REVIEW OF SPIN DEPENDENT TRANSPORT

By

Abdisa Geleta

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PHYSICS

The undersigned hereby certify that they have read and recommend to the Graduate Programs for acceptance a project entitled "**Review of Spin Dependent Transport**" by **Abdisa Geleta** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

Dated: August 2017

Examiner: _____
Dr. Belayneh Mesfin

Examiner: _____
Dr. Tesgera Bedassa

Advisor _____
Dr. Teshome Senbeta

Chairman _____
Dr. Deribe Hirpo

ADDIS ABABA UNIVERSITY

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Author: **Abdisa Geleta**

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Table of Contents

List of Figures

Abstract

Spin based electronics, is based on the use of spin orbit coupling in convectional semiconductors materials. We regard the prediction and discovery of intrinsic spin Hall effect as an important step toward developing integrated spin logic devices and achieving lower energy consumption. To develop and review the three potential means of dissipationless spin transport in semiconductors with and without spin-orbit coupling are the use of spin currents, propagating modes, and orbital currents. Dissipationless spin currents occur in materials with strong spin-orbit coupling, such as GaAs, while orbital currents occur in materials with weak spin-orbit coupling, such as Si, but with degenerate bands characterized by an atomic orbital index. The potential means for achieving dissipationless spin transport constitute a theoretical and associated potential experimental directions with technological implications. A number of alternatives to the current semiconductor technology have recently been proposed, including technologies based on carbon nanotubes, molecular electronics, and dilute magnetic semiconductors. In materials without spin-orbit coupling, one of the current efforts should be to try to detect the orbital Hall effect and to investigate whether the orbital moment can be transferred to spin and hence be used for spin injection. Moreover, experimental techniques should be devised to enhance the amount of spin polarization arising from spin current.

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Abdisa Geleta
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Chapter 1

Introduction

1.1 Background of Spintronics

Basic concepts of a spin-polarized current has been laid by Mott in 1936 [1]. In his work, Mott provided an explanation for an unusual behavior of resistance in ferromagnetic metals. He realized that at sufficiently low temperatures, where magnon scattering becomes vanishingly small, electrons of majority and minority spin, with magnetic moment parallel and antiparallel to the magnetization of a ferromagnet, respectively.

In 1967 I. A. Campbell and coworkers [2] introduced the first experimental demonstration of two current conduction at low temperatures in a ferromagnetic metal. The main finding of their work was that the detail measurements over a range of relative concentration for alloys containing two impurities simultaneously give actual values of $\rho_\uparrow$ is spin up resistivity and $\rho_\downarrow$ is spin down resistivity and their ratio $\rho_\uparrow/\rho_\downarrow$ which in turn give information on the electronic structure of the alloys.

In ferromagnetic metals like Fe, Ni, Co and their alloys, both the $4s$ and $3d$ electron bands contribute to the density of states at the Fermi level E_F. The Fermi level cuts

across more than one band. As the sketch in Fig.1.1, the Fermi surface intersects a free-electron 4s band. However, it also intersects a 3d band which is not a simple parabola. In a ferromagnetic metal, the 3d up-spin and down-spin sub bands are shifted out of symmetry. This Figure 1.1 represents a band model of ferromagnetism, and the shift is called an exchange splitting, U_{ex} [3].

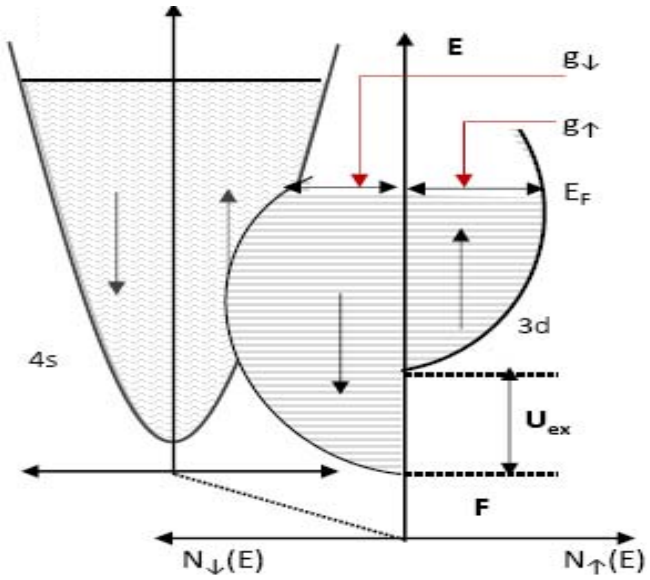

Figure 1.1: Energy bands of metals, density of states N(E) as a function of energy E. In a transition metal ferromagnet, the 4s and 3d bands are intersected by E_F. The 3d band is exchange shifted by energy U_{ex}.

In a ferromagnetic material, the ion cores in the lattice have a net nonzero spin. These magnetic ions can interact with each other when their charge distributions overlap, and such effect is called the exchange interaction. The number of down-spin conduction electrons differs from the number of up-spins, and this difference gives the spontaneous magnetization of the material. These result in shifting of energy band in the spin up and spin down 3d bands. This band splitting creates the imbalance between $n_\uparrow$ and $n_\downarrow$ numbers of density of states for spin up and spin down respectively,

of $3d$ electrons that results in ferromagnetic moment $\mu \approx -(n_\uparrow - n_\downarrow)\mu_B/\mathtt{atm}$ (where μ_B is the Bohr magneton) [4]. The conduction process for such case is dominated by the 4s band because of its much *higher mobility*. Experiments [5] show that at low temperature spin up and spin down carry current in parallel; and this is a base of Giant magnetoresistance.

In 1971, D'yakonov and Perel [6] showed the possibility of orienting electron spin with current. When currents flow through a conductor, the multiple scattering of the carriers should give rise to a spin flux perpendicular to the current and directed from the interior to the periphery of the conductor. This leads to accumulation of spin orientation at the surface of the sample, limited by the spin relaxation. As a result there should exist at the surface of a current-carrying sample spin-layer (a layer in which the electrons spin are oriented). The thickness of this spin layer is determined by the length of spin diffusion.

The spin dependent scattering probability results in very different mean free path (the length for which the spin of an electron conserved) $l_\uparrow$ and $l_\downarrow$, or equivalently relaxation time (the time needed for an electron of velocity v_F to travel the mean free path l) $\tau_\uparrow$ and $\tau_\downarrow$.

As pointed in references [7, 8], Julliè*r* (1975) formulated a model for a change of conductance between the parallel ($\uparrow\uparrow$) and antiparallel ($\uparrow\downarrow$) magnetization in two different ferromagnetic regions. The corresponding *tunneling magnetoresistance* (TMR) in ferromagnet/insulator/ferromagnet (F/I/F) magnetic tunneling junction (M/T/J) is defined as

$$\mathtt{TMR} = \frac{\Delta R}{R_{\uparrow\uparrow}} = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}, \tag{1.1.1}$$

where resistance R and conductance $G = 1/R$ are given by the relative orientations of the magnetization in ferromagnet F_1 and F_2; acts as spin filter and spin detector, respectively. The insulator between the ferromagnets is a barrier.

Figure (1.2) represents the M/T/J, where the parallel configuration has low resistance

than the antiparallel case. The M/T/Js are the basis of Magnetic Random Access Memory (MRAM). It combines two concepts: short access time of semiconductor based on RAM and the non-volatile property of magnetic memories [9]. MRAM is potentially an ideal memory because it has the properties of nonvolatility, high speed, unlimited write endurance, and low cost. These memories use the hysteresis of magnetic materials for storing data and some form of magnetoresistance for reading the data output.

The fundamental properties of ***spintronics*** are closely related to the length scale L characteristic of samples and to the motion of electrons in metals. There are several length scales that characterize the properties of electrons in metals. These are the spin-flip mean free path l and typically takes values in the range 10^2 nm to 10 μm [10], the spin-diffusion length λ_{spin} and the Fermi wave length λ_F, which characterizes the electronic states.

To find the spin-polarized current in non-magnetic metals it is necessary that the system length L be much shorter than λ_{spin}. In ferromagnetic metals, due to the imbalance between the number of electrons with up and down spins, the current may be spin polarized. Because the electrical resistivity is governed by the mean free path l, characterizes the scattering process of electrons, it is necessary that $l \ll \lambda_{spin}$. When this condition is satisfied, the spin polarization of the current is well defined and the up-spin and down-spin electrons may be treated independently. This is called Mott's two-current model [1]. When the $l \ll \lambda_{spin}$ is satisfied, the two-current model holds even in systems for which $L \ll \lambda_{spin}$.

