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In this thesis, we investigated the spin-polarization effects of materials as well as externally applied fields which can be used to induce and manipulate spin-polarized currents in semiconductor materials. Our studies are focused on the current-perpendicular-to-plane (CPP) structures, the two dimensional electron gas (2DEG) transistor heterostructures, the bulk transistor structures, as well as the mesoscopic multiple terminal devices. The general objective of this thesis is thus to study spin transport effects as well as spin-polarization techniques that can be suitably applied to the above devices.

In chapter 2, we studied spin transport within the drift-diffusion regime across a CPP type of ferromagnetic (FM)-semiconductor (SC) device. We proposed using a pillar spin nano-injector to enhance spin injection efficiency, taking into consideration the effects of spreading resistances that arise from current confinement. We also modeled the effect of current-confinement on magnetoresistance in a CPP spin valve. Finally, we developed a model which includes the effect of interfacial potential barriers at the FM-SC interface, and evaluates the spin and charge current self-consistently.

In chapters 3 and 4, we model ballistic spin transport under the influence of magneto-electric barriers within the 2DEG transistor. We study a spinFET with multiple magneto-electric barriers, and the effects of these barriers on spin polarization and electron transmission. We proposed the “zero-gauge” barriers to increase the spin polarization while keeping the electron conductance high. The multi-gate spinFET device shows sufficient versatility for programmable logic function, as well as non-volatile storage to be realized using a single spinFET. These devices compare favorably with practical CMOS devices with respect to power consumption, speed, and size.
In chapters 5 and 6, the Dresselhaus and the Rashba spin orbit coupling (SOC) and its effects on spin transport were studied. Understanding these effects is crucial to harnessing it for enhancing spin-polarized current in the 2DEG as well as bulk transistor devices. We derived the spin-dependent transport model that utilizes these effects, taking into considerations the discrete distribution of magnetic vector potentials, and the energy sub-bands within the 2DEG. For the Dresselhaus effect, we considered III-V materials in a bulk transistor with multiple gates.

In chapter 7, we studied electron transport in a 2DEG system that comprised the Rashba SOC, and spatially continuous magnetic fields. We derived the spin-dependent wave functions that showed the combined effects of SOC, magnetic, and cross electric fields on spin current. Spin polarization within a cyclotron was studied and the effects of electric field on the cyclotron shift were also studied for its possible use as a spin current separator. In chapter 8, we studied spin transport in a mesoscopic quantum dot (QD) device using the Keldysh technique so that lead perturbation and Coulomb blockade effect can be considered. We derived theoretical relations of the spin injection efficiency and spin transfer effects on the magnetized quantum dot, which elucidated the angular dependence of the spin transfer effects with respect to QD magnetization orientation.
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FIG. 2.1. Schematic illustration of the spin injection device with small cylindrical FM injector interfaced with the Cu layer to form a bilayer injector. Two bilayers are used to ensure a symmetrical interface electrochemical splits that simplify calculations.

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FIG. 2.4. Spin injection graphs were plotted for spreading resistance derived from simulated values and that derived from analytically calculated values. Results shows that the discrepancy between simulated value and analytic value has little effect on spin injection.

FIG. 2.5. Spin injection increases with increasing $\sigma_{SC}$, which is achieved by increasing $N_D$. For GaAs materials, $N_D$ of $10^{18}$ cm$^{-3}$ and above could generate spin injection of 20% and above.

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FIG. 2.11. (a) \( R_L \) increases with increasing interfacial potential barrier (at constant ratio split of spin-dependent potential). (b) Spin injection increases with increasing interfacial potential barrier (at constant ratio split of spin-dependent potential). If the split of spin-dependent potential is increased, spin injection rises even more significantly, i.e. graph for \( U_1 = 0.1U_\perp \) has the steepest gradient.

FIG. 3.1. Schematic illustration of a double-pair magneto-electric barrier element that can be realized by magnetizing the periodically spaced ferromagnetic gate stripes deposited on top of a device heterostructure.

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FIG. 3.8. The anti-symmetrical double-pair element is also characterized by symmetrical A distribution across a double-pair element. Breaking this symmetry could induce spin current across the barriers.

FIG. 3.9. Results show spin polarization (red) and transmission probability (green) for \( n=1 \) double-pair, and anti-symmetrical magnetic barriers configuration of \( B=(+2,+2,-2,-2)B_0 \). It is worth noting that the positive and negative potentials applied to region II, IV, respectively are required to induce a net \( P \) value.

FIG. 3.10. Results show spin polarization (red) and transmission probability (green) for \( n=27 \) double-pairs, and anti-symmetrical magnetic barriers configuration of \( B=(+2,+2,-2,-2)B_0 \). It is worth noting that the positive and negative potentials applied to region II, IV, respectively are required to induce a net \( P \) value.

FIG. 3.11. Results show spin polarization (red) and transmission probability (green) for \( n=1 \) double-pair, and anti-symmetrical magnetic barriers configuration of \( B=(+5,+5,-5,-5)B_0 \). It is worth noting that the positive and negative potentials applied to region II, IV, respectively are required to induce a net \( P \) value.

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FIG. 3.13. The total device response time is illustrated above as the time taken for the transmission probability of electrons or the current to reach its steady value right after a remagnetization of the ferromagnetic gate.

FIG. 3.14 (a) Tunneling time decreases with increasing electron kinetic energy. Higher electrical potential barriers increase tunneling time. (b) Tunneling time decreases with increasing electron kinetic energy. Higher magnetic barriers increase tunneling time.

FIG. 3.15. Tunneling time increases with increasing potential barriers.

FIG. 3.16. Tunneling time increases smoothly with increasing magnetic barrier heights at low \( B \) values.

FIG. 4.1. Programmable AND/ NAND gate can be realized with just a single spinFET by remagnetizing FM gates 1&3 of the device. FM gates 2 and 4 are two input to the logic gate. (a) shows the design of an And gate, (b) shows the design of an NAND gate.
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FIG. 4.2. Computation results of device conductance resulting from the input conditions of the FM 2 and 4.

FIG. 4.3. The spinFETs can be adapted to function as a single-transistor non-volatile memory cell, by constructing and removing the symmetrical configuration of discrete magnetic vector potential values within a double-pair element.

FIG. 4.4. Results show the high and low resistance states of the spinFETs when it is toggled between the asymmetrical and symmetrical A configuration. (a)-(b) shows resistance states under the electrical potential of $U=20\ E_0$. (c)-(d) shows resistance states under the electrical potential of $U=10\ E_0$.

FIG. 4.5. The spinFETs can be adapted to function as a single-transistor non-volatile memory cell, by constructing and removing the zero-gauge and non-zero gauge configuration within a double-pair element.

FIG. 4.6. Results show the high and low resistance states of the spinFETs when it is toggled between the zero-gauge and non zero-gauge configuration. Results in (b) show that in the non zero-gauge configuration, resistance increases significantly with increasing number of barriers used.

FIG. 4.7. (a) $P$ modulation can be achieved by varying the electrical potential. (b) Large, monotonic modulation of $P$ by $U$ can be achieved at selected range of electron energies.

FIG. 4.8. Schematic illustration of the magnetic transistor for programmable logic. In logic functions, gates FM 1-4 and NM 1-2 are used.

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FIG. 4.10. The magneto-electric device can be adapted by employing the “weighted” gate concept to perform the function of multi-bit memory within a single transistor.

FIG. 4.11. $T$ curves correspond to the eight binary states of the multi-bit memory device. The vertical (horizontal) dotted line depicts current (voltage) detection modes. In the inset, the x axis shows the eight curves of the main graph, each corresponding to a binary input configuration of FM 4,3,2 of (000)-(111).
FIG. 4.12. The magneto-electric transistor can be realistically fabricated with the above dimensions, as well as material choices.

FIG. 5.1. Schematic structure of a III-V semiconductor materials that generate spin polarization.

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FIG. 5.6. Computation results are shown for $T$ and $P$ curves of the device of GaAs materials. External fields were applied in the form of $n=1$ zero-gauge double-pair gates. Grey curve shows average $P$ of 2% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero, peak $P$ less than 1%.

FIG. 5.7. Computation results are shown for $T$ and $P$ curves of the device of GaSb materials. External fields were applied in the form of $n=1$ zero-A double-pair gates. Grey curve shows average $P$ of 5% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero, peak $P$ around 2%.

FIG. 5.8. Computation results are shown for $T$ and $P$ curves of the device of GaSb materials. External fields were applied in the form of $n=5$ zero-gauge double-pair gates.

FIG. 5.9. Computation results are shown for $T$ and $P$ curves of the device of InSb materials. External fields were applied in the form of $n=5$ zero-gauge double-pair gates. Grey curve shows average $P$ of 10% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero, peak $P$ around 3-4%.

FIG. 5.10. Computation results are shown for $T$ and $P$ curves of the device of InAs materials. External fields were applied in the form of $n=1$ zero-gauge double-pair gates.
FIG. 6.1 (a) Device with delta $B$ field oriented in $y$ direction in the 2DEG. (b) Device with delta $B$ field oriented in the $z$ direction in the 2DEG. The former can utilize RSOC to enhance spin polarization of current. In the latter device, spin polarization could be mitigated by the in-plane RSOC effects.

FIG. 6.2. Electron tunnels through the barriers from region I on the left to region V on the right. $A$-$J$ are wave-function amplitude in different regions. $A_1$-$D_2$ are wave-function amplitudes at the delta barriers.

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Chapter 1

Introduction to spintronic

1.1 Brief history of spin and magnetism

The study of electron spin began with the seminal experiments by Stern and Gerlach [1] in 1922, and Phipps and Taylor in 1927, which recorded two distinct magnetic dipole moment values of an electron beam that passed perpendicularly through a region with an applied magnetic field. The discovery of the additional energy terms reveals an inadequacy of the Schrödinger [2] equation in describing even a single particle system. Such inadequacies were later addressed by Dirac [3] who formulated the Dirac’s equations and predicted from first principles the energy term due to particle spin. The studies of spin were further advanced in the 1950s, into areas of optical orientation, spin relaxation, spin-orbit coupling by D’yakonov, Pikus, Bir Aronov, Rashba, Elliot, Yafet, Dresselhaus and others [4,5,6,7,8,9].

The scientific understanding of the nature of electron spin had not, however, driven a parallel development of applications exploiting the spin property of electrons. Until recently, the harnessing of electron spin for technological purposes was largely confined to the manipulation of the macroscopic spin effect, i.e. the resultant magnetic moment of a large ensemble of individual net atomic magnetic moments aligned in a specific low energy axis, which is a specific property of ferromagnetic materials. The study of magnetism and magnetic materials is a well-established topic, encompassing investigations into the different contributions to the total free energy of a magnetic system, the coupling between applied field and magnetic moment, and the effects of
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various anisotropic effects (e.g. magnetocrystalline, shape and surface) on the magnetization alignment. However, this study can be virtually described within the classical framework (of Maxwell’s equations), with the underlying quantum effects being reduced to phenomenological models (e.g. Heisenberg model to describe exchange interactions).

