Transport features of electron and hole quantum wires with Rashba coupling

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Agraïments

Primer de tot, voldria agrair al meu director de tesi, el Dr. Llorenç Serra Crespi, la seva tasca d’orientació durant el doctorat així com totes les hores que m’ha dedicat per tal que els seus coneixements fossin també meus. Gràcies Llorenç per ser un sac de paciència davant la meva ignorància! No menys atenció es mereixen na Rosa i en David per totes les hores que hem passat junts i per la seva dedicació incondicional. Tampoc em vull oblidar de na Francesca Garcíass, qui indirectament m’ha proporcionat la via l’oportunitat d’obtenir el treball aquí present. Manifestar també agraïment als altres ajudants de professor amb els quals he compartit hores de laboratori i tortuoses correccions i revisions de pràctiques i a tots els doctorants del departament de Física (hem passat tantes hores junts que ja són pràcticament de la família) i, en general, manifestar la gratitud a tot el departament de Física. Per acabar, voldria agrair també el suport d’en Javi i dels meus pares i germans per la seva paciència durant aquests quatre anys.
Abstract

This thesis studies the effects of the Rashba spin-orbit coupling on the transport properties of electron and hole quantum wires. For each case, a specific physical system is considered: the first one is a quantum wire with inhomogeneous Rashba coupling while the second is a quantum wire with homogeneous Rashba intensity and with external magnetic field; they are studied in the first (electrons) and the second (holes) parts of this work, respectively. Both systems are examples of the effects of the Rashba spin-orbit coupling on the physics of transport.

In Part I, for electron systems, we study the conductance and polarization of the outgoing current for an incident unpolarized electron beam. The electron conductance of a quantum wire has a staircase dependence with energy, where each step is a conductance plateau. With the Rashba inhomogeneity a Fano dip appears at the end of each plateau, at specific energies, and we observe how the outgoing current is spin polarized. This current polarization occurs only above the first plateau, since it is due to the interference of two propagating modes with opposite spin. We also study how two conductance dips, in the first plateau, interfere when we have two tunable Rashba regions. We show how this interference evolves from crossing to anticrossing behavior when the distance between the two regions increases. Transport through evanescent states is responsible for this behavior, as we will see.

Continuing Part I, we study the generalization of the Datta-Das transistor for a quasi-one-dimensional system —the original device corresponds to a purely one-dimensional system with a Rashba region attached to polarized leads and its main feature is an oscillatory behavior of the conductance with Rashba strength. In our system we observe how that sinusoidal behavior is strongly affected by the multichannel transport, i.e., transport in a quasi one-dimensional system having a transverse confinement. As a consequence, increasing the number of propagating channels the effect of spin precession is destroyed. Finishing this first part, the limit from quasi one-dimensional to two-dimensional system is considered, when the quantum wire becomes a two-dimensional electron gas with a Rashba stripe.

In the hole-system study, Part II, we present calculations of the g factors for the lower conductance steps of three dimensional quantum wires. We define the g factors from the anomalous half-steps appearing in the conductance in the presence of magnetic field. Our results prove that the anisotropy of g factors for different magnetic field orientations originates in the Rashba spin-orbit coupling. We also analyze the relevance of the deformation, as the wire evolves from 3D towards a flat 2D geometry. For high enough wire deformations, the perpendicular g factors are greatly quenched by the Rashba interaction. On
the contrary, parallel g factors are rather insensitive to the Rashba interaction, resulting in a high g factor anisotropy. Finally, we study the purely one-dimensional hole system.
Resum

En aquesta tesi s’estudien els efectes de l’acoblament d’espí-òrbita sobre les propietats de transport de fils quàntics d’electrons i forats. Per a cada cas s’ha considerat un sistema físic diferent: per als primers (electrons) és un fil quàntic amb una zona inhomogènia d’acoblament de Rashba mentre que en els segons (forats) l’interacció de Rashba és homogènia a l’espai on, a més, s'ha aplicat un camp magnètic uniforme extern. Així la tesi està separada clarament en dues parts, la primera pel cas del transport electrònic i la segona pel transport fet per forats. Els dos sistemes són exemples del efectes que fa l’acoblament d’espí-òrbita de Rashba sobre el transport.

A la Part I, per al sistema d’electrons, estudiam la conductància i la polarització del corrent resultant quan el feix incident d’electrons és no polaritzat. La conductància per un fil quàntic té una dependència escalonada amb l’energia, on cada graó és un plateau de conductància. Amb la inhomogeneïtat de Rashba, apareix un mínim de Fano al final de cada plateau a energies específiques i, a més, el corrent de sortida està polaritzat en espí. Aquest corrent polaritzat només el trobem a partir d’energies del segon plateau, ja que és la conseqüència de la interferència de dos modes propagants amb espins oposats. També estudiam, en aquesta part, com interfereixen aquests dos mínims de conductància quan tenim dues zones seguides d’interacció de Rashba. Observam com els dos deeps passen d’un comportament de creuament a anticreuament quan la distància entre les dues regions augmenta. Els responsables d’aquest comportament no són més que els estats evanescents.

Continuant en aquesta Part I, estudiam la generalització del transistor de Datta i Das per a un sistema quasi-unidimensional –el dispositiu original correspon a un sistema purament 1D amb una regió de Rashba acoblada a uns contactes polaritzats, on la seva principal característica és la del comportament oscil·latori de la conductància en funció de la intensitat del Rashba. En el nostre sistema observam que aquest comportament sinusoïdal es veu fortalement afectat pel transport multicanal, és a dir, transport en un sistema quasi-unidimensional el qual té un confinament transversal. Conseqüentment, augmentant el nombre de canals propagants, l’efecte de precessió d’espí es veu destruït. Per acabar aquesta part d’electrons, es considera el límit d’un sistema quasi-unidimensional a un de bidimensional, on el fil quàntic passa a ser un gas d’electrons bidimensional amb una franja de Rashba.

Per al sistema de forats, Part II, presentem càlculs dels factors giromagnètics per als primers escalons de la conductància per fils quàntics tridimensionals. Definint els factors g com a mitjons escalons “anòmals” que apareixen en la conductància quan s’hi aplica un camp magnètic extern, trobem que l’anisotropia del factors g per a diferents orientacions del camp magnètic és conseqüència.
de l’acoblament de Rashba. També analitzam la rellevància de la deformació, quan el fil passa d’una geometria tridimensional a bidimensional. En un fil molt deformat, el factor g perpendicular disminueix fortament amb l’increment de la interacció de Rashba. D’altra banda, per un camp magnètic paral·lel al fil, els factors g són considerablement insensibles al Rashba. Finalment, estudiam el límit d’un sisema purament unidimensional pel cas de forats.
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Preface

Transport in nanostructures has been attracting a lot of attention for many years [Fer97, Dat02]. The tendency to produce and investigate materials containing smaller and smaller structures, and having low-dimensional features, leads towards the mesoscopic regime. Mesoscopic systems allow the study of basic features of quantum mechanics in a controlled way; their effects are expected to become more and more important in this field of research, since they are very promising for applications as nanoelectronic devices.

In these mesoscopic systems, the coherence of the electron wave function is the unique condition for the ballistic transport. A particularly remarkable illustration of the importance of the quantum phase is the magnetic Aharonov-Bohm effect [Aha59], as may be seen in quasi two-dimensional semiconductor systems. Consequently, the dimensions of the system have to be sufficiently small for conserving the quantum phase; such scale depends on the material but in general is a few nanometers. As a consequence, a general requirement for mesoscopic devices is the need to confine the electrons (or holes) in suitable dimensions.

Confining electrons (holes) in a low-dimensional system keeping phase coherence has been achieved with semiconductor heterostructures, i.e., semiconductor systems composed of a series of different materials. The combination of AlGaAs/GaAs is a suitable material for this ballistic transport; on the other hand this semiconductor creates an energetic dip where the electrons and holes remain confined in a two-dimensional system (2DEG or 2DHG), or in a quasi-one-dimensional system (applying additional gates we obtain quantum wires), in which case the electron (hole) motion is free along the wire.

For mesoscopic systems, the fabrication of this artificial structures and their experiments are usually performed at low temperatures, because under these conditions the current is carried only by electrons (or holes) at the Fermi energy. A variety of mesoscopic phenomena can be understood without the Coulomb interaction. Put it another way, at low-enough electron concentrations transport in a noninteracting approach is often a good enough approximation. Our work was made under these general considerations: non-interacting coherent
ballistic transport.

The control of the conductance using not only the electron charge but the electron spin is studied in recent years [Fer97, Wol01, Dat02, Zut04, Val06, Aws09]. Combining both, charge and spin transmission, a new generation of devices is envisaged [Fie99, Ohn99]. This new technology has been called spintronics, and its aim is thus the creation, manipulation and detection of spin current and, therefore, it requires the knowledge of how the electron spin interacts with its environment. Spin-orbit interaction is a good tool for achieving this goal and, specially, the Rashba type, present in some semiconductor materials used in mesoscopic systems such as AlGaAs/GaAs.

In this new research area, the paradigm is the spin field-effect transistor (SFET) proposed by Datta and Das [Dat90]. Their suggestion exploits the current modulation that arises from spin precession due to the SO coupling in a narrow-gap semiconductor, while magnetized contacts are used to preferentially inject and detect specific spin orientations. Recently, it has been demonstrated its feasibility [Koo09], i.e., that the electron current can be tuned using the electron spin. In Fig. 1 left panel a sketch of the experiment is shown; the electron is injected with a given spin orientation and depending on the orientation of the polarized leads and the spin precession angle the electron is transmitted or not. Using the Rashba strength, right panel of the same figure, conductance is modulated. The first part of this thesis was motivated to a great extent by this recent experiment; specifically, we addressed the question of what happens when the Datta-Das transistor is not the ideal one-dimensional channel.

On the other hand, the Rashba spin-orbit interaction in hole systems is stronger than in electron ones. Holes have the additional properties of having spin 3/2 and kinetic energies described by the $4 \times 4$ Luttinger Hamiltonian, with non-diagonal matrix elements mixing different spin components. In this case, recent experiments [Dan97, Dan06, Klo09, Che10] study how the magnetic field affects the hole conductance in low dimensions, usually in the same semiconductors heterostructures mentioned above, AlGaAs/GaAs. The results of Ref. [Dan06] are shown in Fig. 2: conductance as a function of hole energy ($V_{SG}$) and magnetic field parallel (left panel, $B_{||}$) and perpendicular (right panel, $B_{\perp}$) to the wire. Owing to the magnetic field, the staircase conductance splits its plateaus (in black in the figure); these splittings define the g factors that, as main effect, are highly anisotropic depending on the magnetic field orientation. These experiments motivated the second part of the thesis, where we study what is the effect of the Rashba coupling on the hole conductance in the presence of an external magnetic field.

The aim of this thesis is thus the study of the transport properties of electron
and hole quantum wires with Rashba spin-orbit coupling. In the electron system, the Rashba intensity is localized and acts as a scattering center in the quantum wire; while in the hole system the Rashba coupling is uniform and in addition an external magnetic field is applied in any orientation. Although the two systems are different, in both cases we address the same question: how the Rashba spin-orbit coupling affects the current. The presence of Rashba SO coupling is thus the common property and, as we will see along the thesis, it strongly influences the wire conductance. The different configurations naturally split the thesis in its two parts: the first one corresponding to the electronic transport and the second one to the hole transport.

In the first part, as said, we address electronic transport. The physical system, a quantum wire with a localized Rashba interaction, is introduced in Chap. 1. In the following chapter, Chap. 2, we study the conductance and the outgoing spin polarization as a function of the Fermi energy; as we will demonstrate, a localized Rashba region acts as a polarizer. In this chapter a multi Rashba region is also considered in order to study the conductance as a function of one Rashba strength and the distance between both regions. In Chap. 3 we consider polarized leads in our wire in order to describe the Datta-Das transistor. Firstly we perform a study on the energy dependence of the conductance and polarization in Sec. 3.1; in the following section, Sec. 3.2, we focus our attention on the conductance as a function of the Rashba strength, and how evolving from purely-1D to quasi-1D systems the oscillatory behavior of the conductance is modified. To end the study of the electron transport, in Chap. 4 we consider the limit of vanishing transversal confinement, corresponding
Figure 2: g factor anisotropy from the experiment by Danneau et al. [Dan06].

to a 2DEG with a Rashba stripe. Reviewing all, in Chap. 4.5 we make some general electron conclusions.

In the second part of the thesis, the system under study is a 3D hole quantum wire with uniform Rashba spin-orbit coupling, including an external and uniform magnetic field. We use the $4 \times 4$ Luttinger Hamiltonian in order to describe the kinetic term, which is described in Chap. 5. The main results about the holes are in Chap. 6; firstly we describe the energy bands in presence of Rashba intensity and how they are modified when a magnetic field is applied parallel and perpendicular to the wire, Sec. 6.1. Secondly, the g factors are studied as a function of Rashba strength and wire flatness, in Sec. 6.2; we find that the g factor anisotropy seen in some experiments such as [Dan06], in Fig. 2, originates in the Rashba coupling. In Secs. 6.3 and 6.4 the linear regime of the g factor with the magnetic field and the limit of quasi-one dimensional quantum wire are studied. Finally, we draw some general conclusions on the hole system.

Only mention here that the results from Part I, shown along the thesis, are based on the published proceedings and papers [Gel09, Gel10, Gel10b, Gel11, Gel11b]. For work of Part II, hole quantum wire, the results are submitted.
Part I

Electronic transport
Chapter 1

Rashba coupling and quantum wire

As is well known in atomic physics, the spin-orbit interaction has a relativistic origin [Ber75]. In the presence of an external electric field, the relativistic correction introduces a coupling of the electron spin with its own momentum. The electric field is seen by each electron as a momentum-dependent effective magnetic field. The interaction of the electron spin with this effective magnetic field is called spin-orbit interaction (SOI)

\[
\mathcal{H}_{SO} = -\frac{\hbar}{4m_0^2c^2} \hat{\sigma} \cdot (\vec{p} \times \nabla V(\vec{r})) ,
\]

where \(\hbar\) is the reduced Planck’s constant, \(m_0\) the bare electron mass, \(c\) the velocity of light, \(\hat{\sigma}\) the vector of Pauli matrices and \(V(\vec{r})\) the electrostatic potential in which the electron propagates with momentum \(\vec{p}\). In atomic physics \(V(\vec{r})\) is the Coulomb potential of the atomic nucleus.

In semiconductor physics the electron moves in a periodic crystal and band structure is also affected by this coupling. A paradigmatic example is the topmost valence band in GaAs.

In III-V heterostructures such as GaAs, AlGaAs, InAs, etc., we find two different sources of potential asymmetries that cause the electric field responsible of the spin-orbit interaction:

a) The first one is the bulk inversion asymmetry (BIA), i.e., in the chosen 2DEG plane the semiconductor crystal lacks a center of space inversion. This asymmetry is fixed for a given sample, is intrinsic of the system and it is not possible to manipulate it externally. The spin-orbit coupling caused by this inversion asymmetry is known as Dresselhaus interaction.
b) The second one is only possible in low dimensional systems where the semiconductor loses the symmetry in the growth direction ($z$-direction in our reference). This is the *structural inversion asymmetry* (SIA), and the spin-orbit interaction corresponding to this asymmetry is called *Rashba coupling* [Ras60]. This asymmetry manifests in both valence and conduction bands of the semiconductor and originates spin-orbit coupling as can be seen in $kp$ models [Las84]. The Rashba interaction can be tuned with external electric fields acting on the 2DEG using, e.g., miniaturized electrodes.

The relative importance between both spin-orbit interactions, Dresselhaus and Rashba, varies depending on the band structure of the material, the electron density and the geometry of the sample under investigation. A quantitative comparison of spin-orbit effects induced by the two sources of asymmetry reveals that for some materials one prevails over the other, as in the case of InAs/AlInAs heterostructures, where Dresselhaus spin-orbit interaction is not significant in front of Rashba. Both interactions are intrinsic of the system, but in the case of Rashba its strength can be tuned *in situ* using an external electric field (perpendicular to the bidimensional layer). This external field modifies the intrinsic electric field, modifying in this way the Rashba strength, as was first demonstrated experimentally by Nitta in 1997 [Nit97]. In general there is more interest in the Rashba interaction than in the Dresselhaus, owing to its tunability. Our study concentrates on the Rashba interaction, neglecting the Dresselhaus term.

In the first part of this work, the electronic transport is described when the Rashba spin-orbit coupling is limited to a finite region of a quantum wire. In Chap. 4, vanishing confinement in transversal direction is considered, the bidimensional case, where the localized Rashba region corresponds to an infinite stripe perpendicular to the electron transport.

As Rashba interaction is the common scattering center of this part, a brief introduction about it is given in Sec. 1.1; in Sec. 1.2, we consider the most general system used in our work, which is the quantum wire with a localized Rashba region and with polarized leads.

### 1.1 Rashba coupling

The Rashba spin-orbit coupling has its origin in the asymmetry in the growth direction ($z$). The electrostatic potential, which provides the interaction, Eq. (1.1), has its origin in the valence band. A phenomenological model, well establish in the literature [Cah03, San06, Fab07, Agn10], was given by Rashba
RASHBA COUPLING

[Ras69]. In a bidimensional system this model reads

$$H_R = \frac{\alpha}{\hbar}(p_y \sigma_x - p_x \sigma_y),$$  (1.2)

where $\alpha$ represents the Rashba strength and it is taken as a tunable parameter, physically determined by a tunable external gate. The Hamiltonian in Eq. (1.2) can be interpreted as Zeeman effect

$$H_Z = \mu_B \vec{\sigma} \vec{B}_{\text{eff}}(\vec{k}),$$  (1.3)

with a $k$-dependent effective magnetic field

$$\vec{B}_{\text{eff}}(\vec{k}) = \frac{\alpha}{\mu_B}(-k_y, k_x, 0).$$  (1.4)

In a quasi one-dimensional system with homogeneous Rashba interaction, the Rashba Hamiltonian is the contribution of two terms: the first one is the intersubband coupling $H_{\text{mix}}$ and the second one is the spin precession $H_{\text{prec}}$, given both by

$$H_{\text{prec}} = -\frac{\alpha}{\hbar} p_x \sigma_y,$$  (1.5)

$$H_{\text{mix}} = \frac{\alpha}{\hbar} p_y \sigma_x,$$  (1.6)

respectively, when the electronic transport is along the $x$-direction.

In a purely one-dimensional system, the mixing term vanishes $p_y = 0$, and only the precession term survives. Using this system, Datta and Das proposed the spin field-effect transistor (SFET) [Dat90] introduced in the preface. They considered the usual structure of a transistor, with a drain, a source and a narrow channel with a gate. In the spin transistor, source and drain are ferromagnetic semiconductors with parallel magnetic moments to the transport direction. When the source injects the electrons, they are transported ballistically through the channel and are detected when arriving to the drain. The gate is used to generate an effective magnetic field induced by the Rashba interaction. The Rashba-induced field causes a precession of the electron spin along its transport path that can be controlled tuning the gate voltage, this scenario is sketched in the left panel of Fig. 1 in the Preface. Varying the Rashba strength, conductance is modulated in an oscillatory behavior. Depending on the direction of the electron spin at the end of the transistor channel it can enter the drain (ON) or not (OFF).

This transistor and the effects of the intersubband coupling term are the object of our study in Chap. 3. We will see how these considerations modify strongly the electron conductance.
1.2 Quantum wire confinement

Datta and Das considered a purely one-dimensional system for their transistor, but the experimentalists obtain quasi one-dimensional samples, where the electron motion is free along the axis of the wire (x-direction) but is quantized in the confining direction (y-direction). These quantized energies correspond to transverse modes. Usually the extra confinement needed in a quantum wire is obtained by means of a gate potential. To a good approximation we can model this potential as a parabolic one. The main results of part I of the thesis are for a localized Rashba region in a parabolic confinement, when this system is attached either to normal or to polarized leads.

We consider a quasi-one-dimensional system (a quantum wire) with a localized Rashba interaction (the Rashba dot) coupled to semi-infinite leads. Figure 1.1 shows a sketch of the physical system. Transport occurs along the x-direction. We characterize the Rashba dot as a small region of length ℓ with strong spin-orbit coupling with strength α₀. The spin polarization in the leads in a given direction $\hat{n}$ is described using a Zeeman field $\Delta(x)$ that couples to the spin vector $\vec{\sigma}$.

The system Hamiltonian reads

$$\mathcal{H} = -\frac{\hbar^2}{2m^*_0} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + \frac{1}{2} m^*_0 \omega_0^2 y^2 + |\Delta(x)| + \Delta(x)\hat{n} \cdot \vec{\sigma} + \mathcal{H}_R. \quad (1.7)$$

The confinement along the direction y, perpendicular to the current, is taken as parabolic with oscillator frequency $\omega_0$. This lateral confinement potential defines the energy and lengths units, $\hbar \omega_0$ and $\ell_0 = \sqrt{\hbar/m^*_0 \omega_0}$, respectively, that we use to give the value of the different parameters of our system, see Appendix A. $m^*_0$ is the conduction band effective mass of the semiconductor.