In general, $l \gg \lambda_F$, and such a length scale becomes important when interference occurs between wave functions of electrons. The velocity of electrons on the Fermi surface is given by the Fermi velocity v_F. Hence the time scale for an electron with v_F traveling a distance l is given by $\tau = \frac{l}{v_F}$ and called the relaxation time.

1.2 Gigantic Magnetoresistance

Magnetoresistance (MR) is the change in the electric conductivity of a material in the presence of magnetic field. The MR of metallic, semiconductor and insulator are different. The metallic conductance of ferromagnetic materials depend on the orientation (the angle between electric current and the magnetization) of magnetization. This type of MR is known as anisotropic magnetoresistance (AMR). The ratio of MR when the current is perpendicular to magnetization direction to that of parallel is rather small. Researchers continued to increase this ratio and succeeded in the discovery of giant magnetoresistance (GMR) [11, 12].

The discovery of GMR is considered as the starting point of the *spin based electronics* (spintronics). GMR is the change in electrical resistance in response to applied magnetic field. GMR is a quantum mechanical effect observed in layered magnetic thin-film structures of the order of the nanometer size that are composed of alternating layers of ferromagnetic and nonmagnetic layers. The two main concept observed from GMR experiment are interlayer coupling and spin dependent scattering.

When the magnetic moments of the ferromagnetic layers are parallel, the spin-dependent scattering of the carriers is minimized. When the ferromagnetic layers are antiparallel, the spin-dependent scattering of the carriers increases. The directions of the magnetic moments are manipulated by external magnetic fields that are applied to the materials [13].

1.3 Application of Spin-Dependent Transport

In principle, electron has both charge (e) and spin (1/2). Though, the theory of electronics is always related to the charge (e) of electron, the theory of magnetism is always attached to the spin of electron, and correspondingly, magnetic moment μ_B.

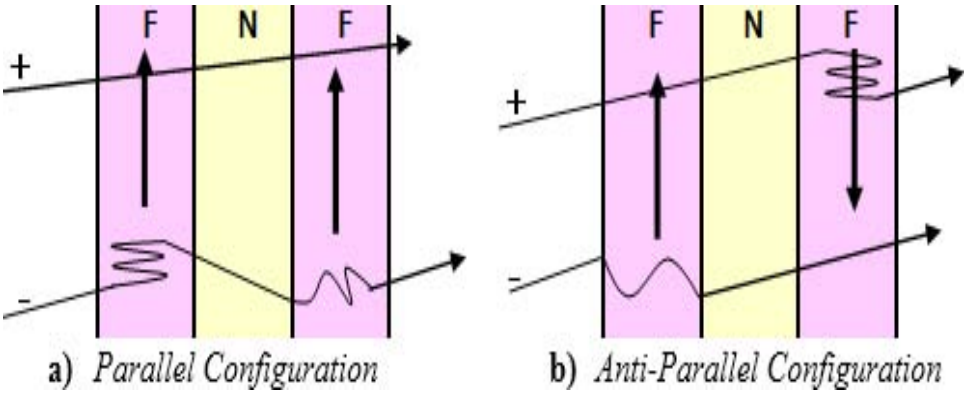

Figure 1.2: Schematic representation of the GMR mechanism.
The electron trajectories are represented by straight lines and the scattering by abrupt changes in direction. The signs + and − are for spins $s_z = 1/2$ and $-1/2$ (majority and minority spin states, identical to ↑ and ↓ of uniform magnetic materials), respectively. The arrow represents majority spin direction in the magnetic layer. F denotes ferromagnetic material and N denotes nonmagnetic material. Adopted from [13].

In electronics, one can control the motion of electron using applied electric field and by magnetic field. In magnetism we control electron motion using its spin, which can be controlled by magnetic field and also by electric field for relativistic case. In general, the transport system which involves spin degree of freedom is known as spin-dependent transport.

Recently, spin transport in microstructure became one of the research potential. The electronic spin degree of freedom is on its way to replace the charge degree of freedom as carrier of information. In addition, the spin-based electronic devices have many advantages over the traditional semiconductor devices such as a long coherent life-time, faster data processing speed, and lower electric-power consumption.

In section 1.1, we have seen that the two-current model and this holds true for ferromagnetic transition metals. This is to mean that the electrical resistivity of ferromagnetic metals depends on spin. This spin dependence of resistivity is governed by

the spin dependence of the electronic states near the Fermi level, and by the spin dependent impurity potentials in ferromagnetic alloys [10, 14]. The simplest expression of electrical conductivity is the Drude formula [15],

$$\sigma = \frac{e^2 n \tau}{m^*}, \tag{1.3.1}$$

where e, n, τ and m^* are electron charge, carrier density, lifetime and effective mass of electrons, respectively. These quantities are spin dependent and the most important is the spin dependence of the lifetime as it affects highly electron scattering. The lifetime is related to the mean free path ℓ through the relation:

$$\ell = v_F \tau, \tag{1.3.2}$$

where v_F is the Fermi velocity. For given ferromagnetic metals, ℓ is much shorter than the spin-diffusion length λ_{spin}, and the spin of the carrier electrons are well conserved in the time scale τ [14].

The spin dependent Drude formula (1.3.1) does not clearly show the contribution to the conductance by spin-up and spin-down, separately. The first attempt to understand the contribution of spin-up states and spin-down states in the conductivity of spin dependent transport was the experimental result of Fert, A., and Cambell, I. A. [16, 17]. They measured the residual resistivity and temperature dependence of various binary and ternary alloys and obtained ($\sigma_\uparrow$ is spin up electric conductivity and $\sigma_\downarrow$ is spin down electric conductivity) the ratio $\rho_\downarrow/\rho_\uparrow$ ($=\sigma_\uparrow/\sigma_\downarrow$) for diluted alloys of Fe, Co and Ni metals. This ratio is called the α-parameter. The MR can be given in terms of this parameter as:

$$MR = \left(\frac{1-\alpha}{1+\alpha}\right)^2 . \tag{1.3.3}$$

where $\alpha = \rho_\downarrow/\rho_\uparrow = \sigma_\uparrow/\sigma_\downarrow$.

Nowadays, spin-dependent transport have different applications. Some of these applications exist in magnetic memory, read/write heads, MRAM, spin transistor, spin

filter, spin diodes and spin quibits for quantum computing [3, 4]. The advantages of spin-dependent transport over the electron charge transport are multi-functionality, non-volatility, increased integration density, increased data processing speeds and low power consumption. An important phenomena of spin transport system is spin injection. Spin injection is defined by Silsbee there in [18] as:

> Spin injection is the transfer of spin-polarized electrons across the first ferromagnetic layer to non-magnetic layer and then to the second ferromagnetic layer. The processes accompanied by diffusion across the non-magnetic metal and enhanced transmission in the second layer.

The use of ferromagnetic metallic electrodes appears to be essential for most practical all-electrical spin-based devices before useful ferromagnet semiconductor are developed [19].

The spin injection system may include ohmic injection, tunnel injection, Ballistic injection, and hot electron injection. Ohmic injection is a method in which we have ohmic contact between a ferromagnetic metal and a semiconductor that produces spin current in semiconductor. Metal-semiconductor ohmic contacts result from heavily doping the semiconductor surface, leading to spin-flipping scattering and loss of the spin polarization. However, this method is not much successful, which is only about 4.5% [20]. Johnson [21, 22] use the advantage of the spin splitting of the spin degeneracy of electrons confined in a semiconductor 2D-Quantum well structure to over come the spin injection problem.

Motivation and Chapters Outline

As we discussed above, having an alternative way of transport system in electronics world is crucial. To this end, we want to review different scholars works in this regard.

After reviewing different works we compare and contarst different alternatives and we recommend the best way of spin transport systems.

The Projet work is organized as follow. In Chapter 2, the quantum theory of spin as well as the mathematical description of Pauli matrices are presented. In Chapter 3, we review three potential means of dissipationless spin transport in semiconductors with and without spin orbit coupling; the use of spin currents, propagating modes, and orbital currents. Finally in Chapter 4, we describe spin torques as a result of an influence in nonmagnetic lead adjacent to the ferromagnetic layer.

Chapter 2

The Quantum Theory of Spin

2.1 Why Spin?

Spin is a phenomena that occurs in quantum mechanics and has no analogy in classical physics. The electron was the first elementary particle whose spin is detected. Several experiments which could not be classically interpreted; motivated Goudismit and Uhlenbeck [23] in 1925 to hypothesize; Every electron has an intrinsic angular momentum (spin) of $\frac{1}{2}\hbar$ which corresponds to a magnetic moment of one Bohr magneton $\mu_B = \frac{|e|\hbar}{2mc}$.