1.2 Metallic spin-based devices

The discovery of the Giant Magneto-Resistive (GMR) effect in the 1980s’ highlighted the importance of understanding the coupling of magnetic moments (orbital / spin) to electron transport. The GMR phenomenon requires the formulation of new theoretical models which consider the individual spins of conduction electrons and not just the collective effect of local magnetic moments. As such, the discovery of the GMR effect is often regarded as the starting point in the field of spin electronics, or spintronics [10]. Fert et al. [11] derived within a semi-classical framework the phenomenological equations which are still widely used in the computation of GMR ratio. The GMR discovery sparked an intense interest in spintronics, and within a few years i.e. in the early 1990’s, S. S. P. Parkin and B. Gurney [10] of IBM has successfully demonstrated the first practical GMR device known as the spin valve, which is used in the hard disk sensor technology.

Another major development in the field of spintronics is the development of the magneto-resistive random access memory (MRAM) which utilizes the magnetoresistive effect of a magnetic tunneling junction for non-volatile storage. Due to the lucrative market in memory devices, there have been intensive efforts by many companies e.g. NVE, IBM, Infineon, Motorola, Altis, and Cypress Semiconductor Inc. to develop MRAM as a viable commercial product. In October 2004, Freescale Semiconductor (formerly the Semiconductor Product Sector of Motorola) became the first company to launch a commercial 4-Mbit MRAM product [12].
1.3 Semiconductor spintronics

In the initial phase, active research in spintronics is focused on metallic spin-based devices. Subsequently, researchers began to investigate the possibility of semiconductor-based spintronics. The main advantage of semiconductors (SC) over metals is that its conductivity can be varied over a wide range by changing its carrier concentration, either by doping, or by an externally applied field, or by some means of carrier excitation (e.g. photo excitation). Thus in SC-based spintronics, spin-dependent effects can become a “gate-able” property of the device.

There are three requirements in achieving SC-based spintronics – i) production of a spin polarized current, ii) external control and manipulation of the spin-polarized current, and iii) detection of spin-polarized current. There are two main routes in producing a spin-polarized current, i.e. either spin injection from a ferromagnetic source electrode into the SC layer, or by inducing ferromagnetism within the SC itself by introducing a transitional metal dopants e.g. Mn. Ferromagnetism in magnetic semiconductor can be controlled by different means, e.g. by changing doping concentration, different doping configurations, or by applying electric field [13]. Magnetic semiconductors can also function as a spin injector into a normal semiconductor. For spin control and manipulation in semiconductor material, we utilize various spin-related phenomena like the Rashba spin orbit coupling, the Dresselhaus spin orbit coupling, and the nuclear field effects. These phenomena have been studied for their abilities to induce spin polarized current, rotate its polarization axis, as well as affect the rate of spin relaxation. Besides these intrinsic effects, spin manipulation achieved by the application of external delta magnetic fields [14,15] through ferromagnetic gate stripes have also been studied. Additionally, the application of continuous magnetic fields can also induce spin-dependent effects on the electron cyclotron motion [16,17]. The combined effects of these fields and the inherent spin orbit coupling on spin-dependent transport in SC materials have thus become an interesting research topic in magneto-electronic
transport. However, in ferromagnetic metals, momentum scattering is spin-dependent because the density of states at the Fermi energy level is spin-dependent. Magneto-transport in the ballistic regime would therefore differ substantially from the scattering regime due to its spin dependent scattering.

1.3.1 Spintronics devices

The application of spin-dependent devices is, however, limited by the fact that a spin-polarized current can only be easily induced in magnetic materials. Since semiconductors are usually nonmagnetic, it has not been equally easy to induce spin-polarized current to flow in them. From the industrial perspective, it is essential not only for a spin-polarized current to be induced in semiconductors, but also be manipulated electrically, in order to achieve a “spin transistor” function. The spin transistor is a key element upon which other more complicated devices (e.g. logic gates, memories, etc.) can be built; the collection of these devices thus constitutes a whole new class of spin-based electronics.

Theoretically, a spin field-effect transistor (spinFET) device has been proposed by Datta and Das [18] as early as 1989. The ferromagnetic source and drain electrodes act as a spin polarizer and spin analyzer, respectively. Electrical voltage ($V_g$) is applied to the Schottky gate to alter the Rashba spin-orbit coupling strength within the InAlAs-InGaAs 2DEG, and thus manipulate the spin polarized current in the semiconductor channel. This device has been experimentally [19,20] shown to function, but at extremely low temperatures. One of the main obstacles to the practical implementation of the Datta-Das spinFET is the low spin injection efficiency between a ferromagnetic metal and semiconductor. Schmidt et al., Rashba [21,22] and other theorists provided explanation that this low spin injection efficiency is caused mainly by the conductivity mismatch between the semiconductor and metal. One possible method to overcome this mismatch
is by using a magnetic semiconductor [23,24] as an injector, since its resistivity is of the same order as that of the semiconductor layer. However, the shortcoming is that magnetic semiconductors lose their ferromagnetic property at temperatures well below room temperature.

1.3.2 Magnetic semiconductor

The surging interest in spintronics research is due, in part, to the recent achievements in fabricating magnetic semiconductors [25,26]. Magnetic semiconductors have been found to exhibit useful magnetic properties like interlayer coupling, giant magneto-resistance (GMR), and tunneling magneto-resistance (TMR). The convergence of semiconductor and magnetic technologies promises a redefinition of present-day electronics. The early work on magnetic semiconductors started in the 1960’s with attention then focused on Eu-Chalcogenide (EuSe, EuS, EuO) and Cr-Chalcogenide spinels (CdCr2Se4, CdCr2S4) [27].

There was a lull in research activities, since the Curie temperature (Tc) of these classes of materials could not be raised beyond 50K despite intense research effort. In the 1980’s, work shifted to the study of the II-VI compounds doped with Mn, e.g. Cd_{1-x}Mn_{x}Te. These materials were also known as the diluted magnetic semiconductors (DMS). Practical applications were limited because most of the II-VI DMS are either paramagnetic or exhibit spin-glass behavior. Finally, in the 1990’s, the pioneering works of H. Ohno [13] and Munekata [28] led to the development of III-V (As, Sb) based DMS doped with e.g. Mn. From the applications standpoint, the advantage of III-V DMS over the other DMS types lies in the fact that ferromagnetism is hole-mediated, with the Mn dopants acting as acceptors [26, 28]. Since the ferromagnetic property of III-V DMS is closely linked to hole carrier concentration, it can thus be controlled by any method which induces a change in the carrier density, e.g. electrical and photonic means. It is this versatility which has made III-V DMS the most intensely-researched DMS group presently.
1.3.3 Spin-related phenomena in semiconductor

Finally we discuss the electron spin-orbit coupling to the semiconductor crystal field [8,19,20,29] which forms the basis of manipulating the spin-polarized current. This spin-orbit coupling naturally arises as a result of inversion asymmetry in the zinc-blende crystal lattice. This is a relativistic phenomenon, which was first described in Dirac’s equation [30]. It has been shown that these spin orbit coupling (SOC) effects can induce spin polarized current in n-doped, III-V semiconductors, and enable electron spin manipulation by electrical means [17,18,31,32]. This constitutes a clear advantage compared with electron spin coupling to local magnetic moments in ferromagnetic materials, or to external magnetic field, for which external electrical manipulation is practically impossible. It is thus important to understand these phenomena, so as to optimize them for achieving spin-manipulation in future spintronic devices.

1.4 Motivations and objectives

The above sections gave an overview of the recent development of spin-based physics, and its applications particularly in semiconductor spintronics. In this thesis, the main research focus is on the theoretical analyses and understanding of the physics involved in efficiently inducing a spin polarized current in CPP structures, semiconductor transistor-like devices, mesoscopic multiple-terminals devices, and the subsequent transport and manipulation of this spin-polarized current through the devices [17,18]. To conceptualize a viable semiconductor based spintronic device, it is important to understand how spin-polarized current as well as charge current can be induced in a semiconductor, transported across the device with little spin loss or relaxation, manipulated externally by either applied magnetic or electric fields, and finally be detected by conduction across magnetic contacts or junctions. Thus, our initial study is focused on the novel use of ferromagnetic nanocontacts, to generate a spin-polarized current and inject it into a semiconductor layer efficiently without causing loss of spin polarization. Since the overriding objective of
spintronics is to create new, more efficient devices based on spin-dependent current, we are next drawn to the analysis and modeling of 2DEG spinFET devices with ferromagnetic gates. Such devices are capable of a high degree of versatility with respect to device design since the charge and spin-polarized currents are strongly dependent on the magneto-electric gate configuration [14,15]. We study the use of spatially-confined ("delta") magneto-electric fields to induce spin-polarized current and manipulate these fields to realize desired device functionalities e.g. programmable logic or multi-level storage. We also investigate the spin-orbit coupling effects due to surface-induced asymmetry (Rashba effect) in a 2DEG system and bulk-induced asymmetry (Dresselhaus effect) in a bulk transistor system. These effects can induce a spin-split in the majority and minority spin carriers. We proposed means of harnessing this spin-split effect to enhance the spin-polarized current polarization, and to control the polarization orientation [33].

We also investigate the effect of applying spatially continuous magnetic fields in the spinFET system [16,17]. This induces the Landau spin orbit coupling, which is yet another effect that can be utilized to enhance the spin polarization of current. In practical devices, it is more convenient to apply and manipulate electric rather than magnetic fields. We re-configured our theoretical model to study the effects of electric fields applied perpendicular to the magnetic field and the 2DEG plane, and analyze the spin polarization of current spin induced by cross magneto-electric fields. Such a configuration has the advantage that the resulting spin-polarized current polarized in the in-plane direction is more resistant to spin dephasing effects e.g. due to the D’yakonov-Perel-like mechanism. The use of cross-fields also enables high spin polarization to be achieved with fewer magneto-electric barriers, thus reducing the device dimension and allowing ballistic transport to be achieved more easily. Finally, for the analysis of spin transport in mesoscopic structures [34,35,36], we apply the Keldysh non-equilibrium technique to study the spin-polarized current across a two-terminal QD device, subject to the effect of perturbations in the leads, various electron correlations, Coulomb blockade charging effect, and finite temperature. The charge and spin-polarized currents were derived in terms of momentum-space Green’s functions. We have
studied the spin-polarized current, spin injection efficiency, and spin transfer torque in the QD device, subject to external influences like biases, coupling to leads, thermal effects, etc.

