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Spin relaxation in semiconductor
nanostructures

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Spin relaxation in semiconductor
nanostructures

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À minha família

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*“what we observe is not nature in itself but nature
exposed to our method of questioning.”*

*PHYSICS AND PHILOSOPHY
WERNER HEISENBERG*

Resumo

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No campo de pesquisa denominado spintrônica é de fundamental importância o entendimento dos mecanismos de relaxação de spin. A fim de contribuir com esse objetivo, estudamos a relaxação de spin em nanoestruturas semicondutoras na presença da interação spin-órbita. Primeiramente, analisamos o decaimento e defasamento do spin eletrônico em pontos quânticos formados no grafeno usando a teoria de Bloch-Redfield. Consideramos um ponto quântico circular com as interações spin-órbita intrínseca e de Rashba. A relaxação de spin ocorre via relaxação de energia pela interação elétron-fônon acompanhado do mecanismo de spin-flip auxiliado pela interação spin-órbita. Previmos a presença de um mínimo no tempo de relaxação de spin T_1 em função do campo magnético externo $\mathbf{B}_{\text{ext}}$ causado pelo acoplamento spin-órbita de Rashba que por sua vez leva a cruzamento evitado de níveis de energia com spins opostos. Em contraste, a interação spin-órbita intrínseca gera um comportamento monotônico de T_1 com $\mathbf{B}_{\text{ext}}$ devido ao acoplamento direto spin-fônon. Demonstramos também que o tempo de decoerência de spin $T_2 \simeq 2T_1$ é dominado por contribuições dos mecanismos de relaxação em primeira ordem na interação spin-órbita e na interação elétron-fônon. Desenvolvemos também um modelo numérico que leva em conta o mecanismo de relaxação de spin de D'yakonov-Perel em fios quânticos com múltiplas subbandas. Consideramos espalhamentos elásticos, que conservam a orientação do spin, no operador evolução temporal. Em seguida, calculamos o valor esperado dos operadores de spin dependentes do tempo para um ensemble de elétrons. Por fim, extraímos o tempo de relaxação de spin em função do campo magnético externo $\mathbf{B}_{\text{ext}}$. Observamos um comportamento não-monotônico da relaxação de spin para um campo $\mathbf{B}_{\text{ext}}$ alinhado perpendicularmente ao fio quântico. Em sistemas com acoplamento spin-órbita fracos, nenhuma ressonância de spin é encontrada quando $\mathbf{B}_{\text{ext}}$ está alinhado paralelamente ao fio quântico. No entanto, previmos o aparecimento de ressonâncias de spin anômalas em sistemas com forte acoplamento spin-órbita mesmo quando $\mathbf{B}_{\text{ext}}$ está alinhado ao canal balístico. Por fim, estudamos a formação de uma densidade de spin helicoidal cruzada e robusta contra espalhamento por impurezas em um gás bi-dimensional de elétrons na presença das interações spin-órbita de Rashba α and Dresselhaus β . Generalizamos o efeito previsto para um poço quântico com uma subbanda para duas subbandas ocupadas quando as interações spin-órbita assumem o mesmo valor em intensidade mas sinais opostos, e.g., $\alpha_1 = +\beta_1$ e $\alpha_2 = -\beta_2$ para a primeira $v = 1$ e segunda $v = 2$ subbandas. Denominamos esse novo padrão de helicóides de spin persistentes e cruzadas. Analisamos as equações de difusão com carga e spin acoplados com o intuito de investigarmos o tempo de vida das densidades de spin helicoidais cruzadas e a possibilidade de medi-las com os experimentos atuais. Estudamos também o efeito da interação spin-órbita interbanda na relaxação dos modos helicoidais de spin, espectro de energia com cruzamentos evitados e

texturas de spin.

Palavras-chaves: Relaxação de spin. Fios quânticos. Pontos quânticos. Computação quântica. Spintrônica. Interações spin-órbita de Rashba e Dresselhaus.

Abstract

HACHIYA, MARCO O. **Spin relaxation in semiconductor nanostructures.** 2013. 114 p. Tese (Doutorado em Ciências) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2014.

In the research field of spintronics, it is essential to have a deep understanding of the relaxation mechanisms of the spin degree of freedom. To this end, we study the spin relaxation in semiconductor nanostructures with spin-orbit interaction. First we analyze the spin decay and dephasing in graphene quantum dots within the framework of the Bloch-Redfield theory. We consider a gate-tunable circular graphene quantum dot where the intrinsic and Rashba spin-orbit interactions are operative. We derive an effective Hamiltonian via the Schrieffer-Wolff transformation describing the coupling of the electron spin to potential fluctuations generated by the lattice vibrations. The spin relaxation occurs with energy relaxation provided by the electron-phonon coupling and the spin-flip transition assisted by spin-orbit interactions. We predict a minimum of the spin relaxation time T_1 as a function of the external magnetic field $\mathbf{B}_{\text{ext}}$ caused by the Rashba spin-orbit coupling-induced anticrossing of opposite spin states. By contrast, the intrinsic spin-orbit interaction leads to monotonic behavior of T_1 with $\mathbf{B}_{\text{ext}}$ due to direct spin-phonon coupling. We also demonstrate that the spin decoherence time $T_2 \simeq 2T_1$ in graphene is dominated by relaxation processes up to leading order in the spin-orbit interaction and the electron-phonon coupling mechanisms. Secondly, we develop a numerical model to account for the D'yakonov-Perel spin relaxation mechanism in multisubband quantum wires. We consider the elastic spin-conserving scattering events in the time-evolution operator and then evaluate the time-dependent expectation value of the spin operators. After averaging these results over an ensemble, we can extract the spin relaxation time as a function of $\mathbf{B}_{\text{ext}}$. We observe a non-monotonic behavior for the spin relaxation time with $\mathbf{B}_{\text{ext}}$ aligned perpendicularly to the quantum wire. This effect is called ballistic spin resonance. In our model, the ballistic spin resonance occurs near the subband anticrossing induced by the subband-spin mixing spin-orbit interaction term. In systems with weak spin-orbit coupling strengths, no spin resonance is observed when $\mathbf{B}_{\text{ext}}$ is parallel to the channel. Nevertheless, we also predict the emergence of anomalous resonances plateaus in systems with strong spin-orbit couplings even when $\mathbf{B}_{\text{ext}}$ is aligned with the quantum wire. Finally, we predict the emergence of a robust spin-density helical crossed pattern in two-dimensional electron gas with Rashba α and Dresselhaus β spin-orbit couplings. This pattern arises in a quantum well with two occupied subbands when the spin-orbit coupling strengths are tuned to have equal absolute strengths but opposite signs, e.g., $\alpha_1 = +\beta_1$ e $\alpha_2 = -\beta_2$ for the first $\nu = 1$ and second $\nu = 2$ subbands. We named this novel pattern as crossed persistent spin helices. We analyze the spin-charge coupled diffusion equations in order to investigate the lifetime of the crossed persistent spin helices and the feasibility of probing the crossed persistent spin helix mode. We also study the interband spin-orbit

interaction effects on the crossed persistent spin helices, energy anticrossings and spin textures induced by the interband spin-orbit coupling.

Key-words: Spin relaxation. Quantum wires. Quantum dots. Quantum computation. Spintronics. Rashba and Dresselhaus spin-orbit couplings.

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CHAPTER 1

INTRODUCTION

1.1 Quantum computation and spintronics

In recent years, theoretical and experimental efforts have been devoted to enhance the quality of our electronic devices. For instance, a burgeoning research field called quantum computation aims to build up a computer faster than its classical counterpart for some dedicated tasks. In quantum computers, the basic unit to hold information is a general two-level quantum system, called a quantum bit (qubit). Notably, a qubit can exist as any superposition combining the states 0 and 1, as opposed to the classical bit which can only assume either the value 0 or 1. If we assume that elementary computation operations can be realized in this superposition, each qubit can perform multiple computations at the same time (high parallelism) increasing significantly its computational speed. In principle, a quantum computer would be composed of an array of these qubits on which quantum gates would perform logical operations successively where the final measurement would be the outcome of a computation. Notice that these operations on the qubit have to be carried out within times much shorter than the timescale that information held by the qubit might be lost to the environment. Thus it is necessary to understand the coupling with the environment in order to reduce its influence on the qubit dynamics. This decoherence mechanism constitutes a serious limitation of a quantum computer's performance. This issue motivates an investigation on a list of physical systems as a potential basic units

to perform this next-level computers. Such proposals to implement a quantum computer were made in distinct systems such as electron spins in semiconductor quantum dots (1), superconductor circuits (11), ion traps (12), nuclear magnetic resonance setups (13), etc.

In the meanwhile, spintronics researchers have proposed a new generation of electronic devices which could be faster and more economical than the current ones (14). As the microelectronic devices get smaller, approaching atomic dimension, spintronics gets more attention from the scientific community. In this research field, the electron spin, instead of (or in combination with) its charge or in combination with, plays a central role. Until the 1990s, in mostly of our devices the concept of information carried out were based on the flow (or the absence of flowing) of electric charge. Nevertheless, the Datta-Das spin-field-effect transistor proposal suggested the possibility of modulating the channel resistivity via control of the spin current flow from a ferromagnetic emitter to another ferromagnetic collector (15, 16). The main idea behind this new device was controlling spin alignment via spin-orbit interaction, which can be tuned by an external gate voltage. Since then, other proposals have been made such as magnetic filters, spin transistors, solar cells, magnetoresistive memories, bipolar spintronic devices, etc (14). All these proposals require the control, manipulation and measurement of the spin as an effort to build efficient spintronic devices. Thus this spin-based technology also rely on long spin relaxation and decoherence times to work properly. To achieve this state-of-the-art performance, it is required a complete understanding of the spin interactions such as spin-orbit and hyperfine couplings and the nature of the environment in these systems.

In short, quantum computation and spintronics are promising research fields that were created as a result of the quest for the quantum computer and/or enhanced devices. So far, these fields have presented to us a deeper understanding of physics and the nature of fundamental interactions in the various systems. We expect that in the near future, real applications from semiconductor spintronics and quantum computation will be available as the fruits of this effort to improve the quality of our everyday lives.

1.2 Quantum dots as spin qubits

A promising candidate to host a solid state qubit is based on semiconductor quantum dots (1) (see illustration in Fig. [1.1]). These systems can be built in semiconductor heterostructures where the electrons are confined along the growth direction. A complete freezing of the remaining spatial degrees of freedom is achieved electrostatically by metallic top gates. Within this so-called Loss-Divicenzo proposal, the qubit is defined by two spin states up $|\uparrow\rangle$ and down $|\downarrow\rangle$ of each electron in a quantum dot. Besides this particular choice of a two-level system as a qubit, the system studied has to fulfill five basic requirements to be possibly implemented as a quantum computer. These conditions, known as DiVincenzo's Criteria, are given by: scalability, initialization, a feasible universal set of quantum gates, measurement capability, and longer relaxation and decoherence times (compared with gate operation times) (17).

Figura 1.1 – Double quantum dots as basic units (qubits) of a universal scalable quantum computer based on the Loss-Divicenzo proposal (1). Electrons are initially confined in a 2D electron gas formed in a semiconductor quantum well. A further lateral confinement is achieved by metallic top gates located on top of the 2D electron gas. Single-qubit rotations can be performed via electron spin resonance where a static B_{ext} and an oscillating magnetic field B_{ac} are combined to coherently manipulate spin orientation (2). Two-qubit gate operations can be achieved lowering the barrier between the quantum dots in a switching time τ . In this case, the spin dynamics is controlled by the time-dependent Heisenberg exchange coupling (1).

Here, we focus on the last requirement which concerns about the timescales involved

in building a quantum computer in quantum dots (1). If this requirement is not fulfilled, then the information stored in each qubit will be lost due to its coupling to the environment, where pure quantum states will evolve in a statistical mixture in a timescale determined by the spin decoherence time. Moreover, the qubit will reach its ground state changing the spin orientation in a timescale given by the spin relaxation time. Yet, multiple one-qubit and two-qubit gate operations in semiconductor quantum dots (such as GaAs) have not been achieved experimentally due to the coupling qubit-environment. The interaction with the surrounding environment could be attributed to two main sources: the phonon bath and the nuclear spin bath. The former, in combination with the spin-orbit interaction, can cause energy relaxation accompanied by a spin-flip process leading to the spin relaxation of the qubit. The latter is due to the hyperfine interaction which couples the electron spin and the nuclear spins of the host material. The spin bath can be viewed as a fluctuating effective magnetic field which is the main source of the spin decoherence in GaAs quantum dots.

Thus this last requirement is a major issue to the feasibility of a quantum computer using quantum dots. It motivated us to investigate different materials where the detrimental effects of the spin-orbit interaction and hyperfine interaction are reduced. Thus carbon-based materials such as graphene (18) and carbon nanotubes (19) arise as natural candidates to host a spin qubit. Notably, single-layer graphene, a one-carbon-atom-thick layer arranged in a honeycomb crystal lattice, has attracted much interest in the last decade due to its unique electronic properties (5). Graphene has a relatively weak hyperfine interaction and spin-orbit (SO) couplings. A graphene sheet is composed naturally of 99% of ^{12}C with nuclear spin 0, and of 1% ^{13}C with nuclear spin 1/2, leading us to expect long dephasing times in carbon-based quantum dots due to a weak hyperfine interaction(20). Moreover, the weak SO couplings in graphene generates a spin-splitting of the order of tens of μeV due to the low atomic weight of carbon atoms (21, 22). In this thesis, we investigate the feasibility of building up a quantum computer using graphene quantum dots in terms of its spin relaxation and decoherence times.

In the next section, we present the proposal of a spintronic device. Its operational limitations will motivate us to investigate the spin relaxation mechanisms in each dimensionality in further sections.

1.3 Datta-Das Spin-Field Effect Transistor

The most remarkable proposal of a spintronic device is the so-called Datta-Das spin-field effect transistor (spin-FET). This new concept, introduced by Datta and Das in 1990 (15), concerns the control the electron spin by electric means via spin-orbit (SO) interaction. The device is comprised of two ferromagnetic electrodes connected by a low-dimensional channel (see Fig. [1.2]). These channels are generated by electrostatic confinement in a 2D electron gas which is formed at the interface of a semiconductor heterostructure, such as AlGaAs/GaAs. One ferromagnetic electrode (source) injects electrons with its spins oriented parallel to the magnetization of the injector, for instance, along $\mathbf{x}$ direction $|\uparrow_x\rangle$. In this low-dimensional channel, two SO couplings are operative depending on whether they originate from the structural and bulk inversion asymmetry, named Rashba $\mathcal{H}_R$ and Dresselhaus $\mathcal{H}_D$, respectively. The SO Hamiltonian $\mathcal{H}_{SO} = \mathcal{H}_R + \mathcal{H}_D$ reads

$$\mathcal{H}_{SO} = \alpha(k_x\sigma_y - k_y\sigma_x) + \beta(k_y\sigma_y - k_x\sigma_x), \quad (1.1)$$

where α and β denotes the Rashba and Dresselhaus SO coupling strengths, respectively. Here, $\mathbf{k}$ is the electron momentum and $\boldsymbol{\sigma}$ the Pauli matrices. Particularly, the Rashba SO interaction strength can be tuned via external gates, $\alpha(V_g)$ (23). For the sake of simplicity, let us restrict ourselves to a strictly 1D channel along x direction where only the Rashba SO $\mathcal{H}_R$ is operative with the time-evolution operator given by $\mathcal{U}(t) = \exp[-i\alpha k_x t \sigma_y]$. Thus the electron spin will precess after entering the channel with its dynamics entirely determined by the time-evolution operator acting on its spin state, i.e., $\mathcal{U}(t)|\uparrow_x\rangle$. In the absence of scattering, the spin will precess with a single frequency defined by the Rashba coupling $\alpha(V_g)$. Since this parameter can be tuned, it is possible to choose the spin orientation when the electron reach the ferromagnetic collector (drain). We assume here that both source and drain have the same magnetization alignment. If the Rashba coupling is chosen such that $2\alpha(V_g)k_x t = (2n + 1)\pi$, with $n = 0, 1, 2, \dots$, each electron will reaches the drain with their spins pointing along $\mathbf{x}$, $|\downarrow_x\rangle$. In this case, the electrons will not enter the ferromagnetic collector increasing the channel resistivity (OFF state). Otherwise, if the Rashba coupling fulfills the condition $2\alpha(V_g)k_x t = (2n)\pi$, each electron

will enter the drain since its state $|\uparrow_x\rangle$ is parallel to ferromagnetic collector decreasing the channel resistivity (ON state).

Notice that spin-orbit interaction is a double-edged sword, since it allows spin manipulation but also causes spin relaxation combined with spin-independent scattering processes. To overcome this problem, the Datta-Das proposal can be implemented in a strictly 1D channel where the spin-independent scattering cannot lead to spin relaxation. However, it is experimentally challenging to realize such specific condition. Relaxing the ballistic requirement has been one of the major efforts of the researchers towards realizing the spin FET of Datta and Das (15). Recently, other proposals have extended the operation of the Datta-Das transistor to the nonballistic regime independently of the channel width(24, 25). This can be achieved by considering the interplay between the Rashba and the Dresselhaus spin-orbit couplings. Their couplings strengths can be tuned to be equal which results in momentum-orientation independent eigenspinors, even in two dimensions. Thus spin-independent scatterings will not be able to randomize the spin orientation thus suppressing the spin relaxation (24).

Figura 1.2 – Schematic of the Datta-Das spin-field-effect transistor. A spin-polarized current is injected in the low-dimensional channel from a ferromagnetic (FM source) with magnetization along the x direction. Each electron spin will precess due to the spin-orbit interaction, which can be controlled by a gate voltage V_g . Depending on the size of the channel and the spin-orbit coupling strength, the electron can reach the ferromagnetic collector (FM drain) with spin aligned in parallel (or anti-parallel) to the collector magnetization, which is also along x direction. Each situation leads to a increase (decrease) of the channel resistivity corresponding to the states ON (OFF) in the transistor. Thus the spin degree of freedom can be controlled indirectly by the spin-orbit interaction via electrical means.

1.4 Spin relaxation mechanisms

In this section, we describe the main sources of spin relaxation in different dimensionalities.

1.4.1 Quantum dots

In order to perform quantum computation using semiconductor quantum dots as qubits, it is required to manipulate coherently the electron spin in longer timescales compared with gate operation times, as explained in Sec.[1.2]. Thus it is necessary to investigate the sources of dissipation and decoherence which strongly affects the spin dynamics. In quantum dots, these are the phonons of the crystal and nuclear spins of the host material.

Phonons does not couple directly to the electron spin. As a result, the Coulomb electron-ion interaction for the atoms that are shifted from their equilibrium positions due to lattice vibrations, also known as electron-phonon interaction $\mathcal{H}_{\text{e-ph}}$, is consequently a spin-independent term, $\langle n, \downarrow | \mathcal{H}_{\text{e-ph}} | n, \uparrow \rangle = 0$, where n indexes the quantum dot orbital numbers. Nevertheless, the SO interaction is able to open a relaxation channel since it can mix states with opposite spins states (admixture mechanism). Treating the SO interaction as a perturbation and using time-independent perturbation theory, we have that

$$|\tilde{n}, \uparrow\rangle = |n, \uparrow\rangle + \sum_{n' \neq n} c_{n,n'} |n', \downarrow\rangle, \quad (1.2)$$

where $\tilde{n}$ denotes the orbital number after performing the perturbation theory and the coefficient $c_{n,n'} \propto \mathcal{H}_{\text{SO}}$. Using these perturbed states, the matrix element $\langle \tilde{n}, \downarrow | \mathcal{H}_{\text{e-ph}} | \tilde{n}, \uparrow \rangle$ is no longer zero. Thus the spin relaxation occurs via phonon emission (energy exchanged with the bath) accompanied by a spin-flip transition due to SO interaction. Specifically, in GaAs quantum dots, the spin relaxation rate depends strongly on the external magnetic field, $1/T_1 \propto B^5$. This dependence was confirmed experimentally revealing also very long spin relaxation times, $T_1 \sim 1 \text{ s}$ (26). In addition, the decoherence time T_2 is on the same order of the spin relaxation time T_1 , i.e., $T_2 = 2T_1$, for the leading order of the electron-

phonon interaction (27). This power law $1/T_1 \propto B^5$ is suppressed for large magnetic fields when the phonon wavelength becomes much smaller than the dot size. Also, spin-orbit-induced energy anticrossing with states with opposite spins can lead to a non-monotonic behaviour of the spin relaxation time as a function of the external magnetic field (28). The magnetic field condition for the enhancement of the spin relaxation rate has to be avoided in order to reduce the qubit errors. Similar mechanism of spin relaxation due to the phonon bath-induced energy relaxation accompanied by a spin-flip assisted by the SO interaction also occurs in graphene- and carbon nanotubes-based spin qubits (18, 19, 29).

The electron spin can also interact with the spins from the nuclear spins of the host material which is described by the hyperfine interaction. In a quantum dot, an electron is confined to lengthscales of the order of the Fermi wave length, which for GaAs is about ~ 100 nm. This size is much larger than the lattice space which is on the order of 1 Å. As a consequence, the electron orbital wavefunction extends over a region much larger than the lattice constant and the electron spin dynamics is strongly affected by the fluctuating magnetic field effectively generated by the many nuclear spins within this region. Hence, the spin decoherence time is reduced to the order of nanoseconds. This very short timescale limits the feasibility of a semiconductor quantum dots-based quantum computer. Several attempts were suggested to overcome this issue such as preparation of the spin bath in a narrowed distribution (30) and high magnetic fields combined with ultra-low temperatures as an effort to polarize the bath (31).

1.4.2 Quantum wires

As mentioned in Sec.[1.3], the Rashba SO interaction originates from the structural inversion asymmetry along the growth direction. On the other hand, the Dresselhaus SO coupling comes from the bulk inversion asymmetry of the lattice. These interactions can be represented by a momentum-dependent effective magnetic field

$$\mathcal{H}_{\text{SO}} = \frac{1}{2}g\mu_B \mathbf{B}_{\text{SO}} \cdot \boldsymbol{\sigma}, \quad \mathbf{B}_{\text{SO}} = \mathbf{B}_{\text{R}} + \mathbf{B}_{\text{D}} \quad (1.3)$$

where the effective Rashba $\mathbf{B}_{\text{R}}$ and Dresselhaus $\mathbf{B}_{\text{D}}$ magnetic fields are given by

$$\mathbf{B}_R = \frac{2\alpha}{g\mu_B} \begin{pmatrix} +k_y \\ -k_x \end{pmatrix}, \quad \mathbf{B}_D = \frac{2\beta}{g\mu_B} \begin{pmatrix} -k_x \\ +k_y \end{pmatrix}. \quad (1.4)$$

In a back-of-the-envelope calculation, there is a simple way to show the electron momentum and SO magnetic field dependence of the spin relaxation time τ_{SR} due to a mechanism called D'yakonov-Perel (32). Consider an electron going through multiple random scatterings generating also a random fluctuating effective magnetic field. So, the spin precession frequency (Larmor frequency) $\Omega_{SO} = |g\mu_B \mathbf{B}_{SO}/\hbar|$ can be different after each scattering event, which will lead to a dephasing of the spin components for an electron ensemble. For simplicity, let us assume that Ω_{SO} can only change between two values, either $+\Omega_{SO}$ or $-\Omega_{SO}$. After a time on the order of the momentum scattering time τ_p , the spin will precess either with the frequency $+\Omega_{SO}$ or $-\Omega_{SO}$ with the same probability. In addition, the phase accumulated between each scattering events is $\delta\phi = \nu\Omega_{SO}\tau_p$, with $\nu = \pm$ depending on the precession orientation around a fixed axis. Notice that this problem can be mapped onto a one-dimensional symmetric random walk with stepsize $\delta\phi$. So, the standard deviation σ of the total phase after N steps is given by $\sigma(\delta\phi) = \delta\phi\sqrt{N}$, where $N = t/\tau_p$. The standard deviation of the total phase becomes relatively large (order of unity $\sigma(\delta\phi) \approx 1$) in a time τ_{SR} , the spin alignment will be significantly different for each electron spin leading to spin relaxation. Mathematically, $\sigma(\delta\phi) = \delta\phi\sqrt{N} \approx 1$, this expression simplifies to

$$\frac{1}{\tau_{SR}} = \frac{\delta\phi^2}{\tau_p} = \Omega_{SO}^2 \tau_p. \quad (1.5)$$

Notice that the spin relaxation time τ_{SR} is inversely proportional to the momentum scattering time τ_p . This mechanism is illustrated in Fig. [1.3].

