UNIVERSIDAD DE INVESTIGACIÓN DE TECNOLOGÍA EXPERIMENTAL YACHAY

Escuela de Ciencias Físicas y Nanotecnología

TÍTULO: Two terminal devices for the CISS effect Analytical and Modeling

Trabajo de integración curricular presentado como requisito para la
obtención
del título de Físico

Autor:

Sanmartin Castillo Miguel Angel

Tutor:

Ph.D. Peralta Arcia Mayra Peralta

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Dedication

To my family who have always been there for me, supporting and giving me all you can to make me the person who I am becoming.

Miguel Angel Sanmartin Castillo

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I want to make two special mentions of gratitude to two people who have made this accomplishment possible. My co-advisor Dr. Ernesto Medina has never quit believing in me and allowing me to work with him learning and growing up as a Physicist and as a person. My other co-advisor Dr. Solmar Varela that have given me the inspiration and the tools to believe that through science and hard work we can be and create the change our country and the world need. Thank you both for being an important part of my academic path and always motivating and spire me to believe and remember the importance of doing science.

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Resumen

Resultados experimentales sobresalientes en moléculas quirales muestran un transporte de espín preferencial dependiendo de la quiralidad en dos mediciones terminales (selectividad de espín inducida quiralmente o CISS). Los teóricos han propuesto que estos dispositivos de espín activo están impulsados por la interacción espín-órbita (SOI). Sin embargo, tal interacción en dispositivos terminales tiene prohibido girar filtros debido a la simetría impuesta por las relaciones de Onsager en el régimen lineal. Mostraremos que los experimentos no corresponden a la configuración teórica de dos terminales, por lo que el "teorema" de dos terminales no se aplica.

En este trabajo, proponemos estudiar un modelo de una molécula acoplada de espín-órbita invariante en el tiempo, como el ADN y los oligopéptidos, que también son espacialmente quirales y, por lo tanto, carecen de un centro de inversión. Comenzaremos derivando los elementos principales, desde un enfoque de matriz de transmisión macroscópica, el comportamiento de un dispositivo de dos terminales, incluida la interfaz sensible al espín. Si bien el tratamiento teórico predice cero magnetorresistencias (MR) de dos terminales sensible al espín, encontramos estos resultados de una mala interpretación de las configuraciones experimentales que de hecho muestran MR sensible al espín.

Palabras Clave:

CISS, espintronica, acomplamiento espin orbita, conductancia

Abstract

Outstanding experimental results in chiral molecules show preferential spin transport depending on the chirality in two terminal measurements (Chirally induced Spin Selectivity or CISS). Theorists have proposed that this spin active devices are driven by the Spin-Orbit interaction (SOI). Nevertheless, such an interaction in terminal devices is forbidden to spin filter due to the symmetry imposed by Onsager relations in the linear regime. We will show that experiments do no correspond to the theoretical two-terminal-setup so that the two terminal "theorem" does not apply.

In this work we propose to study a model of a Time reversal invariant spin-orbit coupled molecule such as DNA and Oligopeptides that are also spatially chiral and thus lack an inversion center. We will begin by deriving the main elements, from a macroscopic transmission matrix approach, the behavior of a two-terminal device, including the spin-sensitive interface. While the theoretical treatment predicts zero two-terminal magnetoresistance (MR) sensitive to spin, we find these results from a misinterpretation of the experimental setups which do indeed show spin-sensitive MR.

Key Words:

CISS, spintronic, spin-orbit coupling, conductance.

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Chapter 1

Introduction

In the early days of science when we just dream on, would it be possible to someday control light? Could it be possible to describe the behavior of such phenomena? well with the development of technologies and human capacities, we have accomplished a lot in a brief period of time. In terms of electrical devices for the last 50 years, the world has experienced a high increment of creation and applications of these devices as well as an increase of attention of researchers around the world. Electronic devices have multiplied their size change rate and little by little integrated circuits as we know would start to reach their limit. Gordon Earl Moore, Intel's co-founder predicts that about every two years the number of transistors in an integrated circuit should double to increase the efficiency, velocity, and power. This is known as Moore's law[6]; an empirical law that is used in industry as an indicator of how fast the computational power is increasing and needed versus the physical capacity of the device.

With the imminent miniaturization of the devices, emergent fields that study electronic structures and electron transmission at really low scales have appeared. As a consequence, in recent years, an attractive idea has emerged, it consists of using an electron intrinsic property known as Spin[7]. The appearance of Spin has brought with it new ideas and ways of deal electronic transport therefore giving birth new fields of study for this area. Spintronics is a resent research field in Physics that studies the detection, manipulation and control of the electric field of the spin. New areas such as spin caloritronics, valleytronics, spin filters, spin valves, spin injection, detection and many others are spin-based electronics that show the importance of spin manipulation and its applications for the future. The field of Spintronics appeared around 1980s, even though spin was discovered several years earlier at the beginning of century, 1920. When researches focused on the description of the behaviors of electrons, they found out that to fully describe those kind of systems, an additional concept was missing. The unknown parameter theorizes about electrons that could rotate about their own axis. Another way to describe the Spin is looking at this phenomena as the angular momentum of an electron, it will make the electron "rotate" clockwise or anticlockwise.

In the experimental setup shown in Figure 1.1 electrons pass through a chiral molecules until they reach the ferromagnet (FM). At the edges, it is obtained a spin selectivity activity that occurs depending on the polarization of the ferromagnet and the chirality of the molecules[8]. The curled shape of the chiral molecule presents a particular affinity with spin. Several experiments with chiral molecules as DNA, oligopeptides, proteins, etc. have shown the same behavior in experiments of photo emission and conduction. The spin-dependent response of organic molecules had not been of interest because these molecules are usually composed of light atoms whose spin-orbit interaction is usually small. However, these results open a new window to the study of these systems.

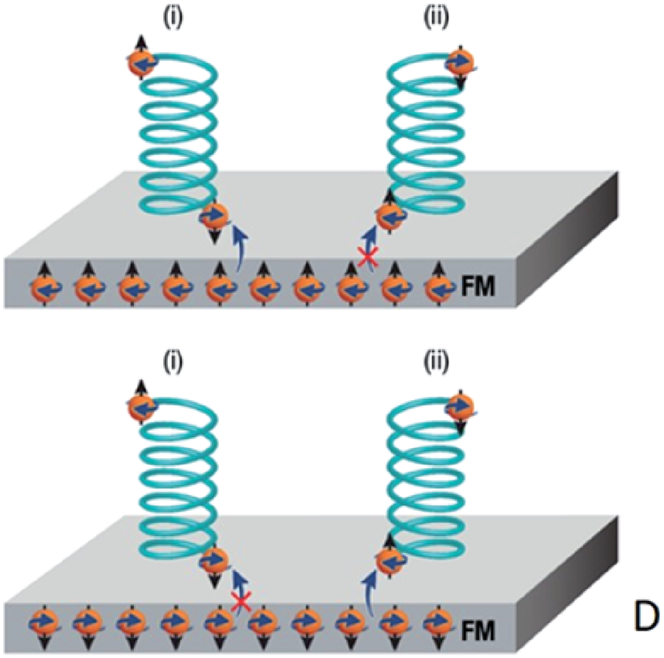

Figure 1.1: Spin-charge contribution of chiral molecules in FM. The spin polarization in the ferromagnetic in (i) is effective to the direction of the chiral molecule. In the bottom (ii), when the direction FM is reversed, the actual spin effective transport changes. Retrieved from: © Ron Naaman/Weizmann Institute of Science

Chiral molecules present a particular curl shape that could be exploited by the electron's degree of freedom, the spin. The molecule would act as a filter creating an effective channel for a specie of spin between the FM and the molecule. This kind of system behaves as if there is a magnetic field acting on it. Therefore, when electrons are transferred into a molecule component one spin state is preferred over the other, generating a preferred component that is directly associated with the enantiomeric nature of the structure. This is known as the Chiral Induced Spin Selectivity (CISS) effect. CISS effect presents a dependency on the symmetry/asymmetry of a chiral molecule, which is an advantage for proposing effective circuit-geometries for spintronic and nanodevices. The CISS effect may provide a novel approach for understanding the role of electron spin in many systems of materials such as magnetic, non magnetic, and biological systems. In recent years the popularity of this effect has increased; so interesting experiments that reveal fundamental information keeps capturing our attention.[9,10].

Typical experiments in the study of electron transport devices are the experimental measurements at 2 terminals/leads, where fundamental cases focus on a spin-dependency in energy. A well used approximation is the model of tight binding. Many theoretical works have been studying CISS effect at molecular level as the group of E. Medina and Gohler presented right now[1,11–13] which present a detailed manipulation molecular transport expressions. An example of a molecular electronic configuration used to described electron transmission through large helical molecules, such as DNA can be observed in figure 1.2[1]. In the experiment, Gohler et al observed that self assemble monolayers of double-stranded DNA molecules show interesting measurements of electron transport passing through the assembly in photoemission experiments.

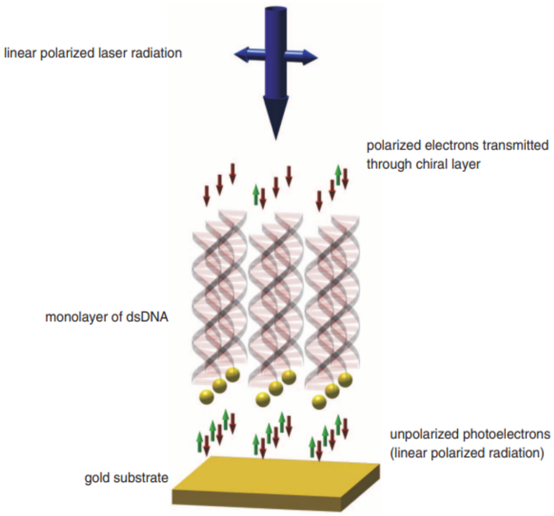

Figure 1.2: Scheme for measurement of spin polarization in photo emission processes. Electrons that are ejected from a gold substrate, with linearly and circularly polarized light, pass through an assembled monolayer of DNA molecules. Retrieved from Gohler[1]

In Figure 1.2, we observe a molecular assemble of DNA above a metal substrate. This kind of experiments could be designed with the use of appropriate molecules which are likely to join the metal or substrate. Molecules with thiol terminations as DNA, oligopeptides, proteins, benzene-1,4-dithiol[9,14,15] have shown high efficiency to get attached to metals. Once the molecule is located at the surface, an external energy source is applied, in this case a laser pulse that produces photo-electrons energetic enough to expel the electrons attached to the substrate with no damage to the molecule. Electrons, before passed trough to the molecule and been subjected to this source get spin polarized with their spin aligned anti-parallel to their speed. Consequently, an assembly of DNA performs an efficient work as a spin filter, which means high affinity to polarized spin with a determined direction.

Other prominent experiments in the field of spintronics are STM-break junction experiments, due to their facilities to add molecules to terminals and get measurements. In order to get information from STM, it needs to fulfill two statements that the sample is conductive and has a molecule embedded. A small metallic bed is submerged into the substrate where we find a molecule, for this example oligopeptide, with magnetic pits for around 10 minutes. Once the molecule gets attached to the metal, it possible can make measurements using the STM tip. When a biased current is applied to the STM, it is observe in the I-V curves the contribution of the spin in the molecule.[2]

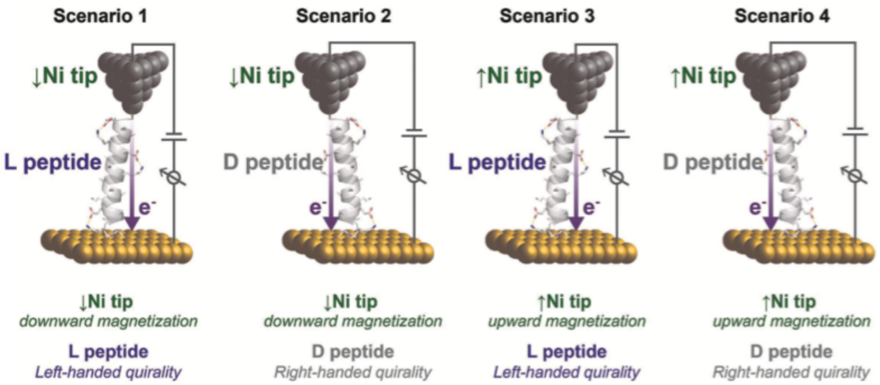

Figure 1.3: Schematic representation and description of the four studied case scenarios combining the three key experimental parameters. Sample bias voltage (defined as sample minus tip voltages) is positive meaning the electrons are flowing from the Ni to the Au electrodes.[2]

As you can notice in the image 1.3 of experimental setup in this context, the measurements have been taken in a two terminals or two leads device. Following the idea of using the spin degree of freedom as an alternative to improve current, Xu Yang, Caspar H. Van der Wal and Bart J. van Wess[9,16,17] proposed an interesting model for two and four terminals for mesoscopic devices taking into account the spin contribution to the current. The possibility to take measurements from this kind of devices is allowed by the breaking of Onsager's reciprocity principles. As we keep going beyond linear regime to a non linear one, Onsager's principle is broken. Usually a spintronic device needs two important components: spin injection and spin detection, through which electrical or optical signals and spin signals can be interconverted and act as a carrier[5,16]. Normally, these kinds of effects are studied in solid-state devices but, as we have shown chiral molecules could present an incredible affinity to provide electron transport. CISS effect suggests that electron going through certain chiral molecules such as sDNA, helicenes, could acquire a specific spin polarization.