The inhomogeneous Rashba coupling $\mathcal{H}_R$ is given by

$$\mathcal{H}_R \equiv \mathcal{H}_R^{(1)} + \mathcal{H}_R^{(2)} = \frac{\alpha(x)}{\hbar} p_y \sigma_x + \left[ -\frac{\alpha(x)}{\hbar} p_x + i \frac{\alpha'(x)}{2} \right] \sigma_y, \quad (1.8)$$

where, as usual, spin is represented by the vector Pauli matrices $\vec{\sigma}$ while $p_x$ and $p_y$ are the Cartesian components of the electron’s linear momentum. The Rashba intensity $\alpha(x)$ varies smoothly taking a constant value $\alpha_0$ inside the Rashba dot and vanishing elsewhere (see Fig. 1.1b)). The term proportional to $p_x$ is responsible for spin precession of an injected electron [Dat90]. The intersubband coupling term proportional to $p_y$ couples adjacent subbands with opposite spins. Both terms are equivalent to the Eqs. (1.5) and (1.6), respectively, for inhomogeneous Rashba strength. Note that the term with
1.2. QUANTUM WIRE CONFINEMENT

the derivative $\alpha'(x)$ is added in Eq. (1.8) to ensure the Hermitian character of the Hamiltonian with the usual symmetrized operator generalization: $\alpha_0 p_x \rightarrow [\alpha(x)p_x + p_x\alpha(x)]/2$.

As mentioned above, the Zeeman field $\Delta(x)$ describes the polarized leads, then it is constant in the left and right asymptotic regions ($\Delta_{L,R}$) and it smoothly vanishes at distances $d_{L,R}$, toward the left and right of the Rashba dot. These are assumed large enough such that all evanescent states at the interface vanish before reaching the leads. This approximation is good at low temperatures and for electron densities large enough so that strong correlations can be safely neglected [Aue94]. A positive scalar potential $|\Delta(x)|$ is also introduced in order to align the majority spin potentials in the contacts with the potential bottom of the central region. This eliminates the effect of a potential mismatch [Sch00] for this spin component and, in practice, it would correspond to use a potential gating of the central region. It allows us to focus on the properties induced purely by the spin-orbit coupling. The potential depth of the central region felt by the other spin component is controlled by the value of the Zeeman field in the contacts. The case of parallel polarized contacts (P) corresponds to $\Delta_L = \Delta_R \equiv \Delta_0$ while the case of antiparallel polarizations (AP) corresponds to $\Delta_L = -\Delta_R \equiv \Delta_0$, where $\Delta_0$ is half of the absolute Zeeman splitting. For simplicity, $\Delta_0$ is assumed equal in both contacts and we take it as a parameter. We use the notation $n\hat{P}$ and $n\hat{AP}$ to indicate parallel and antiparallel configurations along a certain direction $\hat{n}$. Figures 1.1c) and 1.1d) show the potential $v_s$, for $s = \pm$ spins, defined as

$$v_s(x) = s\Delta(x) + |\Delta(x)|.$$  \hspace{1cm} (1.9)

Notice that in the P configuration the $s = -$ spin sees no potential at all while
s = + is confined by a potential well of width \( \ell + d_L + d_R \). On the contrary, in the AP configuration both spins feel a potential step, but in opposite contacts. These differences in potential landscape for + and − spins greatly influence the transport properties of the stripe with polarized contacts. In the simplest case of no polarized leads, the Zeeman splitting value vanishes, \( \Delta_0 = 0 \).

All spatial transitions in \( \alpha(x) \) and \( \Delta(x) \) are described using Fermi-type functions characterized by a small diffusivity \( a_\alpha(x) = \alpha_0 [F(x, \ell/2) - F(x, -\ell/2)] \),

\[
\alpha(x) = \alpha_0 [F(x, \ell/2) - F(x, -\ell/2)],
\]

\[
\Delta(x) = \Delta_L F(x, -d/2) + \Delta_R [1 - F(x, d/2)],
\]

where the Fermi functions are

\[
F(x, x_0) = \frac{1}{1 + e^{(x-x_0)/a}}.
\]

In general, \( a \) is assumed to be small enough although we shall also discuss below the dependence with this parameters in same cases.

### 1.2.1 Coupled Channel Method

For a given energy \( E \) the electron wave function fulfills Schrödinger’s equation

\[
(H - E) \Psi = 0
\]

with the appropriate boundary conditions. Our method of solution combines discretization of the longitudinal variable \( x \) in an uniform grid with a basis expansion in transverse eigenfunctions \( \phi_n(y) \) and in eigenspinors \( \chi_s(\eta) \) along a direction given by a unitary vector \( \hat{n} \)

\[
\Psi = \sum_{s=\pm} \sum_{n=0}^\infty \psi_{ns}(x) \phi_n(y) \chi_s(\eta),
\]

where \( s = \pm \) is the spin quantum number while \( \eta = \uparrow, \downarrow \) denotes the twofold spin discrete variable. In terms of the polar and azimuthal angles (\( \theta, \phi \)) corresponding to the spin quantization axis \( \hat{n} \) we can write

\[
\chi_+ \equiv \left( \begin{array}{c} \cos \left( \frac{\theta}{2} \right) \\ \sin \left( \frac{\theta}{2} \right) e^{i\phi} \end{array} \right); \quad \chi_- \equiv \left( \begin{array}{c} \sin \left( \frac{\theta}{2} \right) \\ -\cos \left( \frac{\theta}{2} \right) e^{i\phi} \end{array} \right).
\]

The transverse eigenfunctions are the solutions of the harmonic 1D oscillator

\[
\left( -\frac{\hbar^2}{2m_0} \frac{d^2}{dy^2} + \frac{1}{2} m_0^* \omega_0^2 y^2 \right) \phi_n(y) = \varepsilon_n \phi_n(y)
\]
with
\[ \varepsilon_n = \left( n - \frac{1}{2} \right) \hbar \omega_0; \quad n = 1, 2, \ldots \] (1.17)

Projecting Eq. (1.13) onto the basis we obtain the equations for the unknown channel amplitudes \( \psi_{ns}(x) \)
\[ -\frac{\hbar^2}{2m_0} \psi''_{ns}(x) + \left[ v_s(x) + \varepsilon_n - E \right] \psi_{ns}(x) + \sum_{n's'} \langle ns|\mathcal{H}_R|n's'\rangle \psi_{n's'}(x) = 0. \] (1.18)

Notice that the Rashba interaction is the only source of interchannel coupling since, in general, the matrix element \( \langle ns|\mathcal{H}_R|n's'\rangle \) will be nondiagonal. Using the separation in two spin-orbit contributions introduced in Eq. (1.8) we can write
\[ \langle ns|\mathcal{H}^{(1)}_R|n's'\rangle = \frac{\alpha(x)}{\hbar} \langle n|p_y|n'\rangle \langle s|\sigma_x|s'\rangle, \] (1.19)
\[ \langle ns|\mathcal{H}^{(2)}_R|n's'\rangle = \left[ -\frac{\alpha(x)}{\hbar} p_x + \frac{i}{2} \alpha'(x) \right] \delta_{nn'} \langle s|\sigma_y|s'\rangle. \] (1.20)

Equations (1.19) and (1.20) clearly show that, in general, both \( \mathcal{H}^{(1)}_R \) and \( \mathcal{H}^{(2)}_R \) couple channels with opposite spins through the matrix elements \( \langle s|\sigma_x|s'\rangle \) and \( \langle s|\sigma_y|s'\rangle \). Of course, if the spin quantization axis \( \hat{n} \) is chosen along the \( x \) or \( y \) axis then either \( \langle s|\sigma_x|s'\rangle \) or \( \langle s|\sigma_y|s'\rangle \) become diagonal. Regarding the coupling between transverse modes, we notice that \( \mathcal{H}^{(2)}_R \) is always diagonal \( \langle \delta_{nn'} \rangle \) while \( \mathcal{H}^{(1)}_R \) is connecting modes differing in one subband index \( n' = n \pm 1 \) through the oscillator matrix element \( \langle n|p_y|n'\rangle \).

If we neglect \( \mathcal{H}^{(1)}_R \) as in strict one-dimensional systems, Eq. (1.18) involves a single mode \( n \). If, in addition, the spin axis is chosen along \( y \) then the two spin modes uncouple and no spin oscillation is allowed; in other directions \( (x \) or \( z \) ) a rigid spin precession should be expected if all the contribution between parenthesis in Eq. (1.20) is assumed constant. This precession is the underlying working mechanism of the Datta-Das spin transistor [Dat90].

### 1.2.2 Landauer formalism

The physical behavior of our system will be analyzed in the linear transport regime, focussing on an experimentally measurable quantity: the linear conductance.
In ballistic nanodevices there are no inelastic processes and Coulomb interaction is neglected, which is valid in systems with low electron concentration ($\lesssim 10^{11}$ cm$^{-2}$). With both simplifications transport properties can be described as a scattering process (scattering approach [But92, Lan57]). The linear-response conductance is given by

$$G = G_0 \sum_{ns, n's'} |t_{n's', ns}|^2,$$

(1.21)

where $G_0 = e^2/h$ is the conductance quantum and $t_{n's', ns}$ is the probability amplitude from a given left incident mode $ns$ to the right mode $n's'$. This probability transmissions are obtained from the channel amplitudes, $\psi_{ns}(x)$, using the corresponding boundary conditions (see Appendix B.1).

In order to study the polarization of the transmitted current, we also define the polarized conductance $G_p$

$$G_p = G_0 \sum_{ns, n's'} s'|t_{n's', ns}|^2,$$

(1.22)

which takes into account the electron spin transmitted $s'$, and the relative polarization $p$

$$p = \frac{G_p}{G},$$

(1.23)

which takes the values form $-1$ to $1$, where $p = -1$ indicates $100\%$ spin down polarization, $p = 1$ corresponds to $100\%$ polarization in spin up and $p = 0$ no polarization is allowed.
Chapter 2

Quantum wire with normal leads

Besides the constant-spin-orbit case, situations where the Rashba coupling acting on a 2DEG is inhomogeneous in space have been theoretically addressed by analyzing interface-induced effects such as, for example, spin accumulation, beam focusing and ‘spin optics’ [Kho04, Mar04, Usa04, Gla05, Nik05b]. A finite SO region in a 2DEG has been shown to contain bound states purely induced by the spin-orbit coupling [Val04]. In a quantum wire, a finite SO region produces quasibound states that quench the wire’s conductance at specific energies, i.e., dips appear in the conductance plateau for a given number of propagating modes [San06]. This Fano-Rashba dips have been studied in the presence of disorder [She08, Wan08] and under the influence of magnetic fields [San08].

In this chapter we focus our attention on a quantum wire with transport along the $x$-direction and parabolic confinement in the $y$-direction attached to normal leads and with localized Rashba interaction. For $\Delta_0 = 0$ the Hamiltonian (1.7) reduces to

$$\mathcal{H} = -\frac{\hbar^2}{2m_0^*} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + \frac{1}{2}m_0^*\omega_0^2 y^2 + \mathcal{H}_R.$$  \hspace{1cm} (2.1)

Using the coupled channel method from Subsec. 1.2.1 the channel amplitudes $\psi_{ns}(x)$, from Eq. (1.18) at $v_s(x) = 0$, are given by

$$-\frac{\hbar^2}{2m_0^*} \psi_{ns}''(x) + (\varepsilon_n - E)\psi_{ns}(x) + \sum_{n's'}\langle ns|\mathcal{H}_R|n's'\rangle \psi_{n's'}(x) = 0.$$ \hspace{1cm} (2.2)

Under this considerations we make a brief review of the conductance in Sec. 2.1, presenting our main result in Sec. 2.2, which is the polarization of the
CHAPTER 2. QUANTUM WIRE WITH NORMAL LEADS

output current. In Sec. 2.3 we provide the study of the conductance when we have two tunable Rashba regions.

2.1 Conductance

In order to gain a better understanding of Sec. 2.3, we present here a small explanation of the conductance as a function of the Fermi energy in our system. Solving numerically the coupled channel equations (2.2), the characteristic conductance curve as a function of the Fermi energy \( E \) (in units of \( \hbar \omega_0 \)) for unpolarized incident electron beam is shown in Fig. 2.1. The parameters for the localized Rashba interaction are \( \alpha_0 = 0.3 \hbar \omega_0 \ell_0 \) and \( \ell = 8 \ell_0 \) (corresponding, in the case of InAs, to \( \alpha_0 = 17 \text{ meV nm} \) and \( \ell_0 = 0.45 \mu \text{m} \) for \( \hbar \omega_0 = 1 \text{ meV} \), see App. A).

The conductance is approximately quantized to integer values of \( 2e^2/h \). This is a consequence of the mode quantization in the electron waveguide. The quantization is not exact only due to the Rashba interaction. First, we observe a damped oscillation for energies close to the onset of each plateau. Second, there exists a dip right before the second conducting channel opens. The conductance dip is related to the backscattering induced by the wave interference between two paths—the channel passing through the quasi-localized level and the nonresonant transmission channel [San06]. The discussion about this quasi-localized level is discussed as follows.

As we explained in Sec. 1.2, the Rashba Hamiltonian consists of two terms, the precession term and the intersubband coupling, \( \mathcal{H}_R^{(1)} \) and \( \mathcal{H}_R^{(2)} \) in equation (1.8). Consider for the moment only the former, which produces a spin rotation as the electron moves along the longitudinal direction. In the case of a constant Rashba strength \( [\alpha(x) = \alpha_0 \text{ for } 0 < x < \ell \text{ and zero elsewhere}] \) and for states with spin direction along \( y \), the Rashba precession term is shown to be equivalent to a square well potential of depth \( \hbar^2 k_R^2/2m^*_0 \) [San06] where

\[
k_R = \frac{m^*_0 \alpha_0}{\hbar^2}.
\] (2.3)

Such potential, thus, sustains bound states. On the other hand, the intersubband coupling term induces transitions between these bound states and the continuum that form the nonresonant channel describing direct transmissions through the Rashba dot. This interaction causes a finite broadening of the bound states. Furthermore, the interference between continuum and quasi-bound states leads to the appearance of characteristic dips in the conductance curves [She04, Zha05b, San06] that can be explained as Fano resonances [Fan61].
2.2. SPIN POLARIZED CURRENT

For a better integration with present semiconductor technologies, it is highly desirable that beams of spin polarized electrons be tunable via electric means only. Several approaches have been explored to produce spin polarized currents in quantum wires when the spin-orbit interaction is of the Rashba type [Kis01, Eto05, Ohe05, Yam05, Cum06, Per07, Zha08]. These are based on branching structures that collect electrons with opposite spin polarization in different leads [Kis01, Ohe05, Yam05, Cum06] or potential constrictions that induce transitions between adjacent subbands with opposite spins [Eto05, Zha08]. Consequently, an interesting subject of study is the polarization of the output current.

The polarization corresponding to an incident beam of unpolarized electrons as a function of the Fermi energy is shown in Fig. 2.2. Here, we take the spin quantization axis along the $y$ direction since the Rashba precession term points precisely along $y$ (the Rashba field axis). In the absence of the intersubband coupling term, the states with spin along $y$ are eigenstates of $H_R$ and do not undergo spin flip processes. As a consequence, a net polarization could arise from a combined effect of both terms entering in Eq. (1.8). However, this condition is not sufficient as we demonstrate below.

We note that the current polarization vanishes for all energies in the first plateau. This energy range corresponds to one propagating mode per spin polarization.
Figure 2.2: Polarization of the transmitted current for a beam of unpolarized electrons. We use the same parameters as in Fig. 2.1. Vertical dashed lines indicate the threshold energies for the first and second conducting mode. Polarization is finite only for energies above the threshold of the second mode.

We see in Fig. 2.2 that the polarization attains a finite value at the onset of the second plateau ($E = \varepsilon_2 = 1.5\hbar\omega_0$). For energies above $\varepsilon_2$ there are now four possible propagating states, each corresponding to distinct mode and spin indices. We thus expect wave interference between them induced by the Rashba intersubband coupling term, leading to finite current polarizations.

We observe that the polarization decreases for increasing $E$ performing a few oscillation cycles as $E$ approaches the middle of the plateau. Although not shown in the figure, we also notice that the polarization is reversed when $\alpha_0$
changes sign. Finally, there is again a sharp increase of \( p \) close to the onset of the third plateau \( (E \lesssim \varepsilon_3) \). This fact can be related to the enhanced coupling to the evanescent states from the third subband as \( E \) approaches the threshold of the third conducting channel. Unlike the first plateau case, this coupling to quasi-bound states can now give rise to a net spin polarization in the conductance because the interaction between the two propagating states can be strongly influenced by the localized state. Nevertheless, the analysis of this particular scenario is more complicated than the previous regime of only one propagating mode. We next discuss the physical mechanism for the net polarization observed at the beginning of the second plateau.

### 2.2.1 The model

Our analysis is based on the coupled channel method for scattering in electron waveguides [Gur93, Noc94] which has been recently extended to treat spin dependent potentials [San06], and which we have introduced in Subsec. 1.2.1 (in Chap. 1). Taking Eq. 2.2 and using the gauge transformation

\[ \psi_{1+}\rightarrow \psi_{1+}\exp(\pm i \int k_R(x')dx'), \]

we obtain the pair of equations,

\[
\begin{align*}
\frac{p_x^2}{2m^*_0} - \frac{\hbar^2 k^2_R}{2m^*_0} - (E - \varepsilon_1) \psi_{1+}(x) &= V_{12}\psi_{2-}(x), \\
\frac{p_x^2}{2m^*_0} - \frac{\hbar^2 k^2_R}{2m^*_0} - (E - \varepsilon_2) \psi_{2-}(x) &= V_{21}\psi_{1+}(x),
\end{align*}
\]

for the two-band model, which neglects contributions from states other than \( n = 1 \) and \( n = 2 \). This approximation is good for energies away from the onset of the third plateau.

We note that \( \psi_{1+} \) couples only to \( \psi_{2-} \) and not to \( \psi_{2+} \). In fact, the states \( \psi_{1-} \) and \( \psi_{2+} \) obey the same coupled channel equations. For energies in the first plateau, \( \varepsilon_1 < E < \varepsilon_2 \), Eq. (2.5) describes a localized state which produces enhanced backscattering reflected in the conductance dip. Here, we focus on the energy range \( E \gtrsim \varepsilon_2 \) for which both wave function coefficients, \( \psi_{1+} \) and \( \psi_{2-} \), correspond to continuum states. Thus, localized states play no significant role in what follows.

The mixing potential elements read

\[ V_{12} = \frac{i\omega_p \alpha}{\hbar} e^{i\int k_R(x')dx'}, \]
and \( V_{21} = V_{12}^* \), where \( \omega_p = \int dy \phi_1^* p_y \phi_2 \). Thus, Eqs. (2.4)-(2.5) take the form of a Hamiltonian matrix with complex coupling potentials due to the phase factors \( e^{2i \int_{x'}^{x} \phi_R'(x') dx'} \).

The coupled channel equations cannot be solved analytically. For the sake of the present discussion we consider a lattice representation of Eqs. (2.4)-(2.5) along two chains of sites (see Fig. 2.3), corresponding to the states \( \psi_{1+} \) (1 \( \uparrow \) in the figure) and \( \psi_{2-} \) (2 \( \downarrow \)), respectively. Since we consider energies \( E > \varepsilon_2 \), both states are propagating and their on-site energies are \( \varepsilon_1 \) and \( \varepsilon_2 \). We restrict the Rashba coupling to two sites only, which we label as 0 and 1. This is the minimal model that correctly describes a localized Rashba interaction [San08].

According to Eqs. (2.4)-(2.5), the coupling potential \( \tilde{V} \) couples sites belonging to adjacent subbands (in the two-band approximation, the subband indices are \( n = 1 \) and \( n = 2 \)) with opposite spins. Thus, \( V_0 = W \) and \( V_1 = W e^{i \phi} \) where \( W = \alpha/\ell_0 \) and \( \phi = 2 k_R a \) with \( a \) the lattice spacing. The latter is related to the intersite hopping parameter via \( t = -\hbar^2/2m^* a^2 \). Hence, the tight-binding Hamiltonian reads

\[
H_{tb} = \sum_{n\mu} E_n c^\dagger_{n\mu} c_{n\mu} + t \sum_{n,(\mu,\nu)} (c^\dagger_{n\mu} c_{n\nu} + \text{H.c.}) \\
+ \left( V_0 c^\dagger_{10} c_{20} + V_1 c^\dagger_{11} c_{21} + \text{H.c.} \right)
\]

where \( \mu \) and \( \nu \) label the wire sites and the hopping sum is restricted to nearest neighbors. The energy spectrum is \( E_n = \varepsilon_n + 2t \cos k_n a \) with wave number \( k_n \).

For an incident electron from the left, scattering at sites 0 or 1 produces reflected and transmitted waves that can propagate through any of the two subbands. We calculate the transmission probability \( T_{n'n',n\sigma} \) that an electron with mode index \( n \) and spin \( \sigma \) is transmitted into the subband \( n' \) with spin \( \sigma' \), where \( n, n' = 1, 2 \) and \( \sigma, \sigma' = \uparrow, \downarrow \). For example, in the case that an electron with spin \( \uparrow \) is injected from mode 1, the wave function outside the scattering
2.2. SPIN POLARIZED CURRENT

Figure 2.4: Current polarization obtained from the simple tight-binding model discussed in the text. We use the parameters \( t = 1 \), \( \hbar \omega_0 = 0.2 \), \( W = 0.4 \) and \( \phi = \pi/4 \). Therefore, \( \varepsilon_2 = 0.3 \) and the second propagating mode opens at \( E = \varepsilon_2 - 2t = -1.7 \).