In dimensionally-constrained semiconductor structures, such as quantum wires, the DP mechanism is partially suppressed. This occurs when the channel width is comparable or shorter than the mean free path. For this reason, the momentum scattering time is reduced leading to an enhancement of the spin relaxation time (33). In addition, the DP mechanism is completely suppressed in the limit of a strictly 1D channel. In this case only scatterings which will reverse the momentum direction are allowed, $+k \rightarrow -k$ and $-k \rightarrow +k$. According to Eq. [1.4], the spin precession axis does not alter its direction

Figura 1.3 – Illustration of the D'yakonov-Perel spin relaxation mechanism. Each electron from an ensemble undergoes multiple random spin-independent scatterings events. In each scattering event, the effective momentum-dependent spin-orbit magnetic will be oriented along a random direction. Considering that each electron undergoes a different sequence and number of scatterings events, the whole ensemble will reach the same region with their spin orientations randomized within a timescale given by τ_{SR} .

under only momentum reversion. It can be interpreted as the rotations performed by the electron spin after each scattering event, described by the time-evolution operator, commute with each other. Consequently, all electrons in an ensemble will reach their final destinations with the same spin orientation independently of the sequence and number of scatterings. Notice that this statement is no longer true if an external magnetic field is applied in the system since the spin precessions will be performed around distinct axis. In this case, the time-evolution operator in each event does not necessarily commute with each other.

There are other spin relaxation mechanisms which play a major role in low-mobility semiconductor quantum wires and 2D electron gases and/or in the high-temperature limit. For instance, the Elliot-Yafet spin relaxation mechanism which the eigenstates of the Hamiltonian [1.1] are an admixture of spin-up and spin-down components. As a result, there is a non-vanishing probability of spin-flip at each scattering considering a spin-independent potential (34, 35). Hence, the Elliot-Yafet spin relaxation rate is proportional to the impurity concentration. For this reason this rate is inversely proportional to the momentum scattering time, in contrast with the D'yakonov-Perel mechanism.

As explained in Sec.1.4.1, the phonon bath in combination with spin-orbit interaction can lead to spin relaxation due to admixture mechanism. So, this mechanism strongly depends on the lattice vibrations which can be represented by a fluctuating magnetic field. Thus the spin relaxation due to phonons is suppressed at low temperatures. The hyperfine interaction also plays a minor role since it is averaged out for itinerant electrons.

1.4.3 Two-dimensional electron gas

All the spin relaxation mechanisms introduced in the previous Subsec.1.4.2 are also operative in a 2D electron gas. As explained previously, the D'yakonov-Perel mechanism is suppressed in confined system when the mean free path becomes comparable with the channel width. Notice that such behaviour is in agreement with Eq. [1.5], where the shorter the momentum scattering time, the longer the spin relaxation time. Nevertheless, even in 2D systems where the Rashba and Dresselhaus SO interactions are operative, it is possible to suppress completely the D'yakonov-Perel and the Elliot-Yafet relaxation mechanisms. This can be achieved by choosing a parameter such as the external gate voltage, electronic density or well width which fulfills the condition $\alpha = \pm\beta$ for the Rashba and Dresselhaus SO coupling strengths is fulfilled. Within this condition, the *linear-in-k* Hamiltonian [1.1] simplifies to

$$\mathcal{H}_{\text{SO}} = -2\beta |k_{\pm}| \Sigma_{\mp}. \quad (1.6)$$

where $k_{\pm} = (k_x \pm k_y)/\sqrt{2}$ and $\Sigma_{\pm} = \text{sgn}(k_{\pm})(\sigma_x \pm \sigma_y)/\sqrt{2}$. Here, we perform a transformation of coordinates where $x_{\pm} = (x - y)/\sqrt{2}$. The quantities $\Sigma_{\pm}$ are conserved since they commute with the Hamiltonian $\mathcal{H}_{\text{SO}} \propto \Sigma_{\pm}$ and define a *k-independent* direction for the spin quantization axis. In another words, it can be interpreted in terms of the effective SO magnetic field

$$\frac{1}{2}g\mu_B \mathbf{B}_{\text{SO}} = -2\beta k_{\pm} \mathbf{x}_{\mp} \quad (1.7)$$

which has a fixed direction along $x_{\mp}$ depending on the choice $\alpha = \pm\beta$. Consequently, even considering elastic scatterings in the electron dynamics, the effective SO magnetic field will be always parallel the same axis. It mimics the strictly one-dimensional chan-

nel limit discussed in Subsec.[1.4.2]. Thus multiple random scatterings will affect the electron momentum orientation, but it will not change the spin alignment thus reducing the D'yakonov-Perel spin relaxation rate. Moreover, the Elliot-Yafet mechanism is also completely suppressed for momentum-orientation independent eigenspinors (24).

A fixed spin quantization axis in a SO-coupled system can overcome a serious limitation of the Datta-Das spin-FET which only operates in the absence of disorder or in a strictly 1D channel, as discussed in Sec.[1.3]. This is the main proposal of a spin-FET which also operates in the nonballistic regime (24). In one of its operating modes, the electron is injected in the channel with its spin pointing along the spin quantization axis and will suffer spin relaxation depending on the external gate voltage. So, let us assume that the ferromagnetic drain and source have the same magnetization oriented along $\mathbf{x}_-$ ($\mathbf{x}_+$). For a gate bias such that $\alpha = +\beta(-\beta)$, the spin current injected from the source parallel to the fixed spin quantization axis will not relax due to momentum-dependent scattering and will enter the drain (ON state). On the other hand, when $\alpha \neq +\beta(-\beta)$, the initially polarized ensemble of electron will have their spins randomized before reaching the ferromagnetic collector and they will not enter into the drain (OFF state).

Figure 1.4 – (a) Persistent spin helix in a 2D electron gas. This spin pattern arises as an interplay of the Rashba α and Dresselhaus β spin-orbit coupling strengths. Within this model, when they are tuned to the case $\alpha = \beta$, the eigenspinors become independent of the momentum orientation leading to a steady spin pattern. It is robust against spin-independent scatterings and electron-electron interaction. In this figure, we consider the situation where the conserved quantity Σ_- is pointing along the $\mathbf{x}_-$ -direction and the spin precession occurs along the orthogonal direction $\mathbf{x}_+$. (b) Propagation of two different particles along distinct paths. The spin precession only depends on the net propagation parallel to the $\mathbf{x}_+$ axis. The spins for each particle recovers the same initial spin alignment after travelling a distance L_+ . Adapted from Koralek et al. (3) and Bernevig et al. (4).

The presence of conserved quantities Σ_- (Σ_+) also leads to a spin precession patterns that depend only on the net displacement along $\mathbf{x}_+$ ($\mathbf{x}_-$), as depicted in Fig. [1.4]. This

effect was named persistent spin helix (PSH) after Bernevig et al. (4). In order to present a simpler physical understanding of the formation of a PSH, consider two electrons with momentum $\mathbf{k}$ propagating in SO-coupled electron gas with $\alpha = \beta$, as shown in Fig. [1.4]. We can interpret the spin precession around the effective SO magnetic field [1.7] as a rotation with angle $\delta_+ = 4\beta k_+ t/\hbar$. The net distance propagate along the $\mathbf{x}_+$ is denoted by X_+ . Using that $X_+ = \hbar k_+ t/m$, the spin precession angle is given by $\delta_+ = 4m\beta X_+/\hbar^2$. Notice that the spin precession angle only depends on the net distance X_+ propagated perpendicularly to fixed SO magnetic field. We have that any ensemble of electrons starting with the same spin orientation will always keep this alignment on condition that they propagate the same distance along the axis $\mathbf{x}_+$. Accordingly, this spin pattern generated by the electron diffusion is robust against spin-independent scattering. Also, spins for each electron in the ensemble returns to the same initial configuration, which allow us to define the persistent spin helix wavevector $\mathbf{q}_{\text{PSH}} = (4m\beta/\hbar^2)\mathbf{x}_+$, where $|\mathbf{q}_{\text{PSH}}| = 2\pi/L_+$.

These helical spin waves were measured using spin grating technique where the decay time is monitored of an out-of-plane spatially modulated spin excitation with an specific wavevector q (3). A robust helix mode survives longer than the other modes and its enhanced lifetime is extracted using a double-fit exponential model following the prediction by Ref. (4). The spatial and time evolution of local out-of-plane spin polarization using Kerr rotation technique has also been measured (36). This uniform spin pattern relaxes following the DP and EY spin relaxation mechanisms, as explained in Sec.[1.4.2]. For $\alpha = \pm\beta$, a single helical spin wave formation lives longer characterizing the PSH regime. At last, we emphasize that $\alpha = +\beta$ and $\alpha = -\beta$ are related to orthogonal spin quantization axis $\mathbf{x}_-$ and $\mathbf{x}_+$, respectively. It could lead to spin patterns created along orthogonal directions depending on the value of the SO coupling strength in each level of a quantum well with two subbands (37, 38).

1.5 Outline

In this thesis, we investigate dimensionally-constrained spin relaxation mechanisms in semiconductor nanostructures. Different mechanisms play a major role in each dimension depending on the electron mobility. Each of these mechanisms has to be understood in

order to harness their detrimental effects. To this end, we analyze the spin relaxation in graphene quantum dots, multisubband quantum wires and two-dimensional electron gas.

In chapter 2, we study the spin relaxation and decoherence in graphene quantum dots. In our model, we consider a circular and gate-tunable quantum dot formed in a graphene sheet with an applied static magnetic field. Our two-level system (qubit) is comprised of the ground state and the first excited state with opposite spin orientation. The spin relaxation occurs between these states with the energy relaxation provided by the phonon emission. Since the electron-phonon interaction is spin-independent, the spin-flip mechanism is assisted by the SO interaction. Here, we take into account long-wavelength acoustic phonons combined with the Rashba and the intrinsic SO coupling. We derive an effective spin-phonon Hamiltonian via the Schrieffer-Wolff transformation to capture this coupling between the electron spin to potential fluctuations generated by the lattice vibrations. After that, we calculate the spin relaxation time T_1 and the decoherence time T_2 in the framework of the Bloch-Redfield theory. We found that T_1 present distinct behaviors with the external magnetic field depending on the relaxation mechanism and the SO coupling considered in the quantum dot. For the Rashba SO interaction, we obtain a minimum of T_1 as a function of the external magnetic field $\mathbf{B}_{\text{ext}}$. This non-monotonic behavior is induced at the energy anticrossing with opposite spin orientations in the graphene quantum dot spectrum. Here, the Rashba SO interaction mixes opposite spin and excited orbital states which combined with phonon emission open a relaxation channel (admixture mechanism). We predict that this mechanism dominates the spin relaxation time for high magnetic field $\mathbf{B}_{\text{ext}} > 5$ T. By contrast, the intrinsic SO interaction has a monotonic magnetic field dependence of T_1 . In this case, the electron spin couples locally to graphene sheet deformations (deflection coupling mechanism). We expect that this contribution dominates the spin relaxation time at low magnetic fields. The Rashba SO interaction is tunable by an electric field applied perpendicularly to the graphene sheet, so is the monotonicity of the magnetic field dependence of T_1 . Moreover, the magnetic field dependence of the spin relaxation time opens up new possibilities to probe the SO interaction in graphene since different behaviors can be attributed to each SO coupling. We demonstrate that the decoherence time $T_2 = 2T_1$ is dominated by the relaxation contribution for one-phonon processes in the leading order of the SO interaction. In contrast with GaAs quantum dots where the hyperfine interaction strongly reduces the

decoherence time, we have that the admixture mechanism can compete with the influence from the nuclear spins of the host material for high magnetic fields. We also analyze the spin dephasing rate in the vicinity of a general energy anticrossing. We find a vanishing dephasing contribution at the level anticrossing for a any super-Ohmic bath.

In chapter 3, we study the spin relaxation in a quasi-one-dimensional channel. Mainly, we focus on the magnetic field dependence of the spin relaxation time due to the D'yakonov-Perel relaxation mechanism. We develop a model to account for elastic spin-conserving impurity scatterings in the time-evolution operator. Thus we are able to extract the spin relaxation time evaluating the time dependent expectation value of the spin operators. The DP spin relaxation time has a monotonic dependence with the external magnetic field when $\mathbf{B}_{\text{ext}}$ is aligned with the quantum wire. Nevertheless, a non-monotonic dependence can arise due to the interplay of static external magnetic field and the oscillating effective spin-orbit field created by periodic specular scatterings of the electrons off the boundaries of a ballistic micrometer-scale channel. Notice that this ballistic spin resonance does not require any external driving fields. In this case, the resonance condition can be find matching the frequency of the spin-orbit field matched that of the Larmor precession frequency around the external magnetic field. Within our model, we predict a spin resonance due to the spin-orbit induced energy anticrossings of the quantum wire subbands with opposite spins. We also observe an enlargement of the BSR dip into a wide plateau, in agreement with the experimental findings (8). This feature arises as a consequence of injection in higher subbands and small-angle scattering. We also predict that anomalous ballistic spin resonance dips, even when $\mathbf{B}_{\text{ext}}$ is aligned with the quantum wire, occurs in system with a strong SO coupling.

In chapter 4, we predict the emergence of a novel robust spin pattern in a SO-coupled two-dimensional electron gas. In this work, we extend the formation of a persistent spin helix in one-subband model (4) for a quantum well with two subbands. Here, we consider a two-subband model where the Rashba α and Dresselhaus β SO interactions are tuned to have equal strenghts, but opposite signs. Thus for the first subband $\alpha_1 = \beta_1$ while for the second subband $\alpha_2 = -\beta_2$. For the SO interaction in each subband, we can find a spin-conserved quantity aligned along orthogonal directions. This property of the SO Hamiltonian in a quantum well with two subbands give rise to a crossed PSHs. We solve spin-charge coupled diffusion equation in order to analyze the spin helix decay. This

allow us to find potential experimental setups to probe the crossed PSHs. Finally, we investigate the role of the interband SO coupling on the lifetime of the crossed persistent spin helices, levels anticrossings and spin textures in the energy spectrum.

CHAPTER 2

SPIN RELAXATION AND DECOHERENCE IN GRAPHENE QUANTUM DOTS

2.1 Introduction

Over the past years, many materials and setups were suggested to host a spin qubit following the original proposal of Loss and DiVincenzo (1). These authors proposed a universal implementation of a quantum computer using spin states of coupled quantum dots (QDs). Since GaAs QDs were extensively studied in the literature in the last decade (39), a first spin qubit was implemented in this system where single and two-qubit operation were carried out (40). Although long spin relaxation times have been achieved in GaAs QDs (26), the fluctuating effective magnetic field generated by the nuclear spin bath strongly reduces its spin decoherence time. Since this may pose severe constraints to practical implementations of solid-state spin qubits (17), new proposals using different materials have appeared in the literature. Thus carbon-based materials such as graphene (18) and carbon nanotubes (19, 41) have emerged as potential candidates to host a spin qubit. These materials consist of 99% of ^{12}C with nuclear spin 0 and of 1% ^{13}C with nuclear spin 1/2. Hence, the hyperfine interaction is rather a weak contribution leading

to longer decoherence times in these systems (20). Moreover, purification techniques can be used to remove the remaining ^{13}C atoms extending even more the number of logical operations that can be performed before the information in the qubit is completely lost to the surrounding environment. Remarkably, graphene also possesses a relatively weak spin-orbit interaction (SO) compared with narrow-gap semiconductors (21, 22, 42, 43). It is noteworthy that since the main mechanism of the spin relaxation in QDs is due to the electron-phonon interaction where the spin-flip transition is provided by the SO interaction. Consequently, even longer spin relaxation times are expected in a graphene-based spin qubit.

In this chapter, we study theoretically the spin relaxation and decoherence in a circular and gate-tunable graphene QDs. In Sec. [2.2], we analyze the quantum dot energy spectrum. In Sec. [2.3], we derive an effective Hamiltonian via the Schrieffer-Wolff which connects the electron spin with the potential fluctuations caused by lattice vibrations. In Sec. [2.4], we calculate the spin relaxation time T_1 and decoherence time T_2 as a function of the external magnetic field in the framework of the Bloch-Redfield theory. The Rashba SO coupling-induced anticrossing of opposite spin states leads to a non-monotonic dependence of T_1 on the external magnetic field. T_1 minimum occurs in the vicinity of the accidental degeneracy between the two first excited states, where the spin relaxation reaches the same order of the orbital relaxation. For realistic parameters, we determine the value of the external magnetic field $\mathbf{B}^*$ where the T_1 minimum takes place. On the other hand, the intrinsic SO coupling, via direct spin-phonon coupling mechanism, presents a monotonic behavior and dominates the spin relaxation at low magnetic fields. In Sec. [2.5], we also demonstrate that $T_2 \simeq 2T_1$ in the leading order of the non-piezoelectric electron-phonon mechanisms considered in this work. Finally, we also demonstrate that in the vicinity of an energy anticrossing, the spin dephasing rate vanishes for these states for any super-Ohmic bath.

2.2 Model for a graphene quantum dot

In this section, we introduce our theoretical model for a circular and gate-tunable graphene quantum dot. We analyze its energy spectrum and the lifted degeneracy by the

presence of the Rashba SO interaction.

2.2.1 Circular and gate-tunable graphene quantum dots

Figure 2.1 – (a) Graphene is a two-dimensional hexagonal structure made of carbon atoms. These atoms can be seen as a triangular Bravais lattice with the lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ with two atoms (A and B) per unit cell with the nearest-neighbor vectors δ_i , $i = 1, 2, 3$. (b) Brillouin zone of graphene’s honeycomb lattice. The Dirac cones characterized by a linear dispersion relation are located at the K and K' . Adapted from Castro Neto et al. (5).

Graphene is a one-carbon-atom-thick layer arranged in a honeycomb crystal lattice. This hexagonal lattice, formed due to sp^2 orbital hybridization, has as sublattice two equivalent carbon atoms per unit cell denoted by the A and B (pseudospin degree of freedom). The in-plane sp^2 mixed orbitals couple to other hybridized orbitals from neighboring carbon atoms generating the σ -band. Similarly, the out-of-plane p_z orbitals form the π -band which is related to the unique electronic properties of graphene. Its electronic structure is particular since it can be mapped onto a Dirac-like Hamiltonian. That is because the energy spectrum simplifies to a linear dispersion after performing a low-energy expansion around the non-equivalent points K and K' (valleys) in the honeycomb lattice Brillouin zone. Thus the low-energy effective Hamiltonian for graphene in the sublattice space and its respective linear dispersion relation is given by (5)

$$\mathcal{H}_d = \hbar v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = \hbar v_F \mathbf{p} \cdot \boldsymbol{\sigma}, \quad \epsilon(k) = \pm \hbar v_F |k| \quad (2.1)$$

where $\mathbf{p} = \hbar \mathbf{k}$ denotes the momentum operator and $\boldsymbol{\sigma}$ denotes the Pauli matrices vector and acts on the pseudospin subspace (A,B sublattices). Notice that this Hamiltonian is equivalent to the massless Dirac equation with the speed of light replaced by the Fermi

velocity $v_F \approx 10^6$ m/s. Thus one can expect analogous quantum relativistic phenomena in the solid-state physics such as Klein tunneling and *Zitterbewegung*. Particularly, Klein tunneling does not allow for confining electrons via an external electrostatic potential. In order to overcome this issue, graphene can be put on top of a substrate, such as SiC (44) and BN (45, 46). The substrate atoms induce a non-equivalent potential for the sublattice atoms A and B parametrized by $+\Delta$ and $-\Delta$, respectively. It is equivalent to add a mass term in the Dirac-like Hamiltonian (2.1) which opens a gap 2Δ at the valleys K and K' . Consider then a graphene on top of substrate-induced energy gap in a external electrostatic potential $U(r)$ which defines the quantum dot circular shape, as shown in Fig. [2.2]. In addition, we consider an external magnetic field $\mathcal{H}_Z$ to, combined with the mass term, break the valley degeneracy allowing us to restrict our model to a single valley, for instance, K valley. This single-valley approximations holds since the the valley splitting $\Delta E_{K,K'}$ for the ground state is much larger than the intervalley coupling $\Delta_{K,K'}$ even for a very small magnetic field. For instance, $\Delta E_{K,K'} \sim 10^2$ meV $\gg \Delta_{K,K'} \sim 10$ meV (47) for $\mathbf{B}_{\text{ext}} = 0.05$ T. The bare quantum dot Hamiltonian $\mathcal{H}_d$ for the K valley and the Zeeman term $\mathcal{H}_Z$ are given by (48),

$$\mathcal{H}_d = \hbar v_F \boldsymbol{\Pi} \cdot \boldsymbol{\sigma} + U(r) + \Delta \sigma_z, \quad \mathcal{H}_Z = \frac{1}{2} g \mu_B \mathbf{B} \cdot \mathbf{s}, \quad (2.2)$$

where $\boldsymbol{\Pi} = \mathbf{p} - e\mathbf{A}$ is the canonical momentum and the spin operator $\mathbf{s}$ denotes the Pauli matrices vector. An external magnetic field $\mathbf{B}_{\text{ext}}$ is applied perpendicularly to the graphene sheet, thus the vector potential is chosen such that $\mathbf{B}_{\text{ext}} = \mathbf{B} = \nabla \times \mathbf{A} = (0, 0, B)$. The electrostatic potential is explicitly given by $U(r) = U_0 \Theta(r - R)$, where $\Theta(x)$ is the Heavside function defined as $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$.

In order to calculate T_1 and T_2 in graphene QDs, we still have to take into account the spin-orbit and the electron-phonon interactions. The electron-phonon interaction couples different orbital states with the same spin orientation. Thus SO interaction provides the spin-flip mechanism connecting the Zeeman spin-splitting states (admixture mechanism) (49). The lattice vibrations can also coupled directly to the electron spin via the curvature-induced SO interaction (deflection coupling mechanism) (50).