In this work, we introduced the importance of the study of the electron spin going through spintronics experiments and models that describe the contribution of spin in electron transport, in the context of CISS observations. We present a model that joins electron and spin transport that comes from an extension of Landauer-Buttiker's formula. Experiments of Yang and Van Wess[17,18] test the CISS effect in different materials such as ferromagnets, non-ferromagnets, chiral and non-chiral molecules. These experiments are valid for linear regimes using the approximation of Onsager reciprocity which consider symmetry theorems to show its validness. Experiments and literature proposals have shown the possible existence of the CISS effect even though information on its origin is still missing.

The main problem to consider is how to measure only the spin or the CISS effect in a specific direction and don't get messed up with other signals such as magnetization. For this, we replicated and analyzed a two-terminal generic example in order to familiarize ourselves with the notation and observed the troubles these kinds of systems could present. The experimental setup of the device contains a geometry of two probes, a ferromagnetic material, and a chiral molecule. This system showed an energy dependency that can be overcome thanks to the chemical reservoirs. After deriving and testing this proposal approximation, we suggest a complete experiment by adding corrections in the way of taking measurements. We proposed alternative calculations where we take into account the presence of spin accumulation, as well as other possible interactions (electron-phonon) which are contained in a metallic layer. This node relaxes the spin and makes possible the existence of currents. Finally, our analysis presents the spin dependence in electric currents in a linear regime because of Onsager's reciprocity. It manifests the fundamental responses of symmetry theorems in a linear regime and how when it is broken spin-orbit phenomenons can take place.

1.1 Problem Statement

Normally, the spin contribution is studied by using tight binding models, which are more accurate for obtaining results at microscopic levels. Even though many theoretical models about molecular structures have been proposed, it is impossible to completely explain how these molecules possess such magnitudes of spin polarization. As presented in several experiments at linear regime and by using only symmetry theorems, there is a possibility of tackling CISS in an effective way. The study of the presence of spin at a linear regime could be used by innovative electronic materials; remember that the injection, detection, and manipulation of spin is the main goal of spintronic devices. The present study proposes an extension of the formalism presented by Yang and Bart[16,17] to distinguish the spin-electron signals of spin-accumulation and how can we measure the spin contribution in device composed from 2 Terminal reservoirs (2T) or 3 Terminal (3T) , from which we can argue an effective theory to manipulate spin-dependent set-ups.

1.2 General and Specific Objectives

Genera Objectives:

The principal objective of this research work is to present a theoretical proposal of effective spin contribution in spintronic devices. Clarify macroscopic approach of 2 terminal devices and evaluate a 3T correction system of transmission and detection of electron-spin.

Specific Objectives:

- Derive a macroscopic approach based on symmetries theorems of transmission and reflection matrices in a two terminal device.
- Display how the measurements of the leads at the contacts can affect the spin contribution measurements.

- Propose an effective three terminal model of spin independent of energy into the linear regime.

Chapter 2

Theoretical Framework

In this chapter, we detailed the discussions and derivations of the theoretical basis and models employed in this work. Starting from the description of electronic conductance, entering into the formalism of Transport Matrix as an extension of Landauer-Buttiker description of electron transport. Then using the model suggested by Yang and Van Wess of a 2 Terminal nanodevice to finally explicate, what and how does time reversal works.

2.1 Electronic conductance

Current studies consistently characterize electron transport by electron conductance (G), claiming that conductance is the most natural observable measure of electron transport. Considering electronic conductance in a solid device, we should be concerned about the nature of the motion of electrical current carriers. Electrical conduction can be summarized as a diffusive process in which an electron can travel really small distances before being involved in some scattering event[19]. Therefore the behavior of these carriers in matter acts depending on the size of the material.

For macroscopic conductors, Ohm's law displays the concept where the current passing through such conductors is proportional to its geometry and an applied voltage, and this is a linear regimen of conduction. Conductance G at this linear-regime is predicted to be proportional to the area S and inverse proportional to its length L[20], where σ is the conductivity of the sample:

$$G = \frac{\sigma S}{L}. \tag{2.1}$$

This equation implies that conductance will vanishes as the conductor becomes narrower. The existent electrical currents follow the principle of use long narrow conductors like transmission lines. It normally represents a big amount of energy consumption which leads us to a second problem. Trough experimental data we have observed that since the dimensions of a conductor approaches atomic scales the homogeneity of conductivity described by Ohm's law does not work anymore.

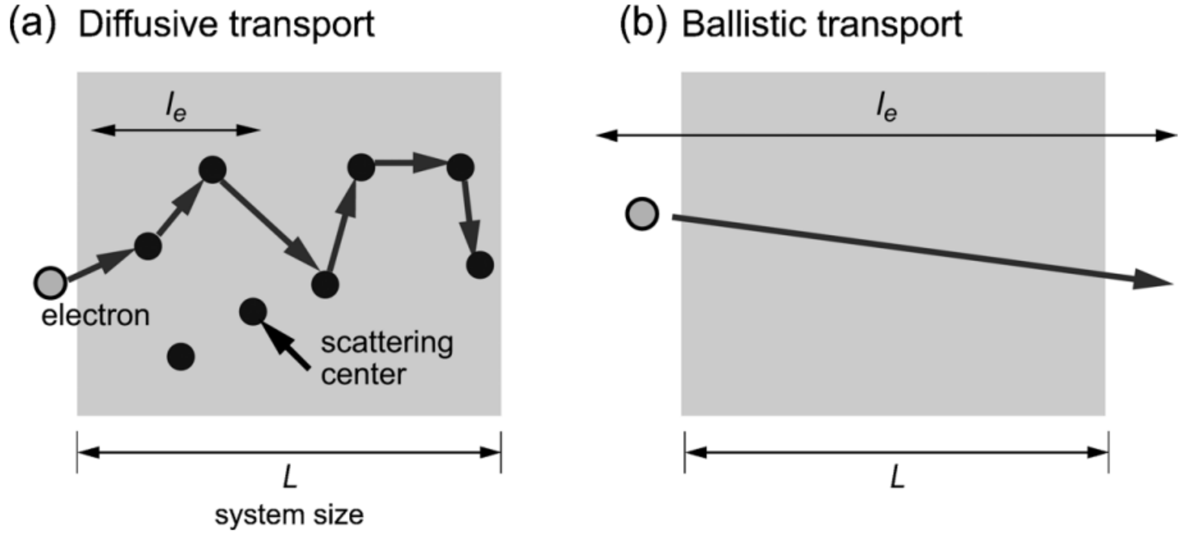

Figure 2.1: In the diffusive transport regime (a) many elastic scattering events occur, while the electron crosses the sample of size L. In the ballistic regime (b) the electron crosses the sample without any elastic scattering event. Retrieved from[3]

An important length scale to take into account is the elastic mean free path l. This scale measures and approximation of the distance between elastic collisions with static impurities. The regime where $L \gg l$ is known as diffusive transport. Here the electron behaves as observed in left of the Figure 2.1, it is to say, the electron can have many interaction before reaching the other side. In a semi-classical picture the electron motion in this regime can be viewed as a random walk of step size among the impurities[20]. On the other hand, when $L < l$ we reach the ballistic regime in which the electron momentum can be assumed to be constant and only limited by scattering with the boundaries of the sample. This approach give us a quantum mechanic behaviour of the electrons[21]. Quantum Mechanics (QM) allows the existence of 1-D channel whose conductance is a simple combination of fundamental constants and does not change with length. Some text called this "quantize conductance".

From here we would be laying at the surface of the fields of quantum transport presenting fundamental concepts like the quantize conductance. G. Rolf Landauer manages this problem by assuming that an obstacle electron suffers elastic scattering[22]. The extended Landauer-Butikker multi-terminal formula that characterized the scattering events as transmission and reflection coefficients is given by:

$$G = \left(e^2/\hbar\right) T. \tag{2.2}$$

This formula defines the characteristic size of the conductor at which macroscopic description no longer applies. An extension of Landauer Formula is called Landauer-Buttiker, which relates scattering events in multi-terminal probes[22]. In the next section you will find how this powerful formula later would be extended to a spin case.

2.2 Transport Matrix Formalism beyond Landauer Formula.

Typically a way to measure transport in a system of two contacts, where the current flows freely, is by the use of an applied bias voltage. The relation between voltage and current from Ohm's law is interpreted as the classical resistance. An intuitive model that will help to understand and give us the chance to measure is the Landauer-Buttiker Formalism, where:

$$R_{mn,ij} = \frac{U_{ij}}{I_{mn}}, \tag{2.3}$$

is the resistance. This model presents an extension version of Ohm's law, which defines resistance R as the ratio of the voltage (U) with it respective subindex important to understand where does the chemical potential or voltage is measured, such as i an j indicates probes state between probes L (left), R (right) and the current (I) that flows between m and n. The definition and understanding of this sub-index will become important along the discussion in order to follow the electron direction transmission or reflection.

Let's propose the analysis of an example. The authors propose a system of 4 points/leads where at each one of the points are at different electrochemical potentials[3,23]. As it will be shown in the discussion part, with the inclusion of multiterminal leads the charges flowing around the terminals could pass through each reservoir, meanwhile just one is going to act as a source and at the same time drained by the influence of the others. The experiment suggests that electrons transported from one lead into whichever reservoir, are going to be attracted into the reservoir no matter the value of its carrier. Keeping in mind that inelastic effects are neglected in the carrier path, energy and momentum are assumed to be preserved.

The derivation of a one-dimensional system with 1 lead geometry, can contribute to the clarification of the all the elements that contributes our net current. Waser propose the measurement of a net current for one of the probes I_1[3,23] . The current injected from reservoir 1 will travel through all the system ans is the only one they tackled. The formula that involves all the elements of the injected current I_{inj} is given by:

$$I_{inj} = e\int_0^{\mu_1} D_{1D}(E)v(E)dE. \tag{2.4}$$

The geometry of our example indicates one-directional way for the current to occur. As the wire is a 1-D material it affects the Density Of States (DOS) because of the use of a 1-D system where DOS is diminished to the middle. $D_{1D}(E)$ and $v(E)$ are constant so we take them out of the integral and obtain the current injection only depending on chemical potential[3,23]. Therefore the new form of the current that refers to Lead 1 has the shape of:

$$I_{inj} = \frac{2e}{h}\mu_1. \tag{2.5}$$

Part of the current supplied by reservoir 1 will be reflected back into the conductor. If R_{ii} is defined as the reflection probability for a reflection of carriers from lead i back into lead i, then the current reflected into lead 1 can be written as:

$$I_R = -\frac{2e}{h}R_{ii}\mu_i, \tag{2.6}$$

which is necessary in order to characterize electron transport. The transport of electrons comes from all the reservoirs into the lead 1. Same as in the resistance, the value of current transmission probability into the first lead is:

$$I_T = -\frac{2e}{h} \sum_{j=2}^{4} T_{1j}\mu_j. \tag{2.7}$$

By summing all of these contributions, it can be seen that the net current flowing into lead 1 is finally given:

$$\begin{aligned} I_1 &= I_{inj} + I_R + I_T, \\ &= \frac{2e}{h}\left[(1 - R_{11})\mu_1 - \sum_{j=2}^{4} T_{1j}\mu_j\right]; \end{aligned} \tag{2.8}$$

We have been studying a 1-D system current behaviour, so to tackle each four leads in a generally way, Wazner introduce I_i. Which will have an important roll to understand and describe spin in the future. The generalized current I_i is presented as:

$$I_i = \frac{2e}{h}\left[(1 - R_{ii})\mu_i - \sum_{j \neq i} T_{ij}\mu_j\right]. \tag{2.9}$$

Finally, Landauer formula is in brief words a relation between the electrical resistance of a quantum conductor and its scattering properties[21] which is our case. The primary study of our case of interest will divide into two parts. The first one will focus on electronic transport, referring to conductance at a mesoscopic level, talking about a specific example: wire's conductance is quantized. The purpose of the study of mesoscopic devices lies in the advances to the complete understanding of the phenomena that involve semiconductors, metals, insulators, and superconductors[10] which here is the spin. Here lies the possibility of building effective nanodevices and possible mesoscopic devices. In the next section, we introduce a model that connects a molecule with a Ferromagnet in a linear regime attempting to measure the magnetoresistance provided by the accumulation of spin.

2.3 2T Model

The (spin-resolved) Landauer formula considers charge voltages as driving forces for electronic charge and spin transport. We will use a formalism derived from Landauer-Butikker that is applied by Yansen and Van Wess[16,17] formula, but extended to the analysis and conversion of electron-spin to describe the model. The formalism of a called *Transport Matrix* include this spin degree of freedom. The model that will be presented also helps to understand the thermodynamic responses of spin-charge converters and assumes conservation of momentum direction.

Figure 2.3 is a picture of the ideal case, being the chiral component located as the blue helix that depends on the current, and electrons with a determined spin-polarization have a preference due to CISS effect. The molecule will act as a filter and electrons that are not polarized in that direction will suffer a reflection of the current. We will observe more of this set ups, but here this kind of components is assumed to favor the transmission of electrons with spin parallel to momentum. Here, we assume that there is no inelastic interaction within the chiral structure, and it implies a conservation of energy and momentum. Following the concepts presented before by equation 2.9, the

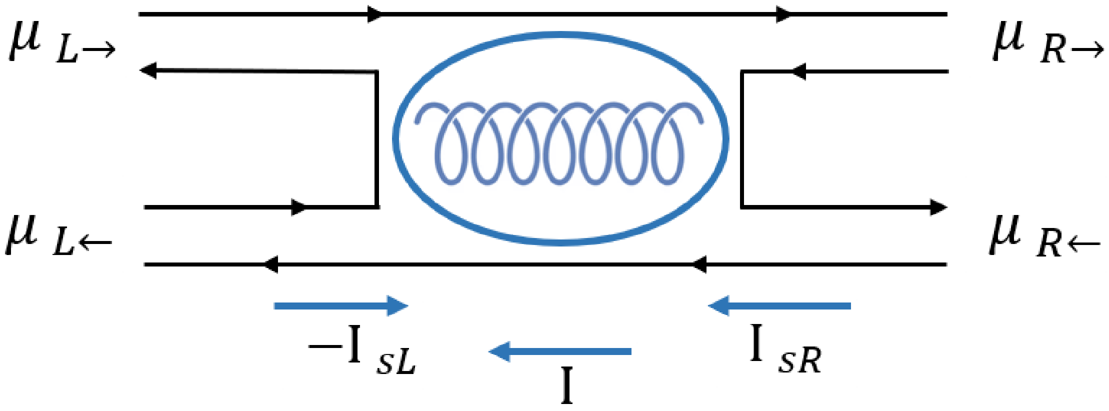

Figure 2.2: Representation of Ideal case of CISS effect in a chiral component.The electrons on both Left (L) and Right (R) of the chiral component labeled with their spin-specific electrochemical potentials $\mu_{L\leftarrow(\rightarrow)}$ or $\mu_{R\leftarrow(\rightarrow)}$ initial state ($\rightarrow$ *or* $\leftarrow$)[4,5]

current that flows in each lead considers crucial parameters involved in the measurement of the conductance. First, we present the nomenclature used to derive this extended formalism of the equations previously mentioned.