The region reads,

\[
\psi = \sum_{\mu < 0} \left[ e^{ik_1\mu a} + r_{1\uparrow} e^{-ik_1\mu a} + r_{2\downarrow} e^{-ik_2\mu a} \right] \\
+ \sum_{\mu > 1} \left[ \tau_{1\uparrow} e^{ik_1\mu a} + \tau_{2\downarrow} e^{ik_2\mu a} \right],
\]

(2.8)

where \( r \) and \( \tau \) are the reflection and transmission amplitudes. Then, \( T_{1\uparrow,1\uparrow} = |\tau_{1\uparrow}|^2 \) and \( T_{2\downarrow,1\uparrow} = |\tau_{2\downarrow}|^2 \).

To determine the current polarization we must obtain the transmitted flux given by \( J_{n'\sigma',n\sigma} = v_n T_{n'\sigma',n\sigma} \), where \( v_n = (1/\hbar)\partial E_n / \partial k_n \) is the electron velocity in the \( n \)-th subband. As a result, the polarization takes the form

\[
p = \frac{\sum_{n'n'\sigma'}(J_{n'\sigma',n\uparrow} - J_{n'\sigma',n\downarrow})}{\sum_{n'n'\sigma'\sigma} J_{n'\sigma',n\sigma'}} \tag{2.9}
\]

where the denominator determines the total conductance,

\[
G = \frac{e^2}{h} \sum_{n'n'\sigma\sigma'} J_{n'\sigma',n\sigma}. \tag{2.10}
\]

We find the exact result

\[
p = \frac{2t^2W^2\Delta}{\Gamma} \sin \phi \sin k_1 \sin k_2 \sec \frac{k_1 - k_2}{2} \tag{2.11}
\]
where
\[
\Delta = 4 \sin \frac{k_1 - k_2}{2} + 2 \sin \frac{3(k_1 - k_2)}{2} \\
+ \sin \frac{3k_1 + k_2}{2} - \sin \frac{k_1 + 3k_2}{2},
\]  
(2.12)

and
\[
\Gamma = 2t^4 (1 + \cos 2k_1 \cos 2k_2) \\
- (2t^4 + W^4)(\cos 2k_1 + \cos 2k_2) \\
+ 2t^2 W^2 \sin k_1 \sin k_2 [1 + \cos \phi \cos(k_1 + k_2)].
\]  
(2.13)

Notably, Eq. (2.11) reproduces most of the results obtained in the numerical simulations (Fig. 2.2). First, \( p \) vanishes if \( k_1 = k_2 \), showing that the polarization effect is due to wave interference between subband states with \textit{different} energy (i.e., different modes). As a result, the working interval of the present spin polarizer lies above the onset of the second plateau, as observed in Fig. 2.1. Second, \( p \) oscillates, at a given energy, with the Rashba strength via \( \phi \), which makes our proposal a \textit{tunable} polarizer just by adjusting the value of \( \alpha \). Third, \( p = 0 \) if \( W = 0 \), i.e., nonzero polarizations arise only due to the intersubband coupling term of the Rashba interaction, as expected. Finally, \( p \) is an odd function of \( \alpha \) since \( p(-\phi) = -p(\phi) \), accounting for the fact that the polarization is inverted when the sign of \( \alpha \) is changed.

In Fig. 2.4, we plot a characteristic polarization curve obtained from Eq. (2.11) as a function of \( E \). Here, the Fermi energy ranges between \( \varepsilon_2 - 2t \) and \( \varepsilon_2 + 2t \) since the bandwidth is \( 4t \). We restrict ourselves in the calculations to energies close to the band bottom \( (E \gtrsim \varepsilon_2 - 2t) \) since in that case the results are more reliable as bandstructure details can be neglected. The peak polarization is attained at energies close to the plateau onset and then slowly decreases with increasing \( E \). This is in agreement with the numerical findings of Fig. 2.2. Obviously, our model cannot explain the oscillatory decaying pattern since the Rashba interaction is restricted to two sites and the oscillations are probably due to interference within the Rashba region. However, our simple model remarkably captures the essential physics.

### 2.3 Multi Rashba region

Our aim in this section is to study the interference of the Fano-Rashba conductance dips of two sequential SO regions in a quantum wire, separated by a distance \( d \) (see Fig. 2.5).
Similar SO modulations, named Rashba superlattices, have been studied in [Zha05b]. Independently tuning $\alpha_1$ and $\alpha_2$, the Rashba intensities of the two regions, the two conductance dips can be brought into close proximity to each other. We show that for large separations $d$ an avoided crossing of the dips is observed. This is reminiscent of the von Neumann-Wigner crossing rule of molecular levels [Bra03]. In our case, the coupling is mediated by evanescent modes around each SO region. If $d$ is larger than the range of the evanescent modes, the dip-dip coupling vanishes and a crossing behavior is seen. On the other hand, for small $d$’s, avoided crossing of the two dips is obtained when transport is enhanced due to transmission from the first to the second region through evanescent modes.

The relevance of evanescent modes in confined (quasi-1D) transmission is well known [Cah90, Kum91, Bar97, Ser07]. For Dirac-delta impurities, Bagwell [Kum91] showed that the dependence of the transmission on the separation between scatterers has two clear regimes: (a) a Fabry-Perot regime for larger separations where the dominant mechanism is the interference between forwards and backwards propagating modes between scatterers and (b) at small separations a regime where transmission occurs predominantly through evanescent modes. This is precisely the physical scenario we have sketched above for the interference of two Fano-Rashba dips. It is also worth stressing that transmission through evanescent modes between scatterers has been proved relevant for the Anderson localization of disordered wires [Cah90].

In this Section, the Rashba intensity $\alpha(x)$ is assumed to vanish everywhere except in two separate regions where it takes the constant values $\alpha_1$ and $\alpha_2$. A sketch of the physical system is given in Fig. 2.5. More precisely,

$$\alpha(x) = \alpha_1 F_{x_1,\ell}(x) + \alpha_2 F_{x_2,\ell}(x) ,$$

where

$$F_{x_0,\ell}(x) = F(x, x_0 + \ell/2) - F(x, x_0 - \ell/2) = \frac{1}{1 + e^{(x-x_0+\ell/2)/a}} - \frac{1}{1 + e^{(x-x_0-\ell/2)/a}}$$

describes a square barrier of length $\ell$ centered at $x_0$, and Fermi functions $F(x, x_0)$ are given in Eq. (1.12). The distance between the two Rashba regions
defined by Eq. (2.14) is \( d = x_2 - x_1 - \ell \) and it is always assumed \( d > 0 \) to avoid overlapping. Experimentally, the Rashba interaction can be controlled with gate electrodes modifying the \( z \)-asymmetry of the quantum well hosting the 2DEG [Nit97, Eng97]. Our model would thus require an independent tuning of the gates defining \( \alpha_1 \) and \( \alpha_2 \). Notice also that no electrostatic in-plane effects, other than the lateral potential \( m_0^* \omega_0^2 y^2/2 \) are contained in the model.

We consider one propagating mode, \( \varepsilon_1 < E < \varepsilon_2 \) and focus our attention on the linear system conductance.

The transmission of the system is obtained numerically (see Subsec. 1.2.1 in Chap. 1 and Appendix B.1). The total number of modes, both propagating and evanescent, in the linear system of Eqs. (2.2) is taken to be large enough to yield converged results. We focus on the Fano-Rashba conductance dips for a fixed \( \alpha_1 \) and varying \( \alpha_2 \), Fig. 2.6. Dark regions represent the position of the conductance dips. The figure clearly shows that for large separation between the two Rashba regions there is a crossing of the two dips that evolves to an anticrossing for small values. Remarkably, for an intermediate distance \( (d = 4 \ell_0) \) the two dips are in a perfectly destructive interference, leading to a high conductance at the position where the crossing would normally occur. We also notice that for very short distances the dips become highly asymmetric, with one of them clearly dominating the other. The scenario presented in Fig. 2.6 can be interpreted in terms of a \( d \)-dependent dip-dip coupling: vanishing for large distances (crossing behavior) and increasing at small \( d \)'s (anticrossing). We present in what follows evidence proving that the quantum wire evanescent modes mediate this coupling using, for this purpose, a scattering matrix formalism.

### 2.3.1 Scattering matrix theory

Scattering phenomena in quantum mechanics with coherent wave functions are described by scattering matrix theory. For a single scatterer there is a matrix of complex numbers relating the flux amplitudes of outgoing channels \( \{b_{c,ns}\} \) to those of incoming ones \( \{a_{c,ns}\} \), where we introduced a “contact” label \( c = L, R \) (referring to left \( L \) or right \( R \)), while \( ns \) are indicating transverse mode and spin as before. Namely,

\[
\begin{pmatrix}
\sqrt{k_n} b_{L,ns} \\
\sqrt{k_n} b_{R,ns}
\end{pmatrix} = \begin{pmatrix}
t_{ns,n's'} & t'_{ns,n's'} \\
\end{pmatrix} \begin{pmatrix}
\sqrt{k_n} a_{L,n's'} \\
\sqrt{k_n} a_{R,n's'}
\end{pmatrix}.
\]

As usual, a sum is implied for repeating indexes in Eq. (2.16) and the factors \( \sqrt{k_n} \) take into account the channel flux by introducing the channel wavenum-
2.3. MULTI RAHSBA REGION

Energy ($\omega_0$)

\begin{align*}
\alpha_2 (\hbar \omega_0 \ell_0)
\end{align*}

\begin{itemize}
\item a) $d=18 \ell_0$
\item b) $d=8 \ell_0$
\item c) $d=4 \ell_0$
\item d) $d=2 \ell_0$
\end{itemize}

\begin{itemize}
\item Dark (bright) color indicates low (high) conductance.
\end{itemize}

**Figure 2.6:** Conductance in units of $e^2/h$ as a function of $\alpha_2$ and $E$ for a fixed $\alpha_1 = 0.3\hbar \omega_0 \ell_0$, $\ell = 8\ell_0$ and $a = 0.1\ell_0$. Each panel corresponds to a different value of $d$, the distance between the two Rashba regions. The wire parabolic confinement fixes our energy $\hbar \omega_0$ and length unit $\ell_0 = \sqrt{\hbar / m^* \omega_0}$. Dark (bright) color indicates low (high) conductance.

In Eq. (2.18) we have introduced the notation $s_L = 1$ and $s_R = -1$ and $x_c$ is indicating the position where the scatterer becomes inactive for contact $c$. 

\begin{equation}
\Psi_c (x, y, \eta) = \sum_{n,s} a_{c,ns} \phi_n(y) \chi_s(\eta) e^{is_c k_n (x-x_c)} + \sum_{n,s} b_{c,ns} \phi_n(y) \chi_s(\eta) e^{-is_c k_n (x-x_c)}. \tag{2.18}
\end{equation}

The idea underlying scattering theory in quasi-1D transmission is that the wave function in the left and right leads ($c = L, R$ regions respectively), where the scatterer is no longer active, is given in terms of channel amplitudes and wavenumbers as

\begin{equation}
k_n = \frac{\sqrt{2m^*_0 (E - \epsilon_n)}}{\hbar}. \tag{2.17}
\end{equation}
For our present purposes, it is essential to realize that the number of channels \( \{ ns \} \) in Eqs. (2.16) and (2.18) is, in principle, infinite [Cah90]. For a given energy \( E \) part of these channels will be propagating \( (E \geq \varepsilon_n) \) and the rest will have an evanescent character. The intrinsic distinction between propagating and evanescent characters is that the wavenumber, Eq. (2.17), is real in the former and purely imaginary in the latter. The physical meaning becomes obvious when looking at the \( x \)-dependence of Eq. (2.18). Though infinite, the number of evanescent channels is truncated in practice and fast convergence is usually obtained.

**Sequential scatterers**

Assuming the scattering matrix of one scatterer is known, the solution for two identical scatterers can be obtained by adequately composing the matrices of each scatterer. This procedure only requires to realize that the right output from the first scatterer becomes left input for the second and vice versa. We need to label now the amplitudes with the “impurity” index \( i = 1, 2 \) as \( \{ a_{c,ns}^{(i)}, b_{c,ns}^{(i)} \} \). Assuming that all the input coefficients vanish except that of mode \( n = 1 \) with spin \( s_i \), \( a_{L,1s_i}^{(1)} = 1 \), the linear system for the output coefficients reads

\[
\begin{align*}
    b_{L,ns}^{(1)} &= \sum_{n's'} t_{ns,n's'} e^{ik_{ns,n's'}d} b_{L,n's'}^{(2)} = r_{ns,1s_i}, \\
    b_{R,ns}^{(1)} &= \sum_{n's'} r_{ns,n's'} e^{ik_{ns,n's'}d} b_{L,n's'}^{(2)} = t_{ns,1s_i}, \\
    b_{L,ns}^{(2)} &= \sum_{n's'} t_{ns,n's'} e^{ik_{ns,n's'}d} b_{R,n's'}^{(1)} = 0, \\
    b_{R,ns}^{(2)} &= \sum_{n's'} t_{ns,n's'} e^{ik_{ns,n's'}d} b_{R,n's'}^{(1)} = 0.
\end{align*}
\]  

Equation (2.19) can be viewed as a sparse linear system for the unknowns \( \{ b_{c,ns}^{(i)} \} \). It can be solved with standard sparse numerical routines for a fairly large number of evanescent modes [Ser09, HSL07]. Reversely, for just one propagating mode, or one propagating and one evanescent mode, analytical solutions can be given that recover known results for the composition of scatterers (see in the following). Of all the output amplitudes of Eq. (2.19), we are interested in the total transmission amplitude \( t_{1s_o,1s_i} = b_{R,1s_o}^{(2)} \), representing the right output from impurity 2 in channel 1\( s_o \) corresponding to a left input in impurity 1 in channel 1\( s_i \), \( a_{L,1s_i}^{(1)} = 1 \).

The method of scatterer composition allows us to investigate the dependence on \( d \), the distance between impurities, in an explicit way from Eq. (2.19). A technical point worth of stressing is that an important simplification occurs for
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![Conductance graph]

**Figure 2.7:** Conductance as a function of distance $d$ between Rashba regions for an energy $E = 1.457\hbar\omega_0$ and $\alpha_1 = 0.3\hbar\omega_0\ell_0$ obtained with the method of scatterer composition. Upper panel is the result including evanescent modes while lower panel only considers the propagating mode.

identical scatterers placed sequentially along $x$; namely, the scattering matrix is the same for each scatterer. Figure 2.7 shows the result obtained as a function of $d$ for the energy and Rashba intensity of the conductance dip of Fig. 2.6. When evanescent modes are fully neglected (lower panel) the transmission of the system vanishes except for a sequence of very narrow, equally spaced peaks. They correspond to a Fabry-Pérot-like regime [Kum91] with constructive interference at distances such that an exact multiple of the electron wavelength fits in between Rashba regions. This behavior changes dramatically for low distances when evanescent modes are included (upper panel): the dip is effectively destroyed by evanescent-mode transmission from the first to the second Rashba region. This effect exactly corresponds to the anti crossing seen in Fig. 2.6 at small distances. With the resolution of Fig. 2.7 upper panel, it is enough to include one evanescent mode, the contribution from higher ones being exceedingly small.

**Analytical**

For only two modes it is possible to obtain analytical solutions to the linear system Eq. (2.19). Let us assume there are only one propagating $n = 1$ and
one evanescent $n = 2$ modes. Taking into account spin, the set of channels splits into two coupled subsets $\{1+, 2-\}$ and $\{1-, 2+\}$. Since both subsets are equivalent we restrict to the first one by considering incidence in mode $1+$. The transmitted output amplitude reads (spin indexes are not explicitly written to simplify notation)

\[
b_{R,1}^{(2)} = \frac{t_{11}t_{12}e^{ik_1d}}{1 - R_{11} - \frac{R_{12}R_{21}}{1 - R_{22}}} + \frac{t_{11}R_{12}t_{21}e^{ik_1d}}{(1 - R_{11})(1 - R_{22}) - R_{12}R_{21}} + \frac{t_{12}t_{21}e^{ik_2d}}{1 - R_{22} - \frac{R_{12}R_{21}}{1 - R_{11}}} + \frac{t_{12}R_{21}t_{11}e^{ik_2d}}{(1 - R_{11})(1 - R_{22}) - R_{12}R_{21}},
\]

(2.20)

where we have defined

\[
R_{n_1n_2} = r'_{n_11}r_{1n_2}e^{i(k_1 + k_{n_2})d} + r'_{n_12}r_{2n_2}e^{i(k_2 + k_{n_2})d},
\]

(2.21)

with $n_{1,2} = 1, 2$.

The explicit dependence on $d$, the distance between Rashba regions, is contained in Eqs. (2.20) and (2.21). To analyze the large-$d$ limit we recall that the evanescent wavenumber is purely imaginary $k_2 = i\kappa_2$ ($\kappa_2 > 0$). As a result we get in that limit $e^{ik_2d} \to 0$ as well as $R_{12} \to 0$, $R_{22} \to 0$ and

\[
R_{11} \to r'_{11}r_{11}e^{ik_1d},
R_{21} \to r'_{21}r_{11}e^{ik_1d}.
\]

(2.22)

The transmitted amplitude is then

\[
b_{R,1}^{(2)} = \frac{t_{11}t_{12}e^{ik_1d}}{1 - r'_{11}r_{11}e^{ik_1d}},
\]

(2.23)

which is a familiar relation frequently used for single mode conductors. Equation (2.20) contains the analytical $d$-dependence that generalizes Eq. (2.23) in the presence of one evanescent channel. This causes, as shown in Fig. 2.7, a modification of the transmission resonances at short distances.

### 2.3.2 Device

The conductance dips discussed above are quite narrow and, therefore, not robust against thermal or disorder fluctuations. Their observation requires the use of very low temperatures and purely ballistic samples. As discussed in the first section, Sec. 2.1, for stronger $\alpha$’s broader dips are induced at the end of each conductance plateau [San06]. For a more robust conductance dip, in this section we analyze the effect discussed in this paper in a device in which
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Figure 2.8: Upper: Conductance as a function of energy for sequential Rashba regions, each one having $\ell = \ell_0$ and $\alpha = \hbar \omega_0 \ell_0$. The different curves correspond to 1 (solid), 2 (dash) and 3 (dash-dot) sequential regions. Upper and lower panels are for small and large separation $d$ between regions, respectively. For comparison, right panels show the result when evanescent channels are not included. Lower panels suggest transistor operation by tuning $\alpha$, for $E \approx 1.25 \hbar \omega_0$, with the OFF and ON states represented by $\alpha \approx 1 \hbar \omega_0 \ell_0$ and $\approx 0$, respectively.

current is controlled by manipulating the intensity of successive Rashba regions (See Fig. 2.8). The idea that a superlattice of this type could be of importance in practical application was already pointed out in Refs. [She08, Wan08]. Our purpose here is to analyze this mechanism from the point of view of interference between Fano-Rashba dips through evanescent modes.

Figure 2.8 displays the conductance for up to 3 regions with a strong ratio $\alpha/\hbar \omega_0 \ell_0$. For a single region there is a sizeable dip which, however, does not extend all the way to zero (solid line). Adding more regions at distance $d = 2\ell_0$ has the effect to enhance the dip forming a quasi gap amenable to practical applications (lower panels). It is remarkable how for just two or three regions with $d = 2\ell_0$ a quasi energy gap clearly develops at the dip position $E \approx 1.25 \hbar \omega_0$. At short distances the coupling through evanescent modes destroys the dip (upper panels) – notice, however, that a second narrow dip appears at $E \approx 1.4 \hbar \omega_0$ for two regions (dashed line, upper left panel) but it is removed for 3 sequential regions (dash-dotted line). A device based on the tuning of $\alpha$ for sequential Rashba regions at a proper distance would not require
the use of polarized leads, as compared to the Datta-Das spin transistor. Its basic shortcoming, however, is the sensitivity to the incoming electron energy which should lie in the region of the quasi gap. Increasing the number of sequential regions makes the quasi gap more robust. The distance between Rashba regions should be chosen appropriately in order to avoid destructive interference through evanescent modes.
Chapter 3

Quantum wire with polarized leads

Since the spin-orbit interaction couples the electron momentum with its spin, the Rashba field behaves as an effective magnetic field that is responsible for spin coherent oscillations, which can be exploited in spintronics. Based on this property, Datta and Das suggested a spin field-effect transistor [Dat90]. It consists of a one-dimensional ballistic channel sandwiched by two ferromagnetic contacts. Their proposal relies on the control of the current along the channel using the Rashba interaction via a third terminal (the gate) and the relative orientation of the leads’ magnetizations. The length of the channel and the intensity of the Rashba strength determine the flow of the current.

Realization of the spin transistor was hindered by some limitations, such as the mismatch problem [Sch00] and the idealization of ballistic transport [Sch03]. However, recent experiments on quasi-two-dimensional structures have overcome these obstacles and have obtained a behavior which looks similar to the spin-transistor effect [Koo09]. Such experimental results are given in Fig. 1 of the Preface.

In reality, strictly one-dimensional channels are hard to fabricate and one must deal mostly with quasi one-dimensional systems containing many propagating channels. Confinement in the transversal direction is accomplished with potentials leading to subband spacings often smaller than a few meV, the order of magnitude of the Fermi energy in low-dimensional systems. As a consequence, multiple subbands are populated and channel mixing effects become relevant in many situations. In fact, the Rashba interaction itself includes an intersubband mixing term which couples adjacent subbands with opposite spins, Eq. (1.19). This coupling has been recently demonstrated to give rise to strongly modulated conductance curves [She04, Zha05b, San06, Lop07], as
shown in the preceding chapter with the conductance dip and polarization of the output current. In presence of in-plane magnetic fields, the intersubband mixing effects induced by the Rashba coupling are shown [Ser05] to reduce the visibility of anomalous conductance steps [Per04] and to produce transmission asymmetric line shapes even in purely one-dimensional systems [San08]. The opposite 2D limit of vanishing transverse confinement was studied for spintronics transport by holes in [Pal04], confirming for this case the feasibility of the spin-transistor effect, and, more recently, in Refs. [Zai10] and [Agn10] to analyze the experiments by Koo et al. [Koo09].