The spin-orbit interactions for the K valley is given by (21)

Figure 2.2 – Setup of a circular and gate-tunable graphene quantum dot. The graphene sheet is put on top a substrate in order to induce an energy gap in the graphene spectrum. The confiment potential is generated by a voltage applied to metallic top gates. Also, an homogeneous magnetic field $\mathbf{B}$ is applied perpendicularly to the graphene sheet.

$$\mathcal{H}_{\text{SO}} = \mathcal{H}_{\text{i}} + \mathcal{H}_{\text{R}} = \lambda_{\text{i}} \sigma_z s_z + \lambda_{\text{R}} (\sigma_x s_y - \sigma_y s_x), \quad (2.3)$$

where $\mathcal{H}_{\text{i}}$ and $\mathcal{H}_{\text{R}}$ denote the intrinsic and Rashba SO effective Hamiltonians, respectively. Here the tensor product notation is implicit, i.e., $\sigma_i s_j \equiv \sigma_i \otimes s_j$, for $i, j = x, y, z$. The intrinsic SO captures the local atomic contribution $\mathcal{H}_{\text{SO}}^{\text{at}} \propto \xi \mathbf{l} \cdot \mathbf{s}$, where ξ is the atomic SO coupling strength $\mathbf{l}$ is the angular momentum. For a while, the correct SO coupling strengths λ_i was under debate. At first, the parameter λ_i was estimated considering the coupling between the π and σ bands formed by the out-of-plane p_z and in-plane p_x, p_y orbitals, respectively. So, the first non-vanishing term appears in second-order perturbation theory resulting in $\lambda_i \sim \xi^2$ (22). However, Gmitra et al. (42) and Konschuh et al. (43) using first-principle calculations and a tight-binding analyzes estimate much higher values for λ_i than those obtained previously in the literature (22). In fact, they claim that the major contribution from λ_i comes from the inclusion of d orbitals in the π -bands in graphene which leads to $\lambda_i \sim \xi$ (43). The Rashba SO coupling arises when an external electric field E is applied perpendicularly to the graphene sheet due to combination of atomic SO interaction and Stark effect. Notice that the Rashba SO coupling λ_{R} is tunable via gate voltage since $\lambda_{\text{R}} \propto E$. The term λ_{R} could be enhanced in curved graphene sheets as a result of hybridization between the in-plane and out-of-plane orbitals (51).

Tabela 2.1 – Electron-phonon constants and sound velocities for longitudinal (LA) and transverse (TA) acoustic phonons.

Modes	a_1	a_2	$s_\mu(10^4 \text{ m/s})$
LA	i	$ie^{2i\phi_q}$	1.95 (53)
TA	0	$e^{2i\phi_q}$	1.22 (53)

The electron-phonon interaction in graphene arises from two main mechanisms. The deformation potential generated by static distortions of the lattice and the bond-length change induced by modifications of the bond-length between neighboring carbon atoms. The electron-phonon Hamiltonian in the sublattice space reads (52)

$$\mathcal{H}_{\text{e-ph}} = \sum_{\mathbf{q}, \mu} \frac{q}{\sqrt{A\rho\omega_{\mathbf{q}, \mu}}} \begin{pmatrix} g_1 a_1 & g_2 a_2^* \\ g_2 a_2 & g_1 a_1 \end{pmatrix} (e^{i\mathbf{q}\mathbf{r}} b_{\mathbf{q}, \mu}^\dagger - e^{-i\mathbf{q}\mathbf{r}} b_{\mathbf{q}, \mu}), \quad (2.4)$$

where g_1 and g_2 are the deformation potential and bond-length change coupling constants, respectively. Here, A is the area of the graphene layer and ρ is the mass area density. These phonon branches have a linear dispersion $\omega_{\mathbf{q}, \mu} = s_\mu |\mathbf{q}|$. The constants a_1 , a_2 (given in terms of the phonon emission angle ϕ_q) and the sound velocities s_μ for the longitudinal-acoustic ($\mu = \text{LA}$) and transverse-acoustic ($\mu = \text{TA}$) modes are given in Table 2.1. Notice that we do not consider the optical phonons since they cannot provide the energy relaxation which leads to spin relaxation assisted by the SO interaction. This is justified since because their energies does not match the Zeeman energy separation for typical laboratory fields.

Finally, we include the free phonon Hamiltonian

$$\mathcal{H}_{\text{ph}} = \sum_{\mathbf{q}, \mu} \hbar \omega_{\mathbf{q}, \mu} b_{\mathbf{q}, \mu}^\dagger b_{\mathbf{q}, \mu} \quad (2.5)$$

where the phonon dispersion relation $\omega_{\mathbf{q}, \mu} = s_\mu |\mathbf{q}|^m$, with $m = 1, 2$ depending on the phonon branch type.

2.2.2 Energy spectrum of graphene quantum dots

Next we analyze the energy spectrum of a circular and gate-tunable graphene quantum dot. Moreover, we will perform a standard degenerate state perturbation theory since the

Rashba SO coupling connects degenerate quantum dot states. First we start with the Hamiltonian $\mathcal{H}_d$ (2.2) rewritten in polar coordinates with $x = r \cos \phi$ and $y = r \sin \phi$ (48)

$$\mathcal{H}_d = -i\hbar v_F \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \partial_r + \hbar v_F \begin{pmatrix} 0 & -e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \left(\frac{1}{r} \partial_\phi + \frac{ieBr}{2} \right) \quad (2.6)$$

where we have used the symmetric gauge $\mathbf{A} = B/2(-y, x, 0)$, with $\mathbf{B} = (0, 0, B) = \nabla \times \mathbf{A}$. Notice that $[\mathcal{H}_d, j_z] = 0$, where $j_z = -i\hbar \partial_\phi + \sigma_z/2$. Using that the commuting operators $\mathcal{H}_d$ and j_z have a common set of eigenspinors, they can be chosen as (48)

$$\langle r, \phi | j, \nu, s \rangle = \psi_{j,\nu,s}(r, \phi) = e^{i(j-1/2)\phi} \begin{pmatrix} \chi_A^{j,\nu,s}(r) \\ \chi_B^{j,\nu,s}(r) e^{i\phi} \end{pmatrix}. \quad (2.7)$$

with $j_z \psi_{j,\nu,s}(r, \phi) = j \psi_{j,\nu,s}(r, \phi)$. Solving the differential equation $\mathcal{H}_d \psi_{j,\nu,s}(r, \phi) = E_{j,\nu,s} \psi_{j,\nu,s}(r, \phi)$, where we have that the spinor components $\chi_{A,B}^{j,\nu,s}(r)$ are given in terms of the confluent hypergeometric functions. Here, the set (j, ν, s) denotes the angular ($j = \pm 1/2, \pm 3/2, \dots$), radial ($\nu = 1, 2, 3, \dots$) and spin $s = \uparrow, \downarrow$ quantum numbers. The bound states $E_{j,\nu,s}$ can be found by matching the solutions at $r = R$ and solving the resulting transcendental equations numerically.

Since we intend to calculate the spin relaxation between transitions from the first excited states to the ground state in a graphene quantum dot, we restrict our analysis to the subspace $\{|+1/2, 1, \downarrow\rangle, |1/2, 1, \uparrow\rangle, |-1/2, 1, \downarrow\rangle\}$. In order to define our qubit states, we perform the degenerate state perturbation theory treating the SO interaction as a perturbative term (6). The selection rules of the Rashba SO interaction for the angular quantum number $|j - j'| = 1$ couples the degenerate states $|1/2, 1, \uparrow\rangle, |-1/2, 1, \downarrow\rangle$ for a certain value of external magnetic field $\mathbf{B}^*$ (29, 48). Whereas the intrinsic SO interaction does not couple these degenerate state since its selection rules are $|j - j'| = 0$ (29). We perform standard degenerate state perturbation theory, where the zero-order eigenstates for the three lowest energy levels

$$\begin{bmatrix} |\gamma_0\rangle \\ |\gamma_1\rangle \\ |\gamma_2\rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\vartheta/2)e^{i\delta} & -\sin(\vartheta/2) \\ 0 & \sin(\vartheta/2)e^{i\delta} & \cos(\vartheta/2) \end{bmatrix} \begin{bmatrix} |1/2, 1, \downarrow\rangle \\ |1/2, 1, \uparrow\rangle \\ |-1/2, 1, \downarrow\rangle \end{bmatrix}, \quad (2.8)$$

$$E_{\gamma_0} = E_{1/2,1} - \frac{\hbar\omega_Z}{2}, \quad E_{\gamma_1, \gamma_2} = \epsilon_{\pm} \mp \sqrt{\epsilon_{\pm}^2 + |\Delta_{SO}|^2}. \quad (2.9)$$

These eigenvalues are plotted in Fig. [2.3]. At the energy anticrossing $\epsilon_- = 0$, we have a energy gap $2\Delta_{SO}$ due to the Rashba SO field. Here, $\epsilon_+ = (E_{1/2,1} + E_{-1/2,1})/2$ and $\epsilon_- = (E_{1/2,1} - E_{-1/2,1} + \hbar\omega_Z)/2$, $\hbar\omega_Z = g\mu_B B$ is the Zeeman energy splitting. We define $\Delta_{SO} = \langle 1/2, 1, \uparrow | \mathcal{H}_R | -1/2, 1, \downarrow \rangle = 4\pi i \lambda_R \int dr r \chi_A^{1/2,1}(r) \chi_B^{-1/2,1}(r)$, $\tan \vartheta = \Delta_{SO}/\epsilon_-$ and $\tan \delta = \Im[\Delta_{SO}]/\Re[\Delta_{SO}]$, where $\Im[x]$ is the imaginary part and $\Re[x]$ the real part of x . Prior to the energy anticrossing region, $\Delta_{SO}/\epsilon_- > 0$, $|\gamma_1\rangle \approx |1/2, 1, \uparrow\rangle + \mathcal{O}(\Delta_{SO}/\epsilon_-)$ and $|\gamma_2\rangle \approx |-1/2, 1, \downarrow\rangle + \mathcal{O}(\Delta_{SO}/\epsilon_-)$. Thus the spin relaxation takes place between $|\gamma_1\rangle \rightarrow |\gamma_0\rangle$. At the anticrossing $\vartheta \rightarrow \pi/2$ since $\epsilon_- = 0$. Then the states from the degenerate subspace hybridize $|\gamma_1\rangle \approx (|1/2, 1, \uparrow\rangle - |-1/2, 1, \downarrow\rangle)/\sqrt{2}$ and $|\gamma_2\rangle \approx (|1/2, 1, \uparrow\rangle + |-1/2, 1, \downarrow\rangle)/\sqrt{2}$. The spin relaxation time reaches the same order of the orbital relaxation in the region of equal weight of spin-up and spin-down (28, 54, 55). Beyond the energy anticrossing region $\Delta_{SO}/\epsilon_- < 0$, $|\gamma_1\rangle \approx |-1/2, 1, \downarrow\rangle + \mathcal{O}(\Delta_{SO}/\epsilon_-)$ and $|\gamma_2\rangle \approx |1/2, 1, \uparrow\rangle + \mathcal{O}(\Delta_{SO}/\epsilon_-)$. In this case, the spin relaxation occurs between $|\gamma_2\rangle \rightarrow |\gamma_0\rangle$.

2.3 Effective spin-phonon interaction

Next we derive an effective Hamiltonian which connects the electron-phonon and the SO interaction. This effective spin-phonon Hamiltonian will be used to calculate T_1 and T_2 in the framework of the Bloch-Redfield theory. We perform a Schrieffer-Wolff transformation (10, 27) in order to remove the SO Hamiltonian in the leading order (6),

Figure 2.3 – Energy difference between the perturbed three lowest energy levels and the ground state vs. magnetic field. From bottom to top, $E_{\gamma_0} - E_{\gamma_0}$ (solid), $E_{\gamma_1} - E_{\gamma_0}$ (dashed) and $E_{\gamma_2} - E_{\gamma_0}$ (dot-dashed). We define our spin qubit as a two-level system composed of the ground state and the first excited state with opposite spin orientation (6). The Rashba SO coupling induces an anticrossing between the bare quantum dot states $E_{1/2,1,\uparrow}$ and $E_{-1/2,1,\downarrow}$, at $B = B^*$ (solid lines in the inset). The spin relaxation is defined as $\Gamma_{\downarrow\uparrow} = \Gamma_{\gamma_0 \leftarrow \gamma_1}$ before the anticrossing, and $\Gamma_{\downarrow\uparrow} = \Gamma_{\gamma_0 \leftarrow \gamma_2}$ after the anticrossing. Inset: Close-up of the energy levels in the vicinity of the crossing region.

$$\tilde{\mathcal{H}} = e^{\mathcal{S}} \mathcal{H} e^{-\mathcal{S}} = \mathcal{H}_d + \mathcal{H}_Z + \mathcal{H}_{ph} + \mathcal{H}_{e-ph} + [\mathcal{S}, \mathcal{H}_{e-ph}], \quad (2.10)$$

where the operator $\mathcal{S}$ is defined as $[\mathcal{H}_d + \mathcal{H}_Z, \mathcal{S}] = \mathcal{H}_{SO}$, with $\mathcal{S} \sim \mathcal{O}(\mathcal{H}_{SO})$. Here we retain terms up to $\mathcal{O}(\mathcal{H}_{SO})$. Notice that the term $[\mathcal{S}, \mathcal{H}_{e-ph}]$ represents the coupling between the electron spin and the potential fluctuations induced by the lattice vibrations. The operator $\mathcal{S}$ can be rewritten in terms of the Liouvillian superoperator defined as $L_i A = [\mathcal{H}_i, A]$, where A denotes an arbitrary operator. We have that $\mathcal{S} = (L_d + L_Z)^{-1} \mathcal{H}_{SO}$, where $\mathcal{S} = \mathcal{S}^R + \mathcal{S}^i$, where $\mathcal{S}^i \propto \lambda_i$ and $\mathcal{S}^R \propto \lambda_R$. Notice that we do not keep the term $[\mathcal{S}, \mathcal{H}_{ph}]$ since $\langle \gamma_0 | \mathcal{H}_{ph} + [\mathcal{S}, \mathcal{H}_{ph}] | \gamma_k \rangle = 0$, and consequently, it does not contribute to the calculation of the spin relaxation and decoherence time.

For the intrinsic SO, we define the matrix element of the effective spin-phonon Hamiltonian as $\langle n_0, \downarrow | \mathcal{H}_{s-ph}^i | n_0, \uparrow \rangle = \langle n_0, \downarrow | [\mathcal{S}^i, \mathcal{H}_{e-ph}] | n_0, \uparrow \rangle$, where $n_0 = (1/2, 1)$ is the ground state angular and radial quantum numbers. This term is given by

$$\langle n_0, \downarrow | \mathcal{H}_{s-ph}^i | n_0, \uparrow \rangle \propto \sum_{n' \neq n_0} \delta_{j,j'} (N_{n_0 n'}^{AA} - N_{n_0 n'}^{BB}), \quad (2.11)$$

with $N_{nn'}^{AA} = \int dr r \chi_A^n(r) \chi_A^{n'}(r)$ and $N_{nn'}^{BB} = \int dr r \chi_B^n(r) \chi_B^{n'}(r)$. Here, we have used the zero and first orders of the dipole expansion of the term $e^{\pm i \mathbf{q} \cdot \mathbf{r}}$ in the deformation potential (LA) and bond-length change (LA, TA), respectively. These terms are compatible with the selection rules for the angular quantum number $|j - j'| = 0$. Interestingly, we can demonstrate that the matrix element $\langle n_0, \downarrow | \mathcal{H}_{s-ph}^i | n_0, \uparrow \rangle$ is identically zero. To this end, we use that the functions $\chi_A^n(r)$ and $\chi_B^n(r)$ purely real and purely imaginary, respectively. As a result, $\langle n_0, \downarrow | \mathcal{H}_{s-ph}^i | n_0, \uparrow \rangle \propto \langle j, \nu | j, \nu' \rangle = 0$ for $\nu \neq \nu'$.

Conversely, the Rashba SO interaction has a non-vanishing contribution to the spin relaxation rate via the admixture mechanism. In this case, the matrix element of the effective spin-phonon interaction is defined as $\langle \gamma_0 | \mathcal{H}_{s-ph}^R | \gamma_k \rangle = \langle \gamma_0 | \mathcal{H}_{e-ph} + [\mathcal{S}^R, \mathcal{H}_{e-ph}] | \gamma_k \rangle$, where $\gamma_k = \gamma_1, \gamma_2$. Explicitly, we have

$$\begin{aligned}
\langle \gamma_0 | \mathcal{H}_{s-\text{ph}}^R | \gamma_k \rangle &= \langle \gamma_0 | \mathcal{H}_{e-\text{ph}} | \gamma_k \rangle \\
&+ \sum_{n, s \neq \gamma_0} \frac{\Omega_1(\gamma_0, n, \gamma_k)}{E_{\gamma_0} - E_n} \\
&+ \sum_{n, s \neq \gamma_k} \frac{\Omega_2(\gamma_0, n, \gamma_k)}{E_{\gamma_k} - E_n},
\end{aligned} \tag{2.12}$$

with the degenerate subspace $\mathfrak{D} = \{|+1/2, 1, \uparrow\rangle, |-1/2, 1, \downarrow\rangle\}$. Also, we define the following product of matrix elements

$$\Omega_1(\gamma_0; n, s; \gamma_k) = \langle \gamma_0 | \mathcal{H}_R | n, s \rangle \langle n, s | \mathcal{H}_{e-\text{ph}} | \gamma_k \rangle, \tag{2.13}$$

$$\Omega_2(\gamma_0; n, s; \gamma_k) = \langle \gamma_0 | \mathcal{H}_{e-\text{ph}} | n, s \rangle \langle n, s | \mathcal{H}_R | \gamma_k \rangle. \tag{2.14}$$

The order of the dipole expansion for the electron-phonon interaction has to be compatible with the selection rules given by the matrix elements of the Rashba SO interaction $|j - j'| = 1$. In this instance, we choose the terms of the first order and zero order of the dipole expansion of the deformation potential (LA) and bond-length change (LA, TA), respectively.

Considering a small amplitudes for the displacement compared to the phonon wavelength, the normal vector to the graphene sheet is $\hat{n}(z) \approx \hat{z} + \nabla u(x, y)$, where the displacement operator is given by $u_z = \sqrt{1/A\rho\omega_q}(e^{i\mathbf{q}\mathbf{r}}b^\dagger - e^{-i\mathbf{q}\mathbf{r}}b)$. We assume a crossover between a linear and quadratic behaviors in the dispersion relation $\hbar\omega_q = \hbar s q + \hbar\mu q^2$, where $\mu = \sqrt{\kappa/\rho}$, with the bending rigidity $\kappa = 1.1$ eV. In this case, the matrix element of the effective spin-phonon Hamiltonian describing the deflection coupling mechanism reads

$$\begin{aligned} \langle n_0, \downarrow | \mathcal{H}_{s-ph}^{ZA} | n_0, \uparrow \rangle &= \frac{i\lambda_i}{\sqrt{A\rho\omega_q}} (q_x + iq_y) \\ &\times (N_{n_0 n_0}^{AA} + N_{n_0 n_0}^{BB}), \end{aligned} \quad (2.15)$$

where we have the sound velocity $s_{ZA} = 0.25 \times 10^3 \text{m/s}$ (29). We only consider the zero-th order of the dipole expansion since this is the first non-vanishing contribution to the spin relaxation rate.

The matrix elements of the spin-phonon Hamiltonian will be used in the next section to calculate the spin relaxation and decoherence time.

2.4 Spin relaxation rates

Next we calculate the spin relaxation rates using the effective spin-phonon Hamiltonians derived in the previous section. First we give a brief introduction of the Bloch-Redfield theory (56, 57). This theory describes the dynamics of a system via time-dependent perturbation theory weakly coupled to a bath. This approach allows us to obtain explicit expressions for the spin relaxation and decoherence times in terms of matrix elements of the observables of the system under study and time-correlation functions of the environment in thermal equilibrium.

Let us start with a general system-bath Hamiltonian $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_{SB}$. Here, $\mathcal{H}_S$ describes the system, $\mathcal{H}_B$ a reservoir in thermal equilibrium (bath) and $\mathcal{H}_{SB}$ describes the system-bath interaction. The system-bath Hamiltonian $\mathcal{H}$ has a direct mapping with our model, i.e., $\mathcal{H}_S \rightarrow \mathcal{H}_d + \mathcal{H}_Z$, $\mathcal{H}_B \rightarrow \mathcal{H}_{ph}$ and $\mathcal{H}_{SB} \rightarrow \mathcal{H}_{s-ph}$. The system dynamics is described by the equation of motion for the reduced density matrix which is called the Nakajima-Zwanzig equation (56). In the interaction picture ($\hat{\rho} = e^{i(\mathcal{H}_d + \mathcal{H}_Z + \mathcal{H}_{ph})t/\hbar} \rho e^{-i(\mathcal{H}_d + \mathcal{H}_Z + \mathcal{H}_{ph})t/\hbar}$), Nakajima-Zwanzig equation reads

$$\frac{d}{dt} \hat{\rho}^S(t) = -\frac{i}{\hbar} \int_0^t dt' \text{Tr}_B \left[\hat{\mathcal{H}}_{s-ph}(t), \left[\hat{\mathcal{H}}_{s-ph}(t'), \hat{\rho}^S(t') \hat{\rho}^B(0) \right] \right] \quad (2.16)$$

where the bath variables are traced out $\hat{\rho}^S = \text{Tr}_B[\hat{\rho}]$. We consider that the system and

the bath are initially uncorrelated, $\rho(0) = \rho_S(0)\rho_B(0)$ where ρ_i denotes a density matrix related with the Hamiltonian $\mathcal{H}_i$. As time evolves, these terms become correlated due to the system-bath interaction Hamiltonian $\mathcal{H}_{s-ph}$. We also assume that the coupling system-bath is weak, so the density matrix in the integral in Eq. [2.16] can be approximated as $\rho(t) = \rho^S(t)\rho^B(0) + \mathcal{O}(\mathcal{H}_{s-ph})$ (Born approximation). Moreover, we assume that $\hat{\rho}(t') \rightarrow \hat{\rho}(t)$ in the integral of Eq. [2.16], i.e., the time evolution of the $\rho_S(t)$ depends only on its present value and not on its past state (Markov approximation). Using that $\mathcal{H}_S|n\rangle = \epsilon_n|n\rangle$ and taking the matrix elements of $\rho^S(t)$ in the Schrödinger picture between the eigenstates $|n\rangle$ of the Nakajima-Zwanzig equation, and Eq. [2.16] simplifies to

$$\frac{d}{dt}\hat{\rho}_{mn}^S(t) = -\frac{i}{\hbar}\omega_{mn}\rho_{mn}^S(t) - \sum_{k,l} R_{nmkl}\rho_{kl}^S(t) \quad (2.17)$$

where $\rho_{mn}^S = \langle m|\rho^S|n\rangle$, $\epsilon_m = \hbar\omega_m$ and $\omega_{nm} = \omega_n - \omega_m$. Here, the Redfield tensor R_{nmkl} reads

$$R_{nmkl} = \delta_{nm} \sum_r \Gamma_{nrrk}^+ + \delta_{nk} \sum_r \Gamma_{lrrm}^- - \Gamma_{lmnk}^+ - \Gamma_{lmnk}^-, \quad (2.18)$$

where $\Gamma_{lmnk}^+ = \frac{1}{\hbar^2} \int_0^\infty dt e^{-i\omega_{nk}t} \overline{\langle l|\mathcal{H}_{s-ph}|m\rangle \langle n|\mathcal{H}_{s-ph}(t)|k\rangle}$, with

$$\mathcal{H}_{s-ph}(t) = \exp(i\mathcal{H}_B t/\hbar) \mathcal{H}_{s-ph} \exp(-i\mathcal{H}_B t/\hbar) \quad (2.19)$$

and $\Gamma_{lmnk}^+ = (\Gamma_{knml}^-)^*$. The overbar symbol denotes the average over a phonon bath in thermal equilibrium at temperature T . To derive this master equation for $\hat{\rho}_{mn}^S(t)$, we also consider the so-called secular approximation. For $\omega_{nm} \gg R_{nmkl}$, we only take into account the secular terms $\epsilon_n - \epsilon_m - \epsilon_k + \epsilon_l = 0$ in Eq. [2.17]. We neglect the non-secular terms $\epsilon_n - \epsilon_m - \epsilon_k + \epsilon_l \neq 0$ since they are fast oscillating terms compared with the system dynamics. Within these approximations, the Bloch equations can be obtained using $\langle dS_z/dt \rangle = \text{Tr}[(d\rho/dt)S]$. Let us analyze the decaying of the a initially non-equilibrium $S_z(0)$ into an equilibrium spin polarization S_z^0 of the component parallel to the external

magnetic field. This spin dynamics is described by $\langle S_z \rangle(t) = S_z^0 - (S_z^0 - S_z(0))e^{-t/T_1}$, where the spin relaxation is explicitly given by (56)

$$\Gamma_{\downarrow\uparrow} = \frac{1}{T_1} = 2\Re(\Gamma_{\gamma_0\gamma_k\gamma_k\gamma_0}^+ + \Gamma_{\gamma_k\gamma_0\gamma_0\gamma_k}^+). \quad (2.20)$$