Physicists and engineers are creating an entirely new generation of microelectronic devices that operate on a quantum mechanical property of electrons, spin. These investigators are racing to use spin effects to create transistors and other circuit elements, including quantum computers, in a field of spintronics [24]. Crucially, researchers and developers of spintronics devices currently take two different approaches:

First, the existing GMR-based technology either by developing new materials with larger populations of oriented spins (called spin polarization) or by making improvements in existing devices to provide better spin filtering.

Second, focuses on finding novel ways both to generate and to utilize spin-polarized current that is, to actively control spin dynamics.

The intent is to thoroughly investigate spin transport in semiconductors and search for ways in which semiconductors can function as spin polarizer and spin valves [19]. This is vital because, unlike semiconductor transistors, existing metal-based devices do not amplify signals (although they are successful switches or valves).
If spintronics devices could be made from semiconductors, however, then in principle they would provide amplification and serve, in general, as multifunctional devices. Perhaps even more importantly, semiconductor based devices could much more easily be integrated with traditional semiconductor technology. More recently, investigators have begun direct investigation of spin transport across interfaces in all-semiconductor devices. In such a scenario a combination of optical manipulation (for example, shining circularly polarized light on a material to create net spin polarization) and material in-homogeneities can be employed to tailor spin transport properties. In addition to the near-term studies of various spin transistors and spin transport properties of semiconductors, a long-term and ambitious subfield of spintronics is the application of electron and nuclear spins to quantum information processing and quantum computation [25].

The late Richard Feynman [26] and others have pointed out that quantum mechanics may provide great advantages over classical physics in computation. However, the real boom started after Peter Shor of Bell Labs devised a quantum algorithm that would factor very large numbers into primes, an immensely difficult task for conventional computers and the basis for modern encryption. It turns out that spin devices may be well suited to such tasks, since spin is an intrinsically quantum property [27].

2.2 Spin Injection

Electrons possess both charge ($-e$) and spin angular momentum ($\pm\frac{\hbar}{2}$). Therefore, when an electron moves in a material, it carries not only a charge but also an angular momentum. Figure 2.1**(a)** shows the schematic of electron transfer from a ferromag-

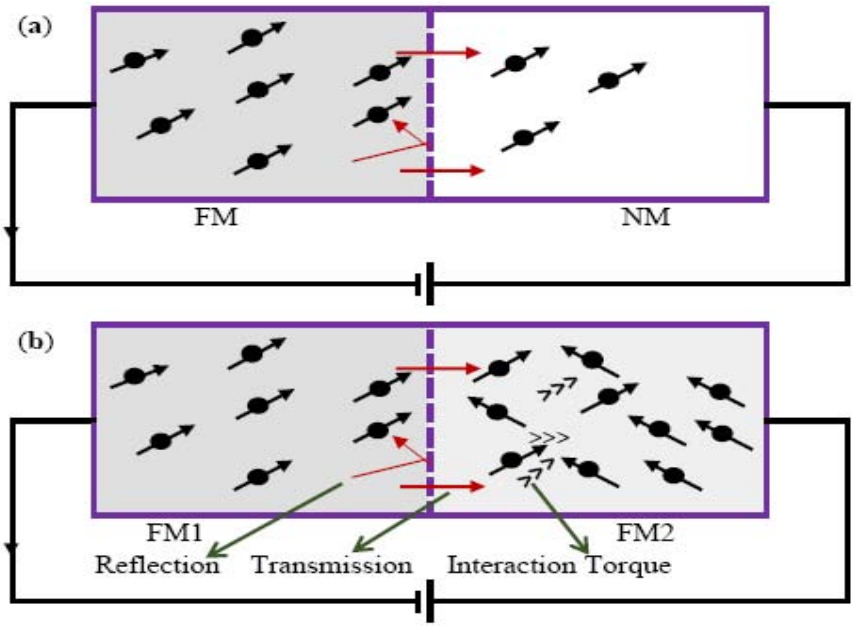

Figure 2.1: Spin injection across an interface.
(**a**) Spin injection from a FM to a NM. Application of an electric current through the interface results in injection of a spin-polarized current into NM. ***(b)*** Spin injection from the FM1 to another FM2 with different magnetization direction. Spin-dependent reflection and transmission at the interface give rise to the MR effect. Injected spins interact with spins of the host material and exert torque on it. Adopted from [22].

netic material (FM) to a non-magnetic material (NM) through an interface [10]. In the FM, since electron spins are polarized, an electric current accompanies the net flow of spins, that is, spin current. The spins traveling as the spin current in the ferromagnetic are then injected (spin injection) into the NM through the interface. The injected spins are subjected to spin relaxation because of spin orbit interaction, and they lose their spin orientations as they move away from the interface. Spin injection phenomena have been observed by detecting the emission of circularly polarized light from injected electrons in semiconductors such as GaAs, and by observing the spin dependent electrochemical potentials in so-called nonlocal magneto resistance geometries or using the magneto resistive/filtering effect [22]. If a current pass through

two FMs with different magnetization orientations, it is well known that the magneto resistance effect occurs. (**b**) In addition, the electron spins injected from the FM on the LHS ($FM1$) into the FM on the RHS ($FM2$) interact with the electron spins in $FM2$ through exchange interaction. As a result, a precession can be excited and the magnetization can be switched on in $FM2$.

2.3 Operator of the Rotation of Spin

In this section we discuss the transformation of the spinors and show how the coefficient of this transformation are expressed in terms of the angles of rotation of the coordinate axes. By the definition of the spin operator $1 + i\delta\varphi \sim \vec{n}.\hat{s}$ is the operator of the rotation through an angle ϕ about a direction specified by the unit vector $\vec{n}$ [28]: for application to the wave function of the particle with spin i.e., spinor of rank one we take $s = \frac{1}{2}\hat{\sigma}$ in this operator. The operator of the rotation through a finite angle $\delta\phi\iota$ about the same direction will be correspondingly given by:

$$\hat{U}_n = e^{\frac{1}{2}i\phi\vec{n}.\hat{\sigma}}. \tag{2.3.1}$$

Like any function of Pauli matrices this expression reduces to one that is lined in this matrices.

$$\hat{U}_n = \hat{I}\cos\phi/2 + i\vec{n}.\hat{\sigma}\sin\phi/2, \tag{2.3.2}$$

where

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.3.3}$$

is the unitary matrix and $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are Pauli matrices, where:

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{2.3.4}$$

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{2.3.5}$$

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.3.6}$$

For example, with a rotation about the $z - axis$

$$\hat{U}_z(\phi) = \hat{I}\cos\phi/2 + i\vec{n}.\hat{\sigma}\sin\phi/2 = \begin{pmatrix} e^{i\frac{1}{2}\phi} & 0 \\ 0 & e^{-i\frac{1}{2}\phi} \end{pmatrix}, \tag{2.3.7}$$

$$R_n(\phi) = \cos(\phi/2)\hat{I} - i\sin(\phi/2)\hat{\sigma}_n. \tag{2.3.8}$$

This means that the component of the spinor are transformed in such a rotation according to:

$$\begin{pmatrix} \psi_1' = & \psi_1 e^{i\frac{1}{2}\phi} \\ \psi_2' = & \psi_2 e^{-i\frac{1}{2}\phi} \end{pmatrix}. \tag{2.3.9}$$

In particular, in a rotation through an angle 2π the spin or components change sign; spinors of any odd rank must therefore have the same property. Similarly, the matrices of transformation consisting of a rotation about the $x - axis$

$$\hat{U}_x(\phi) = \begin{pmatrix} \cos\frac{1}{2}\phi & i\sin\frac{1}{2}\phi \\ i\sin\frac{1}{2}\phi & \cos\frac{1}{2}\phi \end{pmatrix},$$

where we use the transformation of the rotation about the $x - axis$ in the $y - z$ plane by an angle ϕ or $y - axis$

$$\hat{U}_y(\phi) = \begin{pmatrix} \cos\frac{1}{2}\phi & i\sin\frac{1}{2}\phi \\ -i\sin\frac{1}{2}\phi & \cos\frac{1}{2}\phi \end{pmatrix}, \tag{2.3.10}$$

where we use the transformation of the rotation about the $y - axis$ in the $x - z$ plane by an angle ϕ.