REFERENCES


Spin characteristics of electron transport in semiconductor


Chapter 2

Drift diffusion modeling of spin dependent transport

2.1 Spin injection

It has been discussed in chapter 1 that the studies of spin physics have recently extended to the semiconductor materials. The harnessing of spin in transistor-based devices, such as magnetic memory, optoelectronic devices, logic gates has thus become possible. It has also been conceived that semiconductor spintronic research might lead to the development of new devices like the spinFET, or quantum computers. However, the main obstacle to the feasibility of semiconductor (SC) spintronic devices is the difficulty in creating a spin-polarized current in SC materials. As a result spin-polarized current has to be first created in a different medium and injected into the SC materials. Ferromagnetic (FM) materials are natural sources of spin-polarized current. However, the use of FM spin aligners to produce spin-polarized current faces the problem of conductivity mismatch [1,2] between the low resistivity metal and the high resistivity SC. It has been suggested that the diluted magnetic semiconductor (DMS) [3,4] could be used to inject spin-polarized currents into SC materials. However, DMS has low Curie temperature ($T_c$) and efforts to raise the $T_c$ of different DMS have not been successful. Another alternative, following Prof. Rashba's [2] suggestion, is to use a tunnel barrier [5] to solve the conductivity mismatch problem. Experimentally, Zhu et al. [6] reported a spin injection efficiency of 2% at room temperature, using Fe to inject spin polarized current into the SC through a tunnel barrier. Spin injection through tunneling was subsequently replicated by other researchers [7,8] using similar techniques. However, making a thin tunneling barrier with well-characterized spin-split properties remains a formidable engineering challenge. On the theoretical side, there are various other proposed spin
Spin characteristics of electron transport in semiconductor

injection methods that do not rely on using FM metals or tunnel barriers [9,10,11] as spin injectors. These new methods, however, still need experimental verification.

2.2 Small injector device

2.2.1 Device physics

In this chapter, we present a device as shown in Fig. 2.1 for spin injection from a FM-NM bilayer to a SC layer. It is well known that in FM metals, electrons of one spin experience more scattering compared to the other, depending on the intrinsic spin polarization ratio ($\beta_C$ of the FM metal). We conjectured that to maximize the spin injection ratio in the SC layer, the resistance of the FM metal as a fraction of the total device resistance has to increase. This can be accomplished by i) choosing FM metals with high resistivity $\rho$ as a spin aligner; ii) decreasing $A_{FM}$ to achieve minimum $A_{FM}/A_{SC}$. To achieve i), we selected Co, Fe, Ni$_{80}$Fe$_{20}$, Cr, V, or Gd as our FM materials because of their reasonably high values of $\rho$ (for metals). Of these, Co, Fe and Ni$_{80}$Fe$_{20}$ have been reported to have high $\beta$ values. Ni$_{80}$Fe$_{20}$ is used in our computation, because of its higher resistivity of $\rho_F=1.156 \times 10^{-7}$ $\Omega m$ compared to Co and Fe, lower spin diffusion length (SDL) of $\lambda=4$nm than Co (60nm), and a reasonably high $\beta_C$ of 37% compared to Co (42%) and Fe (45%). Similarly Gd$^{3+}$ with $T_c$ at 293K, $\rho_F$ of $14.28 \times 10^{-7}$ $\Omega m$, and $\beta_T$ of 0.14 [12], is also a potentially useful spin injector. To achieve ii), we confined the spin injector to a cylindrical pillar with small cross sectional area ($A_{FM}$), surrounded by insulating material as shown in layer 1 of Fig. 2.1. The small cylindrical cross-section increases total scattering within the ferromagnetic structure. This increases the proportion of spin-dependent scattering as a fraction of total carrier scattering in the device.

The use of a small injector, however, causes current crowding at interfaces 1,4 due to the abrupt discontinuity in $A$, resulting in spreading resistance [13,14,15,16] ($R_{SP}$) which, in our model is
assumed to be non spin-dependent. At the abrupt interface where current radiates in all directions, we used the finite-element software to estimate $R_{SP}$ at the interface and in the Cu region. Finite element analysis shows that after the Cu region, current flows perpendicular to the plane again. $R_{SP}$ found here is then integrated, self-consistently into the spin-drift-diffusion formalism for the device in other regions. In other words, the entire radial current region has been represented by a lumped resistance, while the straight current regions are described by the spin drift-diffusion equations. These regions were then integrated self-consistently.

To minimize $R_{SP}$, which is directly proportional to material resistivity, we conceived that it is important to contain $R_{SP}$ within a low resistivity metallic material instead of the high resistivity SC. Hence a NM (Cu) layer is inserted in layer 2 to form the bilayer injector of FM/Cu. The buffer layer has the same cross-sectional area as the SC, so as to avoid a further $R_{SP}$ contribution. Cu is a suitable material here because it has low resistivity and long SDL of $\kappa=140$ nm. This allows the Cu and SC layers to have a large $A$. The approximate upper limit of $A_{Cu}$ is $(2\kappa)^2$, which ensures that spin-polarized electrons in the Cu layer do not depolarize before entering the SC. To ensure diffusive transport, the lower limit of $A_{FM}$ is set by the mean-free-path (MFP) of the FM metal. Since $\lambda$ is longer than MFP in FM materials, we can approximate the lower limit of $A_{FM}$ to $\pi(\lambda/2)^2$. In FM metals, the Yafet effect [17] is the predominant spin flip mechanism, and the $\lambda$ value given by $(D\tau_{sf})^{1/2}$ where $D$ is the diffusion constant, typically ranges from 10 nm to 1 $\mu$m. For the SC materials, GaAs with SDL of between $\delta=1-5\mu$m is used with thickness $t_{SC}$ restricted to 100 nm to keep resistance low. The SC layer is highly doped so as to lower the resistivity of the SC, and thus its (spin independent) contribution to the overall resistance. Based on the above requirements, device parameter values are calculated using the known SDL values of different materials. Table 2.I contains the conductivity and intrinsic polarization values of materials suitable for spin injection. From the numerical values in Table 2.I, the geometrical
dimensions of the device can be calculated for different material composition. Table 2.II summarizes the geometrical dimensions for different choices of materials, and provides the required minimum values of $A_{FM}/A_{SC}$ for both Co, Ni$_{80}$Fe$_{20}$.

![Schematic illustration of the spin injection device with small cylindrical FM injector interfaced with the Cu layer to form a bilayer injector. Two bilayers are used to ensure a symmetrical interface electrochemical splits that simplify calculations.](image)

**FIG. 2.1.** Schematic illustration of the spin injection device with small cylindrical FM injector interfaced with the Cu layer to form a bilayer injector. Two bilayers are used to ensure a symmetrical interface electrochemical splits that simplify calculations.

**TABLE 2.II.** This table provides bulk conductivity values of some commonly found materials at 20 °C. (Adapted from “Solid State Physics” by Ashcroft and Mermin; “Introduction to Solid State Physics” by Charles Kittel; “Modern Magnetic Materials, Principles and Applications” by R.C.O. Handley). SDL of these materials are listed on the rightmost column. Polarization values were obtained from experimental studies of spin-polarized currents tunneling into Al, $\beta_1$[12], and bulk polarization, $\beta_c$ from Soulen et al. [18].

<table>
<thead>
<tr>
<th>Material</th>
<th>Conductivity, $\sigma \times 10^7 , \Omega^{-1} , m^{-1}$</th>
<th>$\beta_1$ (%)</th>
<th>$\beta_c$ (%)</th>
<th>SDL (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ag</td>
<td>6.29</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cu</td>
<td>5.95</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al</td>
<td>3.77</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tungsten</td>
<td>1.79</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fe</td>
<td>1.03</td>
<td>40</td>
<td>45</td>
<td></td>
</tr>
<tr>
<td>Nichrome (Ni, Fe, Cr alloy)</td>
<td>0.10</td>
<td>23</td>
<td>46.5</td>
<td></td>
</tr>
<tr>
<td>Mn</td>
<td>0.072</td>
<td>35</td>
<td>42</td>
<td>59</td>
</tr>
<tr>
<td>Ni</td>
<td>1.43</td>
<td>35</td>
<td>42</td>
<td>59</td>
</tr>
<tr>
<td>Co</td>
<td>1.72</td>
<td>35</td>
<td>42</td>
<td>59</td>
</tr>
<tr>
<td>Cr</td>
<td>0.78</td>
<td>35</td>
<td>42</td>
<td>59</td>
</tr>
<tr>
<td>V</td>
<td>0.5</td>
<td>35</td>
<td>42</td>
<td>59</td>
</tr>
<tr>
<td>Gd</td>
<td>0.070</td>
<td>14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ni$<em>{0.8}$Fe$</em>{0.2}$</td>
<td>0.865*</td>
<td>32</td>
<td>37</td>
<td>4</td>
</tr>
<tr>
<td>CoFe</td>
<td>50</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
TABLE 2.II. Geometrical dimensions of the device are calculated taking into account the SDL restrictions of various layers. Column 5 shows the minimum $A_{FM}/A_{SC}$ for different FM materials. Both ratios have to be small in order to achieve high spin injection.

<table>
<thead>
<tr>
<th>Device shown in Fig. 1.</th>
<th>Materials</th>
<th>layer thickness (nm)</th>
<th>$A$ of different layers (nm²)</th>
<th>$A_{FM}/A_{SC}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 1</td>
<td>Co</td>
<td>60</td>
<td>900 (πx30x30)</td>
<td>0.00125</td>
</tr>
<tr>
<td>Layer 1</td>
<td>Ni$<em>{80}$Fe$</em>{20}$</td>
<td>4</td>
<td>13 (πx2x2)</td>
<td>0.000166</td>
</tr>
<tr>
<td>Layer 3</td>
<td>GaAs</td>
<td>100</td>
<td>78400 (280x280)</td>
<td></td>
</tr>
<tr>
<td>Layer 3</td>
<td>Ge</td>
<td>100</td>
<td>78400 (280x280)</td>
<td></td>
</tr>
<tr>
<td>Layer 2,4</td>
<td>Cu</td>
<td>140</td>
<td>78400 (280x280)</td>
<td></td>
</tr>
</tbody>
</table>

### 2.2.2 Phenomenological descriptions

It is instructive to derive the equation of spin injection for our device using the phenomenological equations \[1\] for current transport in the diffusive regime. The equations governing spin transport \[19, 20\] for the spin up $J_+$ and spin down $J_-$ currents in a degenerate Fermi gas semiconductor, and their space derivatives are given below:

$$J_+ = -\frac{\sigma_+}{e} \frac{\partial \mu_+}{\partial x}$$

$$\frac{\partial (J_+ - J_-)}{\partial x} = \frac{2eN(E_F) \Delta \mu}{\tau_f}$$

where $\tau_f$ is the spin lifetime; $N(E_F)$ is the density of states at Fermi level $E_F$, $\mu$ is the electrochemical potential; $\Delta \mu = \mu_+ - \mu_-$; $\sigma$ is the conductivity, and $J = J_+ + J_-$ is the total current density. Combining Eqs. (1) and (2) yields:

$$\frac{\partial^2 \Delta \mu}{\partial^2 x} = \frac{\Delta \mu}{(SDL)^2}$$

The solutions to Eq. (3) in the pillar FM layers are given by Eqs. (4):

$$\mu_{\pm} = \mu_0 \pm |c_{\pm}| \exp \left( \frac{(x - x_0)}{\lambda} \right) \quad \mu_{\pm} = \mu_0 \pm |c_{\pm}| \exp \left( - \frac{(x - x_0)}{\lambda} \right)$$
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where subscripts $i$ denote the respective interfaces at the end of layer $i$. The solution to Eq. (3) for the SC layer results in:

$$\mu_{2s} = \mu_{20} \pm |c_{2s}| \exp(-x/\delta)$$  \hspace{1cm} (5)

where $|c_{is}|$ are the spin-split interfacial electrochemical potentials at interfaces $i$; $\mu_i$ is $\mu$ at interface $i$. Because of the thin Cu layers, $|c_{2s}|$ is approximately $|c_{1s}|$, and $|c_{3s}|$ is approximately $|c_{4s}|$. In summary, electrochemical potentials at interfaces $i$ are:

$$\mu_{1s} = \mu_{10} \pm |c_{1s}|; \quad \mu_{2s} = \mu_{20} \pm |c_{2s}|; \quad \mu_{3s} = \mu_{30} \mp |c_{3s}|; \quad \mu_{4s} = \mu_{40} \mp |c_{4s}|$$  \hspace{1cm} (6)