Modelling the reservoir as a bath of harmonic oscillator, we have that (6)

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} \sum_q |\langle \gamma_0 | \mathcal{H}_{s-ph} | \gamma_k \rangle|^2 \delta(\hbar\omega_{\gamma_0\gamma_k} - \hbar\omega_q) \coth\left(\frac{\hbar\omega_{\gamma_0\gamma_k}}{2k_b T}\right). \quad (2.21)$$

Using Eq. [2.21], we calculate T_1 for all the spin-phonon Hamiltonians in Sec. [2.3]. Combining Eqs. [2.21] and [2.12], the relaxation rate due to deformation potential (LA) and the Rashba coupling reads

$$\Gamma_{\gamma_0 \leftarrow \gamma_k}^{g1:LA} = \frac{\pi}{2} \frac{g_1^2}{\hbar \rho s_{LA}^2} \left(\frac{E_{\gamma_k} - E_{\gamma_0}}{\hbar s_{LA}} \right)^4 \int_0^{2\pi} d\phi_q [\Lambda_i^k(A_{g_1})]^2. \quad (2.22)$$

Also, the contribution due to the bond-length change mechanism (LA, TA)

$$\Gamma_{\gamma_0 \leftarrow \gamma_k}^{g2:LA,TA} = 2\pi \frac{g_2^2}{\hbar \rho s_\mu^2} \left(\frac{E_{\gamma_k} - E_{\gamma_0}}{\hbar s_\mu} \right)^2 \int_0^{2\pi} d\phi_q [\Lambda_i^k(A_{g_2})]^2, \quad (2.23)$$

where we use the summation index $i = 1, 2, 3$, and define

$$\Lambda_1^k(A_{g_1,g_2}) = \lambda_1^n \langle 1/2, 1, \downarrow | A_{g_1,g_2} | -1/2, 1, \uparrow \rangle \rho_k, \quad (2.24)$$

$$\begin{aligned} \Lambda_2^k(A_{g_1,g_2}) &= \sum_{n \neq (1/2,1)} \lambda_2^n \langle 1/2, 1, \downarrow | A_{g_1,g_2} | n, \downarrow \rangle \\ &\quad \times \langle n, \downarrow | H_R | 1/2, 1, \uparrow \rangle \sigma_k, \end{aligned} \quad (2.25)$$

$$\Lambda_3^k(A_{g_1, g_2}) = \sum_{n \neq (1/2, 1)} \lambda_3^n \langle 1/2, 1, \downarrow | H_R | n, \uparrow \rangle \times \langle n, \uparrow | A_{g_1, g_2} | 1/2, 1, \uparrow \rangle \sigma_k, \quad (2.26)$$

with $A_{g_1} = a_1 1_{2 \times 2}$, $A_{g_2} = g_2 (\sigma_+ a_2^* + \sigma_- a_2)$, with $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$. Explicitly, the matrix elements read

$$\langle n | A_{g_1} | n' \rangle = M_{nn'} (\delta_{j, j'+1} e^{-i\phi_q} + \delta_{j, j'-1} e^{+i\phi_q}), \quad (2.27)$$

with $M_{nn'} = \int dr r^2 (\chi_A^{n*} \chi_A^{n'} + \chi_B^{n*} \chi_B^{n'})$, and

$$\langle n | A_{g_2} | n' \rangle = (g_2 a_2^* \delta_{j, j'+1} N_{nn'}^{AB} + g_2 a_2 \delta_{j, j'-1} N_{n'n}^{AB}), \quad (2.28)$$

where $N_{nn'}^{AB} = \int dr r \chi_A^n(r) \chi_B^{n'}(r)$. Also, $\rho_{\gamma_1} = -\sin(\vartheta/2)$, $\sigma_{\gamma_1} = \cos(\vartheta/2)$ and $\rho_{\gamma_2} = \cos(\vartheta/2)$, $\sigma_{\gamma_2} = \sin(\vartheta/2)$ and the energy-dependent denominators $\lambda_1^n = 1$, $\lambda_2^n = 1/E_k - E_n + g\mu_B B/2$, $\lambda_3^n = 1/E_{1/2, 1} - E_n - g\mu_B B/2$. Notice that Eqs. (2.22) and (2.23) take into account spin and the orbital relaxation transitions. Thus we have to consider only $\Gamma_{\downarrow\uparrow} = \Gamma_{\gamma_0 \leftarrow \gamma_1}$ before the energy anticrossing, and $\Gamma_{\downarrow\uparrow} = \Gamma_{\gamma_0 \leftarrow \gamma_2}$ after the anticrossing, in order to isolate the contribution to the spin relaxation rate. So, the total contribution due to the Rashba SO coupling and all the electron-phonon mechanisms considered here is $\Gamma_{\downarrow\uparrow}^R = \Gamma_{\gamma_0 \leftarrow \gamma_k}^{g1:LA} + \Gamma_{\gamma_0 \leftarrow \gamma_k}^{g2:LA} + \Gamma_{\gamma_0 \leftarrow \gamma_k}^{g2:TA}$.

As stated in Sec. [2.3], the contribution from the intrinsic SO results only from the deflection coupling mechanism. Thus combining Eqs. (2.21) and (2.16), we have that (6)

$$\Gamma_{\downarrow\uparrow}^{ZA} = \frac{4\pi^2 \lambda_i^2}{\rho} \frac{1}{s_{ZA}^5} (g\mu_B B)^2 \times \left| \int dr r (|\chi_A^n|^2 - |\chi_B^n|^2) \right|^2. \quad (2.29)$$

Here, we have already taken the low magnetic field limit where this contribution plays a major role. We define $Q(B) = \sqrt{s_{ZA}^2 + 4\mu(g\mu_B B/\hbar)}$, with $s_{ZA} = 0.25 \times 10^3 \text{ m/s}$. Finally, summing all the contributions $T_1 = (\Gamma_{\downarrow\uparrow}^R + \Gamma_{\downarrow\uparrow}^{ZA})^{-1}$, we have the magnetic field dependence

of the spin relaxation time in graphene QDs, as shown in Fig. [2.4].

Figura 2.4 – Spin relaxation time T_1 vs. magnetic field $\mathbf{B}$. We account for contributions due to the deformation potential g_1 : LA (dark, dotted), bond-length change mechanism g_2 : LA (dark, dotted) and g_2 : TA (light, dashed) and the out-of-plane phonons ZA (light, dot-dashed). The total contribution (dark, solid lines) is the sum of the spin relaxation rates due to all mechanisms considered in our model. The non-monotonic behavior of T_1 is caused by the Rashba SO coupling-induced anticrossing of opposite spin states at B^* . All the parameters used in the numerical evaluation of the spin relaxation rates are given in Table 2.2. Inset: Blow-up of the low magnetic field regime. Interplay between the deformation potential and deflection coupling mechanisms.

Notice that it is possible to differentiate experimentally the contributions from the intrinsic and Rashba SO interactions by analyzing the spin relaxation time's monotonicity with the external magnetic field. The intrinsic SO leads to a monotonic magnetic field dependence of T_1 via deflection coupling mechanism. A rapid decrease of T_1 occurs due to Rashba SO coupling-induced anticrossing of opposite spin states. Thus it is possible to induce a non-monotonic behavior electrostatically since the Rashba SO coupling is induced by an external electric applied perpendicularly to the graphene sheet.

An alternative analysis of the magnetic field dependence of T_1 can be done calculating the spectral density of the system-bath interaction

$$J_{\gamma_0 \gamma_k}(\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} \overline{\langle \gamma_0 | \mathcal{H}_{s-ph}(0) | \gamma_k \rangle \langle \gamma_k | \mathcal{H}_{s-ph}(t) | \gamma_0 \rangle}. \quad (2.30)$$

This term can be related to Eq. [2.20], i.e., $1/T_1 \propto J_{\gamma_0 \gamma_k}(\omega_{\gamma_0 \gamma_k})$, where $\omega_{\gamma_0 \gamma_k} \propto \omega_Z \propto g\mu_B B$.

Tabela 2.2 – Parameters for the numerical evaluation of the spin relaxation rates. The electron-phonon coupling constants for the deformation potential g_1 and for the bond-length change mechanism g_2 and the coupling strengths for Rashba λ_R for an external electric field E and the intrinsic λ_i SO couplings. The graphene layer is characterized by its mass area density ρ . The quantum dot parameters are its radius R , potential height U_0 and the substrate-induced energy gap Δ . The system is assumed to be in thermal equilibrium with the bath at temperature T .

Parameters	Units
g_1	30 eV (52)
g_2	1.5 eV (52)
λ_R	11 μ eV (22)
E	50 V/300 nm (22)
λ_i	12 μ eV (42)
ρ	7.5×10^{-7} kg/m ² (53)
R	35 nm
$U_0 = \Delta$	260 meV
T	100 mK

Generally,

$$1/T_1 \propto \sum_q K_q \langle \gamma_0 | e^{i\mathbf{q}\cdot\mathbf{r}} | \gamma_k \rangle \langle \gamma_k | \mathcal{H}_{\text{SO}} | \gamma_0 \rangle \delta(\omega_q - \omega_{\gamma_0\gamma_k}), \quad (2.31)$$

with $K_q = q/\sqrt{\omega_q}$ using that $\mathcal{H}_{e-ph} \propto K_q e^{\pm i\mathbf{q}\cdot\mathbf{r}}$. Here, $\sum_q \propto \int d\mathbf{q} q^{d-1}$, where $d = 2$ is the dimensionality of graphene. We find the following results for each SO and electron-phonon couplings: (i) intrinsic SO, $J_{\gamma_0\gamma_k}(\omega_{\gamma_0\gamma_k}) \propto \omega_Z^s$, $s \geq 2$ for the direct spin-phonon coupling (ZA); (ii) Rashba SO, $s = 4$ for the deformation potential (LA) and $s = 2$ for the bond-length change mechanism (LA, TA). Thus for all electron-phonon coupling mechanisms considered here, the spectral density of the system-bath interaction is super-Ohmic ($s > 1$) (6).

In the next section, we calculate the spin decoherence time also within the Bloch-Redfield theory.

2.5 Spin dephasing rates

In this section, we calculate the spin dephasing rates within the Bloch-Redfield theory. We derive the Bloch equation for the spin components perpendicular to the magnetic field. They are given by $\langle S_x \rangle(t) = S_x^0 \cos(\omega_Z t) e^{-t/T_2}$ and $\langle S_y \rangle(t) = S_y^0 \sin(\omega_Z t) e^{-t/T_2}$, where $S_{x,y}^0$

are the initial spin polarizations along the x, y directions. The pure spin dephasing rate is defined by (6, 56)

$$\Gamma_\phi = \frac{1}{T_\phi} = \Re \left(\Gamma_{\gamma_0 \gamma_0 \gamma_0 \gamma_0}^+ + \Gamma_{\gamma_k \gamma_k \gamma_k \gamma_k}^+ - 2\Gamma_{\gamma_0 \gamma_0 \gamma_k \gamma_k}^+ \right). \quad (2.32)$$

The decoherence time is defined as a sum of the spin relaxation rate and the dephasing rate contributions, i.e., $1/T_2 = 1/2T_1 + 1/T_\phi$. Eq. [2.32] can be simplified to

$$\frac{1}{T_\phi} = \lim_{\omega \rightarrow 0} |\langle \gamma_0 | \mathcal{H}_{s-ph} | \gamma_0 \rangle - \langle \gamma_k | \mathcal{H}_{s-ph} | \gamma_k \rangle|^2 \delta(\hbar\omega - \hbar\omega_q) \frac{2\pi k_b T}{\hbar\omega}. \quad (2.33)$$

In terms of the spectral density of the system-bath interaction, the dephasing rate is given by $1/T_\phi \propto \lim_{\omega \rightarrow 0} J(\omega) \coth(\hbar\omega/2k_b T) \propto \lim_{\omega \rightarrow 0} J(\omega)/\omega$. As analyzed in Sec.[2.3], the system-bath spectral density is super-Ohmic for all electron-phonon mechanisms considered here. Then, the spin dephasing rates go to zero when the limit $\omega \rightarrow 0$ is taken, i.e., $1/T_\phi \propto \lim_{\omega \rightarrow 0} \omega^s/\omega \rightarrow 0$, with $s > 1$. Thus the decoherence time $T_2 = 2T_1$ is dominated by relaxation processes due to the electron-phonon coupling mechanisms in graphene up to leading order in the spin-orbit interaction (6). We find that the spin decoherence time due to the admixture mechanism will be the dominant mechanism for high magnetic fields $\mathbf{B} > 5$ T. This contribution will compete with the hyperfine interaction-induced spin decoherence which was predicted to be on the order of tens or hundreds of μs depending on the ^{13}C abundance (20, 58) and the orientation of $\mathbf{B}$ (58).

We also demonstrate that spin dephasing rate also vanishes at the energy anticrossing for a super-Ohmic bath (6). Consider an effective Hamiltonian $\mathcal{H}_\phi = \Delta_+(B)1 + \Delta_-(B)\tau_z$, written in the subspace $\{|+1/2, 1, \uparrow\rangle, |-1/2, 1, \downarrow\rangle\}$, which describes the energy anticrossing. Here, τ_z denote a Pauli matrix and $\Delta_\pm = (E_{\gamma_3} \pm E_{\gamma_2})/2$. Separating the magnetic field into the external contribution B_0 and the internal contribution $\delta B(t)$ caused by bath-induced fluctuations.

$$\mathcal{H}_\phi = (\Delta_-(B_0) + \partial_B \Delta_-(B_0) \delta B(t)) \tau_z, \quad (2.34)$$

where we have assumed small fluctuations of $\delta B(t)$. The term proportional to $\Delta_+ 1_{2 \times 2}$ is not taken into account since it does not lead to spin dephasing. Using the equation for the spin dephasing rate within the Bloch-Redfield theory,

$$\frac{1}{T_\phi} = \left(\frac{2}{\hbar} \partial_B \Delta_-(B_0) \right)^2 \lim_{\omega \rightarrow 0} \Re \int_0^\infty dt' e^{-i\omega t} \overline{\langle \delta B(0) \delta B(t') \rangle}, \quad (2.35)$$

with $\langle A(t) \rangle$ is the thermal equilibrium expectation value of the operator $A(t)$ on the bath. Right at the anticrossing $1/T_\phi \rightarrow 0$ since $\partial_B \Delta_-(B_0) \rightarrow 0$, where we have assumed that the thermal average of the fluctuating magnetic field does not diverge. Far from the anticrossing region, $1/T_\phi$ still could vanish for a super-Ohmic bath, with $J(\omega) \propto \omega^s$, with $s > 1$.

2.6 Conclusions

We calculate the spin relaxation and decoherence time in a graphene quantum dot. The intrinsic SO interaction via the deflection coupling mechanism leads to a monotonic behavior of T_1 with magnetic field and dominates at low magnetic fields. A non-monotonic dependence of the spin relaxation time T_1 as a function of an external magnetic field is related to the Rashba spin-orbit coupling-induced anticrossing of opposite spin states. We emphasize that it is possible to differentiate the contribution to T_1 due to the intrinsic and Rashba SO coupling analyzing its behavior with $\mathbf{B}$. It opens up a possibility to probe the spin-orbit couplings in graphene, which have not been measured in monolayer graphene so far. We demonstrate that the decoherence time is dominated by relaxation processes, i.e., $T_2 = 2T_1$ in the leading order of the electron-phonon interaction. This relation is not necessarily valid for higher-order terms, specially in higher temperatures where the two-phonon processes might dominate the relaxation process. We also prove that the spin dephasing rate vanishes at the energy anticrossing for a super-Ohmic bath.

CHAPTER 3

BALLISTIC SPIN RESONANCE IN MULTISUBBAND QUANTUM WIRES

3.1 Introduction

Spin relaxation in semiconductor nanostructures is one of the main obstacles to the feasibility of spintronic devices. One of the main sources of spin relaxation in high-mobility two-dimensional electron gases is caused by the D'yakonov-Perel (DP) mechanism (32). The spin decay is caused by the interplay between the spin-orbit (SO) interaction and multiple random scattering events. Electrons undergo a series of collision with impurities randomizing their momentum which generates a random effective SO magnetic field. The spin precession frequency vector also changes orientation randomly depending on the sequence of scattering events. So, considering an ensemble of initially spin-polarized electrons, their spins will become more and more misaligned as time goes by. After a relaxation time τ_{SR} , electron spins will be pointing randomly around the Bloch sphere. Also, the spin dynamics in a SO-coupled system strongly depends on the impurity concentration and the dimensionality of the nanostructure. Since the DP spin relaxation time is inversely proportional to the momentum scattering time, dimensional constraints can lead to a suppression of this mechanism. For instance, the experimental observation of the dimensionally constrained DP mechanism in quantum wires has been reported recently

(59). In this case, a progressive decreasing of the channel width in order to reach the same length scale of the electron mean free path also reduces the effectiveness of the DP mechanism until it is finally completely suppression in the strictly one-dimensional limit.

In a quasi-one-dimensional channel, the spin relaxation also can be modified due to the interplay of the SO magnetic field $\mathbf{B}_{\text{SO}}$ and an external static magnetic field $\mathbf{B}_{\text{ext}}$. In general, the spin relaxation has a monotonic dependence on the external magnetic field (60). For typical laboratory fields ($\mathbf{B}_{\text{ext}} > 1$ T), $\mathbf{B}_{\text{ext}}$ dominates over $\mathbf{B}_{\text{SO}}$. As a consequence, the oscillating SO magnetic field is ineffective in causing spin-flip transitions between the Zeeman levels which extends the spin lifetime. Nevertheless, a non-monotonic behavior for $\tau_{\text{SR}}(\mathbf{B}_{\text{ext}})$ can be induced by a combination of an external static magnetic field and the oscillating effective spin-orbit magnetic field due to periodic bouncings of the electrons off of the boundaries of a narrow channel. This effect is called ballistic spin resonance (BSR) after its experimental observation by Frolov et al. (8). Notably, this effect is analog to the ordinary electron spin resonance without the requirement of external oscillating driving fields. Analogously, the spin resonance is reached when the frequency of the oscillating SO field matches the Larmor precession frequency around the external time-independent magnetic field. At resonance, the spin-flip probability is maximized strongly increasing the spin relaxation rate.

In this work, we develop a theoretical model to describe the spin relaxation in quantum wires with Rashba and Dresselhaus SO interactions (61). We account for the dimensionally-constrained D'yakonov-Perel mechanism in a micrometer-scale channel. We consider elastic spin-conserving impurity scatterings in the time-evolution operator. Each electron in the ensemble is redistributed among different subbands with time. Then, we evaluate the time dependent average of the spin operators in the Heisenberg representation which allows us to extract the spin relaxation time τ_{SR} as a function of $\mathbf{B}_{\text{ext}}$. In this quantum-mechanical treatment of the narrow channel, the spin resonance condition is determined by the quantum wire subband anticrossing induced by the SO interaction when the external magnetic field is aligned perpendicular to the wire. On the other hand, the spin relaxation time presents a monotonic behavior when the magnetic field is aligned parallel to the wire and, consequently, to the oscillating SO field. We also predict the presence of BSR dips even when the external magnetic is aligned with the quasi-one-dimensional channel for systems with strong SO couplings. In this case, the SO magnetic

field tilt the initial spin alignment recovering the electron spin resonance configuration.

In the next section, we introduce a semiclassical interpretation of the BSR experiment. This approach was first introduced by the experimentalists in Ref. (8). In further sections, we will introduce our model which consider a more realistic model for DP relaxation mechanism in a multisubband quantum wire. Thus in Sec. [3.3], we present our numerical model which accounts for the DP spin relaxation mechanism. In Sec. [3.4], we analyze our results for the simulation of the BSR experiment. We discuss the presence of anomalous BSR dips in strong SO-coupled system in Sec. [3.5]. Finally, we conclude in Sec. [3.6] with the potential application of our model.

3.2 Semiclassical picture to the spin relaxation in quasi-one-dimensional channels

In order to present a semiclassical interpretation of the BSR, we consider electrons propagate in a strip of a 2D electron gas. This system can be engineered in this system by parallel spatially separated metal gates (split-gate) on top of a 2D electron gas. Then, the electrostatic potential depletes the electrons under the gates forming a quasi-one dimensional channel for the conduction electrons. These electrons are injected via a spin-selective QPC with their spin polarization aligned along the applied static magnetic field $\mathbf{B}_{\text{ext}}$. The term $\mathbf{B}_{\text{ext}}$ defines the spin polarization of the injected electrons and it also serves as a controllable knob for the spin resonance condition. This non-equilibrium spin-polarized current flows to the left and to the right ends of the quantum wire, as depicted in Fig. [3.2]. A charge current flows to the left in direction to the electrical ground. A neutral current diffuses to the right towards the reservoir. Thus a pure spin current is generated in order to keep charge neutrality since no voltage is applied between the injector and the reservoir. In the meanwhile, the spin accumulation generated by the spin current can be detected by another spin-selective QPC located to the right of the QPC-injector. Here, we consider both QPCs fully spin-polarized (conductances equal to e^2/h) with quantization axis defined by the external magnetic field $\mathbf{B}_{\text{ext}}$. The *linear-in-p* Rashba and Dresselhaus SO couplings (62, 63) are operative and they can be represented

by a momentum-dependent effective magnetic field

$$\mathcal{H}_{\text{SO}} = \frac{1}{2}g\mu_B\mathbf{B}_{\text{SO}} \cdot \boldsymbol{\sigma}, \quad \mathbf{B}_{\text{SO}} = \frac{2}{g\mu_B\hbar} \begin{bmatrix} (\alpha - \beta)p_y \\ -(\alpha + \beta)p_x \end{bmatrix}. \quad (3.1)$$

for a coordinate system such that $x||[110]$, $y||[\bar{1}10]$, where $\mathbf{B}_{\text{SO}}$ is a two-component vector. Throughout this chapter, the superscripts $\perp$ and $\parallel$ will denote the components of the momentum, SO and external magnetic fields perpendicular ($\hat{y}$) and parallel ($\hat{x}$) to the channel orientation, respectively. Here, α and β correspond to the Rashba and Dresselhaus SO coupling strengths, respectively. Here, $\mathbf{p} = \hbar\mathbf{k}$ denotes the electron momentum and $\boldsymbol{\sigma}$ the Pauli matrices. We neglect the cubic Dresselhaus SO contribution since its $\mathbf{B}_{\text{SO}}$ can be neglected when compared with *linear-in-p* SO terms (64). Notice that the SO magnetic field is always pointing perpendicularly to the electron momentum for this particular choice of the coordinate system. For a high-mobility 2D electron gas, each electron experiences a periodic trajectory due to specular bouncings of the electrons off the boundaries of a narrow channel. This periodic trajectory due to specular scattering generates a oscillating momentum-dependent effective magnetic field $B_{\text{SO}}^{\parallel}(k_{\perp}(t))$ parallel to the channel orientation. Combined with an $\mathbf{B}_{\text{ext}} \parallel B_{\perp}$ perpendicular to the channel, a electron spin resonance configuration is achieved in the absence of external oscillating fields. Thus we have spin-flip transition between the Zeeman states due to the presence of $\mathbf{B}_{\text{ext}}$ with the energy provided by the small oscillating magnetic field $\mathbf{B}_{\text{SO}}^{\parallel}$. At resonance, the frequency of the SO magnetic field matches the Larmor precession frequency around the external magnetic field

$$f = \frac{g\mu_B B_{\perp}}{h} = \frac{v_F}{2L}, \quad (3.2)$$

where v_F is the Fermi velocity and L is the channel width. Here, we can neglect the SO magnetic field perpendicular to the channel orientation $\mathbf{B}_{\text{SO}}^{\perp}$ when compared with external field $\mathbf{B}_{\text{ext}}$ which gives the resonance condition. This is a valid approximation for the GaAs/AlGaAs heterostructure considered in the experimental work since it posses a weak SO coupling strenghts (8). On the other hand, no spin resonance is expected when $\mathbf{B}_{\text{ext}} \parallel B_{\parallel}$ is parallel to the quantum wire and consequently, to the oscillating SO field $\mathbf{B}_{\text{SO}}^{\parallel}$.