2.4 Spinors

When the spin is zero, the wave function has only one component, $\Psi(0)$. The effect of the spin operator is to reduce it to zero: $\int s\hat{\Psi} = 0$. The relation between $\hat{s}$ and the operator of the infinitesimal rotation implies that the wave function of a particle with zero spin is invariant under the rotation of the coordinate system it is a scalar [29]. The wave function of the particle with spin $\frac{1}{2}$ has two components $\psi(\frac{1}{2})$ and $\psi(-\frac{1}{2})$, for convenience we distinguish these components by the subscripts 1 and 2, respectively. These two component quantity in Eq. 2.4.1 is called *spinor*.

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix}. \tag{2.4.1}$$

In any rotation of the coordinate system, the component of the spinor undergoes a linear transformation

$$\begin{aligned} \psi_{10} &= a\psi_1 + b\psi_2, \\ \psi_{20} &= c\psi_1 + d\psi_2. \end{aligned} \tag{2.4.2}$$

This may be written as,

$$\psi\lambda' = (\hat{U}\psi)_\lambda,\ \lambda = 1,\ 2,\ 3,\ ...,$$

$$\hat{U} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{2.4.3}$$

where $\hat{U}$ is the transformation matrix. Its elements are in general complex function of the angle of rotation of the coordinate axes.

2.5 Wave Function with Spins

By taking the spin into account, we assign the degree of freedom of particle to describe this additional degree of freedom we in introduce in the component of the spin in the $z-$direction as an argument of wave function. The component S_z can only take

two values, namely $\pm\frac{\hbar}{2}$. Therefore, the wave function has the following coordinate representation [30].

$$\Psi = \Psi(\vec{r}, S_z), \tag{2.5.1}$$

while the complete wave function is,

$$\begin{aligned} \psi &= \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_2(\vec{r}) \end{pmatrix}, & (2.5.2)\\ &= \psi_1(\vec{r})\chi_+ + \psi_2(\vec{r})\chi_-, & (2.5.3)\\ &= \psi_1(\vec{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_2(\vec{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}. & (2.5.4) \end{aligned}$$

The introduction of product functions for both components, i.e.,

$$\psi_1(\vec{r})\chi_+ = \psi_1(\vec{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.5.5}$$

$$\psi_2(\vec{r})\chi_- = \psi_2(\vec{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.5.6}$$

is particularly convenient. The functions indicate only the state of the "spin up" or "spin down". $|\Psi_1|$ is obviously the probability of finding an electron with spin up at location $\vec{r}$. $|\Psi_2|$ is the probability of finding an electron with spin down at location $\vec{r}$. The total probability of finding the electron independently is of its spin direction must be 1. Thus,

$$\int (|\Psi_1(\vec{r})|^2 + |\Psi_2(\vec{r})|^2) dV = 1. \tag{2.5.7}$$

The spin operates written as Pauli matrices act on spinors. The Eigen state of the operator σ_z are,

$$\begin{aligned} \sigma_z \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix} = (+1) \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix}, & (2.5.8)\\ \sigma_z \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix} = (-1) \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix}, & (2.5.9) \end{aligned}$$

where $\chi_{\pm}$ are unit spinors

$$\chi_{+}\begin{pmatrix}1\\0\end{pmatrix} \text{ and } \chi_{-}\begin{pmatrix}0\\1\end{pmatrix}. \tag{2.5.10}$$

Therefore;

$$\hat{\sigma}_z\chi_{+} = (+1)\chi_{+}, \tag{2.5.11}$$

$$\hat{\sigma}_z\chi_{-} = (-1)\chi_{+}. \tag{2.5.12}$$

2.6 Pauli Equation

The Pauli equation is also known as the Schrodinger-Pauli equation, is a formulation of Schrodinger equation for spin $\frac{1}{2}$ particle which takes in to account the interaction of particles spin with the electromagnetic field. It is hence non- relativistic limit of Dirac equation and can be used where particles are slow enough that relativistic effect can be neglected [1]. It was formulated by Wolfgang Pauli [31] in 1927.

To describe the quantum dynamics of an electron in a magnetic field, assume that there are no external forces rather than pure magnetic field. The Hamiltonian of an electron in a pure magnetic field is obtained by adding the potential energy of magnetic moment into reaction to the usual expression for the kinetic energy in the magnetic field. The Hamiltonian for the motion of an electron in an electro-magnetic field in the absence of spin is given by,

$$\hat{H}_0 = \frac{1}{2m_e}(\hat{P} + \frac{e}{c}\vec{A})^2 + e\hat{V}, \tag{2.6.1}$$

where $\hat{P} = -i\hbar\vec{\nabla}$, e is charge of electron, $\vec{A}$ is vector potential, V is electrostatic potential.

But in this work it is not important to consider V and the above equation becomes,

$$\hat{H}_0 = \frac{1}{2m_e}(\hat{P} + \frac{e}{c}\vec{A})^2. \tag{2.6.2}$$

Since the spin interacts with the magnetic field the electron gains additional potential energy. The magnetic moment ($\vec{\mu}$) reads,

$$\vec{\mu} = g\left(-\frac{|e|}{2mc}\right)\hat{s}. \tag{2.6.3}$$

$g = 2$ for electron and $\hat{s} = \frac{\hbar}{2}\hat{\sigma}$,

$$\begin{aligned}\vec{\mu} &= 2\left(-\frac{|e|}{2mc}\right)\frac{\hbar}{2}\hat{\sigma} \\ &= -\left(\frac{e\hbar}{2mc}\right)\hat{\sigma}\end{aligned}$$

Therefore, Eq. (2.6.3) becomes,

$$\vec{\mu} = -\mu_B\hat{\sigma}, \tag{2.6.4}$$

where $\hat{\sigma} = \hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$ are Pauli matrices, and

$$\mu_B = \frac{e\hbar}{2mc}, \tag{2.6.5}$$

is the Bhor magneton.

Thus, the potential energy in the magnetic field becomes,

$$\hat{U} = -\vec{\mu}.\vec{B}. \tag{2.6.6}$$

The Hamiltonian of an electron with spin takes the form,

$$\hat{H} = \hat{H}_0 + \hat{U} = \frac{1}{2m_e}(\hat{P} + \frac{e}{c}\vec{A})^2 + \mu_B\hat{\sigma}.\vec{B}. \tag{2.6.7}$$

Finally, we get the Schrodinger equation of particle with spin known as Pauli equation,

$$\left[\frac{1}{2m_e}(\hat{P} + \frac{e}{c}\vec{A})^2 + \mu_B\hat{\sigma}.\vec{B}\right]\vec{\psi} = E\vec{\psi}. \tag{2.6.8}$$

where,

$$\vec{\psi} = \begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix}. \tag{2.6.9}$$

When this is written separately, it becomes

$$\begin{aligned}\hat{H}_1\psi_1 &= \left[\frac{1}{2m_e}(\hat{P}+\frac{e}{c}\vec{A})^2+\mu_B\hat{\sigma}.\vec{B}\right]\vec{\psi_1}=E\vec{\psi_1},\\ \hat{H}_2\psi_2 &= \left[\frac{1}{2m_e}(\hat{P}+\frac{e}{c}\vec{A})^2+\mu_B\hat{\sigma}.\vec{B}\right]\vec{\psi_2}=E\vec{\psi_2}.\end{aligned}$$

The Pauli equation is the system of two coupled differential equations for ψ_1 and ψ_2 describing the electrons with the $z-$component of their spin up or spin down, respectively.

Chapter 3

The Dissipationless Spin Transport in Semiconductors

Spintronics (spin-based electronics) promises a radical alternative, offering the possibility of logic operations with much lower power consumption than equivalent charge-based electronics [32]. One of the fundamental advance in the field of spintronics has been the ground breaking research on solid-state nonvolatile magnetic random access memory (MRAM) [33]. Recent theoretical work suggests that spin transport is different from the transport of charge. Ohms law governing the flow of charge current describes the inevitable dissipation of power in current microelectronic devices. However, the generalized version of Ohms law that governs the flow of spins indicates that the generation of spin current by an electric field can be reversible and non-dissipative. Interestingly, the practical problem of power dissipation in semiconductor devices may be related to the fundamental physics of time-reversal symmetry: *w*hile the charge current is odd under time-reversal symmetry, the spin current is even under time-reversal symmetry. To exploit the energy-saving potential of spin currents, it is essential to control them, in the case of charge flow. Historically, spins have been manipulated by magnetic fields, which will be more difficult to control as we approach the nanometer feature level. Recently it has been recognized theoretically that through intrinsic spin orbit coupling it is possible to manipulate spin

currents via electric fields [34]. New experiments have indeed demonstrated that electron spins may be controlled with traditional electric gates. This would appear to be a significant approach to spin control and manipulation. Control of electric fields forms the basis for integrated circuit technology and highly developed. Electric-field rather than magnetic-field control of spin, via spin-orbit coupling, should provide a more viable path for developing spin-based devices for technological use. The spin-orbit interaction leads to an entirely new set of drift-diffusion equations, in which spin and charge dynamics are tightly coupled. These equations formally resemble Maxwell equations, where spin and charge play the role of electric and magnetic fields [35]. Thus the gradients of spin density drive charge density fluctuations, and vice versa. In particular, the equations predict propagating modes of spin and charge in certain parameter regimes of spin-orbit coupling and spin relaxation. An electric field applied to the system creates a current of holes perpendicular to the field [36]. The holes tend to preferentially occupy atomic orbitals in a direction perpendicular to both the electric field and the direction of movement.

