k_f) = |e^{R}_{\uparrow\downarrow}(k_f) - e^{R}_{\downarrow\uparrow}(k_f)| = 2\alpha k_f.$$  

(3)

The Dresselhaus spin-orbit term,

$$H_D = \gamma (\sigma_x k_x (k_y^2 - k_z^2) + \sigma_y k_y (k_z^2 - k_x^2) + \sigma_z k_z (k_x^2 - k_y^2))$$

(4)

is then included via quasi-degenerate first order perturbation theory. The matrix elements $\langle \Psi_{\uparrow\downarrow}|H_D|\Psi_{\uparrow\downarrow}\rangle$ can be easily calculated (recall though that $\gamma$ is then allowed to vary along $z$ and it is then necessary to symmetrize the corresponding integrals [2]). The obtained splitting, after diagonalization, is given by:

$$\Delta_s(k_f, \theta) = \sqrt{|\Delta_R(k_f) - ((\langle \gamma(z)k_z^2 \rangle)_{\uparrow\downarrow} + (\langle \gamma(z)k_z^2 \rangle)_{\downarrow\uparrow})k_f \sin 2\theta + 1/2 ((\langle \gamma(z) \rangle)_{\uparrow\downarrow} + (\langle \gamma(z) \rangle)_{\downarrow\uparrow})k_f \sin 2\theta |^2 + 4(\langle \gamma(z)k_z^2 \rangle)_{\uparrow\downarrow}k^2_f \cos 2\theta}$$

(5)

where $\langle \gamma(z) \rangle_{\uparrow\downarrow} = \langle \Psi_{\uparrow}\gamma(z)\Psi_{\downarrow}\rangle$, $\langle \gamma(z)k_z^2 \rangle_{\uparrow\downarrow} = \langle \Psi_{\uparrow}|(-id/dz)\gamma(z)(-id/dz)|\Psi_{\downarrow}\rangle$ and so on. It is clear that the anisotropy in such splitting can not be determined with a single parameter. It is easy to show that in the limit of infinite barrier the above splitting reduces to $\Delta_s = 2k_f \sqrt{\alpha^2 + \beta^2 - 2\alpha\beta \sin 2\theta}$ (in the linear approximation), with the anisotropy determined by $\alpha/\beta$. Note that in this limit, $\langle \gamma(z)k_z^2 \rangle_{\uparrow\downarrow} = \langle \gamma(z)k_z^2 \rangle_{\downarrow\uparrow} = \langle \gamma(z)k_z^2 \rangle_{\uparrow\downarrow} = \beta$. However, with barrier penetration these matrix elements present small differences and even with an averaged $\beta$ it is clear that $\alpha/\beta$ does not give in general a good measure of the anisotropy, which must then be studied with the direct ratio between the total splitting along different directions.
Figure 1: (color online). Total spin-splitting (divided by $k_F$) calculated at the Fermi level of a $n_s = 1.1 \times 10^{11} \text{ cm}^{-2}$ GaAs/AlGaAs 2DEG. Angle zero corresponds to the [10] in plane direction. The cases $v_0 = 269 \text{ meV}$ (red line) and $v_0 = 318 \text{ meV}$ (blue line) show the dependence with the band-offset. The linear Dresselhaus approximation (dotted line), the perfect insulating barrier case (dash line) and the ESR data of ref. [5] are also shown. We used the value 23.6 $\text{ eV} \cdot \text{Å}^3$ for the Dresselhaus spin-orbit coupling parameter in the GaAs [8], and the value 19.7 $\text{ eV} \cdot \text{Å}^3$ obtained from a simple linear interpolation for such parameter in the AlGaAs.

Table 1: Comparison with experiment. Note that $\alpha^*/\beta^*$ stands for the ratio between the effective coupling parameters, derived from the total splitting along [11] and [1¯1] in-plane directions, as given by Eq.(6).

| Heterostructure | Ref. | Techn. | $n_s$ ($10^{11} \text{ cm}^{-2}$) | $\alpha^*/\beta^*$ | Theory $\alpha^*/\beta^*$ | $\alpha/\beta$ |
|-----------------|------|--------|-------------------------------|-------------------|-------------------------|-------------|
| $Al_{0.3}Ga_{0.7}As/GaAs$ | [5]  | ESR    | 1.1                          | ~1                | 1.3                     | 0.49        |
|                 | [4]  | SPC    | 1.1                          | 7.6               | 1.3                     | 0.49        |
|                 | [4]  | SPC    | 1.3                          | 2.8               | 1.2                     | 0.52        |
|                 | [4]  | SPC    | 1.8                          | 1.5               | 1.1                     | 0.59        |