A non-local voltage V_{nl} quantifies the chemical potential imbalance between the QPC-

detector and the right reservoir (see Fig. [3.2]). The behavior of V_{nl} can be analyzed by comparison between length scales given by the spin relaxation length λ_{SR} and the distance x_{id} between the QPC-injector and QPC-detector. In the limiting case such that $\lambda_{SR} \gg x_{id}$, the electron ensemble can travel the distance x_{id} with their spins mostly aligned with $\mathbf{B}_{ext}$ which allows them to go through the QPC-detector. As a consequence, V_{nl} increases monotonically reflecting the enhancement of λ_{SR} with $\mathbf{B}_{ext}$. On the other hand, when $\lambda_{SR} \ll x_{id}$, the spin-polarized ensemble relax before reaching the detector. In this case, each electron is equally likely to flow through the QPC detector or to flow towards the reservoir leading to a balanced chemical potential in these two regions. Thus V_{nl} drops when $\tau_{SR}(B_{\perp})$ is strongly reduced at resonance condition for the BSR.

Figure 3.1 – (a) Illustration of the experimental setup used to measure the ballistic spin resonance. Periodic bouncing between the parallel boundaries of the channel creates an effective oscillating spin-orbit magnetic field. This oscillating field combined with an external static magnetic field leads to a spin resonance strongly decreasing the D'yakonov-Perel spin relaxation time. (b) Schematic view of the quasi-one-dimensional channel with width L . A non-equilibrium spin-polarized current is injected via a spin-selective QPC. A charge current flows to the left due to the voltage V_{gr} , while a non-equilibrium spin-polarized carrier diffuses towards the reservoir in order to keep the charge neutrality which originates a pure spin current from the injector QPC to the detector QPC. The injector and detector QPC are separated from a distance x_{id} . The non-local voltage V_{nl} is measured between the QPC-detector region and the equilibrium spin-unpolarized reservoir. Adapted from Frolov et al. (7).

In the next section, we have presented a semiclassical model. However, this simple model does not capture some features of the BSR experiment (8) such as the enlargement of the spin relaxation resonant dip. These limitations motivated us to develop a more realistic model to describe the spin relation in quasi-one-dimensional channels. We introduce our model in the next section.

3.3 Model for D'yakonov-Perel spin relaxation mechanism in a multisubband quantum wire

In this section, we present our model which describes the D'yakonov-Perel in a multisubband quantum wire (61). In order to build a theoretical model to explain the BSR, consider a square wire confinement with width L , the Hamiltonian describing the system reads

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}g\mu_B (\mathbf{B}_{\text{SO}} + \mathbf{B}_{\text{ext}}) \cdot \boldsymbol{\sigma} + V(y), \quad (3.3)$$

with effective mass m , $V(y) = 0$ for $0 \leq y \leq L$ and $V(y) \rightarrow \infty$ elsewhere. This confinement model captures the main features of the BSR experiment (8). In Appendix A, we show the limitations of the harmonic confinement model. Also, the external magnetic field $\mathbf{B}_{\text{ext}}$ applied in the plane of the 2D electron gas.

We intend to analyze the electron spin dynamics by evaluating the time dependent average of the spin operators in the Heisenberg representation. First we have to find the eigenenergies and eigenstates of the Hamiltonian $\mathcal{H}$ 3.3. In a multisubband quantum wire, electrons can only occupy states with a set of well-defined wavevectors given by the dispersion relation of the system. So, for a fixed k , we project the Hamiltonian $\mathcal{H}$ in a truncated subband-spin Hilbert space

$$\mathcal{F} = \{|n, k, s_i\rangle; n = 1, 2, \dots, n_T, k, s_i = \uparrow_i, \downarrow_i\}, \quad (3.4)$$

where $i = x, y, z$, n_T is the total number of subbands in the subspace $\mathcal{F}$ and s_i denotes the spin component along i -th direction. We choose as a basis for $\mathcal{H}$ the solution for square quantum wire in the absence of the SO interaction $\langle \mathbf{r} | n, k, s_i \rangle = \sqrt{2/L} \sin(n\pi y/L) e^{ikx} \chi_i$, where χ_i is the spinor in the σ_i basis, k denotes the wavevector of the plane wave solution along the quantum wire and n is the quantum number related with transverse direction of the quantum wire.

The electron spin dynamics can be determined by the time-evolution operator $\mathcal{U}(k, t) =$

$\exp[-(i/\hbar)\mathcal{H}(k)t]$, where we consider an electron injected initially into the subband labeled n_j of this quantum wire. Then, for an electron initially injected in a general state $|n_j, k, s_i\rangle$, with the spin projection axis aligned with $\mathbf{B}_{\text{ext}}$, its spin dynamics is obtained by numerically calculating the time-dependent expectation value of the respective Pauli spin matrix

$$\bar{\sigma}_i(t) = \langle n_j, k, s_i | \mathcal{U}^\dagger(k, t) \sigma_i \mathcal{U}(k, t) | n_j, k, s_i \rangle = \langle n_j, k, s_i | \sigma_i(t) | n_j, k, s_i \rangle \quad (3.5)$$

in the Heisenberg representation (65, 66). Here we simplify our calculation by performing a similarity transformation such that the time-evolution operator assumes a diagonal form $\tilde{\mathcal{U}}(k, t)$ in the $\mathcal{F}$ -subspace. Using that the time-evolution operator is represented by a square matrix in the truncated subband-spin basis $\mathcal{F}$ with eigenvectors denoted by $\Lambda_1, \Lambda_2, \dots, \Lambda_{2n_T}$ and with respective eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_{2n_T}$. We define a transformation such that $\tilde{\mathcal{U}}(k, t) = \mathbf{P}_k^{-1} \mathcal{U}(k, t) \mathbf{P}_k$, where $\mathbf{P}_k$ is a matrix whose columns are composed of the eigenvector components which diagonalize the Hamiltonian $\mathcal{H}$ for a given k . Explicitly, we have that

$$\mathbf{P}_k \equiv \begin{bmatrix} \Lambda_1 & \Lambda_2 & \cdots & \Lambda_{2n_T} \end{bmatrix}, \quad \lambda_j(t) = \exp[-(i/\hbar)\epsilon_j t]. \quad (3.6)$$

where $\lambda_j(t)$ is the diagonal components of the transformed time-evolution operator $\tilde{\mathcal{U}}(k, t)$. Here, ϵ_j is the eigenenergies of the Hamiltonian [3.3]. After the transformation, Eq. [3.5] reads

$$\bar{\sigma}_i(t) = \langle n_j, k, s_i | \mathbf{P}_k \tilde{\mathcal{U}}^\dagger(k, t) \mathbf{P}_k^{-1} \sigma_i \mathbf{P}_k \tilde{\mathcal{U}}(k, t) \mathbf{P}_k^{-1} | n_j, k, s_i \rangle, \quad (3.7)$$

This calculation does not include transitions between different quantum wire subbands due to scattering events. This generalization will be discussed in the next subsection.

3.3.1 Scattering mechanisms

Now we turn to generalize the evaluation of the time-dependent expectation value of the spin operators $\bar{\sigma}_i(t)$ in order to include scattering mechanisms operative in a narrow

Figure 3.2 – (a) Schematic view of a ballistic channel. A non-equilibrium spin-polarized current is injected in a multisubband quantum wire via a spin-selective QPC with an angular spread Φ and this current flows towards an spin-unpolarized reservoir. Each electron is assumed to be uniformly distributed in the subbands with quantum number n such that $\theta_n < \Phi$. After undergoing multiple random scatterings, the ensemble spin polarization will decay as a consequence of electron spins precessing around distinct fluctuating momentum-dependent effective magnetic fields due to the SO interaction. This is the well-known D'yakonov-Perel mechanism. Energy spectrum of a quantum wire with SO interaction with an external magnetic field (b) parallel $B_{\parallel}$ and (c) perpendicular $B_{\perp}$ to the quantum wire. $B_{\parallel}$ opens a gap at $k = 0$ and $B_{\perp}$ induces an asymmetry of the energy branches depending on the sign of k . The subband-spin mixing term $\mathcal{H}_{SO}^{\parallel} = i(\alpha - \beta)\partial_y\sigma_x$ induces energy anticrossings of the quantum wire subbands with opposite spins. In the absence of $\mathcal{H}_{SO}^{\parallel}$, the magnetic field-tunable level crossing defines the resonance condition for the BSR.

channel. Multiple random scattering events will be included sequentially in the time-evolution operator where the occupied subband will depend on the scattering mechanism that the electron has undergone. During the transition between quantum wire subbands, the electron spin will precess around the SO and external magnetic field. Since each subband can be associated to a distinct effective SO magnetic field, a different sequence of scattering events for each electron will lead to a spin relaxation of a initially spin-polarized ensemble which characterizes the D'yakonov-Perel mechanism. By contrast, in the semiclassical picture, $\mathbf{B}_{\text{SO}}$ keep its absolute value and only change its orientation after each scattering event. Meanwhile in our model, $\mathbf{B}_{\text{SO}}$ can assume a finite set of values depending on the occupied subband.

Let us consider an ensemble of electron where each particle is represented by wave packets propagating freely between collisions. In our model, we consider that these electrons undergo two different mechanisms, namely large-angle and small-angle scatterings. Large-angle scattering is characterized by an elastic spin-conserving impurity scattering that randomizes the electron momentum. We consider that a scattering event occurs with a probability $\delta t/\tau$ within a time interval δt , where τ is the mean free time. Thus we consider that this scattering type allows for transitions to all equally probable subbands at the Fermi energy ϵ_F , where ϵ_F is determined by the electronic density in the wire. Notice that these events are rare since we consider a high-mobility channel such that the mean free path λ is much larger than the quantum wire width, $\lambda \gg L$. On the other hand, the small-angle scattering is the dominant source of scattering in 2D electron gas formed in a modulation-doped quantum well. These spatially separated ionized impurities give up electrons. Consequently, the electrons are affected by a weak screened Coulomb potential which generates a majority of small-angle scattering events (67). This mechanism is very ineffective in creating backscattering events since these involve large momentum transfers. We implement this scattering mechanism by sorting out a random number $\tilde{\Theta}$ for each timestep according to a normal distribution with zero mean and standard deviation Δ . Here we consider an electron coming from the subband n_k and making a transition to the subband n_l at ϵ_F if $\Theta_{n_k, n_{l-1}} \leq \tilde{\Theta} \leq \Theta_{n_k, n_{l+1}}$, where $\Theta_{n_k, n_l} = \theta_{n_k} - \theta_{n_l}$. A set of angles θ_n can be attributed to each quantum wire subband. The angles θ_n are determined by the ratio between the transverse momentum component and its total Fermi momentum k_F , i.e., $\theta_n = \arcsin(k_n/k_F)$, where $k_n = \sqrt{k_F^2 - (n\pi/L)^2}$ (68), as illustrated in Fig. [3.2].

3.3.2 Generalized expectation value of the spin operators

Taking into account the scattering processes discussed in the previous subsection, the generalized time evolution operator after N scatterings for each time interval δt is (61)

$$\begin{aligned} U_N(t) &= U(\gamma_1 k_{n_1}, \delta t) U(\gamma_2 k_{n_2}, \delta t) \dots U(\gamma_N k_{n_N}, \delta t) \\ &= \prod_{v=1}^N U(\gamma_v k_{n_v}, \delta t). \end{aligned} \quad (3.8)$$

We have used that $U(\gamma_v k_{n_v}, t) = P_{\gamma_v k_{n_v}} \tilde{U}(\gamma_v k_{n_v}, t) P_{\gamma_v k_{n_v}}^{-1}$ for v -th scattering event to the subband n_v , where $\gamma_v = \pm 1$ depending whether the electron has scattered backwards $\gamma_v = -1$ or forward $\gamma_v = +1$ at the time $t = v\delta t$. Here, n_v is a integer random number, with $1 \leq n_v \leq n_T$, sorted out according to the type of the scattering event. The generalized spin operator reads

$$\bar{\sigma}_i(t) = \langle n_j, k, s_i | U_N^\dagger(t) \sigma_i U_N(t) | n_j, k, s_i \rangle. \quad (3.9)$$

We point out here that each subband generates a different alignment of the SO magnetic field. So, they can be viewed as spin rotations around random axes depending on the occupied subband. This leads to noncommutativity of the time-evolution operators for successive scatterings (see a simple model for the DP mechanism in a quantum wire with two subbands in Appendix B). Since each electron follows a distinct sequence of scattering events, the electron spin of the ensemble will be pointing along random directions in the Bloch sphere after a time τ_{SR} .

We repeated the above procedure for an ensemble of electrons with their spins initially aligned to $\mathbf{B}_{\text{ext}}$. It allows us to obtain the time dependence of the spin polarization $P_i(t) = \sum_{\mu=1}^{N_{\text{ens}}} \bar{\sigma}_i^\mu(t) / N_{\text{ens}}$, where P_i is the polarization along the i direction for the μ -th electron, and N_{ens} is the total number of electrons considered in our simulation. We have that the average ensemble spin polarization decays exponentially with time τ_{SR} , i.e., $P_i(t) = P_i(t=0) e^{-t/\tau_{SR}}$. This procedure is repeated for different external magnetic fields. Thus we can extract the magnetic dependence of the spin relaxation time $\tau_{SR}(\mathbf{B}_{\text{ext}})$, using

a single-exponential decay fit.

In the next section, we will analyze the magnetic field dependence of the spin relaxation time in a realistic system. We will compare our numerical results with the experimental data from the BSR experiment (8).

3.4 Ballistic spin resonance

In this section we analyze and compare our numerical results to the experimental data obtained in a GaAs quantum well by Ref. (8). We point out that the SO coupling in this system is relatively weak when compared with other semiconductors such as InAs. Thus we restrict ourselves to the weak SO coupling regime through this section (61). In order to understand the role of each term in the Hamiltonian [3.3], we separate it as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{SO}}^{\parallel} + \mathcal{H}_{\text{SO}}^{\perp} + \mathcal{H}_Z^{\parallel} + \mathcal{H}_Z^{\perp}$, where we define the quantum wire Hamiltonian $\mathcal{H}_0 = \frac{\hbar^2 k^2}{2m} + \frac{n^2 \hbar^2 \pi^2}{2mL^2}$, the SO contribution $\mathcal{H}_{\text{SO}}^{\perp} = -(\alpha + \beta)k\sigma_y$, $\mathcal{H}_{\text{SO}}^{\parallel} = i(\alpha - \beta)\partial_y\sigma_x$, and the Zeeman terms $\mathcal{H}_Z^{\parallel} = g\mu_B B_x/2$, $\mathcal{H}_Z^{\perp} = g\mu_B B_y/2$.

In the BSR experiment, electrons are injected using a voltage applied through a QPC (injector) and diffuse along a ballistic channel until their detection by another QPC (detector). Thus we consider an ensemble of electrons injected into the quantum wire with an angular spread Φ relative to the transverse direction (69). We assume that these electrons are uniformly distributed over these subbands as long as they fulfill the condition $\theta_n < \Phi$. In another words, the quantum wires will be equally occupied as long as the injection spread angle Φ is larger than the angle attributed to the subband n (68). This condition is obeyed by the quantum wire subbands with higher values for the quantum number n . Notice that since the small-angle scattering is the dominant source of scattering in our model, the resonance condition will be determined mainly by the occupation in the higher subbands. Another mechanisms, such as the electron-phonon and electron-electron interaction, can be also responsible for redistributing the electrons over the subbands. Using that these mechanism strongly depend on the temperature, we neglect these contribution since the BSR experiment was performed in the low-temperature regime (< 1 K) (7, 8, 70).

We turn our analysis to the cases where the electron is injected with its spin align-

ned to either $B^\parallel$ or $B^\perp$. First let us consider an electron injected in subband n_j with a particular k near the energy anticrossing for a certain value of $B^\perp$ ($B^\parallel = 0$). Its spin dynamics will be strongly affected by the subband-spin mixing term $\mathcal{H}_{\text{SO}}^\parallel$ in the Hamiltonian $\mathcal{H}$ (3.3). This subband-spin mixing term connects different orbital states since it is proportional to the momentum operator along the transverse direction $-i\hbar\partial_y$. Moreover, it can cause a spin-flip transition due to the spin operator σ_x . Explicitly, we have that $\langle n_j, \downarrow_y | \mathcal{H}_{\text{SO}}^\parallel \propto \partial_y \sigma_x | n_j \pm \Lambda, \uparrow_y \rangle \neq 0$, where Λ is an odd integer ($\Lambda = 1, 3, 5, \dots$). Thus the spin-flip probability is maximized near the energy level anticrossing induced spin-orbital mixing caused by the term $\mathcal{H}_{\text{SO}}^\parallel$. As a consequence, the spin relaxation rate is strongly enhanced at the energy anticrossing which is the signature of the BSR. For this reason, the condition for the energy anticrossing is directly related to the resonance condition for the BSR.

For a given ϵ_F , a particular choice for $\mathbf{B}_{\text{ext}}$ defines that the energy anticrossing will occur for a set of quantum numbers $\{n, k\}$. The value of $\mathbf{B}_{\text{ext}}$ which leads to the level anticrossing due to $\mathcal{H}_{\text{SO}}^\parallel$ can be found analyzing the energy-level crossings in the spectrum of $[\mathcal{H}_0 + \mathcal{H}_{\text{SO}}^\perp + \mathcal{H}_Z^\perp] |n, k, s_y\rangle = \epsilon_{n,k,s_y} |n, k, s_y\rangle$. We have that the crossing $\epsilon_{n_j,k,\downarrow_y} = \epsilon_{n_j\pm\Lambda,k,\uparrow_y}$ occurs for the $B_{\text{BSR}}^\perp$ given by

$$\frac{1}{2}g\mu_B B_{\text{BSR}}^\perp = \frac{\pi^2\hbar^2}{4mL^2} [\pm 2n_j\Lambda + \Lambda^2] + (\alpha + \beta)k_F. \quad (3.10)$$

where we have used $k_F = k_F^{n_j} \approx k_F^{n_j+\Lambda}$. Notice that this resonance condition indicates that BSR has multiple resonances depending on the value of Λ . Moreover, each subband n_j also has a slightly different resonance condition which is not captured by the semiclassical picture. Nevertheless, this resonance condition given by Eq. [3.10] can be related to the 2D semiclassical limit obtained in Sec. [3.2] for a large number of subbands in the quantum wire. We have to write the injection subband n_j in terms of the Fermi velocity $v_F^\perp$ and the channel width L as $v_F^\perp = \hbar\pi n_j/mL$. Using that $g\mu_B B_{\text{BSR}}^\perp \gg (\alpha + \beta)k_F$ and $n_j \gg 1$, isolating n_j and substituting into Eq. [3.10], we recover the resonance frequency $f_\Lambda = v_F^\perp/2L \times \Lambda = g\mu_B B^\perp/h$, in agreement with Ref. (8). It simplifies to Eq. [3.2] obtained in the semiclassical picture for the first resonance $\Lambda = 1$.

In the weak SO coupling regime, the spin relaxation has a monotonic dependence with $\mathbf{B}_{\text{ext}}$ and no BSR is expected for the case where the electron spin is initially aligned

along x -axis with $B^\parallel$ ($B^\perp = 0$). Since the electron is injected with its spin pointing along the $\hat{x}$ direction, the term $\mathcal{H}_{\text{SO}}^\parallel$ cannot flip the spin since it acts on its eigenstate, $\langle n_j, \uparrow_x | \mathcal{H}_{\text{SO}}^\parallel \propto \partial_y \sigma_x | n_j \pm \Lambda, \downarrow_x \rangle = 0$. As a consequence, the quantum wire subbands with opposite spins are not connected by the subband-spin mixing term which does not enhance the DP spin relaxation mechanism.

These distinct behaviors of spin relaxation time as a function of the external magnetic field are shown in Fig. [3.3]. Notice that $\tau_{\text{SR}}(\mathbf{B}_{\text{ext}})$ cannot be measured directly by the BSR experiment. Meanwhile, its monotonicity can be quantified experimentally via a non-local measurement (7). This voltage quantifies the chemical potential imbalance between the QPC-detector and the right reservoir, indicated by the regions III and VI in Fig. [3.1], respectively. The explicit expression for the non-local voltage is given by (7)

$$V_{\text{nl}} = \frac{\rho \frac{\lambda_{\text{SR}}}{L} I_{\text{inj}} P_{\text{inj}} P_{\text{det}} \sinh\left(\frac{L_r - x_{\text{id}}}{\lambda_{\text{SR}}}\right)}{\sinh(L_r/\lambda_{\text{SR}}) (\coth(L_r/\lambda_{\text{SR}}) + \coth(L_l/\lambda_{\text{SR}}))} \quad (3.11)$$

where ρ is the channel resistivity and L_r and L_l denotes the distance between the QPC-injector and the right and left ends of the channel, respectively. $I_{\text{inj}} = G_{\text{inj}} V_{\text{inj}}$, where V_{inj} is the voltage applied across the QPC-injector. P_{inj} and P_{det} are the polarization $P = (G_\uparrow - G_\downarrow) / (G_\uparrow + G_\downarrow)$ with the spin quantization axis defined by $\mathbf{B}_{\text{ext}}$. A fully polarized transmission $P \sim 1$ corresponds to a single occupied spin state, i.e., $G_\uparrow \sim e^2/h$ and $G_\downarrow \sim 0$. To obtain this expression for V_{nl} , a general solution to the chemical potential $\mu_\uparrow, \mu_\downarrow$ was found in each region (I-VI) of the experimental setup via the one-dimensional diffusion equation $D \partial^2 V_{\text{nl}} / \partial x^2 = V_{\text{nl}} / \lambda_{\text{SR}}^2$, where D is the diffusion constant and $\lambda_{\text{SR}} = \sqrt{D \tau_{\text{SR}}}$ (71). For the boundary conditions, it was considered an equilibrium spin polarization at the left and right ends of the channel. Also, the continuity of the chemical potential $\mu_\uparrow, \mu_\downarrow$ and conservation of the spin currents $j_\uparrow, j_\downarrow$ across each connected region of the setup (71) were taken into account. Here the spin currents are defined as $j_s = \frac{\sigma_s}{e} \frac{\partial \mu_s}{\partial x}$ for $s = \{\uparrow, \downarrow\}$, where σ_s is the spin-dependent conductivity. Finally, the difference between the chemical potentials in the regions III and VI results in Eq. [3.11].