The blue helix in the figure represent a chiral molecule it could be *parallel* to the momentum of the electron or *anti parallel* to it. This notion of the direction of the momentum allows higher transmission for spins parallel to the momentum. This definition is illustrated in Fig 2.3. The expressions for direction electron transmission $\mathbb{T}$ and reflection $\mathbb{R}$ including each spin contribution, use spin-space matrices that agree with symmetry theorems. This matrix notation is fundamentally used to introduce spin and charge transport in a nonmagnetic chiral component:

$$\mathbb{T}_{\triangleright} = \begin{pmatrix} t_{\rightarrow\rightarrow} & t_{\leftarrow\rightarrow} \\ t_{\rightarrow\leftarrow} & t_{\leftarrow\leftarrow} \end{pmatrix}, \quad \mathbb{R}_{\triangleright} = \begin{pmatrix} r_{\rightarrow\rightarrow} & r_{\leftarrow\rightarrow} \\ r_{\rightarrow\leftarrow} & r_{\leftarrow\leftarrow} \end{pmatrix}. \tag{2.10}$$

The other hand matrices are the time-reversed form of the eq:2.10 for left-moving electrons.

$$\mathbb{T}_{\triangleleft} = \begin{pmatrix} t_{\leftarrow\leftarrow} & t_{\rightarrow\leftarrow} \\ t_{\leftarrow\rightarrow} & t_{\rightarrow\rightarrow} \end{pmatrix}, \quad \mathbb{R}_{\triangleleft} = \begin{pmatrix} r_{\leftarrow\leftarrow} & r_{\rightarrow\leftarrow} \\ r_{\leftarrow\rightarrow} & r_{\rightarrow\rightarrow} \end{pmatrix}. \tag{2.11}$$

Going further with the notation, we define spin-space column vector to the electrochemical potentials and the same with currents. The components of T and R matrices are the representation of spin contribution probability. As you can notice, all the elements from t and r contain sub indices, where the first one represents the initial state and the second the final state of the spin. Furthermore, each vector element describes the independent contribution of one spin component on each side of the molecule (L or R). The equations that are represented from now on are linear combination from this matrices.

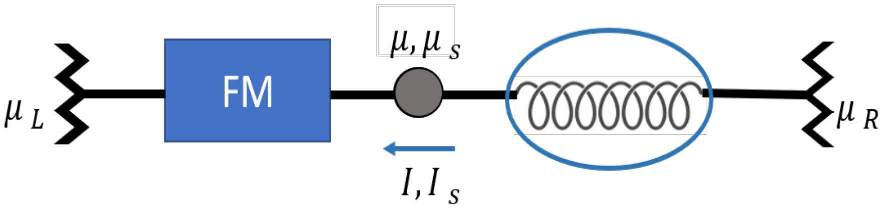

Figure 2.3: Representation of a generic 2T MR measurement geometry. An Ferromagnet (FM) and a chiral component conected in series beetween two spin-unpolarized electrodes Left (L) and Right (R). Charge and spin movement is driven by the difference in electrochemical potentials μ_L- μ_R=-eV.

In the figure 2.3 we present a 2T solid-state mechanism as a electron transport linear-regime circuit segment, whose components are described next by the following rules presented in the text "spin-dependent electron transmission model for chiral molecules in mesoscopic"[24]:

1. First, at the edges as a wavy lines we represent an electron reservoir with its respective chemical potential μ. This potential is the responsible of the energy of the electrons going out of the reservoir. It is not selective in energy or spin and absorbs all incoming electrons.
2. A node pictured as a circle in Fig. 2.3 must be a circuit component where the chemical potential for charge and spin are determined. Here an electron reflects or transmits too, but it gets accumulated which denotes an important role in a 2T CISS device which we will board at the discussion.
3. A CISS molecule represented as an helix as showed in figure 2.2 , a Ferromagnet (FM) as a filled square Fig. 2.3, and the node are viewed as two-terminal circuit constituents with energy-conserving electron transmissions and reflections.
4. The listed components are linked by transport channels represented as a line segment, which conserves both momentum and spin of electrons so it is just used as a wire.

So, following the notation showed in the figure 2.2, we introduce important variables that will be tackle along the text. First we have electrochemical potential as μ=($\mu_\rightarrow$+$\mu_\leftarrow$)/2 and spin accumulation μ_s=($\mu_\rightarrow$-$\mu_\leftarrow$)/2; the same for current vector I=($I_\rightarrow + I_\leftarrow$) and spin current/accumulation I_s=($I_\rightarrow - I_\leftarrow$). We represent the current at each side of the molecule with the use of spin-space column vectors. As showed above in the section 2.2 the current in a linear regime could be described by our system of vectors and matrices. Notice that both $\mathbb{T}$ and $\mathbb{R}$ hold all the transport/reflection information, and relations of each side of the system[4,5]. The expression behind is an extension of the Landauer-Buttikker formula presented in 2.2 with the contribution of spin. This expression will be:

$$\begin{pmatrix} I_{L\rightarrow} \\ I_{L\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[(\mathbb{I}-\mathbb{R}_{\triangleright})\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix} - \mathbb{T}_{\triangleleft}\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix}\right], \tag{2.12}$$

$$-\begin{pmatrix} I_{R\rightarrow} \\ I_{R\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[(\mathbb{I}-\mathbb{R}_{\triangleleft})\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix} - \mathbb{T}_{\triangleright}\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix}\right], \tag{2.13}$$

where N is the number of spin-degenerate channels in a determined surface area, h is the Planck's constant, e is the electron mass and $\mathbb{I}$ being the identity matrix where its elements where obtained from derivations of[4,5].

Using each element of the spin-space column vector we construct our first two equations of current-spin for the left reservoir. Each current equation for the left lead $I_{L\rightarrow}$ and $I_{L\leftarrow}$ represent all the contributions of each electron with spin Left or Right polarization.

$$\begin{pmatrix} I_{L\rightarrow} \\ I_{L\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} r_{\rightarrow\rightarrow} & r_{\leftarrow\rightarrow} \\ r_{\rightarrow\leftarrow} & r_{\leftarrow\leftarrow} \end{pmatrix}\right], \begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix} - \begin{pmatrix} t_{\leftarrow\leftarrow} & t_{\rightarrow\leftarrow} \\ t_{\leftarrow\rightarrow} & t_{\rightarrow\rightarrow} \end{pmatrix}\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix}\right]. \tag{2.14}$$

In the other hand we will need a set of equations to the other side of the reservoir. Later we will dig in the use of this equations which are $I_{R\rightarrow}$ and $I_{R\leftarrow}$. The treatment of this equations are the base of how we can understand and propose the electron-spin inter convention and transmission inside this device. So, the right part is related to the ferromagnet contribution and electron-spin behavior at this point,

$$-\begin{pmatrix} I_{R\rightarrow} \\ I_{R\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} r_{\leftarrow\leftarrow} & r_{\rightarrow\leftarrow} \\ r_{\leftarrow\rightarrow} & r_{\rightarrow\rightarrow} \end{pmatrix}\right]\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix} - \begin{pmatrix} t_{\rightarrow\rightarrow} & t_{\leftarrow\rightarrow} \\ t_{\rightarrow\leftarrow} & t_{\leftarrow\leftarrow} \end{pmatrix}\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix}\right]. \tag{2.15}$$

$$I_{L\rightarrow} = -\frac{Ne}{h}[(1-r_{\rightarrow\rightarrow})(\mu_{L\rightarrow}) - r_{\leftarrow\rightarrow}\mu_{L\leftarrow} - t_{\rightarrow\rightarrow}\mu_{R\rightarrow} - t_{\leftarrow\rightarrow}\mu_{R\leftarrow}], \tag{2.16}$$

$$I_{L\leftarrow} = -\frac{Ne}{h}[-r_{\rightarrow\leftarrow}\mu_{L\rightarrow} + (1-r_{\leftarrow\leftarrow})\mu_{L\leftarrow} - t_{\rightarrow\leftarrow}\mu_{R\rightarrow} - t_{\leftarrow\leftarrow}\mu_{R\leftarrow}]. \tag{2.17}$$

Here we notice the contribution of both spin accumulation and direct spin, using the equations in 12 we relate $\mu_{R\rightarrow}$ with each $\mu_{L\rightarrow} = \mu_L + \mu sL$ and so on with the other important relations that are going to be used along the text:

$$\begin{aligned} \mu_{L\rightarrow} &= \mu_L + \mu_{sL} & \qquad 2\mu_L &= \mu_{L\rightarrow} + \mu_{L\leftarrow} \\ \mu_{L\leftarrow} &= \mu_L - \mu_{sL} & 2\mu_R &= \mu_{R\rightarrow} + \mu_{R\leftarrow} \\ \mu_{R\rightarrow} &= \mu_R + \mu_{sR} & 2\mu_{sR} &= \mu_{L\rightarrow} - \mu_{L\leftarrow} \\ \mu_{R\leftarrow} &= \mu_R - \mu_{sR} & 2\mu_{sL} &= \mu_{R\rightarrow} - \mu_{R\leftarrow} \end{aligned}$$

Now the actual formula I_L represents the current flowing at the left lead (subscript). The expression 2.18 contemplates all the contributions of electrons that are reflected and transmitted and which includes their spin-state:

$$\begin{aligned} I_L = -\frac{Ne}{h}[&(-r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} - r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow} + 2)(\mu_L) + (-r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} + r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow})(\mu_{sL}) \\ &+(t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\leftarrow} - t_{\leftarrow\rightarrow})(\mu_{sR}) + (-t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_R)] \end{aligned} \tag{2.18}$$

Following our spin model we reach to important relations, here we replace the expression by a more simplified one. Here the values of r and t represent probability of being transmitted or reflected from an initial to a final state as their subscripts shows. γ_t represent the contribution of the chiral component that is transmitted and γ_t of being reflected. Notice the sign here is fundamental, because it is related to the chirality of the molecule. Another important factor to take into account is the P_t and P_r, which are intrinsically related to the spin by the polarization. We must be rigorous at the analysis of this polarization because it represents fundamental part at the spin selectivity. All of these relations follow charge conservation rules so we end up with an expression of I_L,

$$\begin{aligned} t &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow} & P_t &= (t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})/t \\ r &= r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow} + r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow} = 2 - t & P_r &= (r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} + r_{\leftarrow\rightarrow} - r_{\leftarrow\leftarrow})/r \\ \gamma_t &= t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow} & s &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow} \\ \gamma_r &= r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} - r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow} - 2 & &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow}, \end{aligned}$$

from[4,5] we obtain:

$$I_L = -\frac{Ne}{h}[\mu_{sL}(S) + \mu_{sR}(S) + \mu_L(t) - \mu_R(t)]. \tag{2.19}$$

Finally, we could write an equation in the form:

$$I_L = -\frac{Ne}{h}[(\mu_L - \mu_R)(t) + \mu_{sL}(S) + \mu_{sR}(S)], \tag{2.20}$$

or in matrix form:

$$I_L = -\frac{Ne}{h}(t \quad s \quad s)\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix}. \tag{2.21}$$

Here we observe a direct dependence that came from spin accumulation and detection.The next term we need to take care of is the accumulation of spin, so we calculate the difference of left and right in each part of the reservoir. The spin accumulation current at the left part of the device is: $I_{sL} = (I_{L\rightarrow} - I_{L\leftarrow})$. Then, to fulfill the derivation of the matrix, we derive and add the contribution of spin accumulation current at the Right $I_{sR} = (I_{R\rightarrow} - I_{R\leftarrow})$ and as previously showed at the Left side (I_{sL}). Replacing by the terms that explains and relates the polarization of spin in different elements we have that: P_t and P_r are the CISS-induced spin polarization of the transmitted T and reflected R electrons:

$$= -\frac{Ne}{h}\left[-\mu_L P_r r - \mu_{sL}\gamma_r + \mu_R P_t t - \mu_{sR}\gamma_t\right]. \tag{2.22}$$

An important assumption that Yang and Van Wess make is that $P_t t = P_r r$, so we can rewrite the equations on the form of a equation with 3 variables. Later on you'll see how it arrive in a 3x3 matrix required by Onsager Reciprocity[19]:

$$-I_{sL} = -\frac{Ne}{h}[(\mu_L - \mu_R)P_r r + \mu_{sL}\gamma_r + \mu_{sR}\gamma_t], \tag{2.23}$$

$$-I_{sL} = \frac{Ne}{h}(P_r r \quad \gamma_r \quad \gamma t)\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix}. \tag{2.24}$$

For the last term of our transport matrix, we will solve for the other part of the current the R side:

$$I_{sR} = \frac{Ne}{h}[(\mu_L - \mu_R)P_t t + \mu_{sL}\gamma_t + \mu_{sR}\gamma_r] \tag{2.25}$$