In this chapter, we analyze the role of intersubband coupling effects in multichannel quantum wires. Our model consists of a quantum wire with localized Rashba spin-orbit interaction coupled to ferromagnetic leads with magnetization perpendicular to the direction of the Rashba field, Eq. (1.7),

\[ \mathcal{H} = -\frac{\hbar^2}{2m_0}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right) + \frac{1}{2}m_0\omega_0^2y^2 + |\Delta(x)| + \Delta(x)\hat{n} \cdot \vec{\sigma} + \mathcal{H}_R, \tag{3.1} \]

where the Rashba coupling \( \mathcal{H}_R \) and the Zeeman field modeling polarized leads \( \Delta(x) \) are described in Sec. 1.2. Using the coupled channel method (Subsec. 1.2.1), expanding in transversal modes, the Rashba interaction contains two terms [Eqs. (1.19) and (1.20)],

\[
\langle ns | \mathcal{H}_R^{(1)} | n's' \rangle = \frac{\alpha(x)}{\hbar} \langle n | p_y | n' \rangle \langle s | \sigma_x | s' \rangle, \tag{3.2} \\
\langle ns | \mathcal{H}_R^{(2)} | n's' \rangle = \left[ -\frac{\alpha(x)}{\hbar}p_x + i\frac{\alpha'(x)}{2}\delta_{nn'} \langle s | \sigma_y | s' \rangle \right], \tag{3.3} 
\]

the intersubband mixing term in Eq. (3.2) and the precession term in Eq. (3.3), where the first one couples adjacent states (transversal modes) with opposite spin and the last one couples the electron motion with its own spin (the Data and Das scenario).

This chapter is split into two parts: in the first one, Sec. 3.1, we study the energy dependence of the conductance and polarization; on the other hand in Sec. 3.2 the interest is on the oscillating conductance of the Datta-Das transistor, i.e., the conductance as a function of the Rashba strength for different configurations of the polarized leads (parallel and antiparallel) along \( x \) and \( y \) directions, and how the multichannel regime modifies this conductance. This section discusses also multichannel effects in spin polarization of the output current as well as the influence of smooth interfaces for the Rashba region.
3.1 Energy dependence

In order to follow the same structure of the previous chapter and to study how the conductance plateaus are modified by the polarized leads, firstly the energy dependence of the conductance and polarization is given in this section. We will distinguish the parallel configuration from the antiparallel one for the spin orientations in $x$ and $y$: $xP$, $xAP$, $yP$ and $yAP$.

**Conductance**

Figure 3.1 displays a comparison of conductances as a function of energy. Black symbols correspond to the results without Rashba coupling while open symbols are for an intensity of $\alpha_0 = 0.3\hbar\omega_0\ell_0$. In the absence of spin-orbit coupling the conductance is characterized by a staircase appearance; each step corresponding to the activation of additional transverse modes. In P configurations steps for up and down spins are shifted by an energy $2\Delta_0$ and, therefore, the conductance jumps by $G_0$ from one step to the next. In the AP case the corresponding increments are doubled, $2G_0$. With the addition of the Rashba coupling (open symbols) we see that in general the conductance displays more oscillation. As a reminiscence of the perfectly clean wires we refer to the energy interval $[n-1/2, n+1/2]\hbar\omega_0$ as the $n$-th conductance plateau. Looking, for instance, at the result for polarization along $x$-axis for the second plateau $[1.5, 2.5]\hbar\omega_0$ we see at the beginning Fano oscillations followed by a sudden increase in conductance for $E \approx 1.9\hbar\omega_0$. Interestingly, a pronounced conductance dip can be seen at the end of the plateau. This is again a Fano resonance but is qualitatively different from those seen at the beginning of the plateau. It originates in a quasibound state shifted by a negative energy from the next plateau by the Rashba coupling. Notice that this is different with respect to the Fano resonances at the beginning of the plateau which stem from quasibound states induced by the polarized contacts. These wire conductance structures are repeated almost regularly in each plateau. Anticipating the stripe case of Chap. 4, Fig. 4.2, we notice that the wire conductance for each conductance plateau resembles the result of the stripe.

Turning to the results for configuration of polarization along $y$ orientation, right column of Fig. 3.1, the Fano oscillations at the beginning of the plateaus are absent while those at the end are still present. It is also worth mentioning that the $yAP$ configuration displays the less-structured conductance of all, the Rashba interaction only inducing dips at energies $E \approx (n + 1/2)\hbar\omega_0$ in this case.
Figure 3.2: Conductance for polarization of the contacts along $x$ (left panels) and $y$ (right panels). Upper and lower rows correspond to parallel (P) and antiparallel (AP) orientations, respectively. We take $\ell = 8\ell_0$ (length of the Rashba region), and $\Delta_0 = 0.2\hbar\omega_0$. Black symbols are for vanishing Rashba coupling while open ones correspond to $\alpha_0 = 0.3\hbar\omega_0\ell_0$.

Polarization

Figure 3.2 displays the energy dependence of the polarization $p$ for selected cases to illustrate the polarization mechanism of the localized Rashba coupling. The stripe is characterized by its full polarization $|p| = 1$ for energies below the Zeeman gap $2\Delta_0$. When exceeding this threshold, the polarization decreases in absolute value and tends to zero for high enough energies. Ramanauer oscillations, discussed in Sec. 4.2 in more detail, can be clearly seen for energies slightly above threshold. Comparing black and open symbols, we notice that the main effect of the Rashba interaction (open symbols) in the stripe geometry is to smooth the transition from full to vanishing polarization in AP configuration.

Focusing on this wire polarization of the transmitted current, the P configuration is characterized by a transition from high absolute polarization at the beginning of the plateau to low polarization towards the plateau end. There is an overall tendency to decrease the polarization when the energy increases.
3.2 Multimode spin transistor

Now we focus our attention on the variations of the conductance with the Rashba strength, $\alpha_0$. Figure 3.3 shows the results for polarized leads oriented along $x$. When $\mathcal{H}_R^{(1)}$ is neglected, intersubband mixing term Eq. (3.2) van-
Figure 3.3: Conductance as a function of Rashba coupling intensity. Black corresponds to the complete Rashba interaction while red-gray to the neglect of $\mathcal{H}_R^{(1)}$. The leads are spin-polarized along $x$ in parallel and antiparallel orientations for left and right panels, respectively. Upper, intermediate and lower panels correspond to $N_p = 1$, 5 and 10 propagating modes, respectively. We take the parameters $\ell = 8\ell_0$, $E = N_p\hbar\omega_0$, $\Delta_L = \Delta_R = 10\hbar\omega_0$, $d_L = d_R = 10\ell_0$, $a = 0.1\ell_0$.

ishes, and the conductance for 5 and 10 propagating modes displays an almost sinusoidal behavior with only minor distortions. These deviations, which are enhanced in the single mode case, can be attributed to the quantum interference with the Rashba dot [San06]. The present results confirm, therefore, the precession scenario mentioned above but only when the number of modes is large enough and interband coupling is neglected. Quite remarkably, however, this scenario is not robust with the inclusion of $\mathcal{H}_R^{(1)}$. When the full Rashba interaction is considered only for small values of $\alpha_0$ the conductance behaves in a regular way. Very rapidly as $\alpha_0$ increases $G$ fluctuates in a staggered way that resembles the conductance fluctuations of disordered systems. The mean value, in units of $G_0$, is $\approx 0.5N_p$, with $N_p$ the number of active channels, while the amplitude of the fluctuation decreases when $N_p$ increases. A similar decreasing behavior was obtained in Refs. [Pal04, Agn10, Zai10] for a vanishing $\omega_0$, but without the disordered fluctuations at strong $\alpha_0$'s due to the absence of interband coupling in the purely 2D geometry.
The existence of the first conductance minimum has been clearly seen in the experiments of Ref. [Koo09], black symbols right panel in Fig. 1 of the Preface. Our results are in agreement with this experiment, but they also predict that successive maxima and minima are heavily distorted or even fully washed out. It is also worth noticing that the first conductance minimum for the black dots occurs at a slightly lower value of $\alpha_0$ than that of the red-gray data, indicating that the minima $\alpha_{\text{min}}$ are somewhat contracted with respect to the simple prediction from the Rashba dot length: $2m_0\ell\alpha_{\text{min}} = n\pi\hbar^2$, with $n = 1, 2, \ldots$ (red-gray symbols).

Right panels of Fig. 3.3 contains the results for polarized leads along $x$ but in antiparallel directions. In this case, when $\alpha_0 \approx 0$ the conductance vanishes due to the spin valve effect. As $\alpha_0$ increases, however, the conductance rises and the spin valve effect is effectively destroyed by the presence of the Rashba dot. For big enough values the system behaves similarly to the case of parallel polarized leads (left panels in same figure), displaying irregular oscillations around a mean value $\approx N_p/2$. For strong spin-orbit couplings and high number of modes no clear distinction between parallel and antiparallel orientations is then to be expected. This is a consequence of the strong subband mixing. In fact, if $\mathcal{H}_R^{(1)}$ is neglected (red-gray symbols) there is a full correspondence between the conductance nodes of the parallel geometry with the maxima of the antiparallel one; as could expected from the simplified rigid precession scenario.

The above results are not modified if other values of $\Delta_{L,R}$ are used, provided they are large enough to ensure full polarization of the leads. The same is true for distances $d_{L,R}$. They should be large enough to allow the decay of evanescent states at the interfaces with the Rashba dot and at the points where Zeeman fields are switched on.

We consider next polarized leads along $y$ and $z$; that is, in directions that are perpendicular to the quantum wire. For $z$ polarizations the results are very similar to the $x$ ones already discussed and thus will not be shown. Figure 3.4 contains the results for $y$-polarized parallel and antiparallel leads. A first conspicuous difference with the results of Fig. 3.3 is that the red-gray symbols do not display wide sinusoidal oscillations. The conductance when $\mathcal{H}_R^{(1)}$ is neglected is actually maximal for the parallel case and stays rather constant with some small oscillations at large $\alpha$’s that disappear when the number of channels increases. On the other hand, $G$ vanishes for the antiparallel orientation. We understand this spin-valve behavior as a complete absence of spin precession, resulting from the fact that $\mathcal{H}_R$ is spin diagonal in this approximation [cf. Eq. (1.20)].

Including $\mathcal{H}_R^{(1)}$ in the $y$-polarized geometry again yields qualitative modifica-
Figure 3.4: Same as Fig. 3.3 for parallel (left panels) and antiparallel (right panels) polarized leads along $y$.

The Rashba coupling is thus quite effective in allowing transmission by flipping spins of the polarized incoming electrons towards the opposite spin orientation of the outgoing ones. The single channel limit (upper right panel of Fig. 3.4) is obviously an exception since even the black symbols vanish in this case. This is easily understood noticing that the incident $ns = 1+$ mode couples in the Rashba dot with modes $2-, 3+, \ldots$, but not with $1-$, which is the only propagating mode in the right lead. Therefore, no conduction is possible under this conditions.

Experimentally, the absence of conductance oscillation in the parallel $y$-oriented configuration has been confirmed [Koo09], second lower curve in Fig. 1 of the Preface. Our results reproduce that behavior (Fig. 3.4) and they also suggest the antiparallel $y$ orientation as an interesting configuration for a spin-orbit-controlled device. Indeed, the initial rise of conductance in the
Figure 3.5: Conductance as a function of $\alpha_0$, for partial polarized leads. The polarization of the contacts is indicated giving the number of propagating down and up spin modes, $(N_-, N_+)$. 

The Datta-Das spin transistor relies on the oscillatory character of the conductance as a function of Rashba intensity. An interest analysis is the robustness of the oscillations in the regime of the partially polarized contacts ($E > 2\Delta_0$), where both spins can propagate. In the wire we always have an integer number of spin-down and spin-up propagating modes $(N_-, N_+)$ and the approximate polarization is given by $|p| \approx (N_+ - N_-)/(N_+ + N_-)$. Of course, partial reflections and transmissions can lead to deviations from this simplified expression. Figure 3.5 shows the conductance as a function of Rashba strength for different degree of parallel polarization in the leads. At full polarization ($(N_-, N_+) = (4_, 0_+)$) there is a clear initial oscillation, but as $\alpha_0$ increases the conductance exhibits an irregular or disordered behavior. When the polarization is reduced the initial oscillation is heavily distorted. At large $\alpha_0$’s the region of irregular conductance is not qualitatively modified when the polarization is reduced.

The results shown above are not much modified if the interfaces with the Zeeman fields at distances $d_L$ and $d_R$ to the left and right of the Rashba
dot, respectively (see Fig. 1.1), are smoothed by increasing the corresponding Fermi-function parameter (see Eq. (1.12), Chap. 1). This confirms that the conductance modifications are an effect of the Rashba dot, and not of the Zeeman field interfaces. Indeed, the more diffuse the interface, the more reflectionless and thus more ideal is the description of the contact. In the next section we shall discuss the case of nonpolarized leads ($\Delta_0 = 0$), but we have also calculated some cases of partial polarization by decreasing $\Delta_0$ when both $s = +$ and $-$ transverse states are active, although their number is not perfectly balanced. We have found that the conductance is qualitatively similar to the fully polarized case, with irregular behavior at large values of $\alpha_0$.

### 3.2.1 Rashba polarizers

In Chap. 2 it was shown that a Rashba dot can act as a current polarizer, in such a way that when a non polarized current enters the dot from the left, the transmitted current to the right may attain an important degree of spin polarization in $y$ direction. For this to occur, we have seen that at least two propagating modes of opposite spin must interfere. In wires with parabolic transverse confinement this means that the energy should at least exceed $1.5\hbar\omega_0$ such that the four modes $\{1+, 1-, 2+, 2-\}$ are active and the interference occurs in subsets $\{1+, 2-\}$ and $\{1-, 2+\}$. The resulting spin polarization is very sensitive to the energy (see Fig. 2.2) and a large enhancement of the polarization $p$, Eq. (1.23) is obtained when the energy is such that a Fano-type resonance with a quasibound state from a higher evanescent band is formed. This type of resonances which lead to the Fano-Rashba effect was investigated in Ref. [San06]. The polarization of the transmitted current is zero if, instead of $y$, other direction for the quantization axis are chosen.

The preference for the transverse $y$ direction in polarization is an example of chirality induced by the Rashba interaction. This is possible even with a time-reversal invariant Hamiltonian such as Eq. (1.8) because our boundary condition (left incidence) is not time reversal invariant. Indeed, if we consider the time reversed boundary condition, i.e., incidence from the right, the current transmitted to the left is polarized in the opposite direction. The superposition of both solutions completely restores the symmetry without any preferred spin direction. The reversal of the polarization for the right-to-left transmission can be seen as a peculiar behavior of Rashba polarizers that makes them fragile in the presence of magnetic barriers like those of Sec. 3.2. Indeed, one could naively think that when the Rashba dot acts as a current polarizer the left-to-right transmission with $y$-magnetized leads should be very high in parallel configuration and very low in antiparallel configuration. This is not the case, however, because of multiple backwards and forwards reflections with their
3.2. MULTIMODE SPIN TRANSISTOR

Figure 3.6: Conductance $G$, black symbols with left scale, and polarization of transmitted current, red-gray symbols with right scale, as a function of the Rashba intensity. We have used the same parameters as in Fig. 3.3, except for the Zeeman fields which are here taken to vanish $\Delta_L = \Delta_R = \Delta_0 = 0$. Upper, intermediate and lower panel correspond to $N_p = 4$, 10 and 20 propagating modes, respectively.

In this section we assume nonmagnetic leads by taking $\Delta_{L,R} = 0$, i.e., vanishing Zeeman fields in Fig. 1.1, and analyze the evolution of the polarization and the conductance when the number of active channels increases. As shown in Fig. 3.6 upper panel, high polarizations $p$ are obtained for the minimal number of channels $N_p = 4$ and strong spin-orbit intensities $\alpha_0$. The clear correlation between $G$ and $p$, conductance minima correspond to maxima in polarization, indicate that this is an effect connected with the formation of quasibound states that tend to block the current for a given spin direction. When the number of channels is increased (lower panel of Fig. 3.6) both $G$ and $p$ show reduced staggering oscillations with increasing $\alpha$, as in Figs. 3.3 and 3.4. There is also an overall tendency to smoothly reduce $G$ and increase $p$ in a linear way with $\alpha$. With increasing number of channels the slopes of these straight lines are reduced and for $\alpha_0 \approx 2\hbar\omega_0\ell_0$ the polarization reaches the values $\approx 0.2$ and $\approx 0.1$ for 10 and 20 propagating channels, respectively.
In almost all cases the polarization is positive, indicating that the transmitted current is preferentially polarized along $+y$.

### 3.2.2 Smooth interfaces

In this subsection we discuss how the results are affected by the way in which the Rashba field is switched on spatially. For this, we vary the parameter $a$ in the Fermi functions describing the transitions shown in Fig. 1.1 (see Sec. 1.2). For large values of $a$ the edges are quite smooth and correspond to an *adiabatic* turn-on or turn-off in space. On the contrary, abrupt changes are given by the limit $a \to 0$. Our method is based on a grid discretization of the variable $x$ and its only requirement is that the grid should be fine enough to describe the spatial variations.

The results discussed above have been obtained using $a = 0.1\ell_0$, a rather small value describing abrupt transitions in space. We have checked that either using a smaller value $a = 0.05\ell_0$ or a larger value $a = \ell_0$ the behaviors of the conductance in the presence of polarized leads discussed, namely the staggering for high values of $\alpha_0$ and the modification due to intersubband coupling, are not qualitatively changed. Of course, it should be fulfilled that
the Rashba dot length $\ell$ is much greater than $a$ in order to still allow the transition to reach to the saturation value $\alpha_0$. More delicate is the polarization $p$ discussed in the preceding subsection and Fig 3.6. In Fig 3.7 we show the evolution with $a$ of $G$ and $p$ when $N_p = 5$ channels are propagating in the wire. The polarization vanishes when $a$ increases, indicating that smooth edges do not favor the appearance of polarized currents. In this diffuse-edge limit the conductance takes the maximal value $G = N_p G_0$ as in a purely ballistic wire without any Rashba dot. The evolution for $\alpha_0 = \hbar \omega_0 \ell_0$ (upper panel) is quite smooth but for $\alpha_0 = 2 \hbar \omega_0 \ell_0$ (lower panel) superimposed to the overall behavior we find irregular maxima and minima as in previous results.
Chapter 4

Two-dimensional limit

The lateral dimension of the transport channel in the experiments by Koo et al [Koo09] was several microns, which indicates a high degree of 2D character, thus deviating from the 1D or quasi-1D regimes. The 2D systems, without confinement in the transversal direction, has been also addressed in [Mat02, Kho04, Mar04, Pal04, She05, Agn10, Ent10, Zai10]. In most cases sharp transitions between the contacts and the channel are assumed and matching of the wave functions at the interfaces is the required condition. As an alternative, our approach assumes smooth transitions and describes transmission and reflection between contacts and channel from the numerical wave function, solution of the complete Schrödinger equation. Our purpose is to provide additional insight on the origin and characteristics of different types of conductance oscillations.

Here we extend the analysis of the previous chapter to the case of vanishing transverse confinement. We thus focus our interest on a two dimensional electron gas (2DEG) with a stripe of spin-orbit interaction perpendicular to the electronic transport and polarized leads. In Section 4.1 we describe the physical system. Section 4.2 discusses the dependence of the conductance and polarization on energy while the Datta-Das transistor configuration is studied in Sec. 4.3. Finally, in Sec. 4.5 we study how the results are affected by a position dependent effective mass.

4.1 Physical system and model

We consider a semiconductor 2DEG in the $xy$-plane with a region of Rashba spin-orbit interaction shaped like an infinite stripe of width $\ell$ oriented along $y$. This case corresponds to the previous system confined by the harmonic
oscillator in the limit of \( \omega_0 \to 0 \).

Figure 4.1a shows a sketch of the physical system. Transport is along \( x \) and the asymptotic leads (contacts) are assumed to be spin polarized along a given direction \( \hat{n} \). The system Hamiltonian reads

\[
\mathcal{H} = -\frac{\hbar^2}{2m^*_0} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + \Delta(x) \hat{n} \cdot \vec{\sigma} + |\Delta(x)| + \mathcal{H}_R, \tag{4.1}
\]

where \( \mathcal{H}_R \) is the well known Rashba Hamiltonian,

\[
\mathcal{H}_R = \frac{\hbar}{2} \left( \alpha(x)p_y \sigma_x - \frac{1}{2} \{\alpha(x), p_x\} \sigma_y \right), \tag{4.2}
\]

polarized leads in direction of \( \hat{n} \) are described by means of a Zeeman field \( \Delta(x) \) and we introduce the scalar potential \( |\Delta(x)| \) in order to align the potential bottom. Such potentials are used in the order to define the spin-dependent potential \( v_s(x) = s\Delta(x) + |\Delta(x)| \) (where \( s = \pm \) spin). Both potentials \( \Delta(x) \) and \( v_s(x) \) are described in Chap. 1.

In Eq. (4.1) the functions determining the Hamiltonian are \( \Delta(x) \) and \( \alpha(x) \). These quantities take a constant value in the three parts of our system: left contact (L), central region and right contact (R), and they vary smoothly, described by a Fermi-type function, at the interfaces, Eqs. (1.10)-(1.12).