As explained in Sec. [3.2], $\tau_{\text{SR}}(B^\parallel)$ and V_{nl} increase monotonically with the external magnetic field. On the other hand, $\tau_{\text{SR}}(B^\perp)$ and V_{nl} are strongly suppressed around the energy anticrossing induced spin-orbit mixing. This suppression in the V_{nl} occurs due to the strong spin relaxation of the injected spin-polarized current. At resonance condition,

the electron spins completely relax before reaching the QPC-detector the electrons flow with the same probability either to the detector or to a large spin-unpolarized reservoir. So, both regions will end up having the same chemical potential and V_{nl} drops to zero. We evaluate V_{nl} numerically where we find a plateau $B^\perp \approx 6 - 8$ T, in agreement with the experimental observation (8). The presence of a wide plateau, and not a sharp dip, indicates that several subbands are contributing to the BSR. According to Eq. [3.10], the resonance condition for each subband has a different value of $B_{BSR}^\perp$. Thus the plateau arises as a combination of injection in higher subbands and small-angle scattering. Notice that this is in contrast with semiclassical Monte Carlo simulation (33, 64) where the electron moves in a strip of a 2D electron gas where the resonance condition has a well-defined value depending on the electron Fermi velocity and the channel width, as given by Eq. [3.2].

In the next section, we will analyze the BSR in systems with strong SO couplings, such as a InAs quantum well. In this case, we have an interplay between the SO and the external magnetic fields which generates anomalous spin resonances when $B^\parallel$ ($B^\perp = 0$).

3.5 Anomalous ballistic spin resonance

In the GaAs/AlGaAs semiconductor heterostructure considered in the experimental work by Frolov et al. (8), the effective SO magnetic field $\mathcal{H}_{SO}^\perp$ can be neglected in comparison with the $\mathbf{B}_{ext}$ for large fields ($\mathbf{B}_{ext} > 0.5$ T). Notwithstanding, in InAs/InAlAs quantum wells this approximation is no longer valid since $\mathbf{B}_{SO} \sim 0.3$ T according to Eq. [3.1] for the higher subbands. In this strong SO coupling regime, we find a non-monotonic behavior also for $\tau_{SR}(B^\parallel)$. We term this emergence of extra resonance dips as “anomalous BSR” (61).

Similarly to Sec. [3.4], we now analyze the two cases depending on the orientation of the in-plane external magnetic field. First considering an external magnetic field applied perpendicular to the wire $B^\perp$ ($B^\parallel = 0$) where the subband-spin mixing term $\mathcal{H}_{SO}^\parallel$ still acts flipping the electron spin and also quickening the spin relaxation. Nevertheless, the resonance condition is modified since it is proportional to the SO magnetic field $g\mu_B B_{SO}^\perp/2 = -(\alpha + \beta)k$. Interestingly, an external magnetic field applied along the

Figure 3.3 – (a) Dependence of the spin relaxation time τ_{SR} ((b) Non-local voltage V_{nl}) with the external magnetic field B_{ext} . For $B^{\perp}$ (light triangles), a clear dip of the spin relaxation time emerges near the SO induced energy anticrossings of the quantum wire subbands with opposite spins. The resonance condition, given by Eq.[3.10], is fulfilled for $B^{\perp} \approx 8$ T for the highest subband. On the other hand, τ_{SR} and consequently V_{nl} increases monotonically with $B^{\parallel}$ (dark circles). (c) Experimental data of the BSR experiment (8) shows the same behavior when compared with our numerical results including the wide plateau at resonance. We have used the following parameters in our simulation: $\delta t = 2$ ps, $N = 1000$, $\Delta = 3^\circ$, $L = 1$ μm , $\Phi = 30^\circ$, number of electrons considered in the ensemble $N_{ens} = 1000$, electronic density $n_{1D} \approx 10^8$ m^{-2} . For the non-local voltage V_{nl} we used the channel resistivity $\rho = 40$ Ω , left (right) end of the channel $L_l = 30$ μm ($L_r = 70$ μm), $x_{id} = 20$ μm , temperature $T = 300$ mK. For the GaAs quantum well, $|(\alpha + \beta)| = 0.05$ meV.nm, $|(\alpha - \beta)| = 0.2$ meV.nm, $|g| = 0.44$ (9) and $m = 0.067$ m_0 (9), where m_0 is the bare electron mass.

channel $B^\parallel$ ($B^\perp = 0$) has two roles. It modifies the resonance condition for the BSR and can tilt the electron spin from $\hat{x}$ direction to new one denoted by $\hat{u}$. Along this new spin orientation, the spin-orbit induced admixture of state with opposite spins allows for the transition $\langle n_j, \downarrow_u | \mathcal{H}_{\text{SO}}^\parallel \propto \partial_y \sigma_x | n_j \pm \Lambda, \uparrow_u \rangle \neq 0$, where $\Lambda = 1, 3, 5, \dots$. The resonance condition is calculated considering the energy spectrum of the Hamiltonian $[\mathcal{H}_0 + \mathcal{H}_{\text{SO}}^\perp + \mathcal{H}_Z^\parallel] |n, k, s_x\rangle = \epsilon_{n,k,s_x} |n, k, s_x\rangle$. The condition for the crossing of energy levels $\epsilon_{n_j,k,\downarrow_x} = \epsilon_{n_j \pm \Lambda, k, \uparrow_x}$ occurs for the $B_{\text{BSR}}^\parallel$ is fulfilled whenever

$$\frac{1}{2} g \mu_B B_{\text{BSR}}^\parallel = \sqrt{\left(\frac{\pi^2 \hbar^2}{4mL^2} [\pm 2n_j \Lambda + \Lambda^2] \right)^2 - ((\alpha + \beta)k_F)^2}. \quad (3.12)$$

Choosing a set of parameters that fulfills this condition, the spin relaxation time $\tau_{\text{SR}}(B^\parallel)$ also has a non-monotonic dependence with the external magnetic field, as showed in Fig. [3.4]. In order to simulate the conditions to generate the anomalous BSR, we choose an InAs quantum well which is characterized by a strong SO coupling when compared with GaAs quantum wells. Moreover, we observe higher harmonics ($\Lambda = 3, 5, \dots$) even at low magnetic fields due to the high gyromagnetic factor in InAs when compared with GaAs. We point out that the square wire confinement used in our model captures the higher harmonics $\Lambda = 3, 5, \dots$ as indicated by the matrix elements of the subband-spin mixing term $\mathcal{H}_{\text{SO}}^\parallel$. In contrast, the harmonic confinement only captures the first resonant dip $\Lambda = 1$ as explained in Appendix A. This particular choice of a square wire was motivated by the experimental findings since these higher harmonics were also observed experimentally in GaAs quantum wells (8). In order to measure these higher harmonics in typical laboratory magnetic fields, the experimentalists used a wider channel ($\sim 3 \mu\text{m}$) which decreases the value of $B_{\text{BSR}}^\perp$ (see Eq.[3.2]). We emphasize that these higher harmonics can be observed experimentally in a micrometer channel engineered in InAs quantum wells even at low magnetic fields. In addition, we predict that BSR can be measured for the two orientation of the external magnetic field, $B^\parallel$ and $B^\perp$, in the strong SO coupling regime.

Figure 3.4 – (a) Dependence of the spin relaxation time τ_{SR} with the external magnetic field $B^{\parallel}$ in InAs quantum well. In this strong SO coupling regime, $\tau_{\text{SR}}(B^{\parallel})$ also presents a non-monotonic behavior. Anomalous BSR dips are observed around $B^{\parallel} \approx 0.6$ T for $\Lambda = 1$ and $B^{\parallel} \approx 1.3$ T for $\Lambda = 3$ (see arrows). (b) τ_{SR} vs. $B^{\perp}$ with the resonance conditions given by $B^{\perp} \approx 0.6$ T for $\Lambda = 1$ and $B^{\perp} \approx 1.9$ T for $\Lambda = 3$. Here we use the same parameters for the numerical simulation as those for GaAs wells in Sec. [3.4]. For InAs we have that $|(\alpha + \beta)| = 2$ meV.nm, $|(\alpha - \beta)| = 5$ meV.nm, $|g| = 14.94$ (10) and $m = 0.026 m_0$ (9).

3.6 Conclusions

We have developed a numerical model to evaluate the spin relaxation time in multisubband quantum wires. We were able to extract the spin relaxation time evaluating the time-dependent average spin operators in the Heisenberg representation. We consider the DP mechanism which arises due to combination of spin precession around the SO magnetic field and random multiple scattering events. In order to consider large- and small-angle mechanisms, we consider momentum-transfer events in the time-evolution operator. By observing the magnetic field dependence of τ_{SR} , we find two distinct behaviors depending on the orientations of the in-plane $\mathbf{B}_{\text{ext}}$. We find that $\tau_{\text{SR}}(B^{\parallel})$ increases monotonically while $\tau_{\text{SR}}(B^{\perp})$ strongly decreases around the energy anticrossing induced spin-orbit mixing as a function of the external magnetic field. In our model, the spin resonance occurs near the spin-orbit induced energy anticrossings of the quantum wire subbands with opposite spins. We also evaluate the non-local voltage which quantifies the behavior of $\tau_{\text{SR}}(\mathbf{B}_{\text{ext}})$. This quantity shows a wide plateau in agreement with the experimental findings (8). This plateau arises due to a combination of injection in higher

quantum wire subbands and small-angle scattering. We also simulate a InAs quantum well which has a strong SO coupling in comparison with GaAs. In this regime, the SO magnetic field along the channel can tilt the initial alignment of the injected electron spin leading to a anomalous BSR. Thus we predict that BSR could be measured for both in-plane directions of $\mathbf{B}_{\text{ext}}$ in the strong SO coupling regime.

CHAPTER 4

CROSSED PERSISTENT SPIN HELICES

4.1 Introduction

The research field of spintronics relies a great deal upon the control of spin via the coupling with its orbital motion provided by the spin-orbit interaction (SO). Nevertheless, the SO interaction is a double-edge sword: on one hand it allows to manipulate electron spin which can be used to carry information, while on other hand it also causes spin relaxation where this information can be lost to the environment. The SO interaction can be viewed as a momentum-dependent effective magnetic field which has its direction randomized after each scattering event. Thus the spin precession orientation for each electron from an ensemble occurs around different axes leading to spin relaxation. This is known as the D'yakonov-Perel (DP) spin relaxation mechanism (32). Also, the eigenspinors are mixed with spin-up and spin-down components in in spin-orbit coupled systems. Thus it leads to a nonzero probability of spin-flip at each scattering event. This spin relaxation mechanism is called Elliot-Yafet (EY) (34, 35). In order to suppress these relaxation mechanisms, many theoretical proposals have been made as an effort to extend the spin lifetime.

A spin lifetime enhancement can be related to the presence of a spin-dependent conserved quantity which leads to a fixed spin quantization axis in the SO eigenspinors - $U(1)$

symmetry (24). This can be achieved in a two-dimensional (2D) electron gas by tuning the Rashba and Dresselhaus coupling to have equal strengths. This feature can be used to build a nonballistic spin-field-effect transistor where the DP and EY mechanism are completely suppressed (24). The presence of this spin-dependent conserved quantity also leads to a spin density textures robust against spin-independent scattering and electron-electron interaction. This pattern is called persistent spin helix (PSH) after Bernevig et al. (4). This spin helix mode arises from the interplay of diffusion and the spin precession around the effective SO magnetic field fixed along a certain direction.

In this chapter, we investigate theoretically the emergence of crossed persistent helices in quantum wells with two subbands. We start with a brief introduction in Sec. [4.2] about the theory presented by Bernevig et al. (4). Also in Sec. [4.2], we derive the average values of the spin components using a quantum-mechanical description accounting for an arbitrary spin-independent potential (24). We solve spin-charge coupled diffusive equations to analyze the decay of the out-of-plane spin component for a spatially-modulated spin excitations. We also analyze some suitable experimental techniques that can be used to test our prediction such as Transient spin-grating spectroscopy and Kerr rotation microscopy. We estimate the D'yakonov-Perel spin relaxation rate due to cubic Dresselhaus and interband SO interaction which reduces the spin helix lifetime. Numerical simulations of the quantum wells provide realistic values for the SO coupling strengths in order to estimate the effect of these symmetry-breaking interactions and the feasibility of this crossed PSHs. In Sec. [4.3], we also study the interband spin-orbit coupling-induced energy anticrossing and unusual spin textures beyond the usual intraband Rashba and Dresselhaus SO coupling model.

4.2 Persistent spin helix

In this section, we will introduce the basics of a persistent spin helix. We will also show that a quantum well with two subbands can host a novel robust spin-density helical pattern with two orthogonal spin quantization axes.

Figure 4.1 – Crossed persistent spin helices in a quantum well with two subbands. This robust pattern is formed in 2D electron gases when the Rashba and Dresselhaus spin-orbit coupling strengths are tuned to have same absolute values but opposite signs. This spin-density helical pattern arises due to interference of PSH in each subband oriented along orthogonal directions. The electrons and their spins are represented by blue spheres and black arrows, respectively.

4.2.1 Introduction to the persistent spin helix

Next we briefly reproduce the calculation presented by Bernevig et al. (4). Consider the linearized Rashba and Dresselhaus SO interactions in a 2D electron gas formed in a semiconductor heterostructure

$$\mathcal{H}_{\text{RD}} = \alpha(k_x \sigma_y - k_y \sigma_x) + \beta(k_y \sigma_y - k_x \sigma_x). \quad (4.1)$$

Further details about these SO couplings will be given in Subsec. [4.2.2]. Within this model, we find a robust spin pattern with infinite lifetime. According to Ref. (4), it is possible to find a set of spin operators which obey the angular momentum commutation rules and commutes with the Hamiltonian $\mathcal{H}_{\text{RD}}$. Thus they found an exact SU(2) symmetry in the *linear-in-k* Rashba and Dresselhaus models.

We start with the definition of the spin density operator $\boldsymbol{\sigma}(\mathbf{r}) = \sum_i \boldsymbol{\sigma}_i \delta(\mathbf{r} - \mathbf{r}')$. This operator can be rewritten in the occupation number representation $\boldsymbol{\sigma}(\mathbf{r}) = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \Psi(\mathbf{r})$. Here, the field operator is given by $\Psi(\mathbf{r}) = \sum_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\sigma}$, where we have chosen plane waves as basis function. Also, the creation $c^\dagger$ and destruction c operators obey the anti-commutation rules for fermions, i.e., $\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}^\dagger\} = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'}$. Thus the second-quantized

spin operator reads

$$\boldsymbol{\sigma}(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{q}\boldsymbol{\sigma}\boldsymbol{\sigma}'} c_{\mathbf{k}\boldsymbol{\sigma}}^\dagger c_{\mathbf{k}+\mathbf{q}\boldsymbol{\sigma}'} e^{i\mathbf{q}\cdot\mathbf{r}} u_{\boldsymbol{\sigma}}^\dagger \boldsymbol{\sigma} u_{\boldsymbol{\sigma}'}, \quad (4.2)$$

where $u_{\uparrow}^\dagger = \begin{pmatrix} 1 & 0 \end{pmatrix}$ and $u_{\downarrow}^\dagger = \begin{pmatrix} 0 & 1 \end{pmatrix}$. Explicitly, we have all spin operator components

$$\sigma_x(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{q}} \{ \sigma_q^+ e^{-i\mathbf{q}\cdot\mathbf{r}} + \sigma_q^- e^{i\mathbf{q}\cdot\mathbf{r}} \}, \quad (4.3)$$

$$\sigma_y(\mathbf{r}) = -i \sum_{\mathbf{k}\mathbf{q}} \{ \sigma_q^+ e^{-i\mathbf{q}\cdot\mathbf{r}} - \sigma_q^- e^{i\mathbf{q}\cdot\mathbf{r}} \}, \quad (4.4)$$

$$\sigma_z(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{q}} \{ c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{q}\downarrow} \} e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (4.5)$$

The coefficients of the Fourier expansion of the spin operators in real space are given by

$$\sigma_q^- = \sum_{\mathbf{k}} c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{q}\uparrow}, \quad \sigma_q^+ = \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger c_{\mathbf{k}\downarrow}, \quad \sigma_0^z = \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\downarrow}. \quad (4.6)$$

These operators obey the angular momentum commutation relations

$$[\sigma_0^z, \sigma_q^\pm] = \pm 2\sigma_q^\mp \quad [\sigma_q^+, \sigma_q^-] = \sigma_0^z. \quad (4.7)$$

Moreover, these operators commute with the Hamiltonian,

$$[\mathcal{H}_{\text{RD}}, \sigma_q^\pm] = (E_{\mathbf{k},\uparrow_{x\pm}}(\mathbf{k} + \mathbf{q}) - E_{\mathbf{k},\downarrow_{x\pm}}(\mathbf{k})) \sigma_q^\pm = 0 \quad (4.8)$$

as long as $\mathbf{q} = \mathbf{q}_{\text{PSH}}$, where $\mathbf{q}_{\text{PSH}} = (4m\beta/\hbar)\mathbf{x}_\pm$ for $\alpha = \pm\beta$. Here, we have used the shifting property of the Rashba and Dresselhaus energy spectrum for $\alpha = \pm\beta$ given by $E_{\mathbf{k},\uparrow_{x\pm}}(\mathbf{k} + \mathbf{q}) = E_{\mathbf{k},\downarrow_{x\pm}}(\mathbf{k})$, as illustrated by Fig. [4.2]. We use that $\mathcal{H}_{\text{RD}} |k, s_{x\pm}\rangle = E_{\mathbf{k},s_{x\pm}} |k, s_{x\pm}\rangle$, where $s = \{\uparrow, \downarrow\}$. Interestingly, this set of spin operators also commute with the SO Hamiltonian even if we include a spin-independent scattering potential and the electron-electron interaction (4).

In the next subsection, we will introduce the model to describe the SO interactions in

a quantum well with two subbands. Also, we verify the feasibility of finding equal Rashba and Dresselhaus SO coupling strengths in realistic systems.

Figure 4.2 – Fermi surfaces for the Rashba and Dresselhaus SO coupling strengths tuned to be equal, (a) $\alpha = -\beta$ and (b) $\alpha = \beta$. The blue (green) curve denotes the spin-up (down) branch. Each spin branch is shifted from each other by a distance q_{PSH} which is given by the PSH wavevector.

4.2.2 Model for a persistent spin helix in a quantum well with two subbands

We account for the intraband Rashba and Dresselhaus SO interactions in a quantum well with two subbands (37, 38). Their derivation starts with the 8×8 Kane model followed by a perturbation theory which obtains an effective SO Hamiltonian for the conduction electrons. The Rashba SO term is induced by the inversion-asymmetry of the confining potential along the semiconductor heterostructure growth direction. This SO coupling strength can be tuned via an external gate voltage. The Dresselhaus SO contribution arises in semiconductors due to inversion asymmetry in bulk. Their *linear-in-k* Hamiltonian reads

$$\mathcal{H}_{RD}^{1,2} = \tau_i \otimes \alpha_i (k_x \sigma_y - k_y \sigma_x) + \tau_i \otimes \beta_i (k_y \sigma_y - k_x \sigma_x), \quad (4.9)$$

where $\mathcal{H}_{RD}^{1,2} = \mathcal{H}_{RD}^1 + \mathcal{H}_{RD}^2$, implying summation over the subband index $i = 1, 2$ corresponding to the first (even) and second (odd) subband, respectively. Here, the pseudospin operators $\tau_{1,2} = (\mathbb{1}_{2 \times 2} \pm \tau_z)/2$ refer to the subspace for each subband. The SO coupling strenghts are given by

$$\eta_{vv'} = \langle \psi_v(z) | \eta(z) | \psi_{v'}(z) \rangle, \quad \gamma_{vv'} = \gamma_D \langle \psi_v(z) | k_z^2 | \psi_{v'}(z) \rangle, \quad (4.10)$$

where $\psi_v(z)$ are the self-consistent calculated wavefunctions along the quantum well growth direction. Thus the intraband Rashba and Dresselhaus SO coupling strenghts are respectively defined as $\alpha_i = \eta_{ii}$ and $\beta_i = \gamma_{ii}$ for the first ($i = 1$) and second subbands ($i = 2$). For now we neglect the contribution from the interband SO interactions where η_{ij} and γ_{ij} , with $i \neq j$. Nevertheless, we will estimate their effects on reducing the spin helix lifetime in a further Subsec. [4.2.4]. The SO couplings were obtained after performing a self-consistent numerical calculations in order to solve the Schrödinger and Poisson equations in the Hartree approximation in realistic quantum wells, as shown in Fig. [4.3].

Fulfilling the condition such that α_i and β_i are tuned to have equal strenghts within the same subband, i.e., $\alpha_i = \pm \beta_i$, the Hamiltonian reduces to $\mathcal{H}_{RD} = -2\tau_i \otimes \beta_i |k_{\pm}| \Sigma_{\mp}$. Here, we define $k_{\pm} = (k_x \pm k_y)/\sqrt{2}$ and $\Sigma_{\pm} = \text{sgn}(k_{\pm})(\sigma_x \pm \sigma_y)/\sqrt{2}$. The quantities $\Sigma_{\pm}$ are conserved since they commute with the Hamiltonian $\mathcal{H}_{RD} \propto \Sigma_{\pm}$ and define a *k-independent* direction for the spin quantization axis - U(1) symmetry (24). Notice that Σ_- and Σ_+ can be related with the orthogonal directions x_- and x_+ are in the 2D electron gas plane which correspond to the $[1\bar{1}0]$ and $[110]$ crystal axes, respectively.

As stated in Sec. [4.1], whenever we have $\alpha_i = \pm \beta_i$, the spin precession patterns becomes robust against spin-independent scattering and depends only on the net displacement along some specific direction. As explained earlier, this persistent spin helix was initially predicted by Bernevig et al. (4) in the one-subband *linear-in-k* Rashba and Dresselhaus SO model. In the next subsection, we extend their results for a two subband case. We study the several tuning conditions for the Rashba and Dresselhaus SO coupling strenghts leading to distinct spin helical patterns. Also, we calculate the average spin operators in order to analyze the formation of unusual spin textures due to crossed PSHs along orthogonal directions.