Eqs. (4) and (5) show that spin accumulation in the device degrades significantly if the thickness of either FM metal or SC is greater than their respective SDL. Currents ($I_{iz}$) for layers 1, 5 can be derived from Eq. (4) in terms of $\mu$ drop across the FM layers (1, 5) as shown in Eq. (7).

$$I_{1s} = -A_{FM} \frac{\sigma_{1s}}{e} \left( \frac{\partial \mu_{10}}{\partial x} \mp |c_{1s}| \right); \quad I_{5s} = -A_{FM} \frac{\sigma_{5s}}{e} \left( \frac{\partial \mu_{40}}{\partial x} \pm |c_{4s}| \right)$$  \hspace{1cm} (7)

Currents in the buffer layers of 2,4 can be modeled with Ohm’s law as shown in Eqs. (8). It is assumed here that the resistances in the Cu layers are dominated by $R_{sp}$, which will be proven by a separate simulation later.

$$I_{2s} = \frac{\mu_{1s} - \mu_{2s}}{2R_{sp}}; \quad I_{4s} = \frac{\mu_{3s} - \mu_{4s}}{2R_{sp}}$$  \hspace{1cm} (8)

To simplify calculations but without jeopardizing our effort to illustrate the usefulness of small injector in increasing spin injection, currents in the SC layer (3) is modeled with Ohm’s law in Eq. (9) but not the drift-diffusion equation of Eq. (5).

$$I_{SC} = \frac{\mu_{2s} - \mu_{3s}}{2R_{SC}}$$  \hspace{1cm} (9)

Substituting Eqs. (7), (8) into (9) yields

$$I_{SC} = \frac{(\mu_{10} \mp |c_{1s}| - 2I_{2s}R_{sp}) - (\mu_{40} \mp |c_{4s}| + 2I_{4s}R_{sp})}{2R_{SC}}$$  \hspace{1cm} (10)
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In layers 1 and 5, the drift-diffusion equation of Eq. (4) can be used to obtain \(|c_{\pm}|\) and \(|c_{\pm}|\). Because of the symmetrical structure of the device, \(|c_{\pm}|=|c_{\pm}|\). As current is continuous across the device, and assuming minimal spin flip in layers 2,3,4 because of deliberate effort to ensure thickness of these layers are much shorter than the SDL in the respective layers, we have

\[ I_{sc\pm} = I_{x\pm} = I_{x\pm}(x = x_i) = I_{s\pm}(x = x_i) \]

The current equation of Eq. (10) becomes

\[ I_{sc\pm} = \frac{\Delta \mu_0 - 4I_{sc\pm}R_{sp} \pm 2|c_{\pm}|}{2R_{sc}} \]  

Substituting Eq. (7) into Eq. (11) (note the change of sign), we obtained

\[ I_{sc\pm} = \frac{\Delta \mu_0 - \left( \frac{\lambda}{\partial \mu_0 / \partial x} \right)}{2R_{sc} + 4R_{sp} + \frac{2\lambda}{\sigma_{s\pm}A_{FM}}} = B \]  

where \(B\) is a constant, independent of spin up / down. Spin injection is defined by:

\[ \gamma = \frac{I_{sc+} - I_{sc-}}{I_{sc+} + I_{sc-}} \]

Derivations for spin injection can be explained with the two-current electrical equivalent circuit of Fig. 2.2 below:

FIG. 2.2. The two-current equivalent circuit is used to illustrate the scattering of spin up / down current through the device.

Substituting Eq. (12) into Eq. (13), noting that \(\sigma_{s} = \sigma_{FM} (1 \pm \beta) / 2\), \(\sigma_{sc\pm} = \sigma_{sc} / 2\) (for degenerate semiconductors), \(R_{sc\pm} = 2R_{sc}, R_{sp\pm} = 2R_{sp}\), spin injection can be derived as shown in Eq. (14), which still bears similarity in form to the spin injection equations derived in Ref. 1. The
Spin characteristics of electron transport in semiconductor

conductivity values used here are bulk values. To derive for thin film conductivity, the relation of
\[ \sigma_{\text{film}} = \sigma_{\text{bulk}}/(1-\beta)^2 \]
is used.

\[ \gamma = \frac{\beta}{1+\left(\frac{R_{\text{SC}} + 2R_{\text{SP}}}{R_{\text{FM}}}\right)(1-\beta^2)} \]  \hspace{1cm} (14)

\( R_{\text{SP}} \) can be approximated to the analytical value [11] of \( 1/4r\sigma_{\text{SP}} \) or \( (\pi/16\sigma_{\text{SP}}^2\Lambda_{\text{FM}})^{1/2} \), which applies in the limit of \( A_{\text{SC}} \rightarrow \infty \). Note that \( \sigma_{\text{SP}} = \sigma_{\text{Cu}} \) and \( r \) is the radius of \( \Lambda_{\text{FM}} \). Substituting \( R_{\text{SP}} \) into Eq. (14) yields

\[ \gamma = \frac{\beta}{1+\left(\frac{l_{\text{SC}}\sigma_{\text{FM}}\Lambda_{\text{FM}}}{\lambda} + \frac{\sigma_{\text{FM}}\sqrt{\pi\Lambda_{\text{FM}}}}{2\lambda}\right)(1-\beta^2)} \]  \hspace{1cm} (15)

Equation (15) confirms that the ratio of \( A_{\text{FM}}/A_{\text{SC}} \) should be kept to the minimum to increase spin injection. It also shows that spin injection can be increased by increasing the conductivity of the SC layer by means of doping. In the case of Si for example, its intrinsic conductivity is \( 3\times10^{-4} \text{ ohm}^{-1}\text{m}^{-1} \). When doping density \( (N_D) \) is increased to \( 1\times10^{18} \text{cm}^{-3} \), two opposing effects occur: i) electron concentration increases, but ii) carrier mobility \( \mu_n \) decreases to just 280cm²/Vs [21] as a result of more impurity scattering. But effect (i) dominates over (ii) so that an overall increase of conductivity to \( \sigma_{\text{Si}} = 4.4\times10^3 \Omega^{-1}\text{m}^{-1} \) occurs. The same trend occurs for Ge and GaAs, which can be doped to achieve even lower resistivities than Si. Hence, Ge and GaAs are chosen as the SC materials in our device. Table 2.III shows that GaAs has better conductivity than Ge and Si at higher doping density.

2.2.3 Simulation of spreading resistance

It is worth noting that the resistance in Cu has been assumed to be dominated by \( R_{\text{SP}} \). We confirmed the dominance of \( R_{\text{SP}} \) in Cu by analyzing the current crowding effect in these two layers using the ANSYS finite element software [22]. The current density distribution in the device is
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calculated numerically by solving the Poisson equation. In the simulation, three layers of materials (Ni$_{80}$Fe$_{20}$, Cu, GaAs) were defined in terms of conductivity values and geometrical dimensions, based on Table 2.1. Figure 2.3 shows current injection from a Ni$_{80}$Fe$_{20}$ spin aligner with $A_{FM}/A_{SC}=0.000166$.

FIG. 2.3. (a) Simulation shows that current crowding effect is restricted to the Cu buffer layer, implying that the non spin-dependent $R_{SP}$ is restricted to the Cu layer. This ensures that $R_{SP}$ would not be very high as Cu has low conductivity. (b) Similar simulations were carried out for Co injector to better show the current crowding effects. Co injector has a larger cylindrical area than the NiFe injector because of its larger mean free path.

These simulation results reveal an inhomogeneous current density distribution in the Ni$_{80}$Fe$_{20}$ and Cu, which is responsible for the $R_{SP}$ effect. As current passes across the Cu buffer layer towards the GaAs region, it initially radiates in all directions out from the small injector interface, but slowly becomes perpendicular to surface plane. At the Cu-GaAs interface, the current density lines become virtually parallel to each other and perpendicular to the interfacial plane. Thus the current crowding effect is almost fully confined to the larger Cu layer, without spilling over to the GaAs layer. This also confirms that Cu with thickness of $t_{FM}=10$nm is thick enough to accommodate $R_{SP}$.

To estimate $R_{SP}$, we first compute the total resistance across the device $R_T$, by passing a known current (20 $\mu$A) and obtaining the voltage difference across the device. In the absence of any
spreading currents, the resistance in the FM layer is given by \( R_{FM} = \rho_{FM} l_{FM} / A_{FM} \), and similar expressions hold for \( R_{Cu} \) and \( R_{SC} \) for the Cu, and SC layers, respectively. The spreading resistance is then obtained from the difference \( R_{SP} = R_I - (R_s + R_{Cu} + R_{SC}) \). \( R_{SP} \) is in our device estimated at 2.85 \( \Omega \), which is substantially lower than the spin dependent resistance of Ni\(_{80}\)Fe\(_{20}\) of 36.8 \( \Omega \). The analytical value of \( R_{SP} \) by Maxwell [20,22] is obtained for an ideal structure of infinite length and cross sectional area [15]. We now investigate how close this analytical result is compared to the actual value for our finite-sized device. There is some discrepancy in the \( R_{SP} \) values compared with Maxwell’s estimate. In the case of Co spin aligner, the Maxwell’s value of \( R_{SP} \) is 0.14 \( \Omega \) while simulation value is 0.16 \( \Omega \), while in the case of Ni\(_{80}\)Fe\(_{20}\), the two \( R_{SP} \) values are 2.1 \( \Omega \) and 5.4 \( \Omega \), respectively. This discrepancy is due to the finite length and surfaces of our devices, for which correction factors to the Maxwell’s formula are required [20,22]. This discrepancy however has little effect on the overall spin polarization \( \gamma \) (Fig. 2.4) since in the presence of the buffer layer \( R_{SP} \) is much smaller than \( R_{SC} \).

![Spin injection vs doping density](image)

**FIG. 2.4.** Spin injection graphs were plotted for spreading resistance derived from simulated values and that derived from analytically calculated values. Results shows that the discrepancy between simulated value and analytic value has little effect on spin injection.
Spin characteristics of electron transport in semiconductor

TABLE 2.III. The first three rows of the table shows the material types, mobility of electrons and holes, and the intrinsic conductivity of these materials. Data were obtained from Ref. 20. The following rows show the increase of conductivity of Ge and GaAs with increasing n type doping concentration.