3.1 Spin Currents

The spin Hall effect is the generation of a transverse spin current by an applied electric field [37]. Recently, considerable interest has been generated by theoretical predictions that under certain conditions the spin Hall current could arise from the intrinsic spin-orbit coupling in the band structure; it would be relatively large and would flow without dissipation, potentially enabling control over spin currents through applied electric rather than magnetic fields. The effect appears in the analysis of semiconductors with spin-orbit coupling; two examples are the $spin-3/2$ valence band of GaAs, described by the Luttinger model, and the conduction band of asymmetric

quantum wells, described by the Rashba model,

$$H_L = \frac{\hbar^2}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(\vec{k}.\vec{S})\right], and \tag{3.1.1}$$

$$H_R = \frac{\hbar^2}{2m}k^2 + \alpha(\vec{k} \times \vec{S}).\hat{z}, \tag{3.1.2}$$

where $\vec{S}$ is a $spin - 3/2$ matrix describing the $P_{3/2}$ valence band state, γ_1 and γ_2 are material constants called Luttinger parameters, and α is the Rashba constant describing the two-dimensional spin-orbit coupling. The origin of the spin current is a topological phase acquired by the carrier wave functions as they move through momentum space. It has been shown [38] that the response of the spin current J_i^j to an electric field E_k has the form

$$J_i^j = \sigma_{sH}\epsilon_{ijk}E_k, \tag{3.1.3}$$

which predicts, an electric field in the x-direction induces a spin current J_y^z (spins polarized along z and flowing in the y direction). In this equation, σ_{sH} is intrinsic transport coefficient and determined by the spin-dependent properties of the ground state, and ε_{ijk} is the totally anti-symmetric tensor in three dimensions. For example, the dissipative ohmic current,

$$J_i = \sigma E_i \ , \tag{3.1.4}$$

having dimensions of charge times velocity, is odd under time reversal. Since the electric field E_i is even under time reversal, the charge conductivity σ is odd and hence dissipative, being dependent on random scattering processes such as momentum scattering. On the other hand, the spin current, having dimensions of angular momentum times velocity, is even. The intrinsic spin Hall conductivity has been predicted for semiconductors with both p-type and n-type doping [38, 39], in both bulk and two-dimensional semiconductors. In bulk p-doped semiconductors, the valence band is split into a light-hole (LH) band and a heavy-hole (HH) band by the spin-orbit

coupling, with Fermi momenta k_F^L and k_F^H, respectively. The associated intrinsic spin Hall conductivity is given by [40]

$$\sigma_{sH} = \frac{e}{6\pi^2}(k_F^H - k_F^L). \tag{3.1.5}$$

For a two-dimensional electron gas, the conduction band can be split because of spin-orbit interaction in systems (such as a two-dimensional gas) that do not have inversion symmetry; this can be of either structural or bulk origin. For the simple Rashba model (structural inversion a symmetry), the spin Hall conductivity, predicted to be universal, is given by

$$\sigma_{sH} = \frac{e}{8\pi}. \tag{3.1.6}$$

It turns out to be the case that in the clean (free of impurities, long momentum relaxation time) limit, all of the two-dimensional n-doped (for which the conduction band is $spin-1/2$) semiconductors with spin-orbit coupling have a universal spin Hall conductivity. These theoretical predictions are valid for systems free of impurities for which the spin splitting is much greater than the lifetime broadening arising from impurity scattering. In the presence of impurity scattering, there are two main contributions, the self-energy correction and the vertex correction. Although the self-energy correction vanishes in the clean limit, and the vertex correction also vanishes has required extensive consideration.

Recently, Wunderlich et al. [41] have reported the detection of spin accumulation in an applied field in semiconductor structures, in n-type and p-type semiconductors, respectively. The spin direction reverses with the applied field E establishing the existence of spin Hall currents leading to nonzero spin accumulation at boundaries. Awschalom and collaborators [42] conducted the experiment in the regime in which the spin splitting is smaller than the lifetime broadening, and concluded that the spin Hall mechanism may be extrinsic (e.g., impurity-related) in their samples. More recent analyses [43, 44] have shown that the experimental results can also be accounted

for on the basis of the intrinsic spin-orbit coupling in the conduction band due to the breaking of bulk inversion symmetry. Wunderlich et al. have conducted the experiment in a hole-doped sample, in a regime in which the spin splitting is larger than the lifetime broadening, and it is commonly believed that in their system the spin Hall currents may have been intrinsic.

3.2 Spin-Charge Propagating Mode-Spintronics without Spin Injection or Spin Detection

The spin-orbit interaction of electrons in GaAs quantum wells is described by Rashba and Dresselhaus terms (H_R and H_D, respectively) in the spin Hamiltonian. These terms describe the magnetic field experienced by electrons arising from static electric fields in the rest frame of the crystal lattice. The strength of the terms determines how the internal magnetic field depends on the electron wave vector $\vec{k}$. The dependence of the precession vector on momentum leads to a strong correlation between the propagation of the electron in position space and its angular momentum in spin space. In a 2D electron gas, the confining potential breaks the inversion symmetry and leads to an electric field perpendicular to the two-dimensional plane of the electron gas. Specifying the confining electric field as being in the z direction in Equation (3.1.3), Rashba [45] has pointed out that there is a spin current in the ground state, of the form of

$$J_i^j = \sigma_S \epsilon_{ij} = \alpha n \varepsilon_{ij}, \tag{3.2.1}$$

where α is the spin-orbit coupling constant, n is the electron density, and i and j take on values of the 2D coordinates x and y. Similarly, one can show that the electron spin also makes a contribution to the charge current, of the form of

$$J_i = \alpha \varepsilon_{ij} S_j, \tag{3.2.2}$$

where S_j is the electron spin density. As Rashba has indicated, the spin current in the ground state in the absence of external fields cannot cause transport or spin accumulation as long as the system is in equilibrium. The existence of the dissipationless ground-state spin current profoundly changes the spin transport in semiconductor devices and leads to the possibility of spin injection purely by electric means. The standard charge and spin transport equations are given by [40].

$$\frac{\partial n}{\partial t} + \partial_i J_i = 0, J_i = -D\partial_i n$$

$$\frac{\partial S_j}{\partial t} + \partial_i J_i^j = -S_j/\tau_s, J_i^j = -D\partial_i S_j \tag{3.2.3}$$

where D is the diffusion constant and τ_s is the spin relaxation time. These equations only account for diffusive behavior as a result of charge and spin transport. However, taking into account the effects of the spin-orbit coupling and substituting the additional contributions of the spin and the charge currents (3.2.1) and (3.2.2) into the standard transport equations (3.2.3), it follows that, in a two dimensional electron gas with Rashba spin-orbit coupling, the equations become

$$\begin{aligned}
&\frac{\partial n}{\partial t} + \partial_i J_i = 0, J_i = -D\partial_i n - \alpha\varepsilon_{ij} S_j, \\
&\frac{\partial S_j}{\partial t} + \partial_i J_i^j = -S_j/\tau_s - \sqrt{D/\tau_s}\partial_j S_3, \\
&J_i^j = -D\partial_i S_j + \alpha\varepsilon_{ij} n + \delta_{ij}\sqrt{D/\tau_s} S_3.
\end{aligned} \tag{3.2.4}$$

The second term in the spin current is the dissipationless spin current. By restricting to the in-plane components of the spin $S_j, j = 1, 2$, the following two continuity equations are easily obtained:

$$\frac{\partial n}{\partial t} = D\partial_i^2 n + \alpha\varepsilon_{ij}\partial_i S_j,$$

$$\frac{\partial S_j}{\partial t} = D\partial_i^2 S_j - \alpha\varepsilon_{ij}\partial_i n - S_j/\tau_s - \frac{1}{2}\sqrt{D/\tau_s}\partial_j S_3, \tag{3.2.5}$$

The first term on the right-hand side of each of the equations represents the usual diffusion current; the second term represents the dissipationless spin-current contribution; the third term of the second equation is the usual Dyakonov-Perel relaxation time, and the last term of that equation represents the coupling of diffusion terms with spin-current terms. If for the moment we neglect the D and τ_s terms, we see that the coupled spin and charge-transport equations formally take the same form as the Maxwell equations in 2D, provided that we interpret the charge density n as being a magnetic field B in 2D and we interpret the two in-plane spins S_x, S_y as being the two electric fields E_x, E_y. The first equation of continuity then becomes Faradays induction law, $\partial_t B = \alpha\varepsilon_{ij}\partial_i E_j$, while the second equation becomes Amperes law, $\partial_t E_i = -\alpha\varepsilon_{ij}\partial_j \vec{B}$. The only difference between the behavior of the system and the behavior of light rests in the value of the speed of light, which in this case is the Rashba coefficient $\alpha \approx 10^{-4}\ c$.