Figure 4.3 – (a) Self-consistent potential V_c for modulation-doped $\text{Al}_{0.12}\text{In}_{0.88}\text{Sb}$ double well with the central barrier $\text{Al}_{0.4}\text{In}_{0.6}\text{Sb}$. This quantum well has two subbands with the corresponding wave functions ψ_1 and ψ_2 . We simulate a well of width $L_w = 50$ nm and one central barrier of width $L_b = 20$ nm. Electrons in the quantum well come from n-doped semi-infinite adjacent regions of width $w = 4$ nm. (b) External gate voltage dependence of the spin-orbit coupling strengths for the Rashba α_i and Dresselhaus β_i for each subband $i = 1, 2$ and the interband Rashba η and the interband Dresselhaus γ ($\gamma \times 10$ for clarity) models. The green lines indicate the gate voltage such that $\alpha_1 = -\beta_1$ and $\alpha_2 = \beta_2$ at $V_g = 0.02$ eV (solid) and $\alpha_1 = \beta_1$ and $\alpha_2 = -\beta_2$ at $V_g = -0.02$ eV (dashed).

4.2.3 Expectation value of the spin operators in the presence of disorder

In this subsection, we will evaluate the expectation value of the spin operators in the presence of the Rashba and Dresselhaus SO interactions. In the symmetric condition $\alpha = \pm\beta$, we are able to write the expectation value of the spin operators in an analytical form even in the presence of a spin-independent scattering potential.

The PSH formation can be traced back to the direction of the spin-conserved quantity in the SO Hamiltonian for each subband. In the trivial case, where the SO coupling for both subbands share the same conserved quantity ($\mathcal{H}_{RD}^{1,2} \propto \Sigma_-$ with $\alpha_{1,2} = \beta_{1,2}$ or $\mathcal{H}_{RD}^{1,2} \propto \Sigma_+$ with $\alpha_{1,2} = -\beta_{1,2}$) a single PSH pattern emerges in the 2D electron gas. Nevertheless, the SO coupling for each subband might also be proportional to different conserved quantities. Thus each subband will be related to orthogonal directions for the spin quantization axes and might create an interference of the PSH patterns. Let us now analyze the case in which $\alpha_1 = \beta_1$ ($\mathcal{H}_{RD}^1 \propto \Sigma_-$) and $\alpha_2 = -\beta_2$ ($\mathcal{H}_{RD}^2 \propto \Sigma_+$). The presence of a different conserved quantity for each subband will lead to a formation of two independent spin patterns oriented along orthogonal directions, as shown in Fig. [4.4] for the first (a) and second (b) subbands. These patterns will interfere creating an unusual spin texture called crossed PSHs. This novel PSH can be understood by evaluating the

expectation value of the spin operators (72). Consider then a general case including a spin-independent scattering potential $V(\mathbf{r})$ (24) in the Hamiltonian $\mathcal{H}_{RD}^{1,2}$ with $\mathbf{k} \rightarrow -i\nabla$. The connection of the PSH with the helical pattern in the spin space is clearer in the x_+x_-z frame of reference. Consider an electron spin initially prepared perpendicularly to the direction of the fixed spin quantization axis for each subband, the steady-state solution taking into account $V(\mathbf{r})$ is given by

$$\psi_1(\mathbf{r}) = e^{-i\frac{\pi}{4}} \frac{\varphi(\mathbf{r})}{\sqrt{2}} e^{+i\delta_-/2} |\uparrow_{x_-}\rangle + e^{+i\frac{\pi}{4}} \frac{\varphi(\mathbf{r})}{\sqrt{2}} e^{-i\delta_-/2} |\downarrow_{x_-}\rangle \quad (4.11)$$

and

$$\psi_2(\mathbf{r}) = e^{+i\frac{\pi}{4}} \frac{\varphi(\mathbf{r})}{\sqrt{2}} e^{+i\delta_+/2} |\uparrow_{x_+}\rangle + e^{-i\frac{\pi}{4}} \frac{\varphi(\mathbf{r})}{\sqrt{2}} e^{-i\delta_+/2} |\downarrow_{x_+}\rangle \quad (4.12)$$

for the first $\psi_1(\mathbf{r})$ and second $\psi_2(\mathbf{r})$ subbands, respectively. Also, the spin precession angles are defined by $\delta_+ = 4m\beta_1x_+/\hbar^2$ and $\delta_- = 4m\beta_2x_-/\hbar^2$. The orbital wavefunction $\varphi(\mathbf{r})$ obeys the single-particle spin-independent Schrödinger equation $\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\varphi(\mathbf{r}) = \left(\epsilon + \frac{2m\beta_i^2}{\hbar^2}\right)\varphi(\mathbf{r})$, where ϵ is the eigenvalues of the wave function $\psi_s(\mathbf{r})$ (24). We found that the expectation values components of the spin operator $\boldsymbol{\sigma} = (\sigma_{x_+}, \sigma_{x_-}, \sigma_z)^T$ are given by

$$\langle \psi_s | \boldsymbol{\sigma} | \psi_s \rangle = |\varphi(\mathbf{r})|^2 \begin{pmatrix} \cos \delta_+ \\ \cos \delta_- \\ (\sin \delta_+ - \sin \delta_-) \end{pmatrix}, \quad (4.13)$$

where $\langle \psi_s | \boldsymbol{\sigma} | \psi_s \rangle = \langle \psi_1 | \boldsymbol{\sigma} | \psi_1 \rangle + \langle \psi_2 | \boldsymbol{\sigma} | \psi_2 \rangle$. The wavefunction $\varphi(\mathbf{r})$ varies over a length scale given by the Fermi wavelength λ_F . For realistic parameters, these wavelengths satisfies $\lambda_Q \gg \lambda_F$, where $\lambda_Q = 2\pi/\delta_i$, $i = +, -$ is the PSH wavelength. So, we have that the modulation induced by the term $|\varphi(\mathbf{r})|^2$ is not accessible experimentally. Thus the only measurable modulation is provided by the emergence of the PSH. This spin pattern exhibits an egg carton-like interference patterns for the PSH along the z direction, as shown in Fig. [4.5]. Notice that this component $\langle \psi_s | \sigma_z | \psi_s \rangle$ vanishes whenever the condition $\delta_+ = \delta_-$ is fulfilled.

Figure 4.4 – Persistent spin helix for the first subband with $\alpha_1 = \beta_1$ (a) and for the second subband with $\alpha_2 = -\beta_2$ (b). They have orthogonal spin quantization axis since $\mathcal{H}_{RD}^1 \propto \Sigma_- \parallel x_- \parallel [1\bar{1}0]$ and $\mathcal{H}_{RD}^2 \propto \Sigma_+ \parallel x_+ \parallel [110]$.

Figure 4.5 – Crossed robust spin-density waves. This robust spin-helical wave density arises due to interference between the orthogonal PSHs in each quantum well subbands.

4.2.4 Spin-charge coupled diffusive equations

Next we solve the diffusive transport equations for the coupled spin and charge densities derived from a quantum Boltzmann-type equation. First we obtain the general solution for a PSH in a single subband quantum well. Then, we generalize our calculation for two subbands.

Here, we give a brief description of derivation of the spin-charge coupled diffusion equations (60). We use semiclassical density matrix (also known as Wigner density matrix) $\rho(\mathbf{r}, \mathbf{p}, t)$. Within this approach, we consider a classical orbital motion. Then, we calculate the Heisenberg equation of motion for $\rho(\mathbf{r}, \mathbf{p}, t)$ using the SO Hamiltonian [4.1] rotated to the frame of reference x_+x_-z . This results in a Boltzman-type equation after including the collision term which account for abrupt changes in the electron momentum due to scattering events. Finally, we calculate the electronic density n and the spin density $\mathbf{S}$ using respectively $n(\rho(\mathbf{r}, t)) = \int d\mathbf{p} \text{Tr}(\rho(\mathbf{r}, \mathbf{p}, t))$ and $\mathbf{S}_i(\rho(\mathbf{r}, t)) = \int d\mathbf{p} \text{Tr}(\mathbf{s}_i \rho(\mathbf{r}, \mathbf{p}, t))$, for $i = x, y, z$ and $\mathbf{s}_i = \hbar \boldsymbol{\sigma}_i / 2$. Thus the spin-charge coupled diffusion equations for a Rashba and Dresselhaus SO-coupled 2D electron gas in the frame of reference x_+x_-z reads

$$\partial_t n = D \partial_i^2 n + B_- \partial_{x_+} S_{x_-} - B_+ \partial_{x_-} S_{x_+} \quad (4.14)$$

$$\partial_t S_{x_-} = D \partial_i^2 S_{x_-} + B_- \partial_{x_+} n - C_- \partial_{x_-} S_z - T_- S_{x_-} \quad (4.15)$$

$$\partial_t S_{x_+} = D \partial_i^2 S_{x_+} - B_+ \partial_{x_-} n - C_+ \partial_{x_+} S_z - T_+ S_{x_+} \quad (4.16)$$

$$\partial_t S_z = D \partial_i^2 S_z + C_- \partial_{x_-} S_{x_-} + C_+ \partial_{x_+} S_{x_+} - T_z S_z, \quad (4.17)$$

with the constants $B_+ = 2(\alpha + \beta)^2(\alpha - \beta)k_F^2\tau^2$, $B_- = 2(\alpha - \beta)^2(\alpha + \beta)k_F^2\tau^2$, $C_+ = 2(\alpha + \beta)k_F^2\tau/m$, $C_- = 2(\alpha - \beta)k_F^2\tau/m$. Here, k_F is the Fermi wavevector, $D = \hbar^2 k_F^2 \tau / 2m^2$ is the diffusion constant, where τ is the mean free time. Also, the spin relaxation rates are denoted by $T_i = 1/\tau_i$, with $i = +, -, z$. Fulfilling the condition $\alpha = \beta$, it results in two pairs of coupled equations, n with S_{x_+} and S_z with S_{x_-} . We can solve these coupled equations after performing a Fourier transform in the space and time. We end up with a second-order equation which gives us two characteristic frequencies $i\omega_{\pm} = \Gamma_{\pm}$. Since the experimental setups are able to monitor the out-of-plane spin components, we explicitly write the solution

$$S_z(\mathbf{q}, t) = A_+(q)e^{-\Gamma_+ t} + A_-(q)e^{-\Gamma_- t}, \quad (4.18)$$

where we have a double exponential decay with the decay rates

$$\Gamma_{\pm}(q) = Dq^2 + T_{\pm} \pm C_{\pm}q. \quad (4.19)$$

The coefficients $A_{\pm}(q)$ are determined after setting the initial condition for the spin polarization. Following the experimental initial condition given by Ref. (3), we set $S_z(x_+, x_-, t = 0) = \cos(q_0 x_+)$, with a well-defined spin polarization wavelength q_0 . It results in the following coefficients $A_{\pm}(q) = [\delta(q + q_0) + \delta(q - q_0)]/4$ where we have already consider the condition $\alpha = \beta$. We also can obtain the solution for the in-plane component

$$S_x(\mathbf{q}, t) = B_+(q)e^{-\Gamma_+ t} + B_-(q)e^{-\Gamma_- t}, \quad (4.20)$$

where the coefficients $B_{\pm}(q) = \mp i[\delta(q + q_0) + \delta(q - q_0)]/4$ satisfy the initial condition $S_x(x_+, x_-, t = 0) = \sin(q_0 x_+)$. Performing a Fourier transform from the q -space to the real space, we have the time-dependent solution

$$S_z(x_+, t) = \frac{1}{2}[e^{-(Dq_0^2 + T_+ + C_+ q_0)t} + e^{-(Dq_0^2 + T_+ - C_+ q_0)t}] \cos(q_0 x_+), \quad (4.21)$$

$$S_x(x_+, t) = \frac{1}{2}[e^{-(Dq_0^2 + T_+ + C_+ q_0)t} + e^{-(Dq_0^2 + T_+ - C_+ q_0)t}] \sin(q_0 x_+). \quad (4.22)$$

For a spin polarization wavelength q_0 matching the PSH wavelength q_{PSH} , i.e., $q_0 = q_{PSH} = 4m\beta^2/\hbar^2$, the decay rates $\Gamma_{\pm}(q_{PSH})$ simplifies to $\Gamma_+(q) = 32\beta^2 k_F^2 \tau$, while $\Gamma_-(q) = 0$. In Ref. (3), preparation and monitoring of the time evolution of the spatially-modulated out-of-plane spin component $S_z(x_+, x_-, t)$ was performed by transient spin grating measurements (3). The enhanced $\tau_E = 1/\Gamma_-(q)$ and the reduced $\tau_R = 1/\Gamma_+(q)$ spin helix lifetime are extracted from the experimental data using a double-exponential fit. Notice that τ_E does not diverge in the realistic case since it is necessary to take into account symmetry-breaking terms such as the cubic Dresselhaus and the interband SO couplings. We will estimate their contributions which limit the spin helix lifetime further

in this section.

Next we consider the same approach applied to a quantum well with two subbands. As stated in Sec. [4.2], we choose an external gate voltage such that $\alpha_1 = \beta_1$ and $\alpha_2 = -\beta_2$ which set the spin conserved quantity to be aligned with x_- for the first subband and x_+ for the second subband. We would like to produce a PSH in each subband, thus we choose as a initial condition $S_z^1(x_+, x_-, t = 0) = \cos(q_0 x_+) + \cos(q_0 x_-)$ and $S_z^2(x_+, x_-, t = 0) = \cos(q_0 x_+) + \cos(q_0 x_-)$. Since the quantum well subbands are decoupled, the total out-of-plane spin polarization is given by $S_z(x_+, x_-, t) = \sum_{i=1,2} S_z^i(x_+, x_-, t) = S_z^1(x_+, x_-, t) + S_z^2(x_+, x_-, t)$, where the superscript denotes the first $i = 1$ and the second $i = 2$ quantum well subbands. Following the procedure described in the one-subband case, the time-dependent solutions are

$$S_z^1(x_+, x_-, t) = \frac{1}{2} [e^{-(Dq_{x+}^2 + T_+ + C_+ q_{x+})t} + e^{-(Dq_{x+}^2 + T_+ - C_+ q_{x+})t}] \cos(q_0 x_+) \quad (4.23)$$

$$+ [e^{-(Dq_{x-}^2 + T_+)}] \cos(q_0 x_-),$$

and

$$S_z^2(x_+, x_-, t) = \frac{1}{2} [e^{-(Dq_{x-}^2 + T_- + C_- q_{x-})t} + e^{-(Dq_{x-}^2 + T_- - C_- q_{x-})t}] \cos(q_0 x_-) \quad (4.24)$$

$$+ [e^{-(Dq_{x+}^2 + T_-)}] \cos(q_0 x_+).$$

Fulfilling the condition $q_0 = q_{PSH}$, where the spin relaxation rates $\Gamma_-(q_{x+}, q_{x-}) = (Dq_{x+}^2 + T_+ - C_+ q_{x+}) \rightarrow 0$ for $\alpha_1 = \beta_1$ and $\Gamma_+(q_{x+}, q_{x-}) = (Dq_{x-}^2 + T_- + C_- q_{x-}) \rightarrow 0$ for $\alpha_2 = -\beta_2$. Thus in the long time limit, only one component will survive for each subband, i.e., $S_z^1(x_+, x_-, t) \propto \cos(q_0 x_-)$ and $S_z^2(x_+, x_-, t) \propto \cos(q_0 x_+)$. Thus in the two-subband case, two robust spin-helical density patterns, related with conserved quantities aligned with orthogonal direction, will interfere $S_z(x_+, x_-, t) \propto \cos(q_0 x_-) + \cos(q_0 x_+)$ leading to a formation of crossed PSHs, as showed in Fig. [4.5].

Another possibility to measure the crossed PSHs is using a technique called Kerr rotation microscopy (36). Within this technique, it is feasible to analyze the time evolution of a initially uniform spin excitation into a PSH. This initial uniform spin pattern can be expanded in terms of cossines with distinct wavelengths $\sum_q [\cos(q x_+) + \cos(q x_-)]$. But in

the long time limit, only the components such that $q_0 = q_{PSH}$ will survive resulting in $S_z(x_+, x_-, t) \propto \cos(q_0 x_-) + \cos(q_0 x_+)$. Thus we expect an emergence of a crossed PSHs in a quantum well with two subbands for an appropriate choice of SO coupling strengths, as discussed previously in this section.

Symmetry-breaking SO couplings.

So far, we found that a PSH has an infinite lifetime within the intraband Rashba and Dresselhaus model. Nevertheless, other SO couplings, such as the cubic Dresselhaus and the interband SO couplings, break the symmetry introduced by the presence of the spin-conserved quantity $\Sigma_{\pm}$ in the intraband Rashba and Dresselhaus model. Thus we need to estimate the spin relaxation time including these symmetry-breaking SO interactions since they limit the PSH lifetime to a finite value. This is because these terms will contribute to the decay rates $\Gamma_{\pm}$. Here, we account for the DP and EY spin relaxation mechanisms.

First consider the cubic Dresselhaus SO coupling

$$\mathcal{H}_{D(3)} = \gamma_D (k_x k_y^2 \sigma_x - k_y k_x^2 \sigma_y) \quad (4.25)$$

Using $k^2 = k_x^2 + k_y^2$, this term can be rewritten as $\mathcal{H}_{D(3)} = \beta_3 (k_y \sigma_y - k_x \sigma_x) + \gamma_D (k_y^3 \sigma_y - k_x^3 \sigma_x)$, where $\beta_3 = -\gamma_D k^2$. Notice that the first term $\propto \beta_3$ can be combined with the linear intraband Dresselhaus (see Eq. [4.9]) which renormalizes the PSH condition to $\alpha = \beta - \beta_3$. The second term $\propto \gamma_D$ breaks the symmetry introduced by the conserved quantities and can cause spin relaxation via DP and EY mechanisms.

Another SU(2) breaking term is the effective SO interband Hamiltonian contains the Rashba and Dresselhaus terms connecting the two subbands subspace (37, 38). Explicitly, it reads

$$\mathcal{H}_{RD}^3 = \tau_3 \otimes \eta (k_x \sigma_y - k_y \sigma_x) + \tau_3 \otimes \gamma (k_y \sigma_y - k_x \sigma_x), \quad (4.26)$$

where $\tau_3 \equiv \tau_x$ and the interband Rashba and Dresselhaus coupling strengths are labelled by η and γ , respectively. Explicitly, they are defined following Eq. [4.10] such that $\eta = \eta_{12} = \eta_{21}$ and $\gamma = \gamma_{12} = \gamma_{21}$. Notice that the interband Rashba coupling is non-vanishing even in symmetric quantum wells (37, 38). Besides, we have to define an effective

SO magnetic field for each subband due to the interband SO couplings. This allow us to calculate the D'yakonov-Perel spin relaxation time following the procedure presented by Ref. (73). To this end, we perform a Schrieffer-Wolff transformation eliminating $\mathcal{H}_{RD}^3$ in first-order from the full SO Hamiltonian $\mathcal{H}_{RD} = \mathcal{H}_{RD}^{1,2} + \mathcal{H}_{RD}^3$. Mathematically, we have that $\tilde{\mathcal{H}}_{RD} = e^{-\mathcal{S}}\mathcal{H}_{RD}e^{\mathcal{S}}$, where the operator $\mathcal{S}$ is chosen such that $[\mathcal{S}, \mathcal{H}_{RD}^{1,2}] = \mathcal{H}_{RD}^3$. The transformed Hamiltonian $\tilde{\mathcal{H}}_{RD}$ up to third order in k is used to calculate the D'yakonov-Perel spin relaxation time (73). We find that the interband SO terms are negligible when compared with the cubic Dresselhaus. The contribution due to the cubic Dresselhaus SO coupling adds an extra term to the spin relaxation rates $T_i = 1/\tau_i$, with $i = +, -, z$. Consequently, the spin decay rates [4.19] is no longer be zero when $\alpha = \pm\beta$ and $q_0 = q_{PSH}$, which limits the PSH lifetime to a finite value.

Hence we estimate the DP mechanism reduces the spin helix lifetime to nanosecond timescales, which is the same order as measured by Koralek et al. (3). Also, the EY mechanism is also dominated by the cubic Dresselhaus SO coupling which was estimated to be on the order of hundreds of nanoseconds (4, 73).