3. Results

The system here considered is a GaAs/AlGaAs heterojunction with varying $n_s$. In Figure 1, we plot the total spin splitting calculated at the Fermi level as a function of wave-vector direction for $n_s = 1.1 \times 10^{11} \text{ cm}^{-2}$. Results obtained within different approximations are compared together with the ESR experimental data of Frolov et al. [5], for the splitting along [11] and [1¯1] directions. The best agreement is obtained with the complete model, i.e. including the finite band offset and the Dresselhaus cubic terms; indicating the importance of both barrier penetration and higher order terms in these structures. In particular, the cubic Dresselhaus terms are seen to be responsible for a strong reduction in the splitting along the [1¯1] direction (45 degrees in the figure). A small sensitivity of the splitting with respect to the most used values for the band-offset is also observed.

In order to best test the present results with the available data, it is convenient to define $\alpha^*/\beta^*$, determined from the calculated (and/or measured) total splitting $\Delta_s$ along the perpendicular [11] and [1¯1] in-plane directions. In the linear approximation, they correspond to the directions with minimum and maximum splitting respectively, and one has:

$$\frac{\alpha^* - \beta^*}{\alpha^* + \beta^*} = \frac{\Delta_s^{[11]}}{\Delta_s^{[1\bar{1}]}},$$

In Table I, we compare both $\alpha^*/\beta^*$ and $\alpha/\beta$ with different experimental data. As indicated, the experimental data correspond to $\alpha^*/\beta^*$ and indeed are seen to agree well with the calculated values including the $n_s$ dependence. Instead, the usual $\alpha/\beta$ parameter presents the opposite behavior and is numerically much less close to the data. We note large
uncertainties in the experimental data, as in the $n_s = 1.1$ case where the different data differ by a large amount. In particular the large 7.6 result for $\alpha^*/\beta^*$ corresponds to a sample with larger potential fluctuations, and in view of the deviations with respect to samples with larger densities might be affected by other effects. We can then conclude that in GaAs/GaAlAs 2DEG systems the anisotropy of the spin-orbit interaction should be studied by looking at the total splitting, rather than at the standard $\alpha/\beta$ parameter.

4. Conclusions

In summary, we have seen that the present variational theory for the Rashba effect, with the Dresselhaus corrections included perturbatively, is able to give a fair description of the spin-orbit anisotropy in GaAs 2DEGs. The correct way to interpret the corresponding measurements has also been discussed, and the use of the standard $\alpha/\beta$ parameter criticized. Good agreement with the experiment indicate that the model may be useful for spintronic applications. Further tests with other III-V semiconductor structures are however needed to fully assess the limits of the present model calculation.

5. Acknowledgments

The authors thank the Brazilian agencies CNPq, CAPES and FAPESB for financial support.

6. References

[1] E. A. de Andrada e Silva, Phys. Rev. B 46, 1921(R) (1992).
[2] R. Eppenga and M.F.H. Schuurmans, Phys. Rev. B 37, 10923(R) (1988).
[3] B. Jusserand, D. Richards, G. Allan, C. Priester and B. Etienne, Phys. Rev. B 51, 4707(R) (1995).
[4] S. Giglberger et al., Phys. Rev. B 75, 035327 (2007).
[5] S.M. Frolov, S. Lüscher, W. Yu, Y. Ren, J.A. Folk, and W. Wegscheider, Nature 458, 868 (2009).
[6] M.A.T. Sandoval, A. Ferreira da Silva, E. A. de Andrada e Silva and G. C. La Rocca, Phys. Rev. B 79, 241305(R) (2009).
[7] M.A.T. Sandoval, A. Ferreira da Silva, E. A. de Andrada e Silva and G. C. La Rocca, Phys. Rev. B 83, 235315 (2011).
[8] J.-M. Jancu, R. Scholz, E. A. de Andrada e Silva and G. C. La Rocca, Phys. Rev. B 72, 193201 (2005).