So in order to find the third row we must analyze the current from the right side of the molecule with defining charge current as: $-I_R = I_{R\rightarrow}+I_{R\leftarrow}$ we have:

$$I_{R\rightarrow} = -\frac{Ne}{h}[(1 - r_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) - r_{\rightarrow\leftarrow}\mu_{R\leftarrow} - t_{\rightarrow\rightarrow}\mu_{L\rightarrow} - t_{\leftarrow\rightarrow}\mu_{L\leftarrow}], \tag{2.26}$$

$$I_{R\leftarrow} = -\frac{Ne}{h}[-r_{\leftarrow\rightarrow}\mu_{R\rightarrow} + (1 - r_{\rightarrow\rightarrow})\mu_{R\leftarrow} - t_{\rightarrow\leftarrow}\mu_{L\rightarrow} - t_{\leftarrow\leftarrow}\mu_{L\leftarrow}]. \tag{2.27}$$

Following charge current equation we denote spin accumulation on the right side of the molecule as:$-I_{sR}$=($I_{R\rightarrow}$-$I_{R\leftarrow}$) and then with the respective changes we obtained:

$$-I_{sR} = -\frac{Ne}{h}[(P_r r)(\mu_R) - (P_t t)(\mu_L) + (-\gamma_t)(\mu_{sL}) + (-\gamma_r)(\mu_{sR})] \tag{2.28}$$

because of the relation $P_t t = P_r r$,

$$I_{sR} = -\frac{Ne}{h}(P_t t \quad \gamma_t \quad \gamma r)\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix}. \tag{2.29}$$

$$\begin{pmatrix} I \\ -I_{sL} \\ I_{sR} \end{pmatrix} = -\frac{Ne}{h}\begin{pmatrix} t & s & s \\ P_r r & \gamma_r & \gamma_t \\ P_t t & \gamma_t & \gamma_r \end{pmatrix}\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{2.30}$$

Once we arrive at our transport matrix we should start to break down each element. The system is summarized in the form of a 3x3 symmetric matrix. Each element is a linear combination of the spin-space matrices of transmission $\mathbb{T}$ and reflection $\mathbb{R}$, t represents the average transmission probability of spin-charge r is the reflection term. P_r and P_t are the spin-polarized electron average transmission or reflection that appears from nowhere. Remember that in a specific space where something is happening, we have to induce the electricity and conductance.

2.3.1 Ferromagnet

Once we have derived correctly the transport Matrix we start by taking apart the ferromagnetic part. As we have a 3x3 Matrix when studying the elements of Figure 2.3 the reciprocity allows us to separate the right and left contributions.

Each contribution would be tackled in an individual way. When we have delimited the direction of the current and by locating the problem to an specific place of the set up we have:

$$I_{\rightarrow} = -\frac{1}{e}G_{\rightarrow}[\mu_L - (\mu_R + \mu_{sR})], \tag{2.31}$$

$$I_{\leftarrow} = -\frac{1}{e}G_{\leftarrow}[\mu_L - (\mu_R - \mu_{sR})], \tag{2.32}$$

$$I = I_{\rightarrow} + I_{\leftarrow} = -\frac{1}{e}[\mu_L(G_{\rightarrow} + G_{\leftarrow}) - \mu_R(G_{\rightarrow} + G_{\leftarrow}) - \mu_{sR}(G_{\rightarrow} - G_{\leftarrow})]. \tag{2.33}$$

In equation 2.32 we present the net contribution current from the spin right electrons. Even if we are located at the left side contemplating the left reservoir part we must take into account both spin right and spin left contributions of the current.

$$I = -\frac{1}{e}[\mu_L(G_{\rightarrow} + G_{\leftarrow}) - \mu_R(G_{\rightarrow} + G_{\leftarrow}) - \mu_{sR}(G_{\rightarrow} - G_{\leftarrow})]. \tag{2.34}$$

Then by separating the perfect transport to a more real one we have: $G_{FM} = T$ and $P_{FM} = \frac{G_{\rightarrow} - G_{\leftarrow}}{G_{\rightarrow} + G_{\leftarrow}}$

$$I = -\frac{1}{e}[\mu_L(G_{FM}) - \mu_R(G_{FM}) - \mu_{sR}(G_{FM})P_{FM}].$$

As we know the total current, taking into account both spins which replacing G_{FM} that represent ideal transport to T and joining terms, we have:

$$I = I_{\rightarrow} + I_{\leftarrow} = -\frac{1}{e}[(\mu_L - \mu_R)T - \mu_{sR}P_{FM}T]. \tag{2.35}$$

Spin accumulation R side transmission coefficient is in the range of $0 \leq T \leq 2$. Remember that the terms of spin transmission accumulation are defined as the difference in the currents of the two different spins at the left side of the system, $I_s = I_{\rightarrow} - I_{\leftarrow}$:

$$I_{sR} = I_{\rightarrow} - I_{\leftarrow} = -\frac{1}{e}[\mu_L(G_{\rightarrow} - G_{\leftarrow}) - \mu_R(G_{\rightarrow} - G_{\leftarrow}) - \mu_{sR}(G_{\rightarrow} + G_{\leftarrow})], \tag{2.36}$$

$$I_{sR} = I_{\rightarrow} - I_{\leftarrow} = -\frac{1}{e}[(\mu_L - \mu_R)(G_{\rightarrow} - G_{\leftarrow}) - \mu_{sR}(G_{\rightarrow} + G_{\leftarrow})],$$

$$I_{sR} = -\frac{1}{e}[P_{FM}(\mu_L - \mu_R)(G_{FM}) - \mu_{sR}(G_{FM})],$$

$$I_{sR} = -\frac{1}{e}[P_{FM}(\mu_L - \mu_R)T - \mu_{sR}T].$$

Finally, we arrive to the matrix 2.37 which is the space-spin set of equations, which are the current and the spin current accumulation:

$$I = -\frac{1}{e}[(\mu_L - \mu_R)T - \mu_{sR}P_{FM}T],$$

$$I_{sR} = -\frac{1}{e}[P_{FM}(\mu_L - \mu_R)T - \mu_{sR}T]$$

Using matrix form we get:

$$\begin{pmatrix} I \\ I_{sR} \end{pmatrix} = -\frac{N'e}{h}\begin{pmatrix} T & -P_{FM}T \\ P_{FM}T & -T \end{pmatrix}\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sR} \end{pmatrix}. \tag{2.37}$$

Where the presence of accumulation of spin in voltage carrier is denoted by μ_{sR}. Until here we have made further analysis of what is happening inside the ferromagnet. What could we infer from these forms of the ferromagnet connected to a reservoir? we explain how is it possible to measure a 2T device spin dependency. As we have mentioned the best way to introduce and explain the problem is by the inclusion of our measurements of the conductance, but first; we include a brief description of how is it possible that an MR signal can occur when an external voltage is applied through the ferromagnet or the chiral component. Lets talk a little bit about how is it possible to measure the spin-charge contribution. As you remember we introduces the conductance as an indicator of electrical conduction, by the extension of this concept of the electric conductance presented in 2.2, we can add the spin freedom degree into the analysis, we apply:

$$\begin{array}{cc} G_1 = \frac{N'e^2}{h}T & G_2 = -\frac{N'e^2}{h}P_{FM}T \\ G_3 = \frac{N'e^2}{h}P_{FM}T & G_4 = -\frac{N'e^2}{h}T \end{array} \tag{2.38}$$

$$\begin{pmatrix} I \\ I_{sR} \end{pmatrix} = -\frac{1}{e}\begin{pmatrix} G_1 & G_2 \\ G_3 & G_4 \end{pmatrix}\begin{pmatrix} \mu_L - \mu \\ \mu_s \end{pmatrix} \tag{2.39}$$

Notice that the measurement from G_2 = -G_3 presents the form of an asymmetric matrix whit its respective different off-diagonal elements. The second part analyzed for FM goes principally at the edge where we can make assumptions from the fragment and the node. We implement a "node" at the problem because at the node we represent phonon-electrons interaction and inelastic events. These events are not specifically analyzed but are the responses to the creation of spin accumulation as well as the final current transport of our systems. As you could observe the FM propose an inversion of spin so we could not observe what is happening at the node because it is located at the center of the device. Moreover we could not say clear what is happening at the node. There is no signal or a total clarification of the node's role in the system.

2.3.2 Chiral Component

spin contribution is studied separately, so we denote $t + r = 2$ to keep the conditions of charge conservation:

$$\begin{aligned} t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} + r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow} &= 1, \\ t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow} &= 1. \end{aligned} \tag{2.40}$$

With these equations, we continue to describe the important roles of the matrix elements. Going on with the calculations we obtained of the scattering matrix at 2.2, to relate with spin and describe the terms of the molecule acting on the system we have:

$$\begin{aligned} \gamma_r &= r - (P_r r + s)/\eta_r - 2 = -t - (P_r r + s)/\eta_r \\ \gamma_t &= -t + (P_t t + s)/\eta_t, \end{aligned} \tag{2.41}$$

$$\begin{aligned} \eta_r &= \frac{r_{\leftarrow\rightarrow} - r_{\rightarrow\leftarrow}}{r_{\leftarrow\rightarrow} + r_{\rightarrow\leftarrow}}, \\ \eta_t &= \frac{t_{\rightarrow\rightarrow} - t_{\leftarrow\leftarrow}}{t_{\rightarrow\rightarrow} + t_{\leftarrow\leftarrow}}, \end{aligned} \tag{2.42}$$

γ_r represent electron-spin reflection contribution probability at the molecule and γ_t the transport probability. These probabilities are quantities that depends of transmission/reflection.

$$\begin{aligned} P_t t = P_r r &= s, \\ t_{\rightarrow\leftarrow} &= t_{\leftarrow\rightarrow,} \\ r_{\rightarrow\rightarrow} &= r_{\leftarrow\leftarrow,} \\ t_{\rightarrow\rightarrow} - t_{\leftarrow\leftarrow} &= r_{\leftarrow\rightarrow} - r_{\rightarrow\leftarrow}. \end{aligned} \tag{2.43}$$

The condition of $P_t t = P_r r = s$ is fundamental to make the transport matrix symmetrical which is a requirement of Onsager Reciprocity to the possible aplication at Yang's work[4,5,19]. Taking advantage of this symmetry at 2.43 the terms of transmission with different spin states are equal by contrast reflection terms with different spin states are different.

$$\begin{aligned} \gamma_r &= -(1 + 2P_t/\eta_r)\,t \\ \gamma_t &= -(1 - 2P_t/\eta_t)\,t \end{aligned} \tag{2.44}$$

$$\begin{pmatrix} I \\ -I_{sL} \\ I_{sR} \end{pmatrix} = -\frac{Ne}{h} \begin{pmatrix} t & P_t t & P_t t \\ P_t t & -(1 + 2P_t/\eta_r)\,t & -(1 - 2P_t/\eta_t)\,t \\ P_t t & -(1 - 2P_t/\eta_t)\,t & -(1 + 2P_t/\eta_r)\,t \end{pmatrix} \begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{2.45}$$

$$\begin{pmatrix} I \\ -I_{sL} \end{pmatrix} = -\frac{Ne}{h} \begin{pmatrix} t & P_t t \\ P_t t & -(1 + 2P_t/\eta_r)\,t \end{pmatrix} \begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \end{pmatrix} \tag{2.46}$$

Now from the chiral components we arrive to the spin contributions :

$$\begin{array}{ll} g_1 = \frac{Ne^2}{h} t & g_2 = \frac{Ne^2}{h} P_t t \\ g_3 = \frac{Ne^2}{h} P_t t & g_4 = -\frac{Ne^2}{h}(1 + \frac{2P_t}{\eta_r})t \end{array} \tag{2.47}$$

$$\begin{pmatrix} I \\ I_{sl} \end{pmatrix} = -\frac{1}{e} \begin{pmatrix} g_1 & g_2 \\ g_3 & g_4 \end{pmatrix} \begin{pmatrix} \mu - \mu_R \\ \mu_s \end{pmatrix} \tag{2.48}$$

Fundamental relations are just used to bring spin-charge. In contrast with the Ferromagnet here we observe a symmetry form of the matrix where g_3 and g_2 are the same, we can observe how in 2.45 the matrix is reduced and equal off-diagonal elements of the matrix suggest a spin selectivity behavior.

2.4 Time Reversal and Magnetization

Lars Onsager developed a general theory capable of handle more than two thermodynamic forces of one system. He presented a relation in the time-reversibly of electrons and its magnetic field as well as its magnetization. The preservation of this reciprocal rules to Onsager are fundamental to the conduction in linear regime and could by magnetic effects[19,22]. Following Buttikker's reasoning, we arrived at the spin-charge transport case, it lets us know that in some parts of the procedure there is an irreversible process that creates an accumulation of voltage. Which is measured by μ_s as accumulation of spin. The importance of the magnetic field in the symmetry theorems seems crucial wherein time-reversal changes and some values stop creating their contribution.

$$T_{ij}(H, M) = T_{ji}(-H, -M) \tag{2.49}$$

The presence of an external magnetic field could mean polarization of the electrons at the contacts, which is explained by the time-reversible process. We must be careful with this interaction of the fields with the electrons, the principal actors P_r and P_t are polarized on reflection and transmission respectively. We do not assume the chiral component to fulfill this reversibility because it has always a positive sign as a result of symmetry. In the case of P_{FM} which notably just takes care of the Ferromagnet. The magnetization direction at the FM is parallel to the magnetic field, we choose an effective direction that follows the current direction to reduce the problem of study. This becomes fundamental in the analysis of transmission. We can notice that at FM polarization changes sign. Which means:

$$\begin{array}{ll} t = t_{\rightarrow\rightarrow} \geq t_{\rightarrow\leftarrow}, & t = t_{\leftarrow\rightarrow} \geq t_{\leftarrow\leftarrow}, \\ t = t_{\rightarrow\rightarrow} \leq t_{\rightarrow\leftarrow}, & t = t_{\leftarrow\rightarrow} \leq t_{\leftarrow\leftarrow} \end{array}$$

$$\begin{array}{ll} g_1 = \frac{Ne^2}{h} t & g_2 = \frac{Ne^2}{h} P_t t \\ g_3 = \frac{Ne^2}{h} P_t t & g_4 = -\frac{Ne^2}{h}(1 + \frac{2P_t}{\eta_r} t) \end{array} \tag{2.50}$$

$$P_t = \frac{(t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})}{t}$$

$$t = (t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow})$$

This allows the chiral component to be independent of the magnetization but and at the ferromagnet we observe that when we have a reversal of magnetic field the P_{FM} = - P_{FM}. Due to the magnetic field which is parallel and that the relations obtained for G_2 = - G_3 could be observed because it happens when we applied and external magnetic field. In terms of the chiral component it is showed that g_2=g_3, creating a direct relation.