<table>
<thead>
<tr>
<th>SC materials</th>
<th>$\mu_n$ (cm$^2$/Vs)</th>
<th>$\mu_p$ (cm$^2$/Vs)</th>
<th>$\sigma$ ($\Omega^{-1}$m$^{-1}$)</th>
<th>$N_D$ doping concentration (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>1.900</td>
<td>500</td>
<td>$3 \times 10^3$</td>
<td>Intrinsic</td>
</tr>
<tr>
<td>Ge</td>
<td>3.800</td>
<td>182</td>
<td>1.8</td>
<td>Intrinsic</td>
</tr>
<tr>
<td>GaAs</td>
<td>9.000</td>
<td>50</td>
<td>$4.6 \times 10^{-7}$</td>
<td>Intrinsic</td>
</tr>
<tr>
<td>Ge</td>
<td></td>
<td></td>
<td>$2.85 \times 10^4$</td>
<td>$1 \times 10^{20}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Ge</td>
<td></td>
<td></td>
<td>$1.44 \times 10^5$</td>
<td>$1 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Ge</td>
<td></td>
<td></td>
<td>$1.72 \times 10^4$</td>
<td>$1 \times 10^{18}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Ge</td>
<td></td>
<td></td>
<td>$2.63 \times 10^3$</td>
<td>$1 \times 10^{17}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Ge</td>
<td></td>
<td></td>
<td>$5.26 \times 10^2$</td>
<td>$1 \times 10^{16}$ cm$^{-3}$</td>
</tr>
<tr>
<td>GaAs</td>
<td></td>
<td></td>
<td>$1.25 \times 10^6$</td>
<td>$1 \times 10^{20}$ cm$^{-3}$</td>
</tr>
<tr>
<td>GaAs</td>
<td></td>
<td></td>
<td>$2.50 \times 10^5$</td>
<td>$1 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>GaAs</td>
<td></td>
<td></td>
<td>$5.00 \times 10^4$</td>
<td>$1 \times 10^{18}$ cm$^{-3}$</td>
</tr>
<tr>
<td>GaAs</td>
<td></td>
<td></td>
<td>$5.26 \times 10^3$</td>
<td>$1 \times 10^{17}$ cm$^{-3}$</td>
</tr>
<tr>
<td>GaAs</td>
<td></td>
<td></td>
<td>$5.55 \times 10^2$</td>
<td>$1 \times 10^{16}$ cm$^{-3}$</td>
</tr>
</tbody>
</table>

2.2.4 Computation results

It can be seen from Eq. (15) that if the Cu buffer layer has not been used, $R_{SP}$ would be large, since $\sigma_{SP}$ would have taken the value of $\sigma_{SC}$ but not $\sigma_{Cu}$. When a NM metal is introduced adjacent to the FM metal to form a bilayer injector, $R_{SP}$ becomes small as $\sigma_{SP}$ has taken the value of $\sigma_{NM}$, which is much greater than $\sigma_{SC}$. Spin injection efficiency is computed using Eq. (15) and parameters in Table 2.II, $\sigma_{SP}=\sigma_{Cu}=5.95 \times 10^7 \Omega^{-1}$m$^{-1}$ and results are shown in Fig. 2.5. It is assumed that changes in the SC doping concentration do not significantly reduce $\delta$, so that $\delta$ is much greater than $t_{SC} = 100$ nm even at the highest doping level. Results in Fig. 2.5 show that spin injection efficiency ($\gamma$) is approximately 20% for $N_D=10^{18}$ cm$^{-3}$, and increases with higher doping concentration of GaAs because of the increases in SC conductivity. Figure 2.5 also shows that without Cu, $\gamma$ is just 1% for the same $N_D$ of $10^{18}$ cm$^{-3}$. The Cu buffer enhances spin injection ratio for GaAs by reducing the $R_{SP}$ effect, such that a $\gamma$ value exceeding 30% is predicted at the highest doping concentration of $N_D$ of $10^{20}$ cm$^{-3}$. For GaAs without Cu, $\gamma$ is just 5% for the same $N_D$. 

[20]
Spin characteristics of electron transport in semiconductor

FIG. 2.5. Spin injection increases with increasing $\sigma_{SC}$, which is achieved by increasing $N_D$. For GaAs materials, $N_D$ of $10^{18} \text{cm}^{-3}$ and above could generate spin injection of 20% and above.

Substituting the lower limit of $A_{FM}$ and the upper limit of $A_{SC}$, Eq. (20) can be expressed in terms of the SDL of the buffer layer:

$$\gamma = \frac{16\beta}{16 + \pi \left( l_{SC} \frac{\sigma_{FM}}{\sigma_{SC}} \frac{\lambda}{(\kappa)^2} + \frac{4\sigma_{FM}}{\sigma_{Cu}} (1 - \beta^2) \right)}$$

(16)

Computation with Eq. (16) shows in Fig. 2.6 that choosing a NM buffer layer of longer SDL enables high spin injection to be achieved at lower $\sigma_{SC}$. This is because for buffer materials with longer SDL, a larger $A$ can be used to further decrease the ratio of $A_{FM}/A_{SC}$. In conclusion, the use of bilayer injector and collector with an embedded pillar FM spin aligner in each bilayer allows high spin injection to be achieved. Such design can also circumvent the decrease of spin injection due to the effect of spreading resistance. Spin injection can be further increased with the use of buffer materials with longer SDL. Spin injection can, however, never exceed the $\beta$ value of the FM materials. For $\beta=100\%$, spin injection in SC is equal in value to $\beta$, regardless of device conductivity and geometrical dimensions.
2.3 Contact resistance

Contact resistance ($R_C$) which occurs at a metal-SC interface. $R_C$ would be significant if the specific contact resistivity $\rho_C$ between SC and Cu is high. This explains our preference for GaAs, Si, or Ge, as these materials are known to form contact of low barriers with non-magnetic metals like Cu or Al. Furthermore, experiments have shown that doping Ge or Si highly with n type impurities can reduce $\rho_C$ quite substantially. Even so, experimental data (Table 2.IV) shows that $R_C$ is substantially higher than $R_{SC}$ and $R_{SP}$ ($\rho_C$ is ~ 20 times higher than $\rho_{SC}$ at doping density $N_D=10^{20}$ cm$^{-3}$) except at very high values of $N_D=10^{21}$ cm$^{-3}$ or higher. This would have an adverse effect on spin injection as described by Eqs. (14) and (15). We conjectured with crude assumptions of symmetrical $R_C$ at both SC-Cu interfaces that Eq. (14) could be modified to:

$$\gamma = \frac{\beta}{1 + \left(\frac{R_{SC} + R_{SP} + R_C}{R_{SP}}\right)(1 - \beta^2)}.$$  

Assuming that scattering at the NM-SC interface is non spin-dependent, this could render as futile all the previous efforts to reduce $R_{SP}$ and $R_{SC}$. Nevertheless, this contact resistance (or Schottky) problem is a long-standing one and various methods have been devised to overcome this problem.

FIG. 2.6. High spin injection is achieved at lower $\sigma_{SC}$ as SDL of the NM buffer layer increases as indicated in the circle region by the arrow.
One possible method is to introduce a delta layer (~5 nm thick) at the SC-Cu interface of high n doping density $N_D = 1 \times 10^{21}$ cm$^{-3}$. Interfacial doping avoids the need for bulk doping. Bulk doping density in excess of $10^{18}$ cm$^{-3}$ would reduce the value of $\kappa$.

<table>
<thead>
<tr>
<th>Materials</th>
<th>$\rho_C$ (Ohm m$^2$)</th>
<th>$(\rho_{SC})<em>t$ (Ohm m$^2$ for $t</em>{SC}=100$nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_B=0.4$eV (Cu and Si or Ge)</td>
<td>$10^{-14}$</td>
<td></td>
</tr>
<tr>
<td>$N_D=1 \times 10^{21}$ cm$^{-3}$</td>
<td>3$\times$10$^{-12}$</td>
<td>1.8$\times$10$^{-13}$</td>
</tr>
<tr>
<td>Ge ($N_D=1 \times 10^{20}$ cm$^{-3}$)</td>
<td>2$\times$10$^{-9}$</td>
<td>3.5$\times$10$^{-13}$</td>
</tr>
<tr>
<td>Ge ($N_D=1 \times 10^{19}$ cm$^{-3}$)</td>
<td>3$\times$10$^{-7}$</td>
<td>3.0$\times$10$^{-12}$</td>
</tr>
<tr>
<td>GaAs ($N_D=1 \times 10^{20}$ cm$^{-3}$)</td>
<td>3$\times$10$^{-12}$</td>
<td>4.0$\times$10$^{-14}$</td>
</tr>
<tr>
<td>GaAs ($N_D=1 \times 10^{19}$ cm$^{-3}$)</td>
<td>2$\times$10$^{-9}$</td>
<td>2.0$\times$10$^{-13}$</td>
</tr>
<tr>
<td>GaAs ($N_D=1 \times 10^{18}$ cm$^{-3}$)</td>
<td>3$\times$10$^{-7}$</td>
<td>1.0$\times$10$^{-12}$</td>
</tr>
</tbody>
</table>

2.4 Magnetoresistance

2.4.1 Current-confined MR

The small injector device described in section 2.2 can be viewed as a form of current-perpendicular-to-plane (CPP) device, similar to the fully-metallic CPP device which has found major usage in the recording heads of hard disk drive. To calculate magnetoresistance (MR) for this device, it has first to be assumed that all layers in the device are thinner than their respective SDL. In previous spin injection computation, FM layers of 1 and 5 are thick and the splitting of electrochemical potentials in each FM layer reaches its maximum at the FM-Cu interface. Further into the FM layer from the interface, electrochemical split narrows and converges at infinity. We therefore conjectured that thick FM layers might result in low MR values although it has no effect on spin injection. This can be seen in Eq. (12) that spin injection is a function of the FM spin diffusion length of $\lambda$ but not FM layer thickness. However, in the analysis of MR, a thick FM layer would complicate computation as due to the effect of drift diffusion, the resistance for spin
up / down current would be an average value that cannot be obtained in a straightforward manner. To simplify calculation, a thin FM layer with thickness on the order of $\lambda$ is used. With small FM thickness, electrochemical drop in this layer is governed by Ohm’s law and not the drift diffusion equation. Spin accumulation thus converges to zero at a distance $\lambda$ projected back from the FM-Cu interface. This simplifies the calculation of FM resistance. MR is defined as follows:

$$MR = \frac{R_{SP} - R_p}{R_p}$$

Neglecting $R_C$, $R_{SP}$, and following the standard derivation steps, the expression for MR is obtained as in Eq. (19), which is similar in form to Eq. (8) of Ref 1.

$$MR = \frac{4\beta^2}{4(1 - \beta^2) + 4 \frac{R_{SC}}{R_{FM}} (1 - \beta^2) + \left( \frac{R_{SC}}{R_{FM}} \right)^2 (1 - \beta^2)^2}$$

As $R_{SC} >> R_{FM}$. Eq. (19) can also be further simplified to Eq. (20) as follows:

$$MR = \frac{4\beta^2}{(1 - \beta^2)^2} \frac{R_{FM}^2}{R_{SC}^2}$$

To include the effect of $R_{SP}$, $R_{SC}$ is replaced by $R_{SC} + 2R_{SP}$. Note that in the derivation of Eq. (19), $2R_{SC}$ was used to describe resistance to electrons of one spin. To include the effect of $R_{SP}$, it is necessary to use the term $2(R_{SC} + 2R_{SP})$ to describe resistance to electrons of one spin in the Cu and SC regions. Therefore $R_{SC}$ of Eq. (19) should be replaced by $R_{SC} + 2R_{SP}$, resulting in Eq. (20).