4.3 Interband spin-orbit coupling-induced spin textures

In this section, we will analyze the spin textures within the full Rashba and Dresselhaus SO coupling models. We consider the intraband and the interband SO Hamiltonian for a quantum well with two subbands. We turn to a particular case where $\alpha_1 = \beta_1$, $\alpha_2 = \beta_2$ and $\eta = -\gamma$ in order to obtain analytical expressions and gain some physical intuition about the interplay of spin textures around the anticrossing region. A more general case will contain the same information as we present here using this simple case but with different spin textures. Within this particular case, the interband SO Hamiltonian $\mathcal{H}_{RD} = \mathcal{H}_{RD}^{1,2} + \mathcal{H}_{RD}^3$ is given by

$$\mathcal{H}_{RD} = -2(\tau_1 \otimes \beta_1 + \tau_2 \otimes \beta_2) |k_+| \Sigma_- \quad (4.27)$$

$$-2\tau_3 \otimes \eta |k_-| \Sigma_+. \quad (4.28)$$

Here, we solve this Hamiltonian in the basis of the decoupled Rashba and Dresselhaus SO Hamiltonian with $\alpha_i = +\beta$, $\mathcal{H}_{RD}^{1,2} = \tau_i \otimes \beta_i |k_+| \Sigma_-$ for $i = 1, 2$, with respective eigenvalues and eigenvectors

$$\begin{aligned} E_{\mathbf{k}_{\parallel}, i, \lambda} &= \epsilon_i^k + 2\lambda\beta_i \left| \tilde{k}_+ \right|, \\ |\mathbf{k}_{\parallel}, i, \lambda\rangle &= \frac{1}{\sqrt{2}} |\mathbf{k}_{\parallel}, i, \uparrow_z\rangle - \lambda \text{sgn}(k_+) e^{-i\pi/4} \frac{1}{\sqrt{2}} |\mathbf{k}_{\parallel}, i, \downarrow_z\rangle, \end{aligned} \quad (4.29)$$

where $\lambda = \pm 1$ is the SO branch index and $s = (\uparrow_z, \downarrow_z)$ denotes the spin quantization axis along the z direction. As a consequence, $\Sigma_+ |\uparrow_{x_-}\rangle = (-i)\text{sgn}(k_+)\text{sgn}(k_-) |\downarrow_{x_-}\rangle$ and $\Sigma_+ |\downarrow_{x_-}\rangle = (+i)\text{sgn}(k_+)\text{sgn}(k_-) |\uparrow_{x_-}\rangle$. The subband subspace Hilbert space $\{|\mathbf{k}_{\parallel}, i, s\rangle; i = e, o, s_u = (\uparrow_{x_-}, \downarrow_{x_-})\}$ which can be divided in two independent subspaces $\mathcal{F}_+ = \{|\mathbf{k}_{\parallel}, e, \uparrow_{x_-}\rangle, |\mathbf{k}_{\parallel}, o, \downarrow_{x_-}\rangle\}$ and $\mathcal{F}_- = \{|\mathbf{k}_{\parallel}, e, \downarrow_{x_-}\rangle, |\mathbf{k}_{\parallel}, o, \uparrow_{x_-}\rangle\}$ combining SO bands with different spin textures. The corresponding eigenvalues are given by

$$\begin{aligned} E_{\mathbf{k}_{\parallel}, \lambda_1, \lambda_2} &= \epsilon_+^k + 2\lambda_1\lambda_2\beta_- \left| \tilde{k}_+ \right| \\ &+ \lambda_1 \sqrt{(\epsilon_-^k + \lambda_1\lambda_2\beta_+ 2|k_+|)^2 + 2\eta^2 \left| \tilde{k}_- \right|^2}, \end{aligned} \quad (4.30)$$

where $\epsilon_{\pm}^k = (\epsilon_o^k \pm \epsilon_e^k)/2$, $\beta_{\pm} = (\beta_2 \pm \beta_1)/2$, $\lambda_1 = \pm 1$ is the subband (pseudospin) index and $\lambda_2 = \pm 1$ defines each SO branch. This energy spectrum is plotted in Fig. [4.6](a). Also, the respective eigenspinors are given by

$$\begin{aligned} |\mathbf{k}_{\parallel}, \lambda_1 = -1, \lambda_2\rangle &= i \cos \frac{\theta}{2} |\mathbf{k}_{\parallel}, e, s_1\rangle \\ &- \lambda_2 \text{sgn}(\tilde{k}_-) \text{sgn}(\tilde{k}_+) \sin \frac{\theta}{2} |\mathbf{k}_{\parallel}, o, s_2\rangle \\ |\mathbf{k}_{\parallel}, \lambda_1 = +1, \lambda_2\rangle &= i \sin \frac{\theta}{2} |\mathbf{k}_{\parallel}, e, s_1\rangle \\ &+ \lambda_2 \text{sgn}(\tilde{k}_-) \text{sgn}(\tilde{k}_+) \cos \frac{\theta}{2} |\mathbf{k}_{\parallel}, o, s_2\rangle \end{aligned} \quad (4.31)$$

where $\tan \theta = 2|k_-| \eta / \Delta\epsilon$ with $\Delta\epsilon = \epsilon_-^k + \lambda_1\lambda_2\beta_+ 2|k_+|$. Here, $(s_1, s_2) = (\uparrow_{x_-}, \downarrow_{x_-})$ for $\lambda_1\lambda_2 = -1$ and $(s_1, s_2) = (\downarrow_{x_-}, \uparrow_{x_-})$ for $\lambda_1\lambda_2 = +1$. Assuming that $\alpha_1 > 0$, $\alpha_2 > 0$ and

$\eta > 0$, the anticrossing will take place between the states with the energies $E_{\mathbf{k}_{||,-1,+1}}$ and $E_{\mathbf{k}_{||,+1,-1}}$. Before the anticrossing, $|\mathbf{k}_{||}, \lambda_1 = -1, \lambda_2 = +1\rangle \approx |\mathbf{k}_{||}, e, \uparrow_{x_-}\rangle + \mathcal{O}(2|k_-| \eta/\Delta\epsilon)$ and $|\mathbf{k}_{||}, \lambda_1 = +1, \lambda_2 = -1\rangle \approx |\mathbf{k}_{||}, o, \downarrow_{x_-}\rangle + \mathcal{O}(2|k_-| \eta/\Delta\epsilon)$. In another words, the lower (upper) SO branch has a dominant component with a spin texture related with the component $|\mathbf{k}_{||}, e, \uparrow_{x_-}\rangle$ ($|\mathbf{k}_{||}, o, \downarrow_{x_-}\rangle$). Increasing the Fermi energy (or equivalently increasing the electronic density), at the anticrossing, the states $|\mathbf{k}_{||}, e, \uparrow_{x_-}\rangle$ and $|\mathbf{k}_{||}, o, \downarrow_{x_-}\rangle$ will hybridize ($\theta \rightarrow \pi/2$ since the energies of the intraband Rashba and Dresselhaus model are equal $E_{\mathbf{k}_{||},e,+1} = E_{\mathbf{k}_{||},o,-1}$). It leads to a energy gap $4|\eta k_-|$ induced by the interband SO coupling. This interband SO-induced energy-level anticrossing takes place between the energies $E_{\mathbf{k}_{||,1,+}}$ and $E_{\mathbf{k}_{||,2,-}}$, as shown in Fig. [4.3] (a). After the anticrossing, $\theta = \pi + \mathcal{O}(2|k_-| \eta/\Delta\epsilon)$, with the dominant spin texture for each component changes place, i.e., $|\mathbf{k}_{||}, \lambda_1 = -1, \lambda_2 = +1\rangle \approx |\mathbf{k}_{||}, o, \downarrow_{x_-}\rangle + \mathcal{O}(2|k_-| \eta/\Delta\epsilon)$ and $|\mathbf{k}_{||}, \lambda_1 = +1, \lambda_2 = -1\rangle \approx |\mathbf{k}_{||}, e, \uparrow_{x_-}\rangle + \mathcal{O}(2|k_-| \eta/\Delta\epsilon)$. Therefore, there is an exchange of spin textures as the Fermi energy goes through the anticrossing region. This interplay of spin textures before and after the anticrossing region also can be understood evaluating the average spin operator for each branch. We found that $\langle \mathbf{k}_{||}, \lambda_1, \lambda_2 | \sigma_x | \mathbf{k}_{||}, \lambda_1, \lambda_2 \rangle = -\langle \mathbf{k}_{||}, \lambda_1, \lambda_2 | \sigma_y | \mathbf{k}_{||}, \lambda_1, \lambda_2 \rangle = -\lambda_2 \text{sgn}(\tilde{k}_+) \cos \theta / \sqrt{2}$ and $\langle \mathbf{k}_{||}, \lambda_1, \lambda_2 | \sigma_z | \mathbf{k}_{||}, \lambda_1, \lambda_2 \rangle = 0$. This average values of the spin component $\langle \mathbf{k}_{||}, \lambda_1, \lambda_2 | \sigma_x | \mathbf{k}_{||}, \lambda_1, \lambda_2 \rangle$ can be seen in Fig. [4.6] (b,c).

Notice that if we have considered the case where $\alpha_1 = \beta_1$, $\alpha_2 = \beta_2$ and $\eta = \gamma$ ($\alpha_1 = -\beta_1$, $\alpha_2 = -\beta_2$ and $\eta = -\gamma$), all the SO terms in the Hamiltonian H_{RD} will be proportional to the same spin-dependent term Σ_- (Σ_+) with the following subspaces $\mathcal{F}_+ = \{|\mathbf{k}_{||}, e, \uparrow_{x_-}\rangle, |\mathbf{k}_{||}, o, \uparrow_{x_-}\rangle\}$ and $\mathcal{F}_- = \{|\mathbf{k}_{||}, e, \downarrow_{x_-}\rangle, |\mathbf{k}_{||}, o, \downarrow_{x_-}\rangle\}$ ($\mathcal{F}_+ = \{|\mathbf{k}_{||}, e, \uparrow_{x_+}\rangle, |\mathbf{k}_{||}, o, \uparrow_{x_+}\rangle\}$ and $\mathcal{F}_- = \{|\mathbf{k}_{||}, e, \downarrow_{x_+}\rangle, |\mathbf{k}_{||}, o, \downarrow_{x_+}\rangle\}$). Thus, the interplay of components within a subspace takes place only between states with the same spin quantization axis. As a consequence, the spin texture for each SO branch will no longer display any change before and after the anticrossing.

Limiting cases: intraband Rashba or Dresselhaus interband Hamiltonian in quantum wells with two subbands

We consider the intraband Rashba interband Hamiltonian given by

$$\mathcal{H}_R = \tau_i \otimes \alpha_i (k_x \sigma_y - k_y \sigma_x), \quad (4.32)$$

Figura 4.6 – (a) Energy spectrum of a quantum well with two subbands with the intraband and the interband Rashba and Dresselhaus are operative. Inset: Blowup of the anticrossing region. Energy crossing in the absence of the interband SO coupling (solid black lines). (b) Average Spin polarization $\langle \sigma_x \rangle$ for the eigenstates related to energies $E_{k_{\parallel},i,\lambda}$ with $i = 1, 2$ and $\lambda = \pm$. The spin orientation changes direction significantly as the Fermi energy goes through the level anticrossing (1 – 4 for $E_{k_{\parallel},2,-}$ and 2 – 3 for $E_{k_{\parallel},1,+}$). (c) Energy spectrum with the size of the markers indicating the degree of the spin polarization along the x-direction. The colors denote the spin-up (red) and spin-down (blue). The SO coupling strenghts are overestimated in order to enhance the visualization of the spin branches and the energy anticrossing.

implying summation over the index $i = 1, 2$. Notice that all the Rashba terms will share the same k -dependent direction for the spin quantization axis since they are proportional to $(k_x \sigma_y - k_y \sigma_x)$, for any values of α_i . For this reason, for a certain value of k , the interband SO Hamiltonian only couples Rashba branches in different subbands with the same spin orientation. Therefore, the interplay between states with the same spin texture will not lead to a exchange of spin orientations as the Fermi energy goes through the anticrossing region. The same conclusions can be obtained in a intraband Dresselhaus interband model $\mathcal{H}_D = \tau_i \otimes \beta_i(k_y \sigma_y - k_x \sigma_x)$, with $i = 1, 2$.

4.4 Conclusions

We developed a model to account for the intraband and interband Rashba and Dresselhaus SO couplings. Within the intraband model, we predict the formation of crossed persistent spin helices in quantum wells with two occupied subbands. This robust spin-helical density pattern arises when the Rashba and Dresselhaus SO coupling are tuned to have equal strenghts but opposite signs. It can be achieved for a well-defined gate voltage confirmed by our self-consistent calculations. The spin patterns formed in each subband have orthogonal fixed spin quantization axes. These spin helices interfere generating this unconventional spin helix mode. We also estimate the effect of including symmetry-breaking SO terms in our model. The cubic Dresselhaus and the interband SO couplings leads to a nanosecond-scale spin relaxation which limits the lifetime of the crossed PSH. We suggest that this robust spin pattern can be experimentally observed using well-tested techniques such as Transient spin-grating spectroscopy and Kerr rotation microscopy. In addition, the Fermi energy can be varied changing the occupation of the quantum well subbands leading to a transition from the ordinary to a crossed PSHs.

We also analyze the non-trivial spin textures near the interband SO-induced energy-level anticrossing. The spin texture varies as the Fermi energy goes through the energy subbands of the quantum well. We estimate the energy anticrossing size using spin-orbit coupling strenghts that were evaluated numerically for realistic semiconductor heterostructure parameters. Non-trivial spin textures have also been experimentally observed in 2D surface electron system of Bi-Ag-Au heterostructures by Bentmann et al. (74).

Nevertheless, their spin textures in a metallic system suggest that a different SO model, compared with ours, is necessary to explain the experimental data.

CHAPTER 5

CONCLUSION

In this thesis, we have studied the spin relaxation in confined geometries such as graphene quantum dots, wires and wells. We have presented distinct mechanisms in each of these dimensions which can affect the information carried and stored by spin in potential spintronic devices and quantum computers.

In a *zero-dimensional structure*, we have investigated the spin relaxation and decoherence in graphene quantum dots with spin-orbit interactions. To this end, we derive an effective Hamiltonian which couples the electron spin to potential fluctuations generated by the lattice vibrations. Then we calculate the spin relaxation time T_1 and the decoherence time T_2 within the framework of the Bloch-Redfield theory. We find a minimum in T_1 as a function of the magnetic field due to the Rashba spin-orbit coupling-induced anticrossing of opposite spin states. The electron-phonon coupling, which allows for energy relaxation between the Zeeman levels via the admixed states with opposite spin due to the Rashba spin-orbit coupling (admixture mechanism), dominates the contribution to the spin relaxation time for high magnetic field $\mathbf{B}_{\text{ext}} > 3$ T. In contrast, the intrinsic spin-orbit interaction gives rise to a monotonic behavior of T_1 with $\mathbf{B}_{\text{ext}}$ and this contribution dominates over the extrinsic's (Rashba SO) at low magnetic fields. Thus the monotonicity of the magnetic field dependence of T_1 is controllable since the Rashba coupling strength is tunable via an external electric field. Notice that both mechanisms depend on the intrinsic or Rashba spin-orbit coupling strengths and each one of them lead to a different monotonicity in the magnetic field dependence of T_1 . This opens up a new pos-

sibility to measure the spin-orbit couplings in graphene, which have not been measured in monolayer graphene so far. We also find that an energy anticrossing has a vanishing dephasing rate for a generic super-Ohmic bath. Since short decoherence times constitute a serious limitation in solid-state-based quantum computing, we believe that it motivates the search for qubits defined in anticrossing levels in semiconductor quantum dots. As a next step, we intend to calculate the spin relaxation and decoherence due to two-phonon processes. Our motivation comes from the recent experimental results in literature which has been obtained for temperatures around 1 K , where the higher-order processes start to play a role (75, 76). Moreover, since the hyperfine coupling in graphene is very weak, the energy-conserving spin dephasing can also compete with the decoherence generated by the nuclear bath under room temperature conditions.

In a *quasi-one-dimensional system*, we have investigated the magnetic field dependence of the spin relaxation in multisubband quantum wires. In particular, we mainly focus on the effect called ballistic spin resonance observed experimentally by Frolov et al.(8). In a semiclassical picture, the spin resonance was produced due to the interplay of static external magnetic field and the oscillating effective spin-orbit field created by periodic specular scatterings of the electrons off the boundaries of a micrometer-scale channel. This spin resonance leads to an increase of the D'yakonov-Perel spin relaxation rate without any external driving fields. We have developed a model to account for the D'yakonov-Perel mechanism taking into account elastic spin-conserving scatterings in combination with the Rashba and Dresselhaus spin-orbit couplings. We consider small- and large-angle scattering mechanisms by hand in the time-evolution operator in each timestep of our calculation. Then, we evaluate the time-dependent average spin-operators in the Heisenberg representation. This procedure allows us to extract the spin relaxation time as a function of the external magnetic field. The ballistic spin resonance occurs when $\mathbf{B}_{\text{ext}}$ is aligned perpendicularly to the quantum wire. This effect is characterized by a non-monotonic behavior for the spin relaxation time with $\mathbf{B}_{\text{ext}}$ can be associated with quantum wire subband anticrossings induced by the SO interaction. Moreover, the magnetic field dependence of the non-local voltage, which is related to the spin relaxation time behavior, shows a wide plateau, in agreement with the experimental findings (8). Conversely, no spin resonance is observed when $\mathbf{B}_{\text{ext}}$ is parallel to the channel in the weak SO coupling regime. Nevertheless, we also predict that a ballistic spin resonance can arise

in systems with strong SO couplings. In this anomalous case, part of the strong spin-orbit field causes admixture of states with opposite spin states oriented along the channel. This leads to a spin resonance induced by the subband-spin mixing spin-orbit term. As a future project, we aim to study the channel width dependence of the spin relaxation time (77). We also emphasize that our numerical model can access the progressively decreasing limit of the number of subbands in the quantum wires up to strictly one-dimensional case. In contrast, the semiclassical Monte Carlo simulation breaks down in this regime.

We predict the emergence of a novel spin pattern in a *two-dimensional electron gas* formed in a quantum well with two subbands where the Rashba α and Dresselhaus β spin-orbit couplings are operative. The electron gas can sustain spin-density waves when the spin-orbit coupling strenghts are tuned to have the same absolute value but opposite signs, $\alpha_1 = +\beta_1$ e $\alpha_2 = -\beta_2$ for the first $\nu = 1$ and second $\nu = 2$ subbands. We can attribute a spin-conserved quantity for each subband, which in this case, are related to orthogonal directions. Thus they lead to the formation of the crossed persistent spin helices. Interestingly, this pattern is robust against spin-independent scattering and electron-electron interaction. We analyze solutions for the spin-charge coupled diffusion equations and discuss experimental techniques that can be used to probe our prediction. We have also investigated the interband spin-orbit coupling in more detail concerning its effects on the lifetime of the crossed persistent spin helices, levels anticrossings and spin textures in the energy spectrum. Within this research topic, future investigations will focus on understanding more clearly the spin relaxation due to Rashba and Dresselhaus SO coupling and their interplay with the interband SO interaction. Moreover, a robust spin-density pattern single-subband quantum well can also be used to design a robust spin-field effect transistor where the ON (OFF) states corresponds to a spin injection parallel (perpendicular) to the spin quantization axis.

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APPENDICES

APPENDIX A

HARMONIC CONFINEMENT IN THE BALLISTIC SPIN RESONANCE: LACK OF HIGHER ORDER RESONANCES

In chapter 3, we have used a square wire confinement in order to explain the experimental features of the spin relaxation in quasi-one-dimensional channels. Nevertheless, the harmonic confinement has also been used extensively in the literature as another simple model for quantum wires. Both confinement models lead to essentially the same qualitative features. In this appendix, we found an example where the harmonic model is not a proper model to describe the spin relaxation in narrow channels. Here we demonstrate that the harmonic confinement model for a quantum wire does not connect multiple orbitals leading to the absence of higher resonance dips in the spin relaxation time. Let us consider the electrostatic potential $V(y)$ modeled by the harmonic confinement

$$\mathcal{H}_h = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}g\mu_B (\mathbf{B}_{\text{SO}} + \mathbf{B}_{\text{ext}}) \cdot \boldsymbol{\sigma} + \frac{1}{2}m\omega^2 y^2, \quad (\text{A.1})$$

where ω is the confinement frequency. We write the Hamiltonian in the truncated subband-spin Hilbert space $\mathcal{F} = \{|nks\rangle; n = 1, 2, \dots, n_T, k, s = \uparrow, \downarrow\}$,

$$\begin{aligned} \mathcal{H}_h = & \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + \frac{\hbar^2 k^2}{2m} + \frac{1}{2} g\mu_B \mathbf{B}_{\text{ext}} \cdot \boldsymbol{\sigma} \\ & -(\alpha + \beta)k\sigma_y + i(\alpha - \beta)\sqrt{\frac{m\omega}{2\hbar}} (a^\dagger - a) \sigma_x, \end{aligned} \quad (\text{A.2})$$

where the creation and annihilation operators are given by $a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$ and $a |n\rangle = \sqrt{n} |n-1\rangle$, respectively. Here, the operator which mixes the spin and orbital states is identified as $\mathcal{H}_{\text{SO}}^\parallel \propto (a^\dagger - a) \sigma_x$. The spin resonance is achieved for a external magnetic field perpendicular to the quantum wire, $B_{\text{BSR}}^\perp$, as long as the the following condition is fulfilled,

$$\frac{1}{2} g\mu_B B_{\text{BSR}}^\perp = \pm \hbar\omega\Lambda + (\alpha + \beta)k, \quad (\text{A.3})$$

where we have that $\Lambda = 1$ solely. Thus we conclude that the harmonic confinement model does not capture the higher resonance dips ($\Lambda = 3, 5, \dots$) as the $B^\perp$ varies.

APPENDIX B

D'YAKONOV-PEREL SPIN RELAXATION MECHANISM IN A QUANTUM WIRE WITH TWO SUBBANDS

In chapter 3, we studied the spin relaxation in multisubband quantum wires. Here we consider a quantum wire with two subbands as a simple model to understand the D'yakonov-Perel spin relaxation mechanism in a narrow channel. Within this simplified model, the the time-evolution operator can be obtained analytically and a more intuitive picture can be used to explain the DP mechanism. Consider the Hamiltonian given by Eq. (3.3) written in the basis composed with two subband-spin Hilbert space $\mathcal{F} = \{|nks\rangle; n = 1, 2, k, s_y = \uparrow_y, \downarrow_y\}$. This truncated Hilbert space can be divided into two decoupled subspaces $\mathcal{F}_{\lambda=+} = \{|1, k, \uparrow_y\rangle, |2, k, \downarrow_y\rangle\}$ and $\mathcal{F}_{\lambda=-} = \{|1, k, \downarrow_y\rangle, |2, k, \uparrow_y\rangle\}$, the Hamiltonian reads

$$\mathcal{H}_\lambda = \epsilon_+ \mathbb{1}_{2 \times 2} + \begin{bmatrix} \epsilon_- - \lambda(\alpha + \beta)k_x & -\lambda i \alpha (p_y)_{12} / \hbar \\ \lambda i \alpha (p_y)_{12} / \hbar & \epsilon_- - \lambda(\alpha + \beta)k_x \end{bmatrix}, \quad (\text{B.1})$$

where $\lambda = \pm$ denotes each subspace, $\epsilon_\pm = (\epsilon_1 \pm \epsilon_2)/2$ for the ϵ_i labelling the i -th subband in the quantum wire, and the matrix element $(p_y)_{12} = \langle 1 | p_y | 2 \rangle$. We will explain that the intersubband transitions combined with spin-independent scatterings are responsible for the spin relaxation in multisubband quantum wires. Notably, in the stricly one-dimensional limit where we consider a quantum wire with a single subband, the DP

mechanism is completely suppressed and the spin lifetime tends to infinite. In order to demonstrate that the intersubband transitions are responsible for spin relaxation, we consider two electrons following distinct semiclassical paths given that they reach the same final position. To do so, we have to prove that an initially ensemble of electrons starting with their spins oriented along the same direction will end up with different orientations for each electron. This is equivalent to demonstrate that the time-evolution operator for different paths does not constitute a set of commuting operators. Physically, we have that the electron spin will precess differently for each path determined by the sequence of random multiple scatterings. For the sake of simplicity, we consider a path such that the electron will move forward a distance Δ with the wavevector $+k$, undergoes an elastic scattering and then move backward the same distance with the wavevector $-k$. The time-evolution operator in the basis $\mathcal{F}$ is given by

$$\mathcal{U}(k) = \exp \left[-(i/\hbar) \mathcal{H}_\lambda(k) (\Delta/v_F^j) \right] = \begin{bmatrix} \Gamma^+(k) & 0 \\ 0 & \Gamma^-(k) \end{bmatrix}, \quad (\text{B.2})$$

where v_F^j is the Fermi velocity considering the injection in the j -th subband, $\Gamma^\lambda(k) = \exp \left[-(i/\hbar) \epsilon_+ (\Delta/v_F^j) \right] \times \exp \left[-(i/\hbar) \hat{\mathbf{n}}^\lambda \cdot \boldsymbol{\sigma} |\boldsymbol{\xi}^\lambda| (\Delta/v_F^j) \right]$ for $\hat{\mathbf{n}}^\lambda = \boldsymbol{\xi}^\lambda / |\boldsymbol{\xi}^\lambda|$, where

$$\boldsymbol{\xi}^\lambda(k) = (0, \xi_y^\lambda, \xi_z^\lambda(k)) = \left(0, \lambda \frac{1}{\hbar} (\alpha - \beta) (p_y)_{12}, (\epsilon_- - \lambda(\alpha + \beta) k_x) \right). \quad (\text{B.3})$$

Once we prove that $[\mathcal{U}(k), \mathcal{U}(-k)] \neq 0$, we have that an electron starting from the position x_0 moving forward that undergoes a backscattering reaching the position x_f will not end up with same spin orientation compared with another electron undergoing the inverse ordering of events. Notice that any path followed by an electron can be divided in a series of forward and backward paths. Calculating this commutator we obtain the relation $\xi_y^\lambda [\xi_z^\lambda(k) - \xi_z^\lambda(-k)]$ which is different from zero since $\xi_y^\lambda \neq 0$. Thus we conclude that intersubband transitions results in the non-commutativity of the time-evolution operator causing spin relaxation in multisubband quantum wires. The limit of a quantum wire with a single subband where no intersubband transitions are allowed, i.e. $\xi_y^\lambda = 0$ and the time-evolution operators for inverse paths commutes $[\mathcal{U}(k), \mathcal{U}(-k)] = 0$. Therefore no spin relaxation due to the DP mechanism takes place in a strictly one-dimensional quantum wire.