Let's note what is happening at the tunnelling model where we only use energy dependency to understand what is happening. Our expressions are proposed to be energy independent, so the use of tunneling is a way to show the breaking of Onsager relations. Even if the contribution will be at a non-linear level, the measurement is at linear regime so we expect fundamental relations. Here at the edge on the left we introduce the chemical potential at left side (L), μ_L who is separated by an energy gap from the right component Which is explained as an energy barrier. The way to overlap the barrier is injecting positive or negative electrons, in the previous section we observed that there are many forms to provide electrons as photo-emission, injection of a bias voltage, Etc.The difference of electrochemical potentials is called spin accumulation, it could also be observed as the contribution of each spin but in one side is opposite to the movement so it gets stuck here creating an accumulation of spin.

Chapter 3

Results & Discussion

3.1 2 Terminal CISS Correction model [*]

For each grouping of results, which may, for example, be from separate publications, the results together with their discussion may be broken into separate sections. Each section heading should include a footnote stating if anyone other than the author was involved in obtaining this group of results and their analysis, and if any publication resulted.

Once the description of the generic 2T circuit is clear and the states of Spin and Charge Transport have been addressed, we go further in the characterization of experimental methods in order to propose complementary calculation and correction of the previously 2T electron transport mechanism proposed. Furthermore to make a proper measurement of the CISS effect we would need to add some elements which will provide a better comprehension of the spin contribution to the total current in the linear regime. In this section we propose an addition to the 2T device which take into account charge distribution and accumulation of spin. In a three-terminal measurement we could tackle this contribution precisely. With the results of the proposed charge-spin signals Bart argues that the voltage generated by the spin accumulation μ_s of a chiral molecule could be conjugated by the voltage generated by the FM that reacts to this voltage.

3.1.1 Proposal of the model

The description exposed in the previous chapters includes the demonstration of possible real solid-devices measured at linear regime. With the presence of a node which was previously exposed as a circle we could identify and understand how could we manage to inter convert spin and charge. As it was stated, because of the existence of 2 different processes that are happening at the same time the current that induces an electron-spin accumulation in fact it becomes the node the responsible to possible measurements.

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[*] "Detecting Chirality in Two-Terminal Electronic Nanodevices *Nano Letters* **2020**, *20(8)*, 6148–6145.

Different Magnetic signals could be taken because of the FM but The first one is caused by the ones that go inside the node. The fact that measurements are taken from the edges of the reservoir from where MR is always presented. Make it impossible to determine the exact contribution of the node to the system. The two processes mentioned before happen inside our circuit, before getting the edges the signal is interconverted and canceled, reaching only one signal. The author judges the total potential difference at the edges of our scheme where the reservoirs are located but not by the potential difference between metal and ferromagnet. They are assuming the accumulation of spin at this part is 0, so they are not taking into account the spin accumulation contribution. See Fig 2.2

We start our the results proposal by presenting Figure 3.1 which is an extended version of a 2T device. Here we have implanted a Metallic gap which we could assume a good conductor (Ag or Ni), next to the Ferromagnet. Is important to be sure how and why do we add this elements. By previous Spintronic experiments[9,18] using molecular junction we notice that to find measurements from molecules we need to join the molecule to an afine metal. Once the molecule is embedded in the metal we could take measurements related to the metal polarization. Chiral molecules have special properties as it inversion center that makes the effect possible, this molecules could be extended with some other molecule or material that have affinity with their edges.

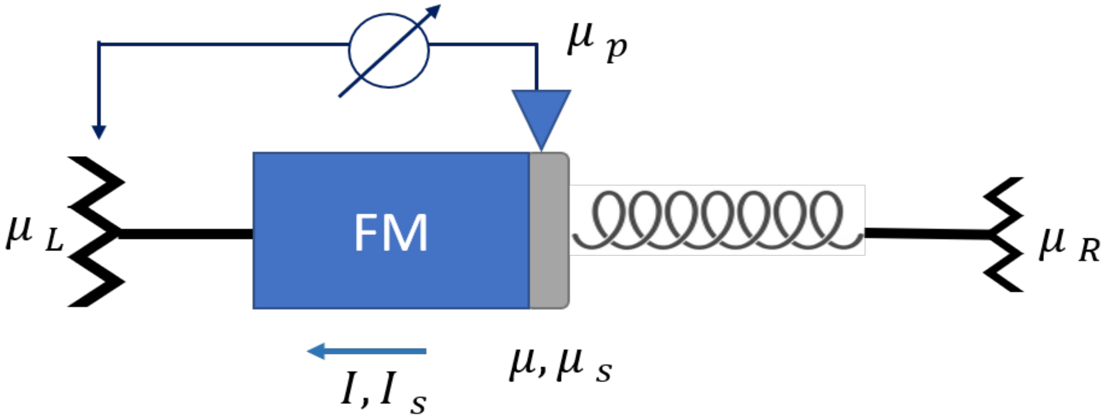

Figure 3.1: 3T device with the measurement of Spin accumulation and the proper treatment of the Node

So we propose to make a measurement at exactly at the joining of metal and ferromagnet. We include a tip at the node from where is possible to could make the measurements of the spin-charge contribution. At the node some interesting processes occurs as: the interaction electron-electron and electron-phonon, we just assume this interaction happens knowing they are part of inelastic collisions and are not going to affect our measurement.

The value of μ_s known as accumulation of spin is located at the so called node and is possible due to CISS effect. Well even they have proposed an "accurate" form of measurements in a probe between μ_L - μ_R We have shown that the presence of constituents with different chirality are fundamental in order to propagates and creates a spin current. As stated before is fundamental to understand the role of spin filtering along the device. At the node we could notice how the spin momentum and charge direction are randomize and we assume nonlinear effects doesn't affect neither energy or momentum direction.

3.1.2 Multi terminal Measurements

The matrix form of the Ferromagnet part:

$$\begin{pmatrix} I \\ I_{sR} \end{pmatrix} = -\frac{N'e}{h}\begin{pmatrix} T & -P_{FM}T \\ P_{FM}T & -T \end{pmatrix}\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sR} \end{pmatrix} \tag{3.1}$$

This equations are energy independent but depend on the spin-charge. To extend the understanding of what is happening with the FMTJ we conclude there are different conductance' to different spins depending on P_{FM} polarization, we include:

$$G_{FM} = G_{\rightarrow} + G_{\leftarrow}$$

$$P_{FM} = \frac{G_{\rightarrow} - G_{\leftarrow}}{G_{\rightarrow} + G_{\leftarrow}}$$

Where P_{FM} Would need the values of the Transport energy and as we keep in the linear part lets say T is independent of ϵ and T as the probability constant where μ_s+μ=$\mu_{\rightarrow}$. The values of $G_{\rightarrow(\leftarrow)}$ are obtained next and they keep their linear behavior. Keeping T constant we find the actual Current spin contribution of the right spin.

$$\int_{\mu_{\rightarrow}}^{\mu_L} T d\epsilon = T(\mu_L - \mu_{\rightarrow}),$$

$$I_{\rightarrow} = -\frac{N'e}{h}\frac{(1 + P_{FM})}{2}T\,(\mu_L - \mu_{\rightarrow})$$

$$I_{\rightarrow} = -\frac{1}{e}G_{\rightarrow}\,(\mu_L - \mu_s - \mu)$$

We wanted to understand $I_{\rightarrow}$ explicitly so we need to find the values of $G_{\rightarrow}$ and $G_{\rightarrow}$:

$$G_{\rightarrow} = \frac{(1 + P_{FM})}{2}T,$$

$$I_{\rightarrow} + I_{\leftarrow} = -\frac{N'e}{h}(T(\mu_L - \mu) - P_{FM}T\,(\mu_S)),$$

$$I_{\rightarrow} - I_{\leftarrow} = -\frac{N'e}{h}(P_{FM}T(\mu_L - \mu) - T\,(\mu_S)),$$

This derivations are fundamental to understand the formalism and take into account the energy Independence of the P_{FM}. Looking at its difference we obtain the pure equation of the right spin state electron contribution. Notice it is happening at the Left reservoir and at the chemical potential difference accounting signals of spin contributions.

$$2I_{\rightarrow} = -\frac{N'e}{h}\left((\mu_L - \mu)\,T\,(1 + P_{FM}) - T\mu_s(1 + P_{FM})\right)$$

$$= -\frac{N'e}{h}\left(T\,(1 + P_{FM})\,(\mu_L - \mu - \mu_s)\right)$$

$$I_{\rightarrow} = -\frac{N'e}{h}\left(\frac{T\,(1 + P_{FM})}{2}\,(\mu_L - \mu_{\rightarrow})\right) \tag{3.2}$$

Where $\frac{(1+P_{FM})}{2}$ is energy independent we Arrive to the equations used to break reciprocity. The meaning of the integral is to account all the windows difference potential that is between μ_L-$\mu_{\rightarrow}$.

$$I_{\rightarrow} = -\frac{N'e}{h}\left(\frac{1 + P_{FM}}{2}\right)\int_{\mu_{\rightarrow}}^{\mu_L} T(\epsilon)d\epsilon \tag{3.3}$$

And the same but opposite to the current state contribution coming from the left:

$$I_{\leftarrow} = -\frac{N'e}{h}\left(\frac{1 - P_{FM}}{2}\right)\int_{\mu_{\leftarrow}}^{\mu_L} T(\epsilon)d\epsilon \tag{3.4}$$

With $G_{\leftarrow}$:

$$G_{\leftarrow} = \frac{(1 - P_{FM})}{2}T,$$

With the inclusion of these parameters that depends on polarization and the energy window we start to get out of the analysis of the linear regime. A further investigation in the microscopic regime is needed in order to fulfill the complete picture of the phenomena happening at the node. The figure included now is a description of spin polarization measurement as a comparison of the two models. In a) there is the ideal node described in the text, next to a ferromagnet. It is not clear how energy could interact with the node. In contrast at the right part b) use a metal to embed the molecule and make it easier and realistic a real transport of spin.

A real 2T measurement where the spin is taken into account and from where we take some part of this analysis could be found in a setup like the one proposed in the Figure 3.3. They follow and accomplish all the important breaking of reciprocity as well as the same way of measurements. Observe that in the work presented by that men the measure directly at the node in this case a Silver probe and the Ferromagnet as the one we propose. Even though there is no other tip involved the Magnetic field of the Niquel-FM provokes a spin reverse and because of the photo exited molecules added to the metal with the addition of a magnetic field they can flow and create the effect through the dye molecules. We choose this model to understand how we can measure the current in that kind of small system. Also, in their study[25] they figure out that there is no real 2T anyways. always the influence of temperature of the environment is going to affect. Neither we or any or the experiments here were taking thermodynamics parameters others than the emission source.

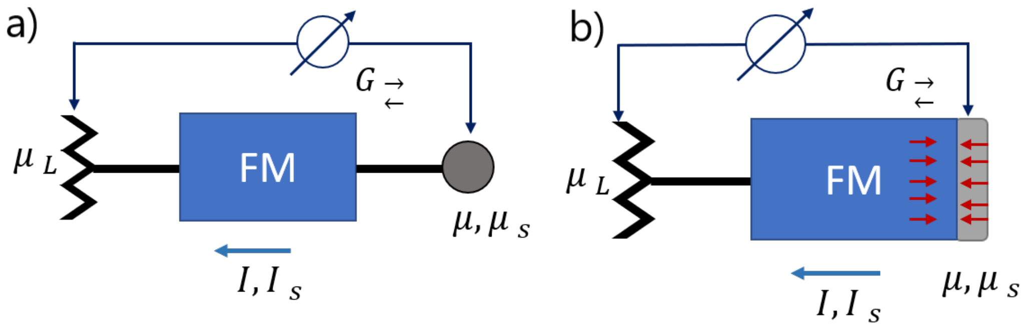

Figure 3.2: Representation of FM Conductance at the Left Reservoir with their spin contribution. Left figure denominated as a) represent hypothetically Yangs model of medition. b) Our transport system which takes into account Polarization of spin at the metal gap.