Taking $A_{cs} = 4\kappa^2$, $A_{fm} = \frac{\pi\lambda^2}{4}$, and ignoring $4(1 - \beta^2)$, Eq. (20) can be expressed as Eq. (21) & (22) as follows:

$$MR = \frac{4\beta^2}{4(1 - \beta^2) + 4 \left[ \frac{R_{SC} + 2R_{SP}}{R_f} \right] (1 - \beta^2) + \left[ \frac{R_{SC} + 2R_{SP}}{R_f} \right]^2 (1 - \beta^2)^2}$$

$$MR = \frac{4\beta^2}{4\pi \left[ \frac{t_{sc} \sigma_{fm}}{16\sigma_{sc} (\kappa)^2} + \frac{\sigma_{fm}}{\sigma_{cs}} \left( 1 - \beta^2 \right) + \frac{t_{sc} \sigma_{fm} \lambda}{16\sigma_{sc} (\kappa)^2} + \frac{\sigma_{fm}}{\sigma_{cs}} \left( 1 - \beta^2 \right)^2 \right] }$$
Computation is conducted for the design that uses Ni$_{80}$Fe$_{20}$ as F metal, Ge or GaAs as semiconductor, and Cu as NM. We follow the geometrical dimensions of Table 2.II and summarized our results in Table 2.V below:

<table>
<thead>
<tr>
<th>Materials</th>
<th>MR (%)</th>
<th>$\sigma$ ((\Omega^{-1}m^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ge ($N_D=1x10^{20}$ cm$^{-3}$)</td>
<td>24.5</td>
<td>2.85x10$^5$</td>
</tr>
<tr>
<td>GaAs ($N_D=1x10^{20}$ cm$^{-3}$)</td>
<td>29.7</td>
<td>1.25x10$^6$</td>
</tr>
<tr>
<td>Ge ($N_D=1x10^{19}$ cm$^{-3}$)</td>
<td>19.8</td>
<td>1.44x10$^5$</td>
</tr>
<tr>
<td>GaAs ($N_D=1x10^{19}$ cm$^{-3}$)</td>
<td>23.6</td>
<td>2.50x10$^5$</td>
</tr>
<tr>
<td>Ge ($N_D=1x10^{18}$ cm$^{-3}$)</td>
<td>4.2</td>
<td>1.72x10$^4$</td>
</tr>
<tr>
<td>GaAs ($N_D=1x10^{18}$ cm$^{-3}$)</td>
<td>11.1</td>
<td>5.00x10$^3$</td>
</tr>
</tbody>
</table>

It can be seen that MR values increase with increasing SC conductivity. In fact MR values for this CPP device can reach 29.7% for highly-doped GaAs ($N_D=1x10^{20}$ cm$^{-3}$), and 24.5% for highly-doped Ge ($N_D=1x10^{20}$ cm$^{-3}$). However, for more achievable doping concentration of $N_D=1x10^{18}$ cm$^{-3}$, MR values are 4.2% and 11.1% for Ge and GaAs, respectively.

2.4.2 Metal-based CPP with half metal insertion

In metal-based spintronic, the CPP device is increasingly used [23,24] as the recording device for high density magnetic storage. The CPP has the advantage that it can be inserted in contact between the two shields, allowing shield gap of the disk head to further reduce. It also has lower areal resistance of 0.05 $\Omega \mu m^2$ compared to the tunneling magnetoresistance (TMR) device of larger than 1 $\Omega \mu m^2$. The CPP device can thus deliver more signal power to the preamplifier that has typical input resistance of 50 $\Omega$. However, the CPP has not been able to produce high MR ratio. Recent experimental works have shown results of MR ratio increasing with the insertion of a heavily oxidized Cu layer that constrict current flow through Cu. Oxidation has been achieved by natural oxidation, as well as ion-argon oxidation, both methods have shown increase of MR ratio with increasing oxidation. The increase of MR has been attributed to the effect of current
confinement, although it is still not fully understood how current confinement causes high MR. We believe the increase of MR is related to the increase of spin injection for parallel magnetizations of the FM contacts, as has been previously described in section 2.2 for the small-injector spin injection device. High spin injection means current for one spin branch far exceeds that of the other spin branch, resulting in low resistance for the spin branch that has the same spin orientation as the parallel magnetization. The overall resistance is thus low. In the anti-parallel configuration, spin injection is zero, resulting in no change of resistance value for the small injector device compared to ordinary-sized injector device. Current-confinement could thus result in high MR in this way.

In this section, we will, however, perform MR modeling for a CPP device without current confinement. Our focus is on studying the effects of inserting half-metallic (HM) materials into the CPP device on MR. Figure 2.7 (a) shows the schematic structure of a CPP device with HM layers inserted between Cu and CoFe. The CPP structures of (CoFe-Fe₃O₄-Cu-Fe₃O₄-CoFe) and (CoFe-CrO₂-Cu-CrO₂-CoFe) correspond to thickness of (4-0.5-2-0.5-4) nm and resistivity of (10-19,000-1.6-19,000-10)x10⁻⁸Ωm and (10-150-1.6-150-10)x10⁻⁸Ωm, respectively. Figure 2.7 (b) shows results of MR increasing with the half metal polarization for different half metal resistivity. Since Fe₃O₄ has much higher resistivity values than CrO₂, i.e. 19,000:50, the former CPP device shows overall higher MR ratio. Figure 2.7 (b) also shows that the HM polarization ratio is important for increasing MR as it increases monotonically with increasing polarization ratio. At very low HM polarization ratio, i.e. 0.3-0.4, MR is consistently low, and the effect of resistivity could hardly result in MR increase. These results were also consistent with our earlier conception that increasing spin-dependent resistance of the device increases spin injection and MR.
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FIG. 2.7. (a) CPP device with insertion of half metal layers (CoFe-HM-Cu-HM-CoFe). (b) MR ratio increases with increasing half metal polarization ratio. Half-metal of higher resistivity value shows significant increase of MR ratio with increasing half metal polarization.

However, the use of half-metal still faces practical problems. The high polarization of close to 90% can only be achieved in crystalline half metal. In actual growth process, the material could become amorphous or partially crystalline, resulting in low polarization. The resistivity of the half metal could also be affected by material structure. In the event of overly high resistance, overall device MR could be suppressed because of the spin flipping effects. Furthermore, the interfacial resistances between the half-metal and adjacent layers have also not been well understood. If the resistance is not spin-anisotropic, overall MR could be affected. In the worst scenario, the resistance could even be spin flipping, thus suppressing MR.

2.5 Asymmetrical interface barriers

It has been mentioned in chapter 1 and section 2.1 of chapter 2 that the tunneling barriers [4,5,6] could be used to overcome the problem of conductivity mismatch, and enhance spin injection. However, the tunneling barriers across most trilayer devices have been assumed to be identical. Figure 2.8 shows a generic trilayer device with barrier height values arbitrarily assumed. In this section, we derived and used a model that removed these assumptions.
The interfacial resistances of $R(0)$ and $R(L)$ were obtained self-consistently. We used the ballistic transmission model to calculate electron transmission across a delta electrical potential at the FM-SC interfaces [25, 26]. Ballistic transport here refers to scattering free transmission of electrons through the interfacial potential barrier. Quantum mechanical tunneling is the method we used to evaluate ballistic transport through the barriers. As our work is theoretical in nature, we have considered single-mode resistance only, i.e. resistance due to one transmission mode only. This is because the purpose of this work is not to simulate transport across this device but to present a new theoretical argument that interfacial resistance is not entirely an intrinsic property of the interface but it is also coupled to external bias effect. We thus need only the simplest representation of the interfacial resistance here.

In the FM, SC, FM layers of our trilayer structure, their thicknesses are larger than the respective SDL. We thus calculated for electron transport through these layers with the spin drift diffusion models. Our trilayer structure is Fe-2DEG-Fe. The 2DEG layer is highly-doped (n++) AlGaAs-GaAs. In the first approximation, we ignore any type of electron scattering within the barriers and assume purely ballistic transport through them. The drift-diffusion equations of Eqs. (3) and (4) are used to generate the spin accumulation equations in the FM and SC as follows:

$$\mu_+ - \mu_- = Ae^{x/\delta} \quad x < 0$$  \hspace{1cm} (23)$$

$$\mu_+ - \mu_- = Be^{-x/\delta} + Ce^{-(x-L)/\delta} \quad 0 < x < L$$ \hspace{1cm} (24)
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\[ \mu_\uparrow - \mu_\downarrow = De^{-x/L/\lambda} \quad x > L \]  

(25)

where \( L \) is the width of the middle layer. The discontinuities of \( \mu_\uparrow, \mu_\downarrow \) across the FM-SC interfaces are given by Eq. (26).

\[ \Delta \mu_{\downarrow\uparrow} = -\frac{e j_{\downarrow\downarrow}(x=0,L)}{G_{\uparrow\downarrow}} \]  

(26)

\( G_{\uparrow\downarrow} \) are the interfacial conductances to be determined self-consistently. For highly doped SC systems in metallic regime, the effect of \( \mu_\uparrow - \mu_\downarrow \) on conductivity change is minimal. This assumption is also in accordance with previous spin transport models of Schmidt, Rashba and van-Son, in which the conductivity of SC layer has been assumed to be constant and spin-independent. Thus based on this approximation, the conductivity polarization parameter \( \alpha \) in the SC is given by:

\[ \alpha = \frac{n_\uparrow}{n_\uparrow + n_\downarrow} = 1/2 \]  

(27)

We introduce \( \alpha \) and \( \beta \) as the spin polarization of conductivity, current, respectively, i.e.

\[ \beta = j_\uparrow / j \quad \text{and} \quad \alpha = \sigma_\uparrow / \sigma, \]  

where \( j = j_\uparrow + j_\downarrow \), \( j \) is constant and continuous across the FM-SC interfaces, \( \alpha \) is not continuous, \( \beta \) is continuously varying across the trilayer, clearly showing the absence of spin-flip scattering at the interfaces and the effect of spin relaxation in the material.

