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# Spin-split Conduction Subbands of III-V Semiconductor Heterojunctions

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**Abstract.** The spin-orbit splitting or Rashba  $\alpha$  parameter at the Fermi energy of 2DEGs in InAlAs/InGaAs heterojunctions is calculated as a function of the electron density, with a variational solution to the multi-band envelope-function model, based on the 8-band Kane model for the bulk. Spin-dependent boundary conditions and mean-field approximation for the electron-electron interaction are used and reasonable good quantitative agreement is obtained with recent Shubnikov-de Haas experimental data.

**Keywords:** Rashba 2DEG, heterojunctions, spin-orbit.

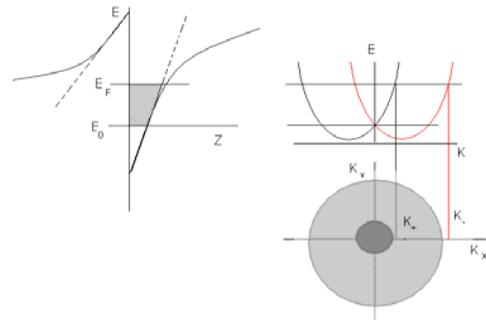
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## INTRODUCTION

The desired control, as in the Datta and Das spin transistor [1], of the spin-orbit splitting (or effective magnetic-field) for 2DEGs in III-V semiconductor heterojunctions, has not been achieved yet. A quantitative agreement between theory and experiment is far from complete. Experimentally, most of the observations have been done with the Shubnikov-de Haas oscillations, and the results are strongly sample dependent and do not always compare well with other techniques [2]. Theoretically, most of the calculations are based on multi-band envelope-function models, but despite reasonably good agreement with different experiments, are not free from concerns like numerical error control, spurious solutions, operator ordering and correct boundary conditions or the use of too many parameters.

Semiconductor heterojunctions form a special class of Rashba split 2DEGs. The electrons are confined by a triangular potential and the strength of the Rashba coupling, together with the carrier density  $n_s$ , can be varied with the gate voltage. In particular, InAs and InGaAs heterojunctions have been much studied. We here consider such heterojunctions, with only the first subband occupied as illustrated in Fig. 1, and calculate the spin-splitting or Rashba  $\alpha$  parameter at the Fermi energy, as a function of the electron density in

particular in a InAlAs/InGaAs heterojunction, using a variational solution to the multi-band envelope-function effective Hamiltonian free from the above mentioned concerns.



**FIGURE 1.** Scheme of the heterojunction and its constant electric field model, with the first subband occupied up to the Fermi energy; and, on the right, the scheme of the Rashba spin-orbit split, with the two Fermi wave vectors  $k_{\pm}$ .

## MODEL AND RESULTS

With the proper choice of the spin quantization and parallel  $k$  directions and some simple algebra, the 8x8 Kane model effective Schrodinger equation for the envelope-functions can be reduced to two independent equations, for each spin quantized along the direction

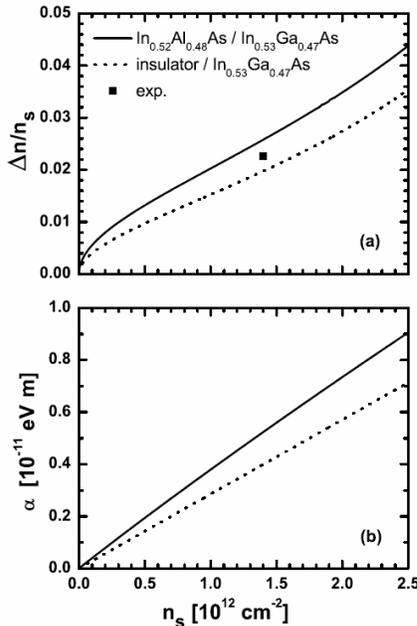
perpendicular to both growth and parallel  $k$  directions [2]. Eliminating the other components, one obtains the following effective Hamiltonian for the conduction band envelope-function:

$$H_{eff.} = -\frac{\hbar}{2} \frac{\partial}{\partial z} \frac{1}{m(E,z)} \frac{\partial}{\partial z} + \frac{\hbar^2 k^2}{2m(E,z)} \pm \alpha(E,z)k + V(z), \quad (1)$$

with simple expressions for the energy dependent effective mass, for the Rashba coupling parameter and for the spin dependent boundary conditions at the interface [3]. Following Ref. [4], we now use different small parameters on both sides of the interface, in order to expand the energy dependent parameters in a power series around the InGaAs conduction band edge, and keep only the leading order terms, what results in energy independent renormalized parameters or non-parabolic corrections, which in turn allow now a variational treatment to the Rashba splitting. For that, we introduce spin-dependent modified Fang-Howard wave-functions, which satisfy the spin-dependent boundary conditions at the interface ( $z=0$ ) and read:

$$\Psi_{\pm}(z) = \begin{cases} A_{\pm} e^{k_b z/2}, & z < 0 \\ B_{\pm} (z + c_{\pm}) e^{-bz/2}, & z > 0 \end{cases} \quad (2)$$

where  $k_b$  is the decaying coefficient given by the effective mass and band-offset in the barrier, and  $b$  is the variational parameter.



**FIGURE 2.** (a) The difference in occupation of the spin-orbit split subbands in an InGaAs/InAlAs heterojunction (solid line) and insulator/InGaAs (dash line). (b) The  $\alpha$  parameter for both case. This is the paragraph spacing that occurs when you use the Enter key.

For every carrier concentration  $n_s$ , we determine the value of  $b$  which minimizes the total energy including e-e interaction in the Hartree approximation. With the obtained dispersion relation then we calculate the frequency of the magneto oscillations semi-classically by the  $k$ -space areas illustrated in Fig.1. The obtained results are shown in Fig. 2, where we plot both the occupation difference in the split subbands and the Rashba parameter at the Fermi energy as a function of  $n_s$ . The band parameters used were  $m^* = 0.041m_e$ ,  $E_g = 0.813$  eV,  $\Delta = 0.326$  eV, and  $\epsilon_{sc} = 13.1\epsilon_0$  for InGaAs; and  $E_g = 1.513$  eV, and  $\Delta = 0.309$  eV for InAlAs barrier. For the conduction band offset we have used 0.5 eV. A constant electric field is assumed and differences in the dielectric constants are neglected. A recent data from Ref.[6] is also included in Fig. 2, showing quantitative good agreement with the present model. The infinite barrier approximation is also shown for comparison.

## CONCLUSIONS

The 8-band Kane model based envelope-function approximation for the Rashba split subbands in III-V semiconductor heterojunctions has been applied here to the 2DEG in a InAlAs/InGaAs heterojunction. With a variational solution, we have calculated the Rashba  $\alpha$  parameter as a function of electron density. The effect of the barrier penetration, including the spin dependent boundary conditions at the interface, is seen to be an enhancement in the Rashba  $\alpha$  parameter of the order of 25%. The model provides simple and accurate analytical results for the spin resolved electron subbands, in good quantitative agreement with the recent experiment in Ref. [6], and should contribute to the semiconductor spintronic development.

## ACKNOWLEDGMENTS

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