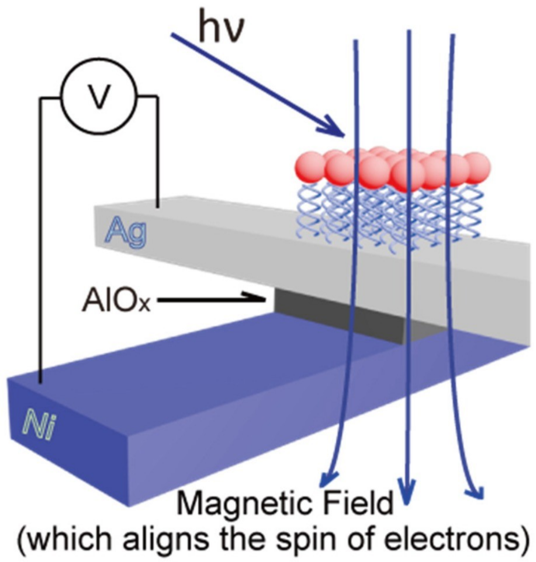

Figure 3.3: (A) Schematic illustration of MEMS application for characterizing the spin selectivity of DNA oligomers

3.1.3 Methodology

We provide a new model, this time it is account for 3 terminals. We want to make the spin contribution surplus so the application and addition of the model is based in our analysis of where and how is the voltage been taken. Lets start by the call of the relations previously obtained for spin-charge transport conductance for the ferromagnet and for the molecule. As we are applying the formalism to a particular set up that uses the same elements from the previously described set ups, we can derive directly from the information provided at the Theoretical Framework.

$$G_1 = \tfrac{N'e^2}{h}T, \qquad G_2 = -\tfrac{N'e^2}{h}P_{FM}T,$$
$$G_3 = \tfrac{N'e^2}{h}P_{FM}T, \qquad G_4 = -\tfrac{N'e^2}{h}T,$$

$$\begin{pmatrix} I \\ I_{sR} \end{pmatrix} = -\frac{1}{e}\begin{pmatrix} G_1 & G_2 \\ G_3 & G_4 \end{pmatrix}\begin{pmatrix} \mu_L - \mu \\ \mu_s \end{pmatrix},$$

$$g_1 = \tfrac{Ne^2}{h}t, \qquad g_2 = \tfrac{Ne^2}{h}P_t t,$$
$$g_3 = \tfrac{Ne^2}{h}P_t t, \quad g_4 = -\tfrac{Ne^2}{h}(1 + \tfrac{2P_t}{\eta_r}t),$$

$$\begin{pmatrix} I \\ I_{sl} \end{pmatrix} = -\frac{1}{e}\begin{pmatrix} g_1 & g_2 \\ g_3 & g_4 \end{pmatrix}\begin{pmatrix} \mu - \mu_R \\ \mu_s \end{pmatrix}.$$

At figure 2.2 we could observe the analysis of the chemical potential where: μ_L-μ_R the interpretation of Yang could be erroneous because he does not present a pure 2T device but as we notice when this kind of measurement happens we neglect the spin contribution and the magneto resistance that couldn't be distinguish. Because the measurement is been taken at the reservoir and the 2 processes active for each component counter each contribution therefore there is no possible CISS measurement.

In contrast the figure 3.1 locates a metal next to the FM making the role of a node but at the same time giving the tip an opportunity to act as a spin valve. So we exposed that in order to pursue the real spin or contribution the real value to be measured or tackle is μ_L-μ due to the fact that at that place we can observe the presence of spin-charge conversion. By combination and derivation of Equations 2.40 and 2.49 we go further and extract new elements that will help us understand the variables inside the node and the FM. Starting by describing μ_s-μ_L where μ_s is described by:

$$\mu_s = [G_3 g_1 + g_3 G_1]\frac{\mu_L - \mu_R}{f},$$

We are looking to obtain a value that connects the Third reservoir described as μ_P. How is it possible? well by the use of this third terminal or reservoir μ_P as it keeps equals to 0 it is only used as a measure point. Where the voltage coming from each side of the reservoir could be differentiate and measured. Then we want to analyse the potential difference of μ_s-μ_L:

$$\begin{aligned} \mu_s - \mu_L &= [G_3 g_1 + g_3 G_1]\frac{\mu_L - \mu_R}{f} - \mu_L, \\ &= \mu_L(\frac{[G_3 g_1 + g_3 G_1]}{f} - 1) - \frac{[G_3 g_1 + g_3 G_1]}{f}\mu_R \end{aligned} \tag{3.5}$$

Notice that for Ferromagnet with the G components we deduce G2=-G3 while for chiral component g2=g3 which show a dependence of the magnetic field that is going to be the responsible of the change of sign and spin-charge movement.[19] The equation 3.1 is a relation that includes the differential potential of $\mu_s - \mu_L$, Even though we now can relate μ_s to μ_L in the node there is still a lack of comprehension of why we need the potential difference from

μ_L - μ_S. We still not have explicitly the value that contributes to this differential potential. We show that in order to fulfil our calculations we need first clarify the contribution at the node.

At the node we introduce the induced characters as spin accumulation μ_s and spin distribution μ their differential potential give us the measurement that normally was taken from[4,24]. The interaction of the chemical potentials at the node is represented:

$$\mu - \mu_s = \mu_R + \Gamma_1(\mu_L - \mu_R) - \Gamma_2(\mu_L - \mu_R), \tag{3.6}$$

where

$$\Gamma_1 = \frac{G_3\,(G_2 - g_2) - G_1\,(G_4 + g_4)}{f},$$
$$\Gamma_2 = \frac{(G_3/G_1 + g_3/g_1)\,G_1 g_1}{f}.$$

Now we present our proposal calculations where at the node we add the contribution of μ_P by the extra tip which is involved only to measure and take into account spin accumulation. Now we may ask to ourselves how can we add the third reservoir and how is it going to influence the spin current. Well the existence of Γ_3 appears naturally from a linear combination of the equations 3.2 and 3.4 but is physically needed in order to explain events that are not measured in Bart's model. The current comes from the left reservoir and the node which shows us the spin contribution in the general form.

$$\begin{aligned}
\mu_s - \Gamma_3(\mu_L - \mu_R) - \mu_L &= \mu_R + \Gamma_1(\mu_L - \mu_R) - \Gamma_2(\mu_L - \mu_R),\\
\mu_s - \mu_L &= \mu_R + \Gamma_1(\mu_L - \mu_R) - \Gamma_2(\mu_L - \mu_R) + \Gamma_3(\mu_L - \mu_R),\\
\mu_s - \mu_L &= \mu_R + \Gamma_1(\mu_L - \mu_R) - \Gamma_2(\mu_L - \mu_R) + \Gamma_3(\mu_L - \mu_R).
\end{aligned} \tag{3.7}$$

We Γ_3 add as an extra contribution coming from μ_P to take in count it comes from the value of μ taking into account the L side. This energy independent value Γ_3 have a chiral dependence at g_3 we have that:

$$\Gamma_3 = \frac{g_3\,(g_2 - G_2) - g_1\,(G_4 + g_4)}{f}.$$

The Γ_3 factor goes in the middle of the chemical differential potential as the 3T would act. Because Metal has an affinity to join molecules which in a dissolved medium get embedded to it by their different charges. In the metal as observed in experiments when electrons are involved in a magnetic field the polarization is presented in their spin. The magnetization aligns with their spin and allows electrons with this polarization a higher probability to transport.

So finally

$$\mu_L - \mu_S = \mu_R + \Gamma_1(\mu_L - \mu_R) - \Gamma_2(\mu_L - \mu_R) + \Gamma_3(\mu_L - \mu_R),$$

$$\mu_L - \mu_S = \mu_R + (\Gamma_1 - \Gamma_2 + \Gamma_3)(\mu_L - \mu_R),$$

$$\mu_L - \mu_S = \mu_R + (\frac{G_3\,(G_2 - g_2) - G_1\,(G_4 + g_4)}{f} + \frac{(G_3/G_1 + g_3/g_1)\,G_1 g_1}{f} + \frac{g_3\,(g_2 - G_2) - g_1\,(G_4 + g_4)}{f})(\mu_L - \mu_R), \tag{3.8}$$

$$\mu_L - \mu_S = \frac{g_3^2 - (g_1 + g_2 + G_2 + g_3)G_3 - g_1 g_4 - g_1 G_4 - G_1(g_3 + g_4 + G_4)}{f}, \tag{3.9}$$

$$\mu_L - \mu_S = g_3^2 - g_3 G_3 - G_1 g_3 + G_3^2. \tag{3.10}$$

3.2 DISCUSSION *

The principal discussion of the document stands in the efficiency of different circuit geometry of solid-state devices capable of measuring and differentiating the CISS effect at a linear regime. The model presented by Yang is not valid to effectively measure. On the other hand, our model adds an extra reservoir, it could measure the spin accumulation. Let's remember how our system could measure something like the CISS effect. Because it measures the accumulation induced by the current coming from the molecule. When electrons pass the molecule they get polarized so a high percentage of the electrons with the same polarization as the molecule is likely to be transported. Once they arrive at the metal electrons are no longer polarized indeed by the magnetization of electrons they could change their direction. In our system due to the Third fictitious TERMINAL/reservoir which preserves its net current equal to 0 and the signals that go in and out of it would create a change in its phase signal. Even our study doesn't take measurements or directly assume dephasing it is extremely ligated to our model.

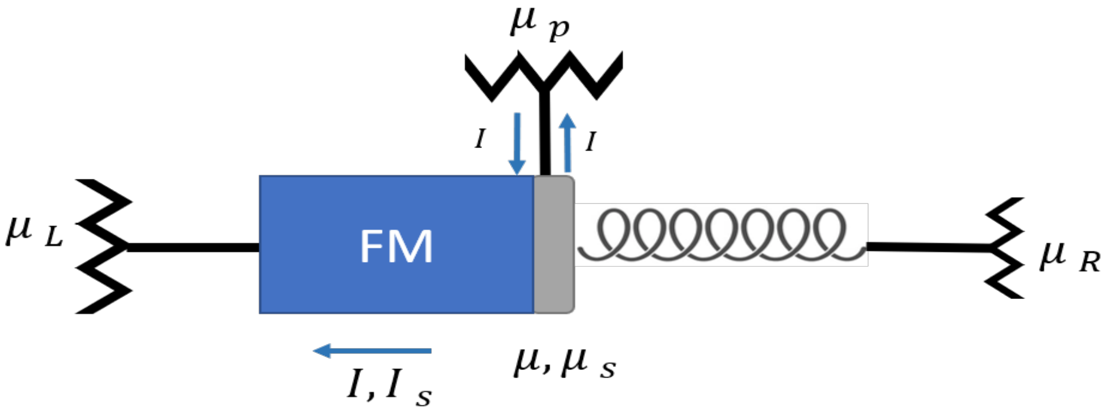

Figure 3.4: (A) Schematic illustration of MEMS application for characterizing the spin selectivity of DNA oligomers

The reciprocity is broken by the addition of a magnetic field, thisaction happens at nonlinear regime, where the dephasing take place. The model compared with the Yang give the reader more information and proper measurements applied to possible future works. This dephasing effect becomes fundamental in our transport system. In a 3 Terminal

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*Footnote stating who the work described in this section was performed in collaboration with, and stating if it is adapted from a publication, e.g., "Photoinduced Absorption within Single-Walled Carbon Nanotube Systems", *J. Phys. Chem. C* **2015**, *120*, 1926–1935.

device that was probing and has a geometry of the triangle. The effect of dephasing is the one in charge of creating current flowing as.[11] Another fact of 3T devices is that depending on their geometry we can find the CISS effect without using FM or magnetic fields and without the presence of these fields, the molecule acts as an active rotor and provokes CISS and are also electrochemical dependence.

Something to add here at the discussion is to clarify the importance of the setup and interaction of the matrix systems with the conduction of electrons with spin. The geometry of the circuit of electron transport proposed is useful even for big molecules. As the metal is joined to the FM the spin accumulation keeps inside metal and is influenced by FM and the chiral molecule. Is evident from here the existence and the possible manipulation of this formalism even there is no complete picture of the physics behind the molecule we can use important characteristic of what we have as its chirality (symetric, asymetric).

Chapter 4

Conclusions & Outlook

We derived a macroscopic circuit model based on symmetries of the elements of the circuit: FM and Molecule, that are reflected in the transmission and reflection matrix equations. The analytical results studied by Yan, Van Wess et al.[16,17,24] present a two terminal device whose elements and equations could be obtained relating transport and reflection matrices and performing linear transformations. The measurements provided was taken at the edges of our device, a signal taken from here is affected by the processes happening inside. Processes such as electron-phonon and scattering events take place in the node where it was represented as the accumulation of spin. The position of the measurement ended up being an important variable, when the signal was taken from the edge of the terminals there was nothing that measures the node so the spin-transport is not successfully measured. A three terminal device model appears when we imply to measure the node, whit the addition of an extra reservoir or a metallic tip. The existence of this extra tip could help us find preciser measurements inside the device including each element separately.

We conclude the circuit-geometry of a spin-charge transport device is fundamental to taking suitable measurements and distinguishing between spin accumulation, spin distribution, and spin contribution of one specific side or any system. The multi-terminals description of the transport for more than 2 reservoirs represents a helpful tool for the efficient correction of the model. With an extra reservoir involved at the node, it will facilitates the information of the change of voltages this reservoir might exhibit is the key to correcting and presenting an efficient 3T model.The future applications and knowledge to obtain from here is enormous.We reproduce a macroscopic approach based on symmetries theorems of transmission for matrices in 2T. The results obtained here present the importance of this formalism and its proper manipulation in order to obtain spin contribution at the linear-regime.

The possibilities of future research are wide open because of the applications in solid devices and spintronics. Our model fuzzed with a chiral molecule extended microscopic theory like the ones provided by[2,9,16,26] which are the pioneers of molecule electronics have shown important advances in the field and is projected to generate more investigation for at least 5 more years. The future contribution of this guidebook lies in the possibility to parametrize the result with thigh binding theory. Also, the results proposed by Yang where the tunneling is reached at a non-linear regime are important in order to understand how the effects of energy dependence can break reciprocity and the application of a bias potential could be an alternative to obtain current transport in molecular components in an efficient way. At our study we have obtain different appears at the example of Yang and is a bias induced transport. To obtain a pure 2T device like the example explained in the introduction of Aragonez et al.[2] we have to fulfill some conductive requirements. We asked ourselves some questions about how it is possible for the molecules to present such a high percentage of transport without really being damaged at all.