The analogy with Maxwells equations for neglecting the D and τ_s terms is useful for two reasons: First, it predicts the existence of a propagating mode of the system in which energy propagates rather than dissipates. This mode is the dissipationless spin current in the ground state. Secondly, in Maxwell physics, a disturbance in the magnetic field (the charge density) creates an electric field (a spin density), that predicting the appearance in spin-orbit-coupled systems of spin density from pure charge density.

A complete analysis of the above equations shows that the existence of a propagating mode is linked to a large spin-orbit coupling given by the condition

$$\alpha \gg \sqrt{D/\tau_s} \approx \sqrt{10^{-2} \times 10^{9}} \approx 3 \times 10^{3} m/s. \tag{3.2.6}$$

For the generic values of $D \approx 10^{-2} m^2/s, \tau_s \approx 1\ ns$ [46], the condition reads $\alpha \gg 3 \times 10^3 m/s$, which is easily realizable with todays experimental techniques [47]. For these values of the parameters, the propagating mode should have weak damping if

its wavelength is within 0.1 $\mu m < \lambda < 10\ \mu m$, and its frequency is within the domain $10\ GHz < \omega < 100\ GHz$. Through spin-orbit coupling, the charge disturbance creates a non-zero spin density. This would not happen in the absence of spin-orbit coupling. As the spin-orbit coupling strength is increased, the induced spin density increases, and its motion changes from a diffusive to a propagating regime. For 2D wells of finite width, it has been shown that the Dyakonov-Perel (DP) spin relaxation time increases as the width is decreased [48]. In the limit when the width is decreased such that the 2D well transforms into a quantum wire, the DP part of the relaxation time $\tau_s \to \infty$. In this limit, a propagating mode should be possible as the condition $\alpha \gg \sqrt{D/\tau_s} \to 0$ becomes easier to realize for increasing spin relaxation times. The

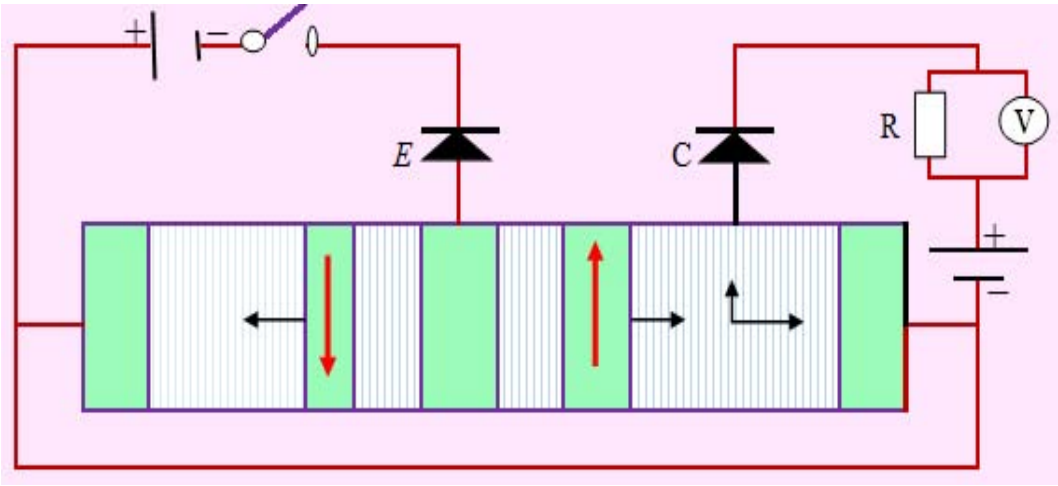

Figure 3.1: A modified version of the classic Haynes-Shockley Experiment. A density packet injected by the emitter (E) spontaneously splits into two counter-propagating packets with opposite spin. One of the two packets propagates to the collector without experiencing a sweeping electric field. The time delay between the injection pulse and the collecting pulse should give a purely electric determination of the Rashba spin-orbit coupling constant.

discovery of the propagating mode would have profound theoretical and experimental implications. First, the mode should facilitate long-range spin manipulation by manipulation of the charge packet. Second, if we are not interested in the spin motion,

we can see that, owing to the reactive coupling to the spin, the charge of the packet should propagate over large distances with little dissipation. This suggests a remarkably simple experiment in the spirit of the classic Haynes-Shockley experiment but without sweeping electric field. Figure 3.1 depicts such a proposed experiment using a narrow sample with light p-doping. Two rectifying metal-to-semiconductor point contacts would respectively be forward-biased and reverse-biased to serve as emitter and collector electrodes. After the emitter pulse was turned on, an electron density packet would be injected into the sample. In conventional Haynes-Shockley setup, the electron packet would be swept to the collector electrode by a electric field. In this case, no sweeping electric field would be applied, but the density packet would spontaneously split into two counter propagating packets with opposite spin orientations, with a velocity directly given by the Rashba coupling constant α. Upon capture of the rightward-moving packet by the collector electrode, a voltage pulse should be registered. From the time delay and the shape of the voltage pulse, one should be able to determine the Rashba coupling constant and the diffusion constant; this could be done by controlling only the charge. This experiment suggests that the injected density pulse should be able to take advantage of the spin current in the ground state and propagate without any applied voltage.

3.3 Silicon Orbitronics

The dominance of silicon in the semiconductor industry, it is important to find a similar dissipationless transport process which does not rely on the spin-orbit coupling. In [36], the possibility of replacing the spin degree of freedom with the orbital spin degree of freedom was investigated, and the associated field of study has been designated as orbitronics. The valence band of Si consists largely of three p-orbitals. The three orbital degrees of freedom transform as a (pseudo) $spin - 1/2$ quantity under rotation, are odd under time reversal, and couple to the crystal momentum of

the holes in the Si. The polarization of the p-orbitals, the direction of flow, and the direction of the electric field are mutually perpendicular. The transport equation is similar in form to the spin Hall equation (3.1.3):

$$J_i^j = \sigma_I \epsilon_{ijk} E_k \ , \tag{3.3.1}$$

where J_i^j is the orbital current flowing along the j direction, and the local orbitals are polarized along the direction perpendicular to both the applied field and the current. For an electric field on the y-axis, we expect an orbital current flowing in the positive x direction to be polarized in the $+z = p_x + ip_y$ direction, while the orbital current flowing in the negative x direction is polarized in the $-z = p_x - ip_y$ direction. As in the case of the spin current, the orbital current is even under time reversal, and the above response equation is dissipationless. The orbital current should appear as a result of the coupling between the hole momentum $\vec{k}$ and the local orbital $\vec{I}$; which is apparent in the Hamiltonian for Si close to the gamma point of the valence band:

$$H = Ak^2 + (A - B)(\vec{k}.\vec{I})^2 \ . \tag{3.3.2}$$

where A and B are material constants. Several recent experiments involving detection of spin currents via the associated spin accumulation at the boundary [46, 41] should provide us with a basis for attempting to detect the intrinsic orbital current in Si. Because Si is an indirect-gap semiconductor with low efficiency for light emission, a LED-type experiment like that described in [41], in which the polarization of the emitted light gives information about the orbital in which the emitting electron resides, is not experimentally viable. However, Kerr and Faraday rotation measurements are insensitive to the Si indirect gap and should be suitable for probing the orbital polarization.