We denote by \( m^*_0 \) the conduction-band effective mass of the semiconductor and by \( \alpha_0 \) the Rashba intensity of the central region. Figure 4.1b) shows the variation of the Rashba intensity \( \alpha(x) \). It also sketches the potentials \( v_s(x) \), for \( s = \pm \) spins. We remark that in the P configuration (\( \Delta_L = \Delta_R = \Delta_0 \)) the \( s = - \) spin sees no potential at all while \( s = + \) is confined by a potential well of width \( d \). On the contrary, in the AP configuration (\( \Delta_L = -\Delta_R = \Delta_0 \)) both spins feel a potential step, but in opposite contacts. As we will discuss below, these differences in potential landscape for \( + \) and \( - \) spins greatly influence the transport properties of the stripe with polarized contacts.

In the absence of transversal confinement the energy unit \( E_U \) can be chosen in two ways (once \( E_U \) is fixed, the length unit \( L_U \) is also fixed as explained in Appendix A): \( E_U = \Delta_0 \) and \( E_U = E \) (Fermi energy). See Appendix A for more details.

Asymptotically, in the 2D contacts, the Hamiltonian eigenfunctions factorize as a plane wave times a spinor in the direction of \( \hat{n} \),

\[
\Phi_{cs}(\vec{r}, \eta; \vec{\kappa}_{cs}) = \exp \left( i\vec{\kappa}_{cs} \cdot \vec{r} \right) \chi_s(\eta), \tag{4.3}
\]

where \( c = L, R \) and \( s = \pm \) are labeling contact and spin, respectively. The wavenumber \( \vec{\kappa}_{cs} \equiv (k_{cs}, q_{cs}) \) is composed of the longitudinal \( (k_{cs}) \) and transverse \( (q_{cs}) \) components. Anticipating a result emphasized below, we note that
the transverse momentum is a good quantum number of the system Hamiltonian, Eq. (4.1). Therefore, $q_{cs}$ must be a characteristic of the wave function not only in an asymptotic region $c$ and for a given spin $s$, but throughout the system, i.e., $q_{cs} \equiv q$. At a given Fermi energy $E$ we then have

$$\kappa_{cs}^2 = k_{cs}^2 + q^2 = \frac{2m_0^*}{\hbar^2}(E - s\Delta_c - |\Delta_c|).$$

Figure 4.1: Sketch of the physical system (a) and of the spatial variation of Rashba intensity $\alpha(x)$ (b) and of the spin-dependent potentials $v_\pm(x)$ (c,d). See Sec. 1.2.

The physically acceptable wave functions fulfill Schrödinger’s equation

$$(\mathcal{H} - E)\Psi = 0.$$  \hspace{1cm} \text{(4.5)}$$

A most general wave function can be taken as a sum on spins and over all transverse momenta (an integral in $q$, while in the transversal confinement we sum over all the transversal states)

$$\Psi(\mathbf{r},\eta) = \sum_{s = \pm} \int dq \psi_{qs}(x) e^{iqy} \chi_s(\eta),$$

where the unknown functions $\psi_{qs}(x)$ can be interpreted as the wave amplitudes in each channel given by $(qs)$.

Projecting Eq. (4.5) we obtain the channel
amplitude equations

\[
\left( -\frac{\hbar^2}{2m^*_0} \frac{d^2}{dx^2} + \frac{\hbar^2 q^2}{2m^*_0} + v_s(x) - E \right) \psi_{qs}(x) + \sum_{s' = \pm} \left\{ \left( \alpha(x) q \langle s | \sigma_x | s' \rangle + \frac{i}{2} \alpha'(x) \langle s | \sigma_y | s' \rangle \right) \psi_{qs'}(x) + i \alpha(x) \langle s | \sigma_y | s' \rangle \frac{d}{dx} \psi_{qs'}(x) \right\} = 0. \tag{4.7}
\]

This equation is equivalent to Eq. (1.18) for infinite transversal momenta. Notice that the channel equations for different \(q\)'s are uncoupled due to the translational invariance of the system in the transverse direction. At a given \(q\), however, the two spin components do couple with each other due to the Rashba spin-orbit interaction. This coupling is described in Eq. (4.7) by the matrix elements \(\langle s | \sigma_{x,y} | s' \rangle\) which can not be diagonalized simultaneously. For any orientation of the spin quantization axis \(\hat{n}\), therefore, there is a Rashba-induced interference of the two spin projections. In the contacts the Rashba coupling vanishes and the wave function recovers the good spin eigenstates \(\Phi_{cs}\) given in Eq. (4.3).

Integration of Eq. (4.7) determines the transmission \(T_{s's}\), which represents an electron entering the system from the left contact with spin \(s\) and going to the right lead with spin \(s'\). It also gives \(T_{s's}\), i.e., from the right contact with spin \(s\) to the left one with spin \(s'\). In terms of these transmissions the total current \(I_x\), per unit of length in the transverse direction \(L_y\), can be obtained by adding up the contributions of all electrons in each contact [Fer97],

\[
\frac{I_x}{L_y} = \frac{e}{(2\pi)^2} \int_{k>0} d^2 \kappa m^*_0 \sum_{ss'} f^{(+)}_{Ls} (\kappa) T_{s's} (\kappa) + \frac{e}{(2\pi)^2} \int_{k<0} d^2 \kappa m^*_0 \sum_{ss'} f^{(-)}_{Rs} (\kappa) T_{s's} (\kappa). \tag{4.8}
\]

In Eq. (4.8), \(f^{(\pm)}_{cs} (\kappa)\) represents the distribution function of electrons in contact \(c\) with spin \(s\), with the upper index indicating right (+) or left (−) direction of motion of the corresponding electron. The distribution of electrons in each contact is given by a Fermi function, characterized by a given chemical potential \(\mu_c\). In the linear response regime the bias \(\delta V = \mu_R - \mu_L\) is very small and it is enough to retain the linear conductance \(I_x = G\delta V\). From Eq. (4.8) we
find the conductance per unit of transverse length

\[
\frac{G}{L_y} = \frac{G_0}{4\pi} \sum_{ss'} \left\{ \kappa_{Ls} \int_{-\pi/2}^{\pi/2} d\theta |\cos \theta| T_{s's}(\kappa_{Ls}, \theta) \right. \\
+ \left. \kappa_{Rs} \int_{\pi/2}^{3\pi/2} d\theta |\cos \theta| T'_{s's}(\kappa_{Rs}, \theta) \right\},
\] (4.9)

where \( G_0 = e^2/h \) is the conductance quantum and \( \kappa_{cs} \) is the Fermi wavevector in contact \( c \), given by Eq. (4.4) when \( E \) is the corresponding Fermi energy.

### 4.2 Numerical energy dependence

**Conductance**

Figure 4.2 show typical results obtained numerically from Eq. (4.9) for \( x \)- and \( y \)-polarized contacts. The case of polarization along \( z \) is similar to the \( x \) one. For each direction \((x \text{ and } y)\) we also compare the situation of parallel and antiparallel Zeeman fields in the contacts.

For a vanishing Rashba field the transmissions can be obtained analytically. If, in addition to \( \alpha_0 = 0 \), the Zeeman fields also vanish \((\Delta_0 = 0)\), the transmissions trivially become one and the exact conductance is then

\[
\frac{G}{L_y} = G_0 \frac{2}{\pi} \sqrt{\frac{2m_0^*E}{h^2}}.
\] (4.10)

When \( \Delta_0 \neq 0 \) we have to distinguish P and AP configurations. The P case is characterized by a perfect transmission of the \(-\) spin, while the \(+\) spin feels the \( v_+ \) potential of Fig. 4.1. Therefore, its transmission switches on only when \( E > 2\Delta_0 \). When this occurs, the underlying potential well makes the transmission of the \(+\) spin oscillate with energy, even with vanishing spin-orbit. Following Ref. [Cah03], we call these variations Ramsauer oscillations, in analogy with the Ramsauer effect in electron scattering [Sch85]. The importance of these oscillations was pointed out in Ref. [Mat02]. Notice also that with vanishing Rashba field the results for \( x \) and \( y \) orientations of the Zeeman fields are identical.

The energy \( 2\Delta_0 \) signals the transition threshold from only one propagating spin when \( E < 2\Delta_0 \), to both spins when \( E > 2\Delta_0 \). At \( \alpha_0 = 0 \), the P conductance below threshold is given by a pure square root behavior, as in Eq. (4.10), while above threshold it shows Ramsauer oscillations of the minority spin transmission. The AP transmission is exactly zero below threshold \((\alpha_0 = 0)\) and above
it begins to increase smoothly, as expected for a spin valve. Note that the Ramsauer effect is not active in the AP configuration since the underlying potential is a step, instead of a well.

Turning now to the spin orbit effects, the most conspicuous one is that for \( E < 2\Delta_0 \), when the contacts are fully polarized, the Rashba field induces the appearance of oscillations in the \( xP \) and \( xAP \) configurations (Fig. 4.2). As we will discuss in detail in the next subsection, these oscillations are due to resonant Fano interferences between the propagating spin and the quasibound states of the opposite evanescent spin. They are qualitatively similar to the Fano-Rashba interferences discussed in Ref. [San06] for quantum wires which we showed in Sec. 2.1. Here, however, the quasibound states are caused by the polarized contacts and not by the Rashba field itself. In the \( y \) orientation, the Fano oscillations below threshold are absent, and only some small variation from the vanishing spin-orbit case can be seen. In general, as shown in Fig. 4.2, for the \( P \) configuration the results with Rashba coupling (red-gray curve)
are slightly below the results without spin-orbit (black curve); while for the AP configuration the situation is reversed.

### 4.2.1 The ansatz model

Let us focus our attention on the oscillations that appear in the fully-polarized-current case, when \( E < 2\Delta_0 \), both in parallel and antiparallel configurations. The upper panel of Fig. 4.3 shows the transmission for vanishing transverse momentum in xP configuration, in comparison with the total transmission obtained by integrating over angle \( \theta \) in Eq. (4.9). We clearly see that the oscillations in \( G \) are due to the deep minima in the transmission for \( q = 0 \). Besides, the position of these minima coincide with the energies of the bound states in the \( v_+ \) potential (dashed lines). At finite \( q \)'s, not shown in the figure, the transmission minima are shifted or they can even disappear. Physically, we indeed expect the \( q = 0 \) contribution to dominate the conductance since in this case all the available energy is used in the longitudinal wavenumber. The present transmission minima are examples of Fano resonances due to the interference with quasibound states. To better understand this behavior this subsection presents a simplified model involving the quasibound states in an explicit way.

Assuming \( q = 0 \) and xP configuration Eq. (4.7) transforms to

\[
\left(-\frac{\hbar^2}{2m_0^*} \frac{d^2}{dx^2} - E\right) \psi_- = V_m \psi_+ , \tag{4.11}
\]

\[
\left(-\frac{\hbar^2}{2m_0^*} \frac{d^2}{dx^2} + v_+ - E\right) \psi_+ = -V_m \psi_- , \tag{4.12}
\]

where we have defined the gradient-dependent mixing potential \( V_m \equiv \alpha'(x)/2 + \alpha(x)d/dx \). Equations (4.11) and (4.12) constitute a two-channel model, where \( \psi_- \) is propagating while \( \psi_+ \) is evanescent, with a localized mixing described by \( V_m \). Similar models were obtained for impurities in quantum wires, where semianalytical solutions were worked out using Green functions [Gur93] or the ansatz by Nockel and Stone [Noc94].

Following Ref. [Noc94] let us make the following ansatz for the evanescent channel amplitude

\[
\psi_+(x) = \sum_n A_n \phi_n(x) , \tag{4.13}
\]

where the \( A_n \)'s are constants and the \( \phi_n \)'s are the bound state wave functions obtained by neglecting interchannel mixing in Eq. (4.12)

\[
\left(-\frac{\hbar^2}{2m_0^*} \frac{d^2}{dx^2} + v_+ - \varepsilon_n\right) \phi_n = 0 . \tag{4.14}
\]
Figure 4.3: Contribution with $q = 0$ to the linear conductance $G/L_y$. The vertical dashed lines signal the bound-state energies of the $v_+$ potential. Except for $\alpha_0 = 0.1 \alpha_U$, we have used the same parameters and units of Fig. 4.2. **Upper panel:** $q = 0$ conductance from Eq. (4.9). For comparison, the red-gray curve shows the full $G/L_y$ of Eq. (4.9). **Lower panel:** $q = 0$ conductance from the ansatz model. Solid and dashed lines are from Eqs. (4.19) and (4.20), respectively.

Notice that if $V_m$ is also neglected in Eq. (4.11) the propagating channel corresponds to a free particle in 1D. Then, in terms of the free-particle Green function, we may write the general solution of Eq. (4.11)

$$\psi_- = e^{ikx} + \frac{m_0^*}{i\hbar^2k} \int_{-\infty}^{\infty} dx' e^{ik|x-x'|}[V_m\psi_+]_{x'},$$  \hspace{1cm} (4.15)$$

where $k = \sqrt{2m_0E/\hbar}$ and $[V_m\psi_+]_{x'}$ denotes the action of the gradient-dependent potential on $\psi_+$ at point $x'$. Using now the ansatz (4.13) in Eq. (4.15), substituting in Eq. (4.12) and projecting on the set of bound states $\{\phi_n, n = 1, \ldots, N_b\}$ we obtain a matrix equation for the $A_n$’s

$$\sum_{n_2=1}^{N_b} [(\varepsilon_{n_1} - E)\delta_{n_1n_2} - M_{n_1n_2}] A_{n_2} = B_{n_1},$$  \hspace{1cm} (4.16)$$
where
\[ M_{mn} = \frac{m_0^*}{i\hbar^2 k} \int dx_1 dx_2 [V_m \phi_{n_1}]_{x_1} [V_m \phi_{n_2}]_{x_2} e^{ik|x_1 - x_2|}, \tag{4.17} \]
and
\[ B_{n_1} = \int dx [V_m \phi_{n_1}]_{x} e^{ikx}. \tag{4.18} \]

Taking the limit \( x \to \infty \) in Eq. (4.15) we find the amplitude of the transmitted wave
\[ t = 1 + \frac{m_0^*}{i\hbar^2 k} \sum_n A_n B_n^*, \tag{4.19} \]
and the corresponding transmission \( T = |t|^2 \). The solid line in Fig. 4.3 lower panel displays numerical results obtained by solving the matrix equation (4.16), showing clear transmission minima when the energy is close to a bound state. A more explicit role of the bound states can be seen neglecting nondiagonal terms of the matrix \( M \). In this case, the transmission amplitude reads
\[ t = 1 + \frac{m_0^*}{i\hbar^2 k} \sum_n |B_n|^2 \varepsilon_n - E - M_{nn}. \tag{4.20} \]

When \( E \approx \varepsilon_n \) the denominator in the right hand side of Eq. (4.20) reaches a minimum, thus yielding the mechanism by which the bound states produce deep minima in transmission. Notice also that \( M_{nn} \) plays the role of a complex “self energy” that slightly distorts the position of the minima. Nevertheless, displacements of the dips from the bound state energies are hardly seen for weak Rashba couplings since \( M_{nn} \approx \alpha_0^2 \). It can also be shown that the relation \( \text{Im} (M_{nn}) = -m_0^* |B_n|^2 / \hbar^2 k \) is fulfilled and that this implies an exactly vanishing conductance at the dip energies.

In the AP configuration no potential well explicitly appears in the Hamiltonian, as shown is the lower panel of Fig. 4.1. Nevertheless, the results of Fig. 4.2 prove that the \( x \)AP configuration also shows clear oscillations, with conductance dips in similar positions to the \( x \)P-polarized case. We can explain this quasibound states as a result of the combination of two effects: a) the reflection on the potential steps in \( v_+ \) and \( v_- \); and b) the Rashba induced spin flip. Indeed, adequately combined, the reflection and the spin flip may lead to a trapped state of the electron. Mathematically, we could describe this mechanism by transforming the Hamiltonian with a local spin rotation \( D(x) = e^{-i\sigma_z \phi(x)} \), where \( \phi(x) \) evolves from zero in the left contact to \( \pi \) in the right one. In the transformed problem one component is then effectively bound by the two original potential steps. The transformation is rather cumbersome, however, due to the noncommutation of the kinetic term with \( \phi(x) \), in addition to the also noncommuting Pauli matrices.
In the $y$ orientation of the contacts there is no coupling between $+$ and $-$ spins for $q = 0$, as immediately noticed from the term $\alpha(x)q\langle s|\sigma_{x}|s'\rangle$ of Eq. (4.7). This explains why there are no clear Fano oscillations for energies below threshold. The minor features, can be attributed to the Rashba-induced coupling for finite $q$’s.

Polarization

Figure 4.4 displays the energy dependence of the polarization $p$ for selected cases to illustrate the polarization mechanism of the localized Rashba coupling. The stripe is characterized by its full polarization $|p| = 1$ for energies below the Zeeman gap $2\Delta_0$. When exceeding this threshold, the polarization decreases in absolute value and tends to zero for high enough energies. Ramsauer oscillations can be clearly seen for energies slightly above threshold. Comparing black and red-gray symbols, we notice that the main effect of the Rashba interaction (red-gray symbols) in the stripe geometry is to smooth the transition from full to vanishing polarization in AP configuration.

4.3 Spin transistor in a 2DEG

The Datta-Das transistor [Dat90] relies on the oscillatory character of the conductance as a function of the Rashba intensity $\alpha_0$. In this section we discuss
4.3. SPIN TRANSISTOR IN A 2DEG

Figure 4.5: Conductance as a function of Rashba coupling intensity for polarization along $x$ and $y$ in P and AP configurations. Solid and open symbols are, respectively, the results with and without the Rashba mixing term $\alpha(x)p_y\sigma_x$ of Eq. (4.2). Differently to the preceding figures, we take here the Fermi energy $E$ as energy unit, with a corresponding length unit $L_U = \sqrt{\hbar^2/m^*_0 E}$. The Rashba-coupling unit is then $\alpha_U = \sqrt{\hbar^2 E/m^*_0}$. The remaining system parameters are: $d = 20\sqrt{5} L_U$, $\ell = 8\sqrt{5} L_U$, $\Delta_0 = 20 E$.

the dependence on $\alpha_0$, considering first fully polarized contacts ($E < 2\Delta_0$) and, subsequently, partial polarization at the end of the section. The fully polarized results agree overall with other theoretical analysis[Pal04, Agn10, Zai10] and, qualitatively, with the experiments of Koo et al. [Koo09], lower line in the right panel of Fig. 1 in the Preface. Quite surprisingly, however, the oscillatory character of the conductance is rapidly washed out if partial polarization is considered in our model by increasing the energy above the Zeeman threshold $E > 2\Delta_0$.

Left column in Fig. 4.5 shows the results of our model for fully polarized leads with spin oriented along $x$. Upper and lower panels correspond, respectively, to $xP$ and $xAP$ configurations. In each case, solid symbols represent the results for the full Rashba Hamiltonian while open symbols correspond to the neglect of the mixing term. The conductance shows a damped sinusoidal behavior in both cases, with decreasing amplitude as $\alpha_0$ rises. These results agree with the expected Datta-Das behavior and, therefore, confirm the precession scenario in the continuum 2D case. Similar damped oscillations were obtained in Refs. [Pal04, Agn10, Zai10]. Notice also that this damping is due to the Rashba mixing since it is absent in the open symbols. The oscillation period changes with the distance $\ell$ and successive minima approximately fulfill the spin precession condition $\ell\alpha_0 = n\pi\hbar^2/m^*_0$, with $n = 1, 2, \ldots$. In AP configuration the conductance vanishes when $\alpha_0 = 0$ as a consequence of the spin mismatch between both contacts, known as spin-valve behavior. In the presence of Rashba
coupling, however, the spin valve behavior is destroyed and we observe that the conductance rapidly increases with $\alpha_0$, at small couplings, and then oscillates in a similar way to the P case (Fig. 4.5 lower panel).

For polarized leads along $z$ the results are very similar to those already discussed for polarization along $x$ and, thus, they will not be shown. On the contrary, right panels of Fig. 4.5 corresponds to the configurations along $y$. As before, upper and lower panels are for $yP$ and $yAP$ configuration while solid and open symbols represent the cases with and without band mixing, respectively. In this case the conductance oscillations are almost absent, specially in the $yP$ arrangement (upper panel), a result that agrees with the experiments [Koo09] (second lower line in right plot of Fig. 1 in the Preface) and with the precessing spin scenario [Dat90]. The $yP$ conductance decreases very slowly with $\alpha_0$ and the effect of mixing is minimal, around a 10% decrease. In $yAP$ orientation we see how the Rashba mixing term again destroys the spin-valve effect at finite $\alpha_0$’s and we observe a small increment in conductance as the Rashba intensity increases. In this configuration there is a reminiscence of the oscillating behavior although much weaker as compared with the $x$ or $z$ orientations.