Appendix A

Conductance for FM and Chiral molecule

We will introduce or at least insert all the calculations and relations that appears with in the node in order to check measurements and so on. Our suggestion is that they are committing an error at the representation of calculations from different experiment and perspectives we have shown an. Also once we have this we can checking the experimental values and ligate this with our experimental results. Let's start by rearranging results and calculations proposed by the notes. Keep explaining with detail each line you plasm. The most part of this modeling could look annoying but finally is interesting and have a great vision to future applications.

So from notes we have to let things clear about the calculation and so on. If you want to get the curves as a probing results is okay. But what we really need is Probes from butikker experiments.Now, let's upload all the experiments and calculations of spin dependence introduced at the matrices level. So first we look at the way the set up is builded:

$$\begin{pmatrix} I \\ -I_{sL} \end{pmatrix} = -\frac{Ne}{h} \begin{pmatrix} t & P_t t \\ P_t t & -(1+2P_t/\eta_r)\,t \end{pmatrix} \begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \end{pmatrix}, \tag{A.1}$$

This first replace or approximation gotten by reduction of the transport Matrix. By a 2x2 Matrix that involves principally the behavior of the chiral component[4,5].

$$\begin{pmatrix} I \\ I_{sR} \end{pmatrix} = -\frac{N'e}{h} \begin{pmatrix} \bar{T}\big|_{\mu}^{\mu_L} & -P_{FM}T|_{\epsilon=\mu} \\ P_{FM}\bar{T}\big|_{\mu}^{\mu_L} & -T|_{\epsilon=\mu} \end{pmatrix} \begin{pmatrix} \mu_L - \mu \\ \mu_s \end{pmatrix}, \tag{A.2}$$

On the other hand we have find a matrix 2x2 that describes the importance of the analysis at the ferromagnet. You can notice the different cog notation of $\mathbb{T}$ where it fully depend on the energy inside the integral or the energy that is enhanced by the chemical potentials. Is interesting to show how the Ferromagnet Polarization is not affected by energy. The value of$\mathbb{T}$ here will depend on a transmission function where scattering is possible to occur.[4]

$$\begin{pmatrix} I \\ I_s \end{pmatrix} = -\frac{1}{e} \begin{pmatrix} G_1 & G_2 \\ G_3 & G_4 \end{pmatrix} \begin{pmatrix} \mu_L - \mu \\ \mu_s \end{pmatrix}, \tag{A.3}$$

So this are the equations after the Transport relations where we can evaluate and principally give one contribution sense in terms of the other. So once we have these the conductance relations obtained from the spin-space matrices we proceed to create a formal relation to enhance this explanation o a general one. So we have:

$$\begin{pmatrix} I \\ I_s \end{pmatrix} = -\frac{1}{e}\begin{pmatrix} g_1 & g_2 \\ g_3 & g_4 \end{pmatrix}\begin{pmatrix} \mu - \mu_R \\ \mu_s \end{pmatrix}, \tag{A.4}$$

Well first introduction to rearrange the equations by the application of some changes and overlooked of how each part provides an unique contribution. Let's introduce the derivations and relations of this matrices in order to convert them into spin-electron signals. I will present and understand the derivations at first. Also remembering taking into account the spin injection,detection and how do we manipulate those signals. In terms of Conductance, Spin-charge accumulation, probes and spin currents taking into account each spin contribution. Joining A.3 to A.4 we could found found the real contribution that can be tacked into account. When we approximate linear regime state we compare and state that they are equal at this part.

$$\begin{aligned} \mu &= \mu_R + \frac{G_3\,(G_2 - g_2) - G_1\,(G_4 + g_4)}{f}\,(\mu_L - \mu_R) \\ &= \mu_L - \frac{g_3\,(g_2 - G_2) - g_1\,(G_4 + g_4)}{f}\,(\mu_L - \mu_R) \end{aligned} \tag{A.5}$$

$$\mu_s = \frac{(G_3/G_1 + g_3/g_1)\,G_1 g_1}{f}\,(\mu_L - \mu_R) \tag{A.6}$$

$$I = \frac{G_1 g_2 g_3 + g_1 G_2 G_3 - G_1 g_1\,(G_4 + g_4)}{f}\,(\mu_L - \mu_R) \tag{A.7}$$

$$f = (G_3 - g_3)\,(G_2 - g_2) - (G_1 + g_1)\,(G_4 + g_4) \tag{A.8}$$

So these are the main formulas that we want to derive. How is it possible because at a steady state the continuity condition requires the currents I and I_s are equal in both subequations^{4,5}. Lets be careful about how we treat them and lets start to analyze and upload the important ones. We observe the dependence of f on $(G_3$-$g_3)(G_2$-$g_2)$ and at linear-regime the conductance values at FM are G_3=-G_2 and the chiral molecule component keeps the same g_2=g_3. We obtain it directly of the Matrix from FM and CISS obtained in Chapter 2.

spin accumulation μ_s depends on G_3 and g_3 but **spin distribution** μ depends on G_3 g_2 or g_3 G_2. So notice that both accumulation and distribution of spin change at magnetization or by the reversibility of the chiral component.

$$\begin{aligned} I &= -\frac{1}{e}\left(G_1(\mu_L - \mu) + G_2\mu_s\right), \qquad & I_s &= -\frac{1}{e}\left(G_3(\mu_L - \mu) + G_4\mu_s\right); \\ I &= -\frac{1}{e}\left(g_1(\mu - \mu_R) + g_2\mu_s\right), \qquad & -I_s &= -\frac{1}{e}\left(g_3(\mu - \mu_R) + g_4\mu_s\right). \end{aligned} \tag{A.9}$$

To understand the possibility of spin-charge transport by the use of the equation here we extend the calculus to obtain a proper interpretation of how spin components behave.

$$
\begin{aligned}
(G_1(\mu_L - \mu) + G_2\mu_s) &= (g_1(\mu - \mu_R) + g_2\mu_s) \\
\mu(-G_1 - g_1) &= -g_1\mu_R + g_2\mu_s - G_1\mu_L) \\
&= \mu_R(-g_1) + \mu_s(g_2 - G_2) - G_1\mu_L
\end{aligned}
$$

$$
\begin{aligned}
(G_3(\mu_L - \mu) + G_4\mu_s) &= -(g_3(\mu - \mu_R) - g_4\mu_s) \\
\mu_s(G_4 + g_4) &= -g_3(\mu - \mu_R) + G_3(\mu_L - \mu) \\
\mu_s &= \frac{-g_3(\mu - \mu_R) + G_3(\mu_L - \mu)}{G_4 + g_4}
\end{aligned}
$$

$$
-\mu(G_1 + g_1) = -g_1\mu_R + (g_2 - G_2)(\frac{-g_3(\mu - \mu_R) + G_3(\mu_L - \mu)}{G_4 + g_4}) - G_1\mu_L
$$

$$
\mu_s = \frac{\mu_l - \mu_r}{f}[G_3g_1 + g_3G_1]
$$

Notice that for ferromagnet with the G components we deduce G2=-G3 while for chiral component g2=g3 which show a dependence of the magnetic field that is going to be the responsible of the change of sign and spin-charge movement. To let things clear we present how is possible a spin charge Transport in a generic 2T circuit. What about Injection of spin current I_s ? We need to understand and formulate the potential difference at μ_L-μ which represent a fraction of the spin accumulation[4,5].

$$
\begin{aligned}
I_s &= -\frac{1}{e}(G_3(\mu_L - \mu) + G_4\mu_s) \\
\Gamma_3 = \mu_L - \mu &= \mu_L - \mu_L + \frac{g_3\,(g_2 - G_2) - g_1\,(G_4 + g_4)}{f}(\mu_L - \mu_R) \\
I_s &= -\frac{1}{e}(G_3(\frac{g_3\,(g_2 - G_2) - g_1\,(G_4 + g_4)}{f})(\mu_L - \mu_R) + G_4\frac{(G_3/G_1 + g_3/g_1)\,G_1g_1}{f}(\mu_L - \mu_R)) \\
I_s &= -\frac{1}{e}[(\frac{G_3g_3\,(g_2 - G_2) - G_3g_1\,(G_4 + g_4)}{f})(\mu_L - \mu_R) + G_4\frac{(G_3/G_1 + g_3/g_1)\,G_1g_1}{f}(\mu_L - \mu_R)] \\
I_s &= -\frac{1}{e}[(\frac{G_3g_3\,(g_2 - G_2) - G_3g_1\,(G_4 + g_4)}{f})(\mu_L - \mu_R) + G_4\frac{G_1g_3 - g_1G_3}{f}(\mu_L - \mu_R)] \\
I_s &= -\frac{1}{e}[(\frac{G_3g_3\,(g_2 - G_2) - G_3g_1\,(G_4 + g_4)) + G_4G_1g_3 - g_1G_3}{f}(\mu_L - \mu_R)] \\
I_s &= -\frac{1}{e}[(\frac{G_3g_3\,(g_2 - G_2) - G_3g_1\,(G_4 + g_4) + G_4(G_1g_3 - g_1G_3)}{f}(\mu_L - \mu_R)]
\end{aligned}
$$

All this derivations comes from Bart and Yang's work[4,5] from where fundamental terms presented in this documents are cautiously analyzed.

Appendix B

Transport Matrix

Here we include the main analysis and calculation of how to obtain a 3x3 transport Matrix using the spin-space matrices of transport. The derivation of this matrix contains all the physics previously explained in the upper part.

This picture provided us by a mesoscopic sample connected to two probes (reserviours,terminals), to be denoted as Left (L) and Right (R). They assume the reservoirs are so large to make possible the characterization of Temperature $T_{L,R}$ and Chemical Potentials $\mu_{L,R}$.

The image shown above is a big picture of an ideal case where the Chiral component is located as the blue helix and is assumed to favor the transmission of electrons with spin parallel to momentum.

The electrons on both Left (L) and Right (R) of the chiral component labeled with their spin-specific electrochemical potentials $\mu_{L\leftarrow(\rightarrow)}$ or $\mu_{R\leftarrow(\rightarrow)}$ initial state($\rightarrow$ or $\leftarrow$).

Following Yaang, we first describe the nomenclature for directional electron transmission $\mathbb{T}$ and reflection $\mathbb{R}$ using SPIN-SPACE matrices.[24] The CISS effect is thus not only relevant for Spintronic applications, but also fundamentally interesting in study of nano-structures and enantiomers. The following matrices represents right moving electrons in a (nonmagnetic) chiral component (1) and (2):

$$\mathbb{T}_{\triangleright} = \begin{pmatrix} t_{\rightarrow\rightarrow} & t_{\leftarrow\rightarrow} \\ t_{\rightarrow\leftarrow} & t_{\leftarrow\leftarrow} \end{pmatrix}, \quad \mathbb{R}_{\triangleright} = \begin{pmatrix} r_{\rightarrow\rightarrow} & r_{\leftarrow\rightarrow} \\ r_{\rightarrow\leftarrow} & r_{\leftarrow\leftarrow} \end{pmatrix} \tag{B.1}$$

Here we have the time-reversed form of the Equation 2.10 for left-moving electrons.

$$\mathbb{T}_{\triangleleft} = \begin{pmatrix} t_{\leftarrow\leftarrow} & t_{\rightarrow\leftarrow} \\ t_{\leftarrow\rightarrow} & t_{\rightarrow\rightarrow} \end{pmatrix}, \quad \mathbb{R}_{\triangleleft} = \begin{pmatrix} r_{\leftarrow\leftarrow} & r_{\rightarrow\leftarrow} \\ r_{\leftarrow\rightarrow} & r_{\rightarrow\rightarrow} \end{pmatrix} \tag{B.2}$$

Following the matrix formalism of transport we define spin-space column vectors using electrochemical potentials and other vectors for currents . Each vector element describe the independent contribution of one spin component in each side of the molecule Left side (L) or Right side (R). Some important facts to notice That by Bart Van Wess "these matrices are spin independent and are fully determined by a transmission probability T.[22]

In Figure 1.1 authors introduced an electrochemical potential μ as a way of transport of our electrons in our device here μ=($\mu_{\rightarrow}$+$\mu_{\leftarrow}$)/2 and the spin accumulation of its chemical potential is represented as μ_s=($\mu_{\rightarrow}$-$\mu_{\leftarrow}$)/2 analogous for current vector I=($I_{\rightarrow} + I_{\leftarrow}$) and spin current/accumulation I_s=($I_{\rightarrow} - I_{\leftarrow}$).

So we start with the representation of the current of each side of the molecule with the use of spin-space column vectors. Notice that both $\mathbb{T}$ and $\mathbb{R}$ which holds all the transport information and relations of each side that we will arrive.

$$\begin{pmatrix} I_{L\rightarrow} \\ I_{L\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[(\mathrm{I} - \mathbb{R}_{\triangleright})\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix} - \mathrm{T}_{\triangleleft}\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix}\right] \tag{B.3}$$

$$-\begin{pmatrix} I_{R\rightarrow} \\ I_{R\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[(\mathrm{I} - \mathbb{R}_{\triangleleft})\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix} - \mathrm{T}_{\triangleright}\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix}\right] \tag{B.4}$$

Where N is the number of spin-degenerate channels, h is the Planck's constant and $\mathbb{I}$ being the Identity Matrix $\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ Now I will shown how we obtain the derivation of the Transport Matrix.