Using the relations of \( \frac{\partial \mu_{\downarrow\uparrow}}{\partial x} = -\frac{e j_{\downarrow\downarrow}}{\sigma_{\downarrow\downarrow}} \) at both interfaces yields Eqs. (28) and (29) for current continuity at \( x=0 \):

\[ \frac{e j}{\sigma_\downarrow} \left[ \beta(0) - \alpha_\downarrow \right] / \alpha_\downarrow \left( 1 - \alpha_\downarrow \right) = \frac{A}{\lambda_\downarrow} \]  

(28)

\[ \frac{e j}{\sigma_\uparrow} \left[ \beta(0) - \alpha_\uparrow(0) \right] / \alpha_\uparrow(0) \left( 1 - \alpha_\uparrow(0) \right) = \frac{-B + C e^{-\nu/\lambda_\downarrow}}{\lambda_\downarrow} \]  

(29)

Similarly, current continuity at \( x=L \) yields Eqs. (30) and (31):
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\[
\frac{e_j}{\sigma} \left[ \frac{\beta(L) - \alpha_j(L)}{\alpha_j(L)(1 - \alpha_j(L))} \right] = -\frac{Be^{-y/\lambda_j} + C}{\lambda_j} \tag{30}
\]

\[
\frac{e_j}{\sigma} \left[ \frac{\beta(L) - \alpha_j}{\alpha_j(1 - \alpha_j)} \right] = -\frac{D}{\lambda_j} \tag{31}
\]

Another set of boundary conditions is obtained by substituting Eqs. (23), (24), (25) into Eq. (26) at the FM-SC interfaces. The electrochemical potential discontinuities for both spin, i.e. \(\Delta\mu_\uparrow\) and \(\Delta\mu_\downarrow\) can be obtained in terms of \(G_{e_j}\) and subtracted from one another to yield:

\[
\frac{e_j}{\sigma} \left( \frac{\beta(0)}{G_j(0)} + \frac{\beta(0) - 1}{G_j(0)} \right) = B + Ce^{-L/\lambda_j} - A \tag{32}
\]

\[
\frac{e_j}{\sigma} \left( \frac{\beta(L)}{G_j(L)} + \frac{\beta(L) - 1}{G_j(L)} \right) = D - Be^{-L/\lambda_j} - C \tag{33}
\]

We have thus obtained 6 boundary relations i.e. Eqs. (28), (29), (30), (31), (32), (33) that completely determine \(A\) through \(D\), as well as \(\beta(0), \beta(L)\). Once the interfacial quantities are known, \(\beta(x)\) can be found. Substituting \(\beta(x)\) into \(\beta = j_j/j\) and integrating, we can then obtain the one-dimensional variation of the \(\mu_{e_j}\) in space. After simplifications, we finally obtained the interfacial discontinuities in \(\mu_{e_j}\) at the two FM-SC interfaces:

\[
\Delta\mu_\uparrow(0) = \frac{ej\beta(0)}{G_j(0)} \tag{34}
\]

\[
\Delta\mu_\downarrow(0) = \frac{ej(1 - \beta(0))}{G_j(0)} \tag{35}
\]

\[
\Delta\mu_\uparrow(L) = \frac{ej\beta(L)}{G_j(L)} \tag{36}
\]

\[
\Delta\mu_\downarrow(L) = \frac{ej(1 - \beta(L))}{G_j(L)} \tag{37}
\]

Eq. (26) shows that the interfacial discontinuity is a function of the interfacial conductance. However, we suggested in this section that the interfacial conductances are themselves functions
of interfacial continuities, and not arbitrary known values as have been assumed in previous literatures [2,25]. Figure 2.9 illustrates the band-structure diagram of electron transmission at various electrochemical levels. The mutual dependences between interfacial $\Delta \mu_{\uparrow\downarrow}$ and $G_{\uparrow\downarrow}$ allows determination of these values in a self-consistent manner.

FIG. 2.9. (a) The electrochemical potential profile of the FM-SC-FM trilayer show that electron kinetic energy / wave-vector depends on the electrochemical potential drop at the interfaces. (b) The energy dispersion curves show that electron of the FM layers have much higher kinetic energies compared to electrons in the SC 2DEG layer. This is because of the significantly higher Fermi energies of metallic materials due to the presence of large number of free conduction band electrons.

We will show in the following derivations using the ballistic transmission models that $G_{\uparrow\downarrow}$ depend on $\Delta \mu_{\uparrow\downarrow}$. The interfacial barrier profiles are described by: $U_{\uparrow\downarrow}^{\pm} \delta(x) + U_{\uparrow\downarrow}^{\pm} \delta(x - L)$ [25,27]. It is assumed that both interfaces are symmetrical i.e. $U_{o}^{\uparrow\downarrow} = U_{l}^{\uparrow\downarrow}$. The absolute values of the Fermi wave vectors in the tri-layer structure are shown in Table 2.VI.
Spin characteristics of electron transport in semiconductor

Table 2.VI. The wave-vectors of electrons in different regions of the device are shown on the left / right column for spin up / down.

<table>
<thead>
<tr>
<th>Spin up</th>
<th>Spin down</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{\uparrow\uparrow} = \sqrt{2m^*<em>{Fe}E</em>{Fe}^{\uparrow\uparrow}/\hbar}$</td>
<td>$k_{\uparrow\downarrow} = \sqrt{2m^*<em>{Fe}(E</em>{Fe}^{\uparrow\downarrow} - \mu_0^d)}/\hbar$</td>
</tr>
<tr>
<td>$k_{\uparrow\downarrow} = \sqrt{2m^*<em>{GaAs}(E</em>{GaAs}^{\uparrow\downarrow} + \Delta\mu_0(0) - E_{Fe}^{\uparrow\downarrow})/\hbar}$</td>
<td>$k_{\uparrow\downarrow} = \sqrt{2m^*<em>{GaAs}(E</em>{GaAs}^{\uparrow\downarrow} + \Delta\mu_0(0) - \mu_0^d)/\hbar}$</td>
</tr>
<tr>
<td>$k_{\downarrow\downarrow} = \sqrt{2m^*<em>{GaAs}(E</em>{GaAs}^{\downarrow\downarrow})/\hbar}$</td>
<td>$k_{\downarrow\downarrow} = \sqrt{2m^*<em>{GaAs}(E</em>{GaAs}^{\downarrow\downarrow})/\hbar}$</td>
</tr>
<tr>
<td>$k_{\downarrow\downarrow} = \sqrt{2m^*<em>{Fe}(E</em>{Fe}^{\downarrow\downarrow} + \Delta\mu_1(L))/\hbar}$</td>
<td>$k_{\downarrow\downarrow} = \sqrt{2m^*<em>{Fe}(E</em>{Fe}^{\downarrow\downarrow} + \Delta\mu_1(L) - \mu_0^d)/\hbar}$</td>
</tr>
</tbody>
</table>

By matching the wave functions at the two interfaces, we obtained the transmission probabilities for the up/ down spin at the two interfaces as:

$$T^{\uparrow\downarrow}(0) = \frac{k_{\uparrow\downarrow}m_{Fe}^{*}}{k_{\downarrow\downarrow}m_{GaAs}^{*}} \left| \frac{2ik_{\downarrow\downarrow}}{ik_{\downarrow\downarrow} + i(m_{Fe}^{*}/m_{GaAs}^{*})k_{\downarrow\downarrow} - \frac{2m_{Fe}^{*}U^{\uparrow\downarrow}(0)}{\hbar^2}} \right|^2 \quad (38)$$

$$T^{\uparrow\downarrow}(L) = \frac{k_{\downarrow\downarrow}m_{GaAs}^{*}}{k_{\downarrow\downarrow}m_{Fe}^{*}} \left| \frac{2ik_{\downarrow\downarrow}}{ik_{\downarrow\downarrow} + i(m_{GaAs}^{*}/m_{Fe}^{*})k_{\downarrow\downarrow} - \frac{2m_{GaAs}^{*}U^{\uparrow\downarrow}(L)}{\hbar^2}} \right|^2 \quad (39)$$

The interfacial conductance can then be derived from the Landau’s formula in the simple form as:

$$\frac{1}{R^{\uparrow\downarrow}(0,L)} = G^{\uparrow\downarrow}(0,L) = \frac{e^2}{\hbar}T^{\uparrow\downarrow}(0,L) \quad (40)$$

Table 2.VII shows the parameters used in the self-consistent determination of interfacial conductances, interfacial discontinuities, spin accumulation, and spin injection.
TABLE 2.VII. The device and material parameters used to compute the interfacial resistances and its effects on spin injection.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j$, current density</td>
<td>1 A/cm$^2$</td>
</tr>
<tr>
<td>$m$ (GaAs), effective mass of 2 DEG GaAs</td>
<td>0.067 $m_e$ ($m_e = 9.1 \times 10^{-34}$ kg)</td>
</tr>
<tr>
<td>$m$ (Fe), effective mass of Fe</td>
<td>$1 m_e$</td>
</tr>
<tr>
<td>$T$, temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>$\lambda_s$, SC spin diffusion length</td>
<td>1 µm</td>
</tr>
<tr>
<td>$\lambda_c$, contact spin diffusion length</td>
<td>100 nm</td>
</tr>
<tr>
<td>$\sigma_s$, 2DEG conductivity</td>
<td>5.55 $\Omega^{-1}$ cm$^{-1}$</td>
</tr>
<tr>
<td>$\sigma_c$, contact conductivity</td>
<td>$10^6 \Omega^{-1}$ cm$^{-1}$</td>
</tr>
<tr>
<td>$\alpha_c^L = \alpha_c^R$, contact polarization parameter</td>
<td>0.7</td>
</tr>
<tr>
<td>$E_F$ (Fe), Fermi level of Fe</td>
<td>11.10 eV</td>
</tr>
<tr>
<td>$E_F$ (GaAs), Fermi level of GaAs 2DEG</td>
<td>3.5 meV</td>
</tr>
<tr>
<td>$h_B$, molecular field</td>
<td>0.25 eV</td>
</tr>
<tr>
<td>$E_B$, $E_F$ (Fe) – $E_F$ (2 DEG GaAs)</td>
<td>11.06 eV</td>
</tr>
<tr>
<td>$w$, SC layer width</td>
<td>100 nm</td>
</tr>
<tr>
<td>$h$, Planck’s constant</td>
<td>$6.6 \times 10^{-34}$ J/s</td>
</tr>
<tr>
<td>$k$, Boltzmann constant</td>
<td>$1.38 \times 10^{-23}$ J/K</td>
</tr>
</tbody>
</table>

In Fig. 2.10 (a), we plot the asymmetry of $R_I$’s as a function of logarithmic bias current. For brevity, $R_L$ denotes $R_I(0)$ and $R_R$ denotes $R_I(L)$. It is seen that as the bias current increases from 1 A/cm$^2$ to $10^3$ A/cm$^2$, the asymmetry in $R_I$’s increases from 0 to 30%. In current-induced magnetization (CIM) switching [28], typical current density requirement ranges from $10^7$ to $10^8$ A/cm$^2$. It can thus be deduced that asymmetry in $R_I$’s should be taken into account in the design of CIM devices. Figure 2.10 (a) illustrates that the degree of asymmetry is determined by the applied bias voltage and hence current density across the tunneling barriers, which in turn determines the size of the discontinuity in the electrochemical potential and spin accumulation at the two interfaces. Of the two contributions, it is the discontinuity in the electrochemical potentials which dominates. It can also be inferred that the asymmetry changes sign (i.e. with $R_R$ being larger than $R_L$) when the electron current direction is reversed.