Chapter 4

Spin Torques as a Result of Spin Accumulation

When a current incident on a thin ferromagnetic (FM) layer is polarized non-collinear with respect to the layer magnetization direction, it exerts a spin-transfer torque on the magnetic layer and may change its magnetization direction [49]. Such phenomenon is therefore referred to as the *Current Induced Magnetization Switching* (CIMS). A successful quantitative descriptions of this process is based on Valet-Fert model, which has been recently extended to non-collinear spin structures [50]. It rests heavily on two additional properties of spin currents:

First, the transverse component of the spin current inside a FM becomes rapidly damped on a typical distance of a few interatomic spacings [51]. Such a very short magnetic coherence length is a result of a large exchange splitting which leads to mostly destructive interference effects due to all contributions of wave vectors on the two Fermi surfaces of the FM metal. Consequently, the spin torque experienced by a FM layer can be identified with the transverse spin current at its interface with a neighboring non-magnetic (NM) layer.

Second, the proper boundary conditions inevitable for a full solution of the diffusion equations must be formulated in terms of properties of individual interfaces and it

comes out that more information is needed than contained in the spin-resolved conductances of the interfaces.

The magneto-electronic circuit theory [52, 53] represents another flexible approach to the transport properties of non-collinear magnetic systems consisting of FM and NM elements (nodes). The theory is based on the semiclassical concept of spin accumulation. With in the developed formalism, the chemical potentials and spin accumulations of the nodes are contained in 2×2 distribution matrices in the spin space. The steady-state currents, spin currents and spin torques in a device can be obtained from applied voltages by solving a set of linear equations quite similar to the Kirchhoffs laws for usual electronic circuits.

A truly microscopic (quantum mechanical) approach to all aspects of CIMS be prohibitively complicated having in mind the large layer thicknesses and the quality of interfaces in presently used multilayers and spin valves. A reasonable compromise between the accuracy and the complexity has been adopted by several authors in addressing the spin polarized electronic and transport properties of a single ferromagnet/non-magnet interface [51, 54] with emphasis put on the conductances and their sensitivity, e.g., to interface alloying. Since the traditional scheme for the transport, namely the Landauer-Buttiker scattering theory [55, 56], has been used in majority of papers, the effect of disorder was included by a supercell technique[52, 57].

Next an alternative approach to the mixing conductances that employs the Non Equilibrium Green's function (NEGF) formalism [55] is introduced. This is applied to a FM layer embedded between two semi-infinite NM leads (where the spin accumulation is present in one of these). The derived general formula is implemented in an *ab initio* technique.

4.1 Spin Accumulation and Spin Torques

Conductance electrons passing transversally through a `FM1|NM|FM2` junction experience spin-dependent reflections at interfaces which leads to spin-polarization of electrons even in NM layer. This can be represented by spin-dependent chemical potential in the NM layer, which corresponds to the spin accumulation. Figure 4.1 assumes the spin accumulation to be uniform across NM layer and it can be described by its direction $\vec{s}$ and size. The *spin-transfer torque* can be related directly to the spin accumulation, and a model with only one FM layer is sufficient to describe the problem. One can examine the linear response of the spin torque to the spin accumulation, thus only infinitesimal spin accumulation is taken into account (see Fig.4.2).

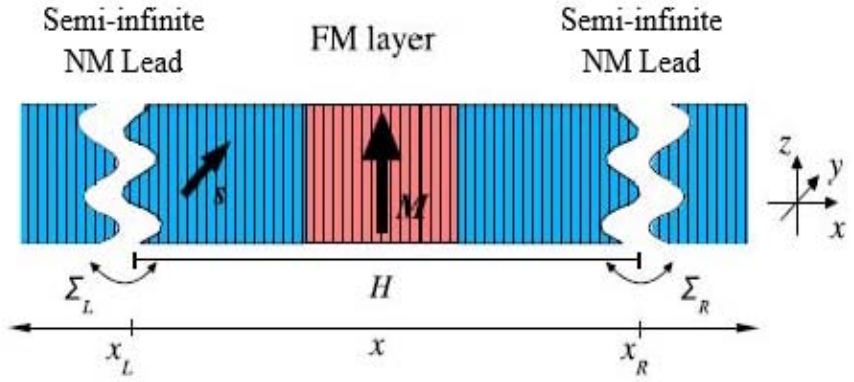

Figure 4.1: `NM|FM|NM` junction with spin accumulation s parallel to the y-axis in the left lead.
The spin accumulation is assumed to be uniform across NM layer and it can be described by its direction **s** and size. The spin-transfer torque can then be related directly to this spin accumulation.

The Hamiltonian is given as

$$\widehat{H} = H_0 + \gamma(\vec{\sigma}.\vec{n}), \tag{4.1.1}$$

where H_0 represents a spin-independent Hamiltonian, $\vec{\sigma} = (\hat{\sigma_x}, \hat{\sigma_y}, \hat{\sigma_z})$, is the vector of Pauli matrices, $\vec{n}$ defines the direction of the exchange field of the FM layer and γ

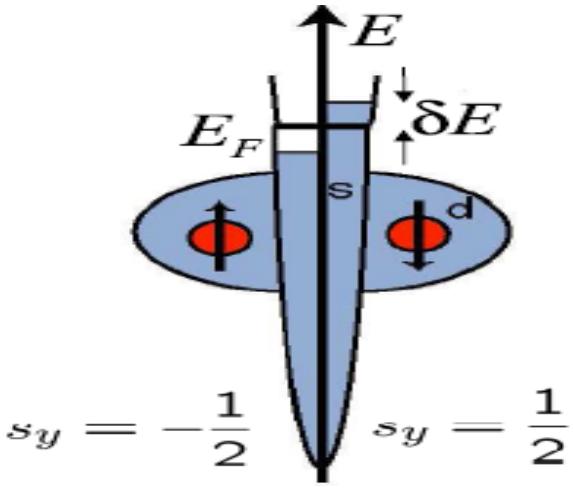

Figure 4.2: Infinitesimally small spin accumulation parallel to the direction of y-axis. The Hamiltonian H is limited to the so called intermediate region and semi-infinite NM leads are included in the system Hamiltonian as a self-energy.

its corresponding exchange splitting (nonzero only inside the FM layer). Matrices in spin space are denoted by hat(^).

For the purpose of CIMS the *spin torque* is defined as a time derivative of the total spin moment and this quantity of interest is obtained directly using its operator given as:

$$\vec{\tau} = -i[\vec{\sigma}, \hat{H}] \ . \tag{4.1.2}$$

This approach is formally different, but physically equivalent to existing approaches based on evaluation of difference between spin currents on both sides of the FM layer [52].

The well known algebraic rules for the Pauli matrices

$$(\vec{\sigma}.\vec{p})(\vec{\sigma}.\vec{q}) = \vec{p}.\vec{q} + i(\vec{p} \times \vec{q}).\vec{\sigma}, \tag{4.1.3a}$$

$$(\vec{\sigma}.\vec{p})\vec{\sigma} = \vec{p} + i\vec{\sigma} \times \vec{p}, \tag{4.1.3b}$$

$$\vec{\sigma}(\vec{\sigma}.\vec{q}) = \vec{q} + i\vec{q} \times \vec{\sigma}. \tag{4.1.3c}$$

valid for arbitrary classical vectors $\vec{p}$ and $\vec{q}$, yield an explicit form of the torque operator

$$\vec{\tau} = 2\gamma\vec{n} \times \vec{\sigma} \ . \tag{4.1.4}$$

This relation shows that the spin torque is a local operator non-zero only inside the intermediate region. *Ab initio* expression for the response C_L of the spin torque to the spin accumulation can be found using NEGF.