First using each element of the spin-space column vector we construct our first equations of current-spin:

$$\begin{pmatrix} I_{L\rightarrow} \\ I_{L\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} r_{\rightarrow\rightarrow} & r_{\leftarrow\rightarrow} \\ r_{\rightarrow\leftarrow} & r_{\leftarrow\leftarrow} \end{pmatrix}\right]\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix} - \begin{pmatrix} t_{\leftarrow\leftarrow} & t_{\rightarrow\leftarrow} \\ t_{\leftarrow\rightarrow} & t_{\rightarrow\rightarrow} \end{pmatrix}\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix}\right] \tag{B.5}$$

In the other hand we will need a set of equations to the other side of the reservoir later we will deep in the use of this equations which are $I_{R\rightarrow}$ and $I_{R\leftarrow}$:

$$\begin{pmatrix} I_{R\rightarrow} \\ I_{R\leftarrow} \end{pmatrix} = -\frac{Ne}{h}\left[\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} r_{\leftarrow\leftarrow} & r_{\rightarrow\leftarrow} \\ r_{\leftarrow\rightarrow} & r_{\rightarrow\rightarrow} \end{pmatrix}\right]\begin{pmatrix} \mu_{R\rightarrow} \\ \mu_{R\leftarrow} \end{pmatrix} - \begin{pmatrix} t_{\rightarrow\rightarrow} & t_{\leftarrow\rightarrow} \\ t_{\rightarrow\leftarrow} & t_{\leftarrow\leftarrow} \end{pmatrix}\begin{pmatrix} \mu_{L\rightarrow} \\ \mu_{L\leftarrow} \end{pmatrix}\right] \tag{B.6}$$

$$I_{L\rightarrow} = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow})(\mu_{L\rightarrow}) - r_{\leftarrow\rightarrow}\mu_{L\leftarrow} - t_{\rightarrow\rightarrow}\mu_{R\rightarrow} - t_{\leftarrow\rightarrow}\mu_{R\leftarrow}] \tag{B.7}$$

$$I_{L\leftarrow} = -\frac{Ne}{h}[-(r_{\rightarrow\leftarrow})(\mu_{L\rightarrow}) + (1 - r_{\leftarrow\leftarrow})\mu_{L\leftarrow} - t_{\rightarrow\leftarrow}\mu_{R\rightarrow} - t_{\leftarrow\leftarrow}\mu_{R\leftarrow}] \tag{B.8}$$

Equation B.6 can be rewrite as the sum of Eq B.7 and B.8 $I_L = (I_{L\rightarrow} + I_{L\leftarrow})$ showing us a part of how the current flows:

$$\begin{aligned} I_L = -\frac{Ne}{h}[&(1 - r_{\rightarrow\rightarrow})(\mu_{L\rightarrow}) - (r_{\leftarrow\rightarrow})(\mu_{L\leftarrow}) - (t_{\rightarrow\rightarrow})(\mu_{R\rightarrow}) - (t_{\leftarrow\rightarrow})(\mu_{R\leftarrow}) + (-r_{\rightarrow\leftarrow})(\mu_{L\rightarrow}) \\ &+(1 - r_{\leftarrow\leftarrow})(\mu_{L\leftarrow}) - (t_{\rightarrow\leftarrow})(\mu_{R\rightarrow}) - (t_{\leftarrow\leftarrow})(\mu_{R\leftarrow})] \end{aligned} \tag{B.9}$$

$$I_L = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow})(\mu_{L\rightarrow}) + (1 - r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow})(\mu_{L\leftarrow}) - (t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) - (t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow})(\mu_{R\leftarrow})] \tag{B.10}$$

Now following the relation of that the chemical potentials of total contribution of spin at each side $2\mu_L = (\mu_{L\rightarrow} + \mu_{L\leftarrow})$ Following to $2\mu_L - \mu_{L\rightarrow} = \mu_{L\leftarrow}$ the same for the other side $2\mu_R - \mu_{R\rightarrow} = \mu_{R\leftarrow}$

$$\begin{aligned} I_L = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow})(\mu_{L\rightarrow}) + (1 - r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow})(2\mu_L - \mu_{L\rightarrow}) + (-t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) \\ +(-t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow})(2\mu_R - \mu_{R\rightarrow})] \end{aligned} \tag{B.11}$$

keep going in calculations:

$$\begin{aligned} I_L = -\frac{Ne}{h}[(-r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} + r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow})(\mu_{L\rightarrow}) + (1 - r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow})(2\mu_L) + (t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\leftarrow} - t_{\leftarrow\rightarrow})(\mu_{R\rightarrow}) \\ +(-t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow})(2\mu_R)] \end{aligned} \tag{B.12}$$

Here we notice the contribution of both spin accumulation and direct spin, using the equations in 12 we relate $\mu_{R\rightarrow}$ with each $\mu_{L\rightarrow} = \mu_L + \mu s L$
and so on with the other important relations:

$$\begin{aligned} \mu_{L\rightarrow} &= \mu_L + \mu_{sL} & 2\mu_L &= \mu_{L\rightarrow} + \mu_{L\leftarrow} \\ \mu_{L\leftarrow} &= \mu_L - \mu_{sL} & 2\mu_R &= \mu_{R\rightarrow} + \mu_{R\leftarrow} \\ \mu_{R\rightarrow} &= \mu_R + \mu_{sR} & 2\mu_{sR} &= \mu_{L\rightarrow} - \mu_{L\leftarrow} \\ \mu_{R\leftarrow} &= \mu_R - \mu_{sR} & 2\mu_{sL} &= \mu_{R\rightarrow} - \mu_{R\leftarrow} \end{aligned}$$

With this change we obtain a Current expressed in terms of chemical spin contribution and spin accumulation:

$$\begin{aligned} I_L = -\frac{Ne}{h}[(-r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} - r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow} + 2)(\mu_L) + (-r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} + r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow})(\mu_{sL}) \\ +(t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\leftarrow} - t_{\leftarrow\rightarrow})(\mu_{sR}) + (-t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_R)] \end{aligned} \tag{B.13}$$

Replacing by:

$$\begin{aligned} t &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow} & P_t &= (t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})\,/t \\ r &= r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow} + r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow} = 2 - t & P_r &= (r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} + r_{\leftarrow\rightarrow} - r_{\leftarrow\leftarrow})\,/r \\ \gamma_t &= t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow} & s &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow} \\ \gamma_r &= r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow} - r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow} - 2 & &= t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow} \end{aligned}$$

.

We obtained:

$$I_L = -\frac{Ne}{h}[\mu_{sL}(S) + \mu_{sR}(S) + \mu_L(t) - \mu_R(t)] \tag{B.14}$$

Finally we obtained and equation with the form of:

$$I_L = -\frac{Ne}{h}[(\mu_L - \mu_R)(t) + \mu_{sL}(S) + \mu_{sR}(S)] \tag{B.15}$$

Or in matrix form:

$$I_L = -\frac{Ne}{h}(t \quad s \quad s)\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{B.16}$$

The next term we need to take care is the accumulation of spin so we calculate the difference of spin up and down or left and right: $I_{sL} = (I_{L\rightarrow} - I_{L\leftarrow})$:

$$\begin{aligned} I_{sL} = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow})(\mu_{L\rightarrow}) - (r_{\leftarrow\rightarrow})(\mu_{L\leftarrow}) - (t_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) - (t_{\rightarrow\leftarrow})(\mu_{R\leftarrow}) + (r_{\rightarrow\rightarrow})(\mu_{L\rightarrow}) - (1 - r_{\rightarrow\rightarrow})(\mu_{L\leftarrow}) \\ +(t_{\leftarrow\rightarrow})(\mu_{R\rightarrow}) + (t_{\leftarrow\leftarrow})(\mu_{R\leftarrow})] \end{aligned} \tag{B.17}$$

$$\begin{aligned} = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow})(\mu_{L\rightarrow}) + (r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow} - 1)(\mu_{L\leftarrow}) + (t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) \\ +(t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow})(\mu_{R\leftarrow})] \end{aligned}$$

$$\begin{aligned} = -\frac{Ne}{h}[(1 - r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow})(\mu_L + \mu_{sL}) + (r_{\leftarrow\leftarrow} - r_{\leftarrow\rightarrow} - 1)(\mu_L - \mu sL) + (t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_R + \mu_{sR}) \\ +(t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow})(\mu_R - \mu_{sR})] \end{aligned}$$

$$\begin{aligned} = -\frac{Ne}{h}[(-r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow} - r_{\leftarrow\rightarrow} + r_{\leftarrow\leftarrow})(\mu_L) + (1 - r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow} + r_{\leftarrow\rightarrow} - r_{\leftarrow\leftarrow} - 1)(\mu sL) \\ +(t_{\rightarrow\rightarrow} - t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_R) + (-t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow} + t_{\leftarrow\rightarrow} - t_{\leftarrow\leftarrow})(\mu_{sR})] \end{aligned}$$

Replacing by the terms from equation 13 where P_t and P_r are the CISS-induced spin polarization of the transmitted T and reflected R electrons:

$$= -\frac{Ne}{h}\,[-\mu_L P_r r - \mu_{sL}\gamma_r + \mu_R P_t t - \mu_{sR}\gamma_t] \tag{B.18}$$

We notices that in equation 13 that $P_t t$ and $P_r r$ so we rewrite:

$$-I_{sL} = -\frac{Ne}{h}[(\mu_L - \mu_R)P_r r + \mu_{sL}\gamma_r + \mu_{sR}\gamma_t] \tag{B.19}$$

$$-I_{sL} = \frac{Ne}{h}\begin{pmatrix} P_r r & \gamma_r & \gamma t \end{pmatrix}\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{B.20}$$

For the last term of our Transport Matrix we will solve for the other part of the current the R side:

$$I_{sR} = \frac{Ne}{h}[(\mu_L - \mu_R)P_t t + \mu_{sL}\gamma_t + \mu_{sR}\gamma_r] \tag{B.21}$$

So in order to find the third row we must analyzed the current from the right side of the molecule with defining charge current as :$-I_R$ =$I_{R\rightarrow}$+$I_{R\leftarrow}$ we have::

$$I_{R\rightarrow} = -\frac{Ne}{h}[(1 - r_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) - r_{\rightarrow\leftarrow}\mu_{R\leftarrow} - t_{\rightarrow\rightarrow}\mu_{L\rightarrow} - t_{\leftarrow\rightarrow}\mu_{L\leftarrow}] \tag{B.22}$$

$$I_{R\leftarrow} = -\frac{Ne}{h}[-r_{\leftarrow\rightarrow}\mu_{R\rightarrow} + (1 - r_{\rightarrow\rightarrow})\mu_{R\leftarrow} - t_{\rightarrow\leftarrow}\mu_{L\rightarrow} - t_{\leftarrow\leftarrow}\mu_{L\leftarrow}] \tag{B.23}$$

Following charge current equation we denote spin accumulation on the right side of the molecule as:$-I_{sR}$=($I_{R\rightarrow}$-$I_{R\leftarrow}$) we have:

$$I_{sR} = -\frac{Ne}{h}[(1 - r_{\leftarrow\leftarrow})(\mu_{R\rightarrow}) - r_{\rightarrow\leftarrow}\mu_{R\leftarrow} - t_{\rightarrow\rightarrow}\mu_{L\rightarrow} - t_{\leftarrow\rightarrow}\mu_{L\leftarrow} + r_{\leftarrow\rightarrow}\mu_{R\rightarrow} - (1 - r_{\rightarrow\rightarrow})\mu_{R\leftarrow} + t_{\rightarrow\leftarrow}\mu_{L\rightarrow} + t_{\leftarrow\leftarrow}\mu_{L\leftarrow})] \tag{B.24}$$

$$I_{sR} = -\frac{Ne}{h}[(1 - r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow})(\mu_{R\rightarrow}) + (-t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow})\mu_{L\rightarrow} + (t_{\leftarrow\leftarrow} - t_{\leftarrow\rightarrow})\mu_{L\leftarrow} + (-1 + r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow})\mu_{R\leftarrow}] \tag{B.25}$$

$$\begin{aligned} I_{sR} = -\frac{Ne}{h}[(1 - r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow})(\mu_R + \mu_{sR}) + (-t_{\rightarrow\rightarrow} + t_{\rightarrow\leftarrow})(\mu_L + \mu_{sL}) + (-t_{\leftarrow\rightarrow} + t_{\leftarrow\leftarrow})(\mu_L - \mu_{sL}) \\ +(-1 + r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow})(\mu_R - \mu_{sR})] \end{aligned} \tag{B.26}$$

$$\begin{aligned} I_{sR} = -\frac{Ne}{h}[(-r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow} + r_{\rightarrow\rightarrow} - r_{\rightarrow\leftarrow})(\mu_R) + (+t_{\leftarrow\leftarrow} - t_{\leftarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\rightarrow\rightarrow})(\mu_L) + (-t_{\leftarrow\leftarrow} + t_{\leftarrow\rightarrow} + t_{\rightarrow\leftarrow} - t_{\rightarrow\rightarrow})(\mu_{sL}) \\ +(2 - r_{\leftarrow\leftarrow} + r_{\leftarrow\rightarrow} - r_{\rightarrow\rightarrow} + r_{\rightarrow\leftarrow})(\mu_{sR})] \end{aligned} \tag{B.27}$$

$$-I_{sR} = -\frac{Ne}{h}[(P_r r)(\mu_R) - (P_t t)(\mu_L) + (-\gamma_t)(\mu_{sL}) + (-\gamma_r)(\mu_{sR})] \tag{B.28}$$

because of the relation $P_t t = P_r r$

$$I_{sR} = -\frac{Ne}{h}(P_t t \quad \gamma_t \quad \gamma r)\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{B.29}$$

We have found the Transport Matrix by our derivations.

$$\begin{pmatrix} I \\ -I_{sL} \\ I_{sR} \end{pmatrix} = -\frac{Ne}{h}\begin{pmatrix} t & s & s \\ P_r r & \gamma_r & \gamma_t \\ P_t t & \gamma_t & \gamma_r \end{pmatrix}\begin{pmatrix} \mu_L - \mu_R \\ \mu_{sL} \\ \mu_{sR} \end{pmatrix} \tag{B.30}$$

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