We turn now to the partially polarized cases, when the energy condition $E > 2\Delta_0$ allows both spins to propagate in the contacts. First notice that the polarization in a given contact $c = L, R$ is given by

$$p_c(E, \Delta_c) = \begin{cases} 
-\frac{\Delta_c}{E - |\Delta_c|} & (E \geq 2|\Delta_c|), \\
-\frac{\Delta_c}{|\Delta_c|} & (E \leq 2|\Delta_c|),
\end{cases} \tag{4.21}$$

where, as already mentioned in Sec. 4.1, we define $(\Delta_L, \Delta_R)$ to be $(\Delta_0, -\Delta_0)$ in the P configuration and $(\Delta_0, -\Delta_0)$ in the AP configuration and $\Delta_0$ is assumed positive. The $xP$ results for partial polarizations are presented in Fig. 4.6. Notice that the oscillatory behavior is greatly quenched when the polarization is decreased, being heavily damped at $|p| = 0.5$ and totally washed out at $|p| = 0.2$. Thus, at low polarizations, our model predicts a monotonous decrease of the conductance with the intensity of the Rashba coupling that is not consistent with the operation of the Datta-Das device [Dat90]. This result shows the importance of having a high degree of polarization in the ferromagnetic contacts for obtaining a robust sinusoidal behavior.

The above results are not substantially modified when using other system parameters, such as changing the energy or the distance between the leads $d$. The monotonous decrease of the conductance, without oscillations, at low polarizations is also seen in $xAP$, $yP$ and $yAP$ configurations.
4.4 Comparing quasi-1D with 2D

As mentioned along the thesis, this chapter is understood as the limit of vanishing transversal confinement in the quantum wire, i.e., $\omega_0 \to 0$. In order to emphasize this idea, in this section we discuss similarities and differences between both systems: wire (referring to harmonic transversal confinement with a Rashba dot) and stripe (corresponding to the bidimensional system with a Rashba stripe).

As we have seen, the units are not the same for both systems; nevertheless the results can be compared in a qualitative way from the graphs of this chapter and the previous one. The limit of vanishing confinement potential affects, in addition, the resolution method and its treatment. The discrete set of transversal modes in the quantum wire (causing the step-like behavior of the conductance) becomes a continuum and the sum over all the infinite transversal modes becomes an integral in the two-dimensional case. This difference is seen in the expansion of the eigenfunction of the Schrödinger equation in terms of the transversal modes (coupled channel method); the wire Eq. (1.14) has a sum for infinite transversal modes, while the stripe Eq. (4.6) has an integral for the transversal momenta $q$. As a consequence, the current as well as the conductance are defined per unit of transverse length $L_y$.

Looking at the energy dependence, we find than the conductance of the wire has a well-defined pattern that repeats itself in each plateau. For the $n$-th plateau the corresponding energy interval is $[n - 1/2, n + 1/2] \hbar \omega_0$, as consid-
CHAPTER 4. TWO-DIMENSIONAL LIMIT

In Chap. 3, comparing Fig. 3.1 (wire) and Fig. 4.2 (stripe) we identify the pattern in a given plateau with the behavior of the stripe, for any orientation of the lead polarization. The main difference between both systems is the Fano-Rashba dip [San06] introduced in Chap. 2 at the end of each conductance plateau, which is not present in the stripe. This dip still remains in the quantum wire with polarized leads. In \( xP \) and \( xAP \) configurations, Fano oscillations for fully polarized leads \( E < 2\Delta_0 \) both in stripe and quantum wire are present for ranges of energy \( \varepsilon_n < E < \varepsilon_n + 2\Delta_0 \), corresponding to the \( n \)-th plateau. Ramsauer oscillations are present just above the energy threshold \( E = 2\Delta_0 \) in the stripe and \( E = \varepsilon_n + 2\Delta_0 \) for \( n \)-th plateau in the wire.

For the current polarization we have a similar behavior to the conductance: for each energy plateau in the wire (Fig. 3.2), the polarization shape is the same than in the stripe (Fig. 4.4). The main difference between both systems is that while in the stripe the degree of polarization varies in a continuum way, in the wire this degree is quantized and depends on the number of propagating bands for each spin; this, along with reflections in the leads, causes oscillations in polarization.

Concluding this section, we refer to the conductance dependence on Rashba strength (Datta-Das transistor). Comparing the plots of wire, Figs. 3.3 and 3.4, and stripe, Fig. 4.5, we observe how both behaviors become identical as the number of propagating channels in the wire increases. In both cases, the sinusoidal behavior of the conductance vanishes when increasing the Rashba strength for \( xP \) and \( xAP \), no oscillations are allowed in \( yP \) and \( yAP \), while the spin valve effect is destroyed in AP configurations owing to the Rashba coupling. The main differences are found for a small number of propagating channels in the quantum wire; when fluctuations become stronger. In the limit of a large number of propagating channels in the wire, reached at high energies, both systems behave identically.

4.5 Space-dependent effective mass

In this section we investigate the relevance of having different effective masses in the semiconductor central region and the polarized contacts. Till now the contacts were considered semiconductor materials with a Zeeman field in a given direction. A generalization towards ferromagnetic materials in the contacts has to include the different effective masses of ferromagnet and semiconductor. As in Ref. [Mir02], we then consider the effective mass in the contacts is the bare electron mass \( m_0 \) while in the central region it is given by the conduction band effective mass of the semiconductor, \( 0.023m_0 \) for InAs and \( 0.063m_0 \) for GaAs. Our aim is not a realistic modeling of ferromagnetic con-
4.5. SPACE-DEPENDENT EFFECTIVE MASS

Figure 4.7: Same as Fig. 4.2 assuming the effective mass in the contacts is given by $m_c = 15m_0^s$ ($c = L, R$).

In the spirit of the model, we now use a generalized kinetic term with a position dependent effective mass $m(x)$,

$$ m(x) = m_L F(x, -d/2) + m_R [1 - F(x, d/2)] + m_0^s [F(x, d/2) - F(x, -d/2)], \quad (4.22) $$

The big jump in effective mass at the interface is smoothed using Fermi functions, $F(x, x_0)$, defined in Eq. (1.12) The presence of these effective-mass interfaces is an additional source of conductance oscillations, as compared to the discussion of the preceding sections. Indeed, in this case even the $\alpha_0 = 0$
conductance with fully polarized contacts displays Ramsauer oscillations, as shown by the black symbols in the upper panel of Fig. 4.7. Based on the preceding section results, the addition of the spin orbit coupling is expected to introduce new oscillations of Fano type due to the coupling with quasibound states. Surprisingly, both types of oscillations interfere destructively, specially in the vicinity of the polarization threshold $E = 2\Delta_0$, as shown by the red-gray symbols in Fig. 4.7 upper panel. Another conspicuous effect of the effective mass discontinuity is the big enhancement of conductance when the energy exceeds $2\Delta_0$. This is clearly noticed when comparing the upper panels of Figs 4.7 and 4.2.

The lower panel of Fig. 4.7 shows the $x$AP conductance with position dependent effective mass. As a difference with Fig. 4.2 (lower panel), there are Ramsauer oscillations due to the mass jumps for $E > 2\Delta_0$ even for a vanishing $\alpha_0$. Below threshold we find Rashba-induced oscillations that look very similar to the $x$P ones in the upper panel. For $y$ oriented contacts the results (not shown), as compared to those of right panels in Fig. 4.2, are also characterized by the appearance of clear Ramsauer oscillations below threshold in the $y$P configuration while in the $y$AP orientation the variations are much smaller.

A natural question to ask is whether the effective mass modification affects the conductance oscillations with $\alpha_0$ discussed in Sec. 4.3. This is addressed in Fig. 4.8 for the fully polarized $x$P configuration. There are small changes, of course, but the overall behavior with damped oscillations is well preserved. Another result we should check is the disappearance of the oscillations at partial polarizations of the contacts (Fig. 4.6). As proved by Fig. 4.8, this result is also robust with respect to effective mass changes. Actually, the quenching of the oscillations at partial polarization is enhanced when the mass in the contacts is taken to be the bare mass: already for $|p| < 0.8$ the conductance becomes monotonous, having only a slight decrease with $\alpha_0$.
Part I: Conclusions

In the first part of this thesis we have studied the ballistic electron transport in a quantum wire with a localized Rashba region. Firstly, we considered this system attached to normal leads. In this case, the conductance shows similarities with the staircase behavior typical of a clean quantum wire without scattering center, but some differences are present. The most conspicuous one is the appearance of a Fano-Rashba conductance dip [San06]. In addition, the Rashba dot acts as a polarizer for unpolarized incident current. Generation of spin polarized current is obtained above the onset of the second conductance plateau; this effect is interpreted as arising from the interference between propagating states from adjacent bands and opposite spins coupled via the Rashba inter-subband coupling term. Using a simple tight-binding model we put forward a simple description of the coupled-channel equations that correctly reproduces the effects observed in the numerical simulations. The interest of this behavior lies in the possibility of obtaining polarized current without external magnetic field.

We also studied the interference of Fano-Rashba dips for two tunable Rashba regions. The two conductance dips have been analyzed, finding how they interfere depending on the Rashba strength and the distance between both spin-orbit coupling regions. As a function of the separation, the two dips evolve from an anticrossing behavior at large distances to a crossing when the two regions are close. The physics has been interpreted in terms of a dip-dip coupling mediated by the wire’s evanescent modes.

Next step was focusing our attention onto the Datta and Das transistor [Dat90], motivated by the results of Koo et al. [Koo09]. This way, we considered the previous system attached to two polarized leads and performed two different lines of study, one corresponding to the energy dependence and the other to the oscillations with Rashba coupling. In this case, the spin splitting of the polarized contacts was modeled by means of position-dependent Zeeman fields.

In the energy dependence, we find two different conductance oscillations. For energies below the Zeeman energy gap, the spin selective barriers of the con-
tacts induce the formation of quasibound states. These quasibound states couple with propagating states via the Rashba coupling and manifest as Fano resonances of the conductance. These Fano resonances appear at the beginning of each conductance plateau. At the end of each plateau we also find a second class of Fano resonances; conductance dips due to quasibound states which are not induced by the polarized leads, but they originate in the Rashba interaction alone [San06]. For energies above the Zeeman gap the conductance shows Ramsauer oscillations due to the underlying potential. These behaviors are present in the energy range of each conductance plateau, like a periodic behavior. We have also discussed the variations for $x$ and $y$ orientation of the polarized contacts in both parallel and antiparallel configurations.

Motivated by the experiment [Koo09], we also studied the conductance as a function of the Rashba strength, focussing on the effects of the multichannel regime onto the paradigmatic one-dimensional transistor. These aspects are related to the intersubband coupling of the Rashba spin-orbit interaction, quite relevant for a better understanding of the physical mechanisms behind the spin transistors and spin polarizers.

Assuming the wire with the Rashba dot oriented along $x$, we analyzed next the transmission in the presence of polarized leads along $x$, $y$ or $z$, with increasing number of propagating channels as a function of Rashba strength. The evolution with Rashba intensity shows dramatic modifications when the Rashba intersubband coupling is included. These modifications are especially relevant at strong values of $\alpha_0$, where staggering oscillations of $G$ have been found. In general, only the first smooth oscillation of $G(\alpha_0)$ remains when the full Rashba interaction is considered, while successive ones are heavily distorted or even fully washed out. This behavior becomes dramatic when the incident current is not fully polarized, since for small polarizations even the first oscillation is damped. The spin-valve behavior is effectively destroyed by the Rashba dot and the conductance for both parallel and antiparallel leads is relatively high.

The role of Rashba dots as spin polarizers has been discussed and explicitly calculated assuming the leads to be nonpolarized. A smooth linear increase of the polarization with Rashba intensity has been observed in the multichannel case. In the limit of adiabatic transitions the polarization vanishes. These overall smooth behaviors are superimposed by irregular changes for high values of $\alpha_0$.

The limit of infinite transversal modes was also studied. This is the 2DEG case, where the Rashba region becomes a stripe. In the analysis of the conductance as a function of the Fermi energy, we identified two types of oscillations: Ramsauer oscillations due to discontinuities in the effective potential and effective
mass; and Fano oscillations due to the coupling with quasibound states. We find similar oscillations in each plateau of the wire system, evidencing a similar underlying physics. The comparison between both system was also presented.

Finally we have considered the case of space-dependent effective mass. The addition of mass jumps at the interfaces modifies the conductance oscillations; the energy dependence is quenched; a result that we attribute to a destructive interference between Fano and Ramsauer oscillations. Regarding the oscillations in conductance as a function of Rashba coupling, our main result is the rapid damping of the oscillations when the contacts are partially polarized. This oscillation quenching is even more pronounced when the effective mass increases in the contacts.
Part II

Hole transport
Chapter 5

Luttinger Hamiltonian in low dimensional hole systems

As discussed in Part I of this thesis, the spin-orbit interaction in semiconductor materials offers interesting possibilities of spin control in nanostructures. Furthermore, the Rashba-type SO is most promising due to its tunability. This spin-orbit coupling not only acts on the electron conduction band, but it also has a profound effect on the hole bands; in a semiconductor such as GaAs, this effect consists in a splitting of the topmost valence band (see Fig. 5.1) into different energy states with total angular momentum $j = 3/2$ and $j = 1/2$, separated by an energy gap $\Delta_0$ (spin-orbit gap). The hole transport is expected to provide new phenomena, as compared with electron transport, because of the total angular momentum of the high-energy holes with $j = 3/2$. In addition transport by holes is anisotropic; i.e., it varies with the orientation in space.

In this part of the thesis we study transport in a low dimensional hole-system. More precisely, our interest focusses on how hole transport in a quantum wire is affected by the presence of a Rashba spin-orbit coupling and an external magnetic field. These results are shown in Chap. 6 but, before that, in this chapter we make a brief introduction to the Luttinger $4 \times 4$ Hamiltonian used to describe the hole kinetic term in Sec. 5.1. This chapter last section, Sec. 5.2, presents the system as well as the resolution method we have used to numerically solve the Schrödinger equation.
Figure 5.1: Schematic picture of the conduction and valence bands of GaAs. In this semiconductor, the spin-orbit gap and energy gap are \( \Delta_0 = 0.341 \text{ eV} \) and \( E_0 = 1.519 \text{ eV} \), respectively.

5.1 Luttinger Hamiltonian

In the high-energy hole band the total angular momentum is \( j = 3/2 \), yielding a four-fold hole spin projection \( \eta = \pm 3/2, \pm 1/2 \). For hole energies below the energy gap \( \Delta_0 \) a very good characterization of the kinetic term is given by the \( 4 \times 4 \) Luttinger Hamiltonian [Lut56]. This is a well established description [Gol93, Kyr00, Win00, Har06, Cso08b, Cso09, Qua10] that does not take into account either conduction or \( j = 1/2 \) valence bands. In this section we make a brief qualitative discussion of the origin of this Hamiltonian. A detailed account can be found in Refs. [Win03, Fab07].

The kp model is derived from the Schrödinger equation for the Bloch functions, expanding the eigenfunctions in terms of the band-edge Bloch functions around band extrema. On the other hand, the envelope function approximation (EFA) can be seen as a sort of generalization of the kp model to the case in which slowly varying electric and magnetic fields, on the length scale of the lattice constant, are present. An interesting thing in the expansion of Bloch functions is the assumption of an intelligent basis, reflecting the symmetry of the bands, such as in s-like and p-like states. A better approximation than the direct application of perturbation theory, in order to solve the resulting equations from the kp model and EFA, is the reduction of the Hilbert space by treating perturbatively remote bands; this was proposed by Kane [Kan57, Kan80]. Owing to the high matrix dimensions, and the irrelevance of the remote conduction bands, the extended Kane model is usually reduced to the \( 8 \times 8 \) Kane model, whose Hamiltonian contains the mixing terms between the lower conduction
band and the two split higher valence bands with total angular momentum \( j = 3/2 \) and \( j = 1/2 \) (see a sketch in Fig. 5.1).

An additional simplification, valid in the limit of strong atomic spin-orbit interaction, \( \Delta_0 \to \infty \), assumes that the hole kinetic Hamiltonian can be further reduced to the \( 4 \times 4 \) Luttinger Hamiltonian \( \mathcal{H}^{(\text{kin})} \), containing only the valence band with \( j = 3/2 \). As an example, for GaAs, the SO gap is \( \Delta_0 = 0.341 \) eV, and the gap from valence to conduction band is \( E_0 = 1.519 \) eV, both much larger than the few meV energies typical of confined systems [Fer97, Dat02, Kod08, Qua10].

This full hamiltonian reads

\[
\mathcal{H}^{(\text{kin})} = \\
\begin{pmatrix}
-\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\| & -\frac{1}{2} C k^+ & -\frac{\sqrt{3} \gamma_1 k^+}{\hbar} & -\frac{\sqrt{3} \gamma_2 k^+}{\hbar} \\
-\frac{\hbar^2}{2m_0} (\gamma_1 - 2\gamma_2) k^2_\perp & -\frac{\hbar^2}{2m_0} (\gamma_1 - 2\gamma_2) k^2_\perp & \sqrt{3} \frac{\hbar^2}{2m_0} \gamma_2 k^+ & -\frac{3\sqrt{3} \gamma_2 k^+}{\hbar} \\
\frac{\hbar^2}{2m_0} (\gamma_1 - \gamma_2) k^2_\| & -\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\| & \frac{\sqrt{3} \gamma_1 k^+}{\hbar} & -\frac{\sqrt{3} \gamma_2 k^+}{\hbar} \\
\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\perp & -\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\perp & -\frac{\sqrt{3} \gamma_1 k^+}{\hbar} & -\frac{\sqrt{3} \gamma_2 k^+}{\hbar} \\
\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\perp & -\frac{\hbar^2}{2m_0} (\gamma_1 - \gamma_2) k^2_\perp & -\frac{\sqrt{3} \gamma_1 k^+}{\hbar} & -\frac{\sqrt{3} \gamma_2 k^+}{\hbar} \\
\frac{\hbar^2}{2m_0} (\gamma_1 - \gamma_2) k^2_\| & -\frac{\hbar^2}{2m_0} (\gamma_1 + \gamma_2) k^2_\| & -\frac{\sqrt{3} \gamma_1 k^+}{\hbar} & -\frac{\sqrt{3} \gamma_2 k^+}{\hbar}
\end{pmatrix}
\]

(5.1)

where \( m_0 \) is the bare electron mass; \( \gamma_1, \gamma_2, \gamma_3 \) and \( C \) are the kp parameters, all of them are material dependent; \( \hat{k} \) is the 3D wavenumber and \( k^2_\|, k_\pm \) and \( \hat{K} \) are given by

\[
k^2_\| = k_x^2 + k_y^2, \\
k_\pm = k_x \pm i k_y, \\
\hat{K} = k_x^2 - k_y^2.
\]

(5.2) \hspace{1cm} (5.3) \hspace{1cm} (5.4)

We shall assume GaAs parameters \( \gamma_1 = 6.85, \gamma_2 = 2.10, \gamma_3 = 2.90 \) and set \( C \) to zero to simplify the representation. We stress that \( C \) is too small to affect our results and that neglecting this parameter is a usual approximation, such as in [Gol93, Kyr00, Har06, Qua10]. The use of this \( 4 \times 4 \) Luttinger Hamiltonian for GaAs is well established in the literature [Gol93, Kyr00, Win00, Har06, Cso08b, Cso09, Qua10].
5.2 The system

Our system consists in a deformed hole quantum wire with homogeneous Rashba spin-orbit interaction in an external magnetic field with arbitrary orientation. The Hamiltonian contains three contributions: the kinetic, the Rashba spin-orbit coupling and the Zeeman terms.

We describe the anisotropic kinetic energies $H^{(\text{kin})}$ of the holes in the 4-band kp model introduced in the previous section, the Luttinger Hamiltonian of Eq. (5.1). We distinguish two different coordinate systems: one corresponding to the crystallographic axis given by $O = \{x, y, z\}$ in which the 3D wave vector $\vec{k}$ entering $H^{(\text{kin})}$ is defined; the other coordinate system is taken from the growth direction ($z'$) and the quantum wire orientation ($x'$), $O' = \{x', y', z'\}$, as pictured in Fig. 5.2a. This $O'$-axes are very important since not all wavevector components $\vec{k}$ have the same prefactor in the kinetic terms; the reason for the well known anisotropy of hole transport [Kod08]. The matrix of coordinate transformations, from one to the other axis configuration, is given by the following set of equations

$$
x = A_1 x' + B_1 y' + C_1 z',
$$
$$
y = A_2 x' + B_2 y' + C_2 z',
$$
$$
z = A_3 x' + B_3 y' + C_3 z',
$$

(5.5)

with the matrix elements $A_i$, $B_i$ and $C_i$ for $i = 1, 2, 3$.

Hole transport will be along the $x'$ direction. In the primed-axis configuration, $O'$, we define the wire confinement represented by a deformed 2D harmonic oscillator,

$$
H^{(\text{conf})} = \frac{1}{2} m_0 \omega_0^2 (y'^2 + a z'^2).
$$

(5.6)

The adimensional parameter $a$ of Eq. (5.6), corresponding to the ratio of confinement strengths in $z'$ and $y'$, controls the flatness or 2D character of the wire. A schematic representation of this parabolic potential can be seen in the contour plot in Fig. 5.2b, where this deformation is clearly shown. The strong confinement along $z'$ corresponds to $a \gg 1$.