4.2 Derivation Based on Non Equilibrium Green's Function

The thermodynamic average of the spin torque $\langle\vec{\tau}\rangle$ for the NM‖FM‖NM system in a stationary non-equilibrium state is given by [58]

$$\langle\vec{\tau}\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} Tr\{\vec{\tau}G^{<}(E)\}dE, \tag{4.2.1}$$

where $G^{<}(E)$ is the lesser component of the NEGF. This quantity is related to the retarded and advanced Green's functions $G^{r}(E)$ and $G^{a}(E)$ through the kinetic equation

$$G^{<}(E) = G^{r}(E)\sum{}^{<}(E)G^{a}(E) \ , \tag{4.2.2a}$$

$$G^{r}(E) = [E - H - \sum{}^{r}(E)]^{-1} \ , \tag{4.2.2b}$$

$$G^{a}(E) = [E - H - \sum{}^{a}(E)]^{-1} \ , \tag{4.2.2c}$$

where $\sum{}^{<}(E)$, $\sum{}^{r}(E)$ and $\sum{}^{a}(E)$ denote the lesser, retarded and advanced components of the self-energy, respectively, which are usually defined in NEGF formalism. The total self-energies are given as sums of separate contributions due to the left (L) and the right (R) leads,

$$\sum{}^{x}(E) = \sum{}_{L}^{x}(E) + \sum{}_{R}^{x}(E), \quad x = r, a, < \ . \tag{4.2.3}$$

These self-energies therefore correspond to embedding potentials once the tight-binding linear muffin-tin orbital (TB-LMTO) formulation is defined in the Hilbert space of the intermediate region. The spin accumulation in the NM leads results in a change of the lesser self-energy $\delta \sum^{<}(E)$, which induces the following first-order change of the thermodynamic average (4.2.1):

$$\delta\langle\vec{\tau}\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} Tr\{G^a(E)\vec{\tau}G^r(E)\delta\sum{}^{<}(E)\}dE \ . \tag{4.2.4}$$

The special form of the torque operator, Eq.4.1.2, together with the expression for $G^{r,a}(E)$, Eq. 4.2.2, provide a relation

$$G^a(E)\vec{\tau}G^r(E) = -i[\vec{\sigma}G^r(E) - G^a(E)\vec{\sigma}] + G^a(E)\vec{\sigma}B(E)G^r(E) \ , \tag{4.2.5}$$

where the abbreviation for the anti-hermitean part of self-energy due to leads. In deriving Eq. 4.2.5, use was made of the fact that the self-energies of the unperturbed NM leads are spin-independent, so that $[\sigma, \sum^{r,a}(E)] = 0$. For stationary non-equilibrium systems without spin accumulation, the lesser self-energies are given by

$$\sum{}^{<}_{L,R}(E) = f_{L,R}(E)B_{L,R}(E), \tag{4.2.6}$$

*w*here the functions $f_{L,R}(E)$ refer to the Fermi-Dirac distributions of the two leads. In presence of the spin accumulation in one of the leads (L), the system is driven out of equilibrium by adding a spin-dependent shift δE_L to the Fermi energy of the lead. This yields the first-order change of the lesser self-energy in a form

$$\delta\Sigma^{<}(E) = \delta\Sigma^{<}_{L}(E) = f'(E)(\vec{\sigma}.\vec{s})B_L(E)\delta E_L, \tag{4.2.7}$$

where $f'(E)$ means the derivative of the Fermi-Dirac distribution and $\vec{s}$ is a unit vector pointing in direction of the spin accumulation. For systems at zero temperature, which will be considered in the following, $f'(E) = -\delta(E - E_F)$ where E_F is the Fermi energy. Substitution of Eqs. (4.2.5, 4.2.7) into Eq. 4.2.4 provides a starting expression for

the corresponding response coefficient C_L:

$$\vec{C}_L \equiv \frac{\delta\overline{\tau}}{\delta E_L} = \frac{1}{2\pi} Tr[i(\vec{\sigma}G^r - G^a\vec{\sigma})(\vec{\sigma}.\vec{s})B_L - \vec{\sigma}BG^r(\vec{\sigma}.\vec{s})B_L G^a], \tag{4.2.8}$$

where all omitted energy arguments equal the Fermi energy E_F. In order to extract the dependence of the response coefficient $\vec{C}_L$ on orientation of the spin accumulation $\vec{s}$ and the magnetization direction $\vec{n}$, the explicit structure of the Greenfs functions $G^{r,a}$ of the Hamiltonian (4.1.1) with respect to the spin must be used,

$$G^{r,a} = \left(\frac{G^{r,a}_\uparrow + G^{r,a}_\downarrow}{2} + \frac{G^{r,a}_\uparrow - G^{r,a}_\downarrow}{2}\right)(\vec{\sigma}.\vec{n}), \tag{4.2.9}$$

where the spin-resolved Greenfs functions are defined by [54]

$$G^{r,a}_s(E) = [E - H_s - \sum{}^{r,a}(E)]^{-1}, s = \uparrow, \downarrow . \tag{4.2.10}$$

The resulting expression for $\vec{C}_L$ follows after a lengthy but straightforward manipulation:

$$\vec{C}_L = D_1 s + D_2 s \times \vec{n} - D_3(\vec{n}.\vec{s})\vec{n}, \tag{4.2.11}$$

where the prefactors D_1, D_2 and D_3 are given by

$$D_1 = \frac{1}{2\pi} tr[i(G^r_\uparrow + G^r_\downarrow - G^a_\uparrow - G^a_\downarrow)B_L - BG^r_\uparrow B_L G^a_\downarrow - BG^r_\downarrow B_L G^a_\uparrow], \tag{4.2.12}$$

$$D_2 = \frac{1}{2\pi} tr[(G^r_\uparrow - G^r_\downarrow + G^a_\uparrow - G^a_\downarrow)B_L + i(BG^r_\uparrow B_L G^a_\downarrow - BG^r_\downarrow B_L G^a_\uparrow)], \tag{4.2.13}$$

$$D_3 = \frac{1}{2\pi} tr[B(G^r_\uparrow - G^r_\downarrow)B_L(G^a_\uparrow - G^a_\downarrow)]. \tag{4.2.14}$$

The form of Eq. (4.2.11) can be simplified by using a general relation

$$i[G^r(E) - G^a(E)] = G^a(E)B(E)G^r(E), \tag{4.2.15}$$

in the expression (4.2.12) for D_1 one obtains $D_3 = D_1$. The previous formula (4.2.11) for the response coefficient C_L can thus be rewritten as

$$\vec{C}_L = D_1\vec{n} \times (\vec{s} \times \vec{n}) + D_2\vec{s} \times \vec{n}. \tag{4.2.16}$$

Note that this results has a general form of a vector perpendicular to $\vec{n}$, in agreement with Eq. (4.1.4). A closer inspection of the real quantities D_1 and D_2, Eq. (4.2.12), reveals their simple relation to a single complex quantity. The spin-mixing conductance C_L^{mix}:

$$C_L^{mix} = \frac{1}{2\pi} tr[i(G_\uparrow^r - G_\downarrow^a)B_L - BG_\uparrow^r B_L G_\downarrow^a], \tag{4.2.17}$$

which yields

$$D_1 = D_3 = 2ReC_L^{mix},\ D_2 = 2ImC_L^{mix}. \tag{4.2.18}$$

The formulas (4.2.16), (4.2.17), and (4.2.18) represents the central result of this Chapter. It is interesting to compare them to the well-known spin-resolved charge conductance. We have shown that these formulas are invariant with respect to the position of boundaries between the leads and the intermediate region, which is an important feature for the consistency of the theory and for practical calculations.

Chapter 5

Summary and Conclusion

We have discussed the basic concepts that should be understood, generally in spintronics and particularly in GMR effects. The spin dependent transport in ferromagnetic metals originate from the electronic structures of the materials. In rare earth metals, electrons responsible for transport and magnetism can be distinguished. All materials which have imbalance of the spin populations at the Fermi level perform spin-polarized transport. This imbalance commonly occurs in ferromagnetic metals because the density of states available to spin-up and spin-down electrons is often nearly identical, but the states are shifted in energy with respect to each other. The electrical resistivity of ferromagnetic metals depends on spin. This spin dependence of resistivity is governed by the spin dependence of the electronic states near the Fermi level, and by the spin dependent impurity potentials in ferromagnetic alloys.
Every electron has an intrinsic angular momentum (spin) of $\frac{1}{2}\hbar$ which corresponds to a magnetic moment of one Bohr magneton $\mu_B = \frac{|e|\hbar}{2mc}$.
Dissipationless spin currents occur in materials with strong spin-orbit coupling, such as GaAs, while orbital currents occur in materials with weak spin-orbit coupling, such as Si, but with degenerate bands characterized by an atomic orbital index. Spin currents have recently been observed experimentally. Propagating modes are the coupled spin-charge movement that occurs in semiconductors with spin-orbit coupling.

This opens the possibility for spin-based transport without either spin injection or spin detection.

The potential means for achieving dissipationless spin transport constitute a theoretical and associated, potential experimental directions with technological implications. A number of alternatives to the current semiconductor technology have recently been proposed, including technologies based on carbon nanotubes, molecular electronics, and dilute magnetic semiconductors. The spin-charge-propagating mode predicted in systems with strong spin-orbit coupling should be another way of manipulating spin. Because of its propagating character, it should almost conserve energy. Moreover, it should be possible to use the mode without regard to the spin: Use would be made of only its propagating charge packet. The experimental detection of this mode, as well as proposals for real devices, constitutes a focus for future research in spin-based electronics.

Ab initio expression for the response C_L of the spin torque to the spin accumulation can be found using NEGF.

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