The direct coupling with the magnetic field $\vec{B}$ is given by the Zeeman term

$$
H^{(Z)} = -2 \kappa \mu_B \vec{B} \cdot \vec{J}
$$

$$
= -2 \kappa \mu_B \begin{pmatrix}
\frac{3}{2} B_z & \frac{\sqrt{3}}{2} B_- & 0 & 0 \\
\frac{\sqrt{3}}{2} B_+ & \frac{1}{2} B_z & B_- & 0 \\
0 & B_+ & -\frac{1}{2} B_z & \frac{3}{2} B_- \\
0 & 0 & \frac{\sqrt{3}}{2} B_+ & -\frac{3}{2} B_z
\end{pmatrix},
$$

(5.7)
where $\kappa$ is a kp parameter, $\mu_B$ represents the Bohr magneton, $\vec{J}$ is the angular momentum operator for a spin $3/2$ and $B_{\pm} = B_x \pm iB_y$. We always refer the magnetic field to the wire system $O'$ using the spherical angles $\theta'$ and $\phi'$,

\begin{align*}
B_{x'} &= B \sin \theta' \cos \phi', \\
B_{y'} &= B \sin \theta' \sin \phi', \\
B_{z'} &= B \cos \theta'.
\end{align*}

(5.8)

We follow the convention that parallel field means parallel to the wire (along $x'$, with $\theta' = \pi/2$ and $\phi' = 0$), while perpendicular refers to perpendicular to the wire but in the plane (along $y'$ with $\theta' = \phi' = \pi/2$). The magnetic kp parameter in GaAs is $\kappa = 1.20$ [Win03].

Finally, the Rashba interaction is described by

$$H^{(R)} = (\vec{k} \times \vec{R}) \cdot \vec{J},$$

(5.9)

where we defined a vector constant $\vec{R} \equiv \alpha \vec{E}$, related to the effective electric field $\vec{E}$ and kp parameter $\alpha$. We shall treat $\vec{R}$ as a two-parameter vector with dominant component along the growth direction, i.e., $\vec{R} = R_{x'} \hat{u}_{x'} + R_{y'} \hat{u}_{y'}$ with $R_{x'} > R_{y'}$. The full matrix representation of $H^{(R)}$ is not given since the expressions for the matrix elements are straightforward but too large.

In the presence of magnetic field, the orbital motion effects of the field are taken into account by means of the substitution

$$\vec{k} \rightarrow -i\nabla - \frac{e}{\hbar c} \vec{A},$$

with the vector potential $\vec{A} = (-yB_z + zB_y, -B_xz/2, B_xy/2)$, where $e$ is the electron charge and $c$ the velocity of light in the vacuum. In this process, Hermiticity is enforced in the cross terms by using the symmetrized forms, such as $k_xk_y \rightarrow (k_xk_y + k_yk_x)/2$.

Summarizing all contributions, the total Hamiltonian reads

$$H \equiv H^{(\text{kin})} + H^{(\text{conf})} + H^{(Z)} + H^{(R)}.$$

(5.10)

5.2.1 Resolution method

Our main interest is to compute the energy dispersion in order to study the conductance and the splitting of the bands in presence of the magnetic field and Rashba spin-orbit coupling. In essence, the Schrödinger equation has to be solved to obtain the energy bands.
As a difference with previous chapters on electron systems, there are now mixing terms between ±3/2 and ±1/2 spins, not only as a consequence of the Rashba Hamiltonian, but to the kinetic term also, as shown by the nondiagonal contributions to the Luttinger matrix Eq. (5.1).

The wire Hamiltonian eigenvalues can be labeled with \( q \), a real number representing the longitudinal momentum along the wire and an index \( I = 1, 2, \ldots \) as

\[
\mathcal{H}(q)|Iq\rangle = \varepsilon_I(q)|Iq\rangle, \tag{5.11}
\]

where \( \varepsilon_I(q) \) are the discrete energy bands of the nanostructure. The eigenvalues are ordered as \( \varepsilon_1(q) \geq \varepsilon_2(q) \geq \cdots \) since the spectrum is not bounded from below due to the negative kinetic terms.

We have obtained the solutions of the eigenvalue problem given by Eq. (5.11) by discretizing in harmonic oscillator states for the two transverse oscillators along \( y' \) and \( z' \),

\[
|Iq\rangle = \sum_{nm\eta} C_{nm\eta}^{(Iq)}|nm\eta\rangle, \tag{5.12}
\]

where \( n, m = 0, 1, \ldots \) represent the number of quanta in each oscillator, respectively. The resulting matrix eigenvalue problem reads

\[
\sum_{nm\eta} \langle n'm'\eta'|\mathcal{H}(q)|nm\eta\rangle C_{nm\eta}^{(Iq)} = \varepsilon_I(q) C_{n'm'\eta'}^{(Iq)}. \tag{5.13}
\]

\( C_{nm\eta}^{(Iq)} \) are the channel amplitudes corresponding to the state \( |nm\eta\rangle \) for a given longitudinal momentum \( q \) and energy band \( I \).
In practice the number of oscillator states in expansion Eq. (5.12) can be truncated once convergence of the results is ensured. In all the numerical simulations of the hole part, the number of transversal bands are taken as $(N_{y'}, N_{z'}) = (20, 20)$, for which there is a rather good convergence. Even so, an interesting point is the limit of purely-1D or quasi-1D channels, truncating to only one band per direction $(N_{y'}, N_{z'}) = (1, 1)$ or taking only one band in the most confined direction, $z'$. The limitations of such severe truncations are considered at the end of the following chapter.

As usual along the thesis, the units are taken from the transversal confinement, with the energy unit $E_U = \hbar \omega_0$ corresponding to the $y'$ frequency, as in chapters 2 and 3. The Rashba strength is also given relative to the confinement, defining a unit of SO coupling $\alpha_U = \hbar \omega_0 \ell_0$. More details are given in App. A.
Chapter 6

Magnetic properties: g-factor anisotropy

In semiconductor hole systems like p-type GaAs nanostructures, transport is mediated by holes in the valence band. As compared to electrons, holes are characterized by a spin $\frac{3}{2}$, besides a sign difference in charge. The corresponding fourfold discrete space is a source of qualitative differences with respect to the more usual twofold spin of electrons. In 2D hole gases different splittings for normal and in-plane fields have been observed, as well as for different in-plane orientations [Win00]. By further confining the hole gas it is possible to generate nanostructures with the shape of quantum wires. In this case, the splitting varies, in principle, with both wire and magnetic field orientations [Dan06, Kod08, Klo09, Che10]. One of these results is shown in Fig. 2 in the Preface, where the splitting of each conductance plateau (in black) visibly changes for magnetic fields in parallel (left panel) or perpendicular (right panel) orientation to the wire. We mention here that theoretical analysis of the spin splittings in hole quantum wires can be found in the literature [Har06, Cso07, Har08, Cso08, Cso08b, Cso09], but to our knowledge the Rashba interaction was not treated specifically in any of these works.

In this part of the thesis we prove that the Rashba interaction is an important source of spin anisotropy in hole quantum wires. This anisotropy manifests in large differences between the energy splittings for magnetic fields parallel and perpendicular to the wire [Dan97, Dan06, Kod08, Klo09, Che10]. Our calculations show that in the presence of Rashba interaction the perpendicular field becomes much less effective in generating spin splitting than the parallel one.

For a better understanding of the hole states, in Sec. 6.1 we show an illustrative example of the energy bands of a hole quantum wire with Rashba spin-orbit
CHAPTER 6. MAGNETIC PROPERTIES

coupling, focusing on the effect of the magnetic field. The main results of this chapter are given in the following section, Sec. 6.2, where the study of the linear conductance g-factor is made as a function of the Rashba coupling and the wire deformation. Interesting points are the study of the band splitting as a function of magnetic field, as well as of the condition when the linear regime is lost. Some examples are given in Sec. 6.3. Concluding this chapter, in Sec. 6.4 low dimensional systems are considered, in the sense of only a few bands in transversal direction to transport; this study revealing that band mixings from all confinement directions are quite important in general and affect the conductance.

6.1 Energy bands with Rashba and magnetic field

Energy bands in 2D hole system are well established [Win03]. The hole bands show a characteristic energy inversion, as compared to the electrons, caused by a negative mass (curvature of the bands) and a strong orientation dependence. Other important features are the crossing/anticrossing behavior between different bands at finite \( q \). In this section we sketch how this scenario refers to our system: the hole quantum wire with Rashba interaction. We will see how the dispersion bands are affected by in-plane magnetic field when this is either parallel or perpendicular to the wire.

As illustrative examples, Fig. 6.1 displays the energy bands of selected cases. As is well known, the Rashba interaction causes a characteristic band structure easily recognizable by the pairs of subbands crossing at \( q = 0 \) and with maxima at opposite \( q \) values (left panel). These maxima correspond to band energy minima for the case of electrons. In the presence of a magnetic field, when this points along the wire (\( x' \), central panel), anticrossing of the bands appears at \( q = 0 \). This anticrossing may lead to anomalous conductance steps, similar to those recently measured in Ref. [Qua10]. In Fig. 6.1 this behavior can be seen for \( (E, q) \approx (-11\hbar\omega_0, 0) \) between bands \( I = 9 \) and \( I = 10 \). For \( B \) in the transverse direction (\( y' \), right panel) the band crossings persist, but the two central maxima for each pair of bands are shifted differently in energy, the band structure becoming asymmetric with respect to \( q \) inversion.

The \( B \)-induced modifications of the band structure, as seen in Fig. 6.1, cause a change in the conductance of the wire. This modification of the conductance, in the limit of weak magnetic field, is conveniently summarized by a number called the g factor of each conductance split level. At \( B = 0 \), time reversal invariance of the system causes the conductance \( G \) to increase in steps of \( 2G_0 \).
6.2 G-FACTOR ANISOTROPY

Figure 6.1: Energy bands for $a = 64$, $R_{z'} = 2.6\hbar\omega_0\ell_0$ and $R_{y'} = 0$. Left panel is for $B = 0$ while center and right ones are for $\mu_B B = 0.1\hbar\omega_0$ in the parallel and transverse directions, respectively. The wire is oriented along $(-2,3,3)$ and the growth direction is $(3,1,1)$.

as the Fermi energy of the leads is reduced (linear conductance regime), where $G_0 = e^2/h$ is the conductance quantum. The evolution of the wire conductance with energy can be understood if we imagine a horizontal line, indicating the position of the Fermi energy, in the left panel of Fig. 6.1; as this line is moved to lower energies it sweeps the band maxima always in pairs, each maximum corresponding to an increase of $G_0$ in the conductance for hole transport. The result is the typical staircase conductance, with step heights of $2G_0$. A similar procedure for the central and right panels of Fig. 6.1 convince ourselves that intermediate half-steps in conductance are caused by the magnetic field. They are smaller than the full steps and proportional to the intensity of the magnetic field. An example of this staircase conductance for the parallel (solid line) and vanishing (dashed line) magnetic field is shown in Fig. 6.2.

6.2 g-factor in lineal magnetic field

The main results of the hole system are found in this section. As already introduced at the beginning of this chapter, recent experiments have found anisotropic g factors when the magnetic field is in parallel or perpendicular direction to the wire [Dan97, Dan06, Kod08, Klo09, Che10]. In all these studies the semiconductor material is GaAs, which is a source of Rashba spin-orbit coupling as discussed above in the thesis. To our knowledge, theoretical studies
such as [Har08, Cso09] have not considered the Rashba term; possibly due to the complexity of the Hamiltonian. In this section we study the anisotropy of the g factors in the presence of a tunable Rashba strength, $R_{x'}$, and as a function of the wire deformation, $a$.

In the limit of weak magnetic fields we can conveniently summarize the $B$-induced $N$th half-step in the conductance, appearing between steps at $2(N-1)G_0$ and $2NG_0$, in terms of a single number called the g factor. As this number depends on the conductance step and the magnetic field orientation, we use the notation $g_{\parallel}^{(N)}$ and $g_{\perp}^{(N)}$ to indicate the g factor of the $N$th step, for $B$ along $x'$ and $y'$, respectively. Of course, other orientations are in principle possible, but we will restrict to these two as they are the relevant ones in the measurements of spin hole anisotropy. Our precise definition is

$$g_{\parallel}^{(N)} = \frac{\Delta_{\parallel}^{(N)}}{3\mu_B B},$$

(6.1)

where $\Delta_{\parallel}^{(N)}$ is the energy range for the $N$th half step in a magnetic field $B$. In Eq. (6.1), the factor 3 in the denominator is introduced by convention [Pin10] and the definition of $g_{\perp}^{(N)}$ is obtained replacing $\Delta_{\parallel}^{(N)}$ by $\Delta_{\perp}^{(N)}$. A graphical definition of the g factor, using parallel magnetic field, is sketched in Fig. 6.2.

**Figure 6.2:** Definition of the g factor. In the left panel, energy bands for vanishing (dashed line) and small (solid line) magnetic fields are shown. The corresponding conductances are shown in the right panel. Without magnetic field, the conductance increases in even multiples of the conductance quantum $G_0$; with a weak magnetic field intermediate half-steps appear with an energy range proportional to the g factor for each specific half-step.
6.2. G-FACTOR ANISOTROPY

Figure 6.3: Parallel and perpendicular g factors as a function of wire deformation for different values of the Rashba strength: $R_{z'} = 0$ (circles), $1.5\hbar \omega_0 \ell_0$ (triangles) and $2.6\hbar \omega_0 \ell_0$ (squares). Upper and lower rows are for parallel and perpendicular fields while columns from left to right correspond to increasing conductance half step $N$ (see text). The results for $N = 1$ are not shown due to their similarity with the displayed $N = 2$ case. The orientation of the wire is the same of Fig. 6.1.

With vanishing magnetic field (dashed line), the conductance increases in steps of $2G_0$. Small magnetic fields (solid line) split the maxima of the energy bands, with an energy range for the $N$th step $\Delta^{(N)}_{||,\perp}$ proportional to the g factor; as a consequence conductance steps are now of a single conductance quantum $G_0$. We remark that in the case of perpendicular magnetic field, the maxima of the energy bands are to be found at finite $q$'s. Notice also that not all the half-steps have the same g factor, i.e., there is a nontrivial $N$ dependence.

Figure 6.3 displays the perpendicular (lower row) and parallel (upper row) g factors for the lower conductance steps, as a function of the wire deformation $a$ and for different values of the Rashba coupling $R_{z'}$. These are the main results of our work. They were obtained for a specific wire orientation ($x'$) and direction of crystallographic growth ($z'$), the same as Fig. 6.1. We have checked, however, that a qualitatively similar influence of the Rashba intensity and confinement deformation (for strong $a$'s) are obtained assuming other arbitrary orientations. The g factors show a general tendency to decrease as $a$ increases, except for smaller deformations ($a < 100$) for which $g$ may increase or even show irregular behavior in some cases. Focussing first on $g_{||}$, we notice that this component does not change significantly when the Rashba intensity
increases, specially at large \( a \)'s, for which the results are almost overlapping in the upper panels of Fig. 6.3. Very remarkably, however, for magnetic field in the perpendicular direction small variations in \( R_{z'} \) are enough to strongly modify the values of \( g_\perp \).

There is a general Rashba-induced quenching of \( g_\perp^{(N)} \) in Fig. 6.3 and 6.4, quite conspicuous for \( N = 4 \) and 5. This effect is so strong that it can reverse the relative importance of \( g_\parallel \) and \( g_\perp \); from \( g_\perp > g_\parallel \) when \( R_{z'} = 0 \) to \( g_\perp \ll g_\parallel \) for increasing \( R_{z'} (> 2.5\hbar\omega_0\ell_0) \). With the chosen values of \( R_{z'} \) we even find a range of \( a \)'s for which \( g_\perp^{(5)} \) essentially vanishes. It is interesting to point out that a similar quenching of conductance plateaus in transverse field was discussed in Ref. [Ser05] for parabolic wires with electron conduction, as opposed to the present hole conduction. In both cases the Rashba spin-orbit coupling is the underlying mechanism. For strong values of Rashba intensity the anisotropy of g factors \( g_\parallel \gg g_\perp \), typical for strong confinement, is not found in any of the halfsteps \( N = 3, 4, 5 \) for small \( a \)'s, such as \( a = 64 \), despite the strong dependence of \( g_\perp \) with \( R_{z'} \). This behavior reflects the sensitivity of the g-anisotropy to the quantum wire confinement, and not only to the Rashba strength.

Turning to the comparison with experiments, this is somewhat complicate due to the sample dependence. In general, however, a large g-factor anisotropy between parallel and perpendicular orientations has indeed been observed in Refs. [Dan06, Kod08, Klo09, Che10]. This was generally attributed to a preferential orientation of the spins along the wire for strong confinements. Our results prove with detailed calculations that the Rashba interaction for holes is the specific mechanism allowing the appearance of this anisotropy. As this interaction is sample dependent and may vary with external field, our results also predict that the hole g factors may be tunable to a certain degree, what may be relevant for spintronic applications. The experimental values of wire deformation \( a \) are somewhat uncertain in general, which is an additional source of difficulty for comparison. In general, however, experimental wire deformations are \( a < 100 \), which in our calculations corresponds to a regime with rather large fluctuations (Fig. 6.3). Only for larger \( a \)'s the value of \( g_\perp^{(N)} \) is consistently below \( g_\parallel^{(N)} \) at high enough \( R_{z'} \). We believe that detailed comparison in this regime is quite involved due to the fluctuations. On the other hand, these sharp variations of \( g_\parallel \) in the small-\( a \) regime and of \( g_\perp \) at all \( a \)'s can be seen as a manifestation of magnetoconductance tunability via the Rashba coupling.
6.3 Nonlinearity of the band splittings with magnetic field

With the purpose to check the limits of the magnetic field linear regime in the previous results, this section considers briefly this question. Of course not all cases can be shown here; only a few representative ones for selected values of wire deformation, \( a \), and Rashba strength, \( R_z' \), will be displayed for the fifth half-step, \( N = 5 \). The splitting energies \( \Delta^{(5)}(\parallel) \) for a parallel (perpendicular) orientation of the applied magnetic field are plotted as a function of magnetic field \( \mu_B B \) in the upper (lower) row of Fig. 6.5. In the linear regime, there is a strict proportionality between both magnitudes, \( \Delta^{(5)}(\parallel,\perp) \) and \( \mu_B B \), reflected in a straight line of slope \( 3g^{(5)}_{\parallel(\perp)} \) in Fig. 6.5. The magnetic values range from \( \mu_B B = 0.01 \) to \( 0.3\hbar\omega_0 \). If at high field the bands for different halfsteps \( N \) are close to crossing the energy splitting \( \Delta^{(5)} \) is not calculated since we cannot easily identify both bands (we call this effect \textit{crossing bands}) and our definition of half step does not apply.

For vanishing Rashba coupling in a parallel magnetic field, crossing bands are not allowed for \( a = 64 \), while strong values \( a = 200 \) and \( 400 \) exhibit crossing between two successive half-steps (in which case the conductance goes from \( 5G_0 \) to \( 7G_0 \)). This crossing is found at \( \mu_B B \approx 0.3\hbar\omega_0 \). The linear regime is then valid for \( \mu_B B < 0.2\hbar\omega_0 \); it is a robust behavior as compared with the perpendicular case, as we will see below. Including Rashba coupling, \( \mathcal{R}_{z'} = \)
2.6ℏω₀ℓ₀ in upper right panel, no big differences between this case and the preceding vanishing Rashba coupling is seen for strong a’s. In fact, the slope in both cases are very similar, including the robustness of the magnetic linearity. An exception is given by the low-deformation case (a = 64) for which the g factor, g(||), strongly decreases and, in addition, its linearity regime is sensible reduced (it finishes at μ₄B ≈ 0.1ℏω₀). We recall that the independence of the parallel g factor on the Rashba intensity for high deformations of the wire was found in the preceding section.

Consider now perpendicular magnetic field, lower row in Fig. 6.5. For this orientation and the energy of the N = 5 halfstep, crossing bands are found for lower magnetic field than for the parallel case, around 0.1 − 0.2ℏω₀. Linearity regime is somewhat stronger for a = 200, 400 [μ₄B₄lin ≤ 0.1ℏω₀] than for a = 64, where it is lost before [μ₄B₄lin ≤ 0.05ℏω₀]. A rather different behavior is seen when the Rashba coupling is considered. In perpendicular magnetic field a very small g factor is found for strong confinements a = 200, 400; seen as an almost vanishing slope in the magnetic linear regime. In any of the three confinements no crossing bands are found and the linear regime just reaches the
value \( \mu_B B_{lin} \leq 0.05\hbar \omega_0 \), emphasizing by contrast the robustness of the linear behavior for the parallel case. The splitting energy increases monotonously for \( a = 200 \) and \( 400 \) while for \( a = 64 \) it reaches a maximum at \( \mu_B B \approx 0.1\hbar \omega_0 \) and finally decreases.

### 6.4 Low dimensional systems: 1 band limit

Our resolution method (Subsec. 5.2.1) consists in expanding the eigenvectors of the Schrödinger equation, \(|Iq\rangle\), in transversal modes of frequency \( \omega_0 \) and \( a\omega_0 \) for the \( y' \) and \( z' \) oscillators, respectively, and in terms of the spin index \( \eta = \pm 3/2, \pm 1/2 \). This expansion, already given in Sec. 5.2.1, reads

\[
|Iq\rangle = \sum_{nm\eta} C_{nm\eta}^{(Iq)} |nm\eta\rangle.
\]

[Eq. (5.12)]

A good question is how does the number of bands in transversal directions \((N_{y'}, N_{z'})\) affects the conductance. For all the previous results we used \((N_{y'}, N_{z'}) = (20, 20)\), which ensures the convergence of the higher energy bands. On the other hand, in electron systems it is a usual approximation to truncate to the lowest energy band in the most confined transversal direction \((z')\) giving a 2DEG; besides, confining in the remaining direction \(y'\) with a parabolic potential corresponds to the quasi-1D electron system; while taking only the lowest \( y' \) band we have the purely-1D system [Fer97, Dat02]. We saw in the first part of this thesis that a purely-1D truncation is not the best approximation for mixing-band interactions, such as the spin-orbit coupling in an inhomogeneous strength (Sec. 3.2). Nevertheless, this approximation describes in a qualitative way some features of the conductance. These kind of approximations are also used in the literature for hole systems [Qua10], and our purpose here is to investigate whether this reduction can become realistic, or just valid, in the purely-1D case, when the wire becomes very confined, \((N_{y'}, N_{z'}) = (1, 1)\), or in quasi-1D, \((N_{y'}, N_{z'}) = (10, 1)\).

Figure 6.6 shows all those situations. In the upper row, the wire deformation is \( a = 30 \) and from left to right panels the number of bands considered are \((N_{y'}, N_{z'}) = (1, 1), (10, 1), (10, 2), (10, 10)\). In all cases no magnetic field is considered, but the Rashba coupling is present \( \mathcal{R}_{z'} = 2.6\hbar \omega_0 \ell_0 \). The wire orientation and growth direction are taken from Ref. [Qua10], corresponding to \((001)\) and \((110)\) respectively. For a better comparison, all plots are represented in the same energy and linear momentum range. In the \((1, 1)\) case the Hamiltonian matrix is a scalar 4 \times 4 matrix yielding only 4 eigenvalues or bands. For the other plots, \((10, 1), (10, 2)\) and \((10, 10)\), there are a very large
number of eigenvalues \((4N_y N_z')\) and the figure only shows the higher ones; the light gray region being actually full of bands in reality.

We observe how from left to right panels the change in energy bands is quite important, specially in the transitions \((1, 1) \rightarrow (10, 1) \rightarrow (10, 2)\); these transitions reflect the space truncations from the purely-1D, to quasi-1D and to quasi-2D hole systems. Increasing the number of bands, the conductance steps tend to be closer in energy (they are shorter), with important differences between the first plot and the last one with \((10,10)\) bands. This is as a consequence of the relevance of the mixing terms, not only in the Rashba Hamiltonian, but also in the kinetic non-diagonal matrix elements, Eqs. (5.1). In the \((10,10)\) plot, a zoom of the same picture is made. We observe that not only the energy spacing between bands is changed; their shape and crossing/anticrossing behaviors also show considerable differences between purely-1D and quasi-1D truncations. Second and third rows are for the same cases, but for flatness degrees \(a = 100\) and \(400\), respectively. We observe a qualitatively similar situation, however the shape for the \((10,10)\) bands becomes somewhat more regular with the increase of the \(z'\) confinement. We have checked that these variations when increasing the number of oscillator bands are qualitatively similar for other wire orientations and growth directions.

From our results, we conclude that it is important to consider more than one energy band in \(z'\) direction, even for strong wire deformations.
Figure 6.6: Energy bands for different number of transversal bands \((N_{y'}, N_{z'})\) for \(a = 30, 100, 400\) (upper, middle and lower rows respectively). In the (1, 1) case, the shown 4 bands form the complete Hilbert space. For the remaining cases only the higher bands are shown, and the gray region is actually full of additional bands. Parameters: \(B = 0, R_z' = 2.6\hbar\omega_0\ell_0, R_y' = 0\), growth direction (001) and wire orientation (110).
Part II: Conclusions

In the second part of this thesis we have studied the g factors of a hole quantum wire with uniform Rashba SO coupling. Several recent experiments [Kod08, Klo09] have studied this topic, emphasizing the spatial anisotropy of the g factor. Some theoretical papers [Har08, Cso08] have also addressed the subject, but the difference between these papers and our work is that we introduced in an explicit way the Rashba spin-orbit coupling. How this kind of interaction affects the g factor was our first question. In addition, our quantum wire is not symmetric in both transversal confined directions, a parameter $a$ controls the wire flatness (for $a \to \infty$ the system approaches the quasi-1D limit).

Firstly, the study of the energy dispersion was considered in presence of Rashba coupling and magnetic field in parallel and perpendicular directions. As in the electron system, when the magnetic field is applied along the wire the energy bands show an anticrossing point at $q = 0$; while in the perpendicular direction the energy bands become asymmetric with respect to $q$ inversion.

Our main study reveals that the g factor anisotropy depends on two parameters. The first one is the wire deformation $a$, such that for a low degree of flatness ($a < 100$) we find a fluctuating, sample-dependent behavior of the g factors; as $a$ increases this behavior becomes increasingly more regular. The second one is the Rashba strength, $\mathcal{R}_z'$ that dominates the anisotropy in the following way. When the wire deformation and Rashba interaction are both large enough ($a > 100$, $\mathcal{R}_z' > 2.5\hbar\omega_0\ell_0$) $g_{\perp}^{(N)}$ is greatly quenched by the Rashba interaction while $g_{\parallel}^{(N)}$ is almost unaffected; the anisotropy ratio $g_{\perp}^{(N)}/g_{\parallel}^{(N)}$ can even be reversed by manipulating $\mathcal{R}_z'$. On the other hand, for small wire deformation (such as $a = 64$) the presence of strong oscillations make this anisotropy inversion due to the Rashba coupling much less clear. Summarizing, we attribute the anisotropy of magnetotransport g factors in hole quantum wires to the Rashba interaction for strong confinements.

The precise limits of the energy-splitting linear regime with the applied field were studied using some selected examples. We observed that the linear regime is robust when the magnetic field is parallel to the wire, while in perpendic-
ular direction linearity becomes greatly reduced when increasing the Rashba strength. An interesting behavior is the no crossing bands with the increase of perpendicular field in the presence of Rashba coupling.

Finally, the limit of very low dimensional systems is studied by severely truncating the number of transversal modes considered. For the purely one-dimensional system we found that such approximation is not valid when we compare this case with the multiband one, i.e., qualitative differences remain even for high values of the deformation $a$. For the quasi one-dimensional system the energy bands are better reproduced in the limit of large $a$, but we should take more than one energy band in $z'$ in order to obtain key features of the energy bands, such as crossing and anticrossing behaviors characteristics of the hole systems.
Outlook

The aim of this thesis was the study of how the Rashba spin-orbit coupling affects transport. We have considered two different systems, one for transport by electrons and another for transport by holes. As we have seen, in both cases the Rashba effect makes important changes on the conductance and can become a source of novel physical phenomena. In this Conclusions a small review of the main results is given as well as a sketch of possible future works that would extend this study.

For the electron case, the physical system considered was a quantum wire with a localized Rashba region. We found Fano-Rashba dips at the end of each conductance plateau and we studied the Rashba dot as a polarizer, when the output current is spin polarized. On the other hand, we considered the Datta and Das transistor, which we modeled using the previous system attached to polarized leads. We demonstrated how going from purely to quasi one-dimensional system the characteristic sinusoidal behavior of the conductance with Rashba strength is not robust. In fact, the multichannel transport destroys this behavior, and we also checked it in the bidimensional system. An extension of this work could be for the sequential Rashba regions: the study of the Fano-Rashba dip for energies below the second plateau and the current polarization it produces. An interesting point would be to clarify whether the polarization peaks, that we find for one region, can become much more robust in multi-Rashba regions or not.

In transport with holes, the physical system we considered is a three dimensional quantum wire with uniform Rashba coupling. The study focused on the gyromagnetic factors when a uniform magnetic field is applied, as a function of the flatness of the wire and Rashba strength. We understand these g factors as the splitting of energy bands owing to the external magnetic field. The main result was how the Rashba strength dominates these g factors and, in this way, determines the anisotropy of the system for strong wire confinement. We also referred to the approximations in low-dimensional hole systems; the truncation to only one band in the most confined direction (quasi-1D holes), as in electron systems, is not a good approximation as we demonstrated.
Part II of the thesis is only the beginning of more detailed investigations. An accurate study for small values of wire deformation could be a good starting point, since the main experiments are in that regime. The study of the $g$ factors when the magnetic field is applied perpendicular to the wire, but out of plane (along $z'$), could be also interesting, comparing with the $g$ factors in the other directions ($x'$ and $y'$). On the other hand, systematic results about the linear regime, the crossing bands and the effect of the orbital motion due to the magnetic field, can be interesting in order to extend the present study. Similarly to the electron part, the study of hole transport along an inhomogeneous Rashba region might provide new transport phenomena, generalizing to the hole case the Fano-Rashba dips of the first part.
Appendices
Appendix A

Units

In order to give the most general results as possible, we consider adimensional units for our parameters. These units, for length and energy, are taken from one parameter of the system. If $E_U$ is our energy unit, then the length unit is given by $L_U = \sqrt{\hbar^2/m^*_0 E_U}$. Notice that the Rashba unit is given by the product of both, $\alpha_U = E_U L_U$. How we choose this parameter will depend on the particular physical system.

In the quasi one-dimensional system, the lateral confinement potential naturally defines the energy and lengths units as

\begin{align*}
E_U &= \hbar \omega_0, \\
L_U &= \ell_0 = \sqrt{\hbar/m^*_0 \omega_0},
\end{align*}

respectively. The Rashba strength is then given by $\alpha_U \equiv \hbar \omega_0 \ell_0$. $m^*_0$ is the semiconductor effective mass of the electron.

Physically, typical values for, e.g., an InAs system are $\alpha_0 = 10 - 50$ meVnm [Gru00], $\ell_0 \lesssim 1$ µm and $\hbar \omega_0 \lesssim 1$ meV. The correspondence between our units and the physical values for InAs with $\hbar \omega_0 = 1$ meV, $\alpha_0 = 17$ meV nm and $\ell_0 = 0.45$ µm, can thus be $\alpha_0 = 0.3 \hbar \omega_0 \ell_0$ and $\ell = 8 \ell_0$. Notice that strong adimensional values of Rashba coupling are described by the same physical value of $\alpha_0$ provided the confinement is weak enough. For instance, assuming InAs parameters [Eng97, Nit97] $\alpha_0 = 10$ meV nm corresponds to $\alpha_0 = 2 \hbar \omega_0 \ell_0$ for $\hbar \omega_0 \approx 0.001$ meV and $\ell_0 \approx 0.5$ µm. This is a wire width which is within the scope of present experimental techniques [Sch04].

In the bidimensional case, we take the energy unit in two different ways, depending on the specific focus of interest. When the interest is in the energy dependence of the conductance or polarization, the energy unit, taken as a
parameter in the Zeeman field $\Delta_0$, and the corresponding length unit $L_U$, read

\begin{align*}
E_U &= \Delta_0, \\
L_U &= \ell_0 = \sqrt{\hbar^2/m^*_0 \Delta_0}.
\end{align*}

In this case, the Rashba unit corresponds to $\alpha_U = \sqrt{\hbar^2 \Delta_0 / m^*_0}$. For InAs-based semiconductors the Rashba coupling can be tuned around $\alpha_0 \approx 10 \text{ meV nm}$, with about one order of magnitude range. Assuming a system length of $\ell_0 \approx 1 \mu\text{m}$ and a Zeeman splitting of $\Delta_0 \approx 0.3 \text{ meV}$ this implies that, in adimensional units, one has $\alpha_0 \approx 0.3 \sqrt{\hbar^2 \Delta_0 / m^*_0}$ and $\ell \approx 10 \ell_0$.

When the focus of interest is the Rashba strength dependence, such as the oscillating behavior of the conductance, we take as energy unit the Fermi energy $E$ and for full polarized leads the Zeeman field is taken, for example, $\Delta_0 = 20E$. The corresponding energy units are then given by

\begin{align*}
E_U &= E, \\
L_U &= \ell_0 = \sqrt{\hbar^2/m^*_0 E},
\end{align*}

with the usual Rashba strength unit $\alpha_U = \sqrt{\hbar^2 E / m^*_0}$.

For the hole case, the energy unit is taken from the in plane transversal confinement ($\gamma'$)

\begin{align*}
E_U &= \hbar \omega_0, \\
L_U &= \ell_0 = \sqrt{\hbar / m_0 \omega_0}.
\end{align*}

This is not the same of the electron case; for holes the mass used in the definition of units is the bare electron mass.
Appendix B

Resolution method

B.1 Quantum wire confinement

This appendix gives some details of the practical method to solve Eq. (1.18) and the corresponding boundary conditions. We use a method based on the quantum transmitting boundary algorithm [Len90, Ser08]. A fictitious partitioning of the system in central and asymptotic regions (contacts) is introduced. The boundaries for the left and right contacts are at $x_L$ and $x_R$, respectively. In the contacts the band amplitudes take the form

$$\psi_{ns}(x) = a_{c,ns} e^{isck_{c,ns}(x-x_c)} + b_{c,ns} e^{-isck_{c,ns}(x-x_c)},$$

where $c = L, R$ is a label referring to left ($L$) and right ($R$) contacts, respectively, and we defined $s_L = 1$ and $s_R = -1$. The incident and reflected amplitudes for a given mode $ns$ and contact $c$ are given by $a_{c,ns}$ and $b_{c,ns}$, respectively. This expression is for a propagating channel in contact $c$, for which $\varepsilon_n + |\Delta_c| + s\Delta_c < E$ and its corresponding wavenumber

$$k_{c,ns} = \sqrt{2m_0^* (E - \varepsilon_n - |\Delta_c| - s\Delta_c)}/\hbar ,$$

is a real number. Equation (B.1) also applies to evanescent modes, $\varepsilon_n + |\Delta_c| + s\Delta_c > E$, if we assume in this case $a_{c,ns} = 0$ and a purely imaginary wavenumber

$$k_{c,ns} = i\sqrt{2m_0^* (\varepsilon_n + |\Delta_c| + s\Delta_c - E)}/\hbar .$$

Notice that the output amplitudes can be obtained from the wave function right at the interface,

$$b_{c,ns} = \psi_{ns}(x_c) - a_{c,ns} .$$

Substituting Eq. (B.4) in Eq. (B.1) we obtain

$$\psi_{ns}(x) - \psi_{ns}(x_c) e^{-isck_{c,ns}(x-x_c)} = 2ia_{c,ns} \sin(sck_{c,ns}(x-x_c)) ,$$

where $c = L, R$ is a label referring to left ($L$) and right ($R$) contacts, respectively, and we defined $s_L = 1$ and $s_R = -1$. The incident and reflected amplitudes for a given mode $ns$ and contact $c$ are given by $a_{c,ns}$ and $b_{c,ns}$, respectively. This expression is for a propagating channel in contact $c$, for which $\varepsilon_n + |\Delta_c| + s\Delta_c < E$ and its corresponding wavenumber

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is a real number. Equation (B.1) also applies to evanescent modes, $\varepsilon_n + |\Delta_c| + s\Delta_c > E$, if we assume in this case $a_{c,ns} = 0$ and a purely imaginary wavenumber

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where $c = L, R$ is a label referring to left ($L$) and right ($R$) contacts, respectively, and we defined $s_L = 1$ and $s_R = -1$. The incident and reflected amplitudes for a given mode $ns$ and contact $c$ are given by $a_{c,ns}$ and $b_{c,ns}$, respectively. This expression is for a propagating channel in contact $c$, for which $\varepsilon_n + |\Delta_c| + s\Delta_c < E$ and its corresponding wavenumber

$$k_{c,ns} = \sqrt{2m_0^* (E - \varepsilon_n - |\Delta_c| - s\Delta_c)}/\hbar ,$$

is a real number. Equation (B.1) also applies to evanescent modes, $\varepsilon_n + |\Delta_c| + s\Delta_c > E$, if we assume in this case $a_{c,ns} = 0$ and a purely imaginary wavenumber

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$$\psi_{ns}(x) - \psi_{ns}(x_c) e^{-isck_{c,ns}(x-x_c)} = 2ia_{c,ns} \sin(sck_{c,ns}(x-x_c)) ,$$

where $c = L, R$ is a label referring to left ($L$) and right ($R$) contacts, respectively, and we defined $s_L = 1$ and $s_R = -1$. The incident and reflected amplitudes for a given mode $ns$ and contact $c$ are given by $a_{c,ns}$ and $b_{c,ns}$, respectively. This expression is for a propagating channel in contact $c$, for which $\varepsilon_n + |\Delta_c| + s\Delta_c < E$ and its corresponding wavenumber

$$k_{c,ns} = \sqrt{2m_0^* (E - \varepsilon_n - |\Delta_c| - s\Delta_c)}/\hbar ,$$

is a real number. Equation (B.1) also applies to evanescent modes, $\varepsilon_n + |\Delta_c| + s\Delta_c > E$, if we assume in this case $a_{c,ns} = 0$ and a purely imaginary wavenumber

$$k_{c,ns} = i\sqrt{2m_0^* (\varepsilon_n + |\Delta_c| + s\Delta_c - E)}/\hbar .$$

Notice that the output amplitudes can be obtained from the wave function right at the interface,

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Substituting Eq. (B.4) in Eq. (B.1) we obtain

$$\psi_{ns}(x) - \psi_{ns}(x_c) e^{-isck_{c,ns}(x-x_c)} = 2ia_{c,ns} \sin(sck_{c,ns}(x-x_c)) ,$$
that is the quantum-transmitting-boundary equation for the contacts.

Equations (1.18) and (B.5), for the central and contact regions, respectively, form a closed set that does not invoke the wave function at any external point. Of course, this is not true for any of these two subsets separately, since central and contact regions are connected through the derivative in Eq. (1.18) and of $\psi_{ns}(x_c)$ in Eq. (B.5). In practice, we use a uniform grid in $x$ with $n$-point formulae for the derivatives $(n \approx 5 - 11)$ and truncate the expansion in transverse bands, Eq. (1.14), to include typically 30-60 terms. The resulting sparse linear problem is then solved using routine ME48 [HSL07].

### B.2 Bidimensional electron system

The numerical calculation of the linear conductance Eq. (4.9) at a given energy $E$ involves two steps. First, for a certain angle $\theta$, or what is equivalent, a certain transverse momentum $q$, the coupled equations for $\psi_{q+}$ and $\psi_{q-}$, Eqs. (4.7), are solved to obtain the transmissions $T_{s's'}$ and $T'_{s's'}$. This is accomplished using the transmitting-boundary algorithm as in quantum wire (previous section). This calculation is for quantum wires, with a confinement potential in the transverse direction, where the system of coupled equations is infinite and had to be truncated. The present case is, in this respect, simpler since only the two spin components of a given transverse momentum need to be considered. Nevertheless, the reader is addressed to Sec. B.1 for the technical details on how the differential equations with open boundary conditions are transformed into a linear system of equations [Fab07].

Once the transmissions at a fixed $\theta$ are obtained, a second step of the calculation requires to integrate over the angle to calculate the linear conductance from Eq. (4.9). This integral turns out to be somewhat delicate due to the presence of resonances as discussed in the quasi-analytical solution by ansatz of Subsec. 4.2.1. The $\theta$-integration is then carried out using Gauss-Legendre quadratures with a certain set of abscissae and weights. To make sure that the integral is well converged we keep increasing the number of Gauss-Legendre points until a required accuracy is reached in a stable way. Typically, we require the error to be $\Delta G/G_0 \leq 10^{-3}$. 

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Curriculum vitae

Education

Degree in Physics (February 2007)
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Publications

• g-FACTOR ANISOTROPY OF HOLE QUANTUM WIRES INDUCED BY THE RASHBA INTERACTION
  Submitted.

• INTERFERENCE OF FANO-RASHBA CONDUCTANCE DIPS

• CONDUCTANCE OSCILLATIONS OF A SPIN-ORBIT STRIPE WITH POLARIZED CONTACTS

• LINEAR CONDUCTANCE OSCILLATIONS IN QUANTUM WIRES AND STRIPES WITH RASHBA INTERACTION

• MULTICHLANNEL EFFECTS IN RASHBA QUANTUM WIRES
• MAGNETIZATION FLUCTUATIONS IN MESOSCOPIC CONDUCTORS OUT OF EQUILIBRIUM

• SPIN POLARIZED CURRENT FROM LOCALIZED RASHBA INTERACTION IN A QUANTUM WIRE

Congresses attendance and schools

• QUANTUM SPINTRONICS. MARATEA WORKSHOP.
Acquafredda di Maratea (Italy): October, 18th-21th, 2010.
Poster presentation: Current polarization and multichannel effects in quantum wire with Rashba interaction.

• SPINTRONICS DAYS AT UPV-EHU.
Oral presentation: Spin transistor and polarization effects in multiple subband quantum wires.

• SECOND WORKSHOP ON NANOELECTRONICS FOR RESEARCHERS OF THE MEDITERRANEAN AREA (NANOMEDITERRANEO II).
Alicante (Spain): June, 18th-19th, 2010.
Oral presentation: Multichannel effects in Rashba quantum wires.

• 5th INTERNATIONAL SCHOOL AND CONFERENCE ON SPINTRONICS AND QUANTUM INFORMATION TECHNOLOGY.
Poster presentation: Localized Rashba interaction in quantum wires: current modulation and spin polarization.

• 20TH INTERNATIONAL CONFERENCE ON NOISE AND FLUCTUATIONS (ICNF).
Pisa (Italy) : June, 14th-19th, 2009.
Poster presentation: Fluctuations of Magnetization in F-N-F systems
• MATERIALS WITH NOVEL ELECTRONIC PROPERTIES WINTER SCHOOL 2009 (MANEP).
  Saas-Fee (Switzerland): January, 11th-16th, 2009.

• XIV INTERNATIONAL SYMPOSIUM ON SMALL PARTICLES AND INORGANIC CLUSTERS (ISSPIC XIV).
  Poser presentation: Localized Rashba interaction and current polarization in quantum wires.

• V REUNIÓN DEL GRUPO ESPECIALIZADO DE FÍSICA DE ESTADO SÓLIDO.
  Santiago de Compostela (Spain): February, 6th-8th, 2008.
  Poster presentation: Current Polarization induced by the Rashba interaction in quantum wires.