In Fig. 2.10 (b), we have plotted $R_L$ for different values of 2DEG GaAs Fermi levels at $U_{l(t)} = 500$ (250) meV. This figure shows that when the SC layer is very heavily doped i.e. with Fermi-level within the conduction band, $R_L$ increases exponentially. This corresponds to steep increase in
interfacial resistance at low values of Fermi-level as shown in the figure. Similar trend is also observed for \( R_R \) since the transmission probabilities are symmetrical with respect to the Fermi-levels. The value of \( R_R \) at \( E_F=3.5\text{meV} \) (GaAs 2DEG) as obtained from our model is \( 5.66 \times 10^{-5} \Omega\text{-cm}^2 \). This value is about 2 orders of magnitude higher than the value of interfacial resistance assumed by Yu and Flatté [25], and Hammar et al. [29]. Higher interfacial resistance should be useful for improving low (~0.01) spin-injection.

![Graph](image)

**FIG. 2.10.** (a) Log plot of interfacial resistance asymmetry vs. current density \( j \). (b) \( R_L \) decreases with increasing Fermi level due to doping.

It should also be noted that spin-split tunnel barriers \( U \) at the two interfaces induces ‘spin-asymmetry’ at \( R_L \) and \( R_R \), that enhance spin injection and magnetoresistance. At barrier heights of \( U_{\uparrow,\downarrow}=500(250)\text{meV} \), the spin asymmetry of \( R_{L,R} \) given by \( \left( \frac{\Delta R}{R} \right)_{L,R} = \left( R_{L,R}^{\uparrow} - R_{L,R}^{\downarrow} \right) / \left( R_{L,R}^{\uparrow} + R_{L,R}^{\downarrow} \right) \), is found to vary from 10% to 15%. This variation remains fairly constant with the change of 2DEG Fermi levels. To increase this ratio and hence spin injection efficiency, we need to study the effect of different barrier heights \( U_{\uparrow,\downarrow} \) on the spin asymmetry of \( R_L \). In Fig. 2.11 (a), \( R_L^{\uparrow,\downarrow} \) as well as the ratio of \( \left( R_L^{\uparrow} / R_L^{\downarrow} \right) \) are plotted for different \( U_\uparrow \) and \( U_\downarrow \), while keeping the relative ratio of \( (U_\uparrow/U_\downarrow) \) constant at 0.5, and \( E_F \) at 3.5 meV. Both \( R_L^{\uparrow} \)
and \( R_L^\uparrow \) increase with increasing barrier height \( U_{\uparrow,\downarrow} \). However, the spin-asymmetry in \( R_L \) increases even more significantly because the effect of \( U_{\uparrow,\downarrow} \) on the electron \( k \)-wavevectors is greater with increasing barrier height. This results in an increase in the spin asymmetry of the transmission probability \( T \) and thus \( R_L \). Figure 2.11 (b) shows that the spin asymmetry of \( R_L \) translates into a large increase in the spin-injection efficiency from \( \sim 1\% \) at \( U_\downarrow = 0.1 \) eV to about 33\% at \( U_\downarrow = 1 \) eV, keeping \( U_\uparrow = 0.5U_\downarrow \). Spin injection can be further enhanced to 50\% by increasing the spin asymmetry of \( U \) to \( U_\uparrow = 0.1U_\downarrow \).

![Graph showing the increase in spin injection efficiency](image)

**FIG. 2.11.** (a) \( R_L \) increases with increasing interfacial potential barrier (at constant ratio split of spin-dependent potential). (b) Spin injection increases with increasing interfacial potential barrier (at constant ratio split of spin-dependent potential). If the split of spin-dependent potential is increased, spin injection rises even more significantly, i.e. graph for \( U_\uparrow = 0.1U_\downarrow \) has the steepest gradient.

**2.6 Conclusion**

We have investigated the spin injection as well as the interfacial resistance means to induce spin-polarized current and ensure its coherent transport across, perpendicular-to-plane, or transistor-like devices. We have found that by using a bilayer injector structure consisting of a nanopillar ferromagnetic (FM) spin injector with a non-magnetic spacer between the FM injector and the semiconductor, spin injection into semiconductors can be enhanced. Our method could be a possible solution to the problem of spin injection currently facing device with hybrid FM-SC.
Spin characteristics of electron transport in semiconductor materials. In this chapter, we have also studied the interface effects of a FM-SC-FM structure on the overall spin polarization of electron current passing through the device. Our contribution here is that we developed a theoretical model that self-consistently describes the effects of current density of interfacial resistance. We suggested that the interfacial resistance is not only an intrinsic property of the material system, but is also coupled to the external bias voltage or current density. Our theoretical model can be used for future simulation work.

REFERENCES

Spin characteristics of electron transport in semiconductor

Chapter 3

Spin-polarized current induced by external fields

3.1 External field effects

It is well known that the application of external magnetic fields causes electron to precess about the field axis and eventually relaxes in its direction. Electron with spin aligned parallel to the field contains lower energy than electron with spin aligned anti-parallel to it. This effect is also known as the Zeeman splitting of electronic energy that lifts spin degeneracy. It is known through the Lagrangian of the system that electron cyclotron motion, and discrete energy levels are resulted from the coupling of the electron momentum to the magnetic vector potential, or gauge. This gives rise to the notion that if the Lorential pulse type of magnetic field (instead of uniform field) is applied periodically across a device structure, electron momentum will be coupled to a constant gauge field that varies in discrete steps across the periodic field system. Besides spin dependent filtering of electron wave vector also becomes possible in the delta field system.

3.2 Device with delta magneto-electric barriers

3.2.1 Field induced spin-polarized current

In this chapter, we would harness the effect of wave vector coupling to the discrete gauge field in a periodic delta field system to generate spin-polarized current. In the context of a transistor like device, in which current is traditionally injected from the device source to its drain, the periodic delta field system has to be established across the source-drain current conduction path, $x$. It is obvious that this method does not require the use of ferromagnetic materials as the spin injectors [1,2,3,4,5]. We are therefore able to avoid dealing with the long-standing problem of spin injection
that exists between ferromagnetic metal and non-magnetic semiconductor. The above conception is supported by recent publications [6,7] that showed that spin polarization ($P$) of electrons can be achieved by passing a current across a two-dimensional electron gas (2DEG) plane under the influence of spatially non-uniform, perpendicular-to-pane, delta magneto-electric barriers. Periodic delta fields that penetrate the 2DEG vertically can be obtained from the fringe fields of periodically spaced ferromagnetic gate stripes deposited on top of the heterostructure across $x$ as shown in Fig. 3.1. The stripes can be magnetized in-plane to realize different combinations of magnetic barriers within a double-pair element. Electric barriers within a double-pair are induced by applying voltage to the magnetized stripes. The delta potential is assumed in this region so that physical analysis can be carried out to study the ability of the magnetic barrier to induce spin polarization. The main focus of studies here is on its ability to induce spin polarization. If a delta barrier can induce spin polarization, so would barriers with finite width generally. Thus the delta barrier is only a mathematical representation to facilitate a clear and simple analysis of the physics. Real barriers would not be delta in shape and the effect of finite barrier width on the accuracy of our results would be studied at a later stage, but beyond the scope of this thesis.

FIG. 3.1. Schematic illustration of a double-pair magneto-electric barrier element that can be realized by magnetizing the periodically spaced ferromagnetic gate stripes deposited on top of a device heterostructure.
Spin characteristics of electron transport in semiconductor

In the ballistic limit, electron conductance for a single transverse mode is simply the product of transmission ($T$) probability and its basic conductance of $\frac{2e^2}{h}$. Spin dependent conductance can therefore be realized by intentionally configuring the magneto-electric barriers to effect a spin-dependent transmission of electrons through the barriers. However, the spin-polarized current device described in recent works are fraught with practical problems that include producing current with sufficiently large spin polarization, low resistance, and producing fringe fields that are strong but narrow enough so as not to limit future shrinking of the device gate length. Computation results of some publications have shown that delta magnetic barriers that are applied in an anti-symmetric fashion across $x$ (Fig. 3.2), cannot induce spin-polarized current [8,9,10] contrary to belief. Figure 3.2 (a) and 3.2 (b) show the schematic of a single-pair element of anti-symmetric and symmetric magnetic barrier configurations, respectively.

![Diagram](image)

**FIG. 3.2.** (a) The anti-symmetric magnetic barriers cannot induce spin polarization. (b) The symmetric barriers can induce a net, finite spin polarization.

where $A, B, C, D, E, F$ are the electron wave amplitude; $k_1, k_2, k_3$ are the electron wave-vectors; $L$ is the width of the single-pair magnetic barrier. Keeping in mind that the single-particle Hamiltonian that describes electron behavior in this system is given by $H = \frac{p_x^2}{2m^*} + \frac{(p_y + (e/c)A_y(x))^2}{2m^*} + U(x) + \frac{eg_y}{2m_0} \sigma^y B_y(x)$, we defined a transmission matrix in the first of Eq. (1) that describes transmission probability through the barriers of Fig. 3.2 and derived the expression of the matrix component $a_1$ in the second of Eq. (1).

$$
\begin{bmatrix}
A \\
B
\end{bmatrix} = \begin{bmatrix}
a_1 & b_1 \\
c_1 & d_1
\end{bmatrix} \begin{bmatrix}
E \\
F
\end{bmatrix}; \quad a_1 = \frac{4k_1 k_2 \cos k_2 L - 2i(k_1^2 + k_2^2 + \sigma^2) \sin k_2 L}{4k_2 k_1 e^{-ik_1 L}}
$$

(1)
where $\sigma$ is the symbol denoting spin (+1 for up spin, -1 for down spin). The magnitude of the matrix component $a_i$ is directly related to $T$ if $F$, the reflection wave in region $x>L$ is taken as zero. $T$ is thus given by:

\[
\frac{|E|}{A} = \frac{4k_1 k_3}{\sqrt{16k_1^2 k_3^2 \cos^2 k_2 L + 4(k_1^2 + k_3^2 + \sigma^2)^2 \sin^2 k_2 L}}
\]  

(2)

\[
\frac{|E|}{A} = \frac{4k_1 k_3}{4k_1^2 k_3^2 \cos^2 k_2 L + (k_1^2 + k_3^2 + \sigma^2)^2 \sin^2 k_2 L}
\]  

(3)

It is seen that the term $\sigma$ in Eq. (2) and Eq. (3) is always positive. This shows that transmission across the anti-symmetrical barrier shows no spin dependence. However, Yong Guo et al. [11] showed that delta barriers configured in the symmetric configuration is able to induce a small, net value of spin-polarized current. Because of the term $\sigma$ in Eq. (4), $T$ is spin dependent. The symmetric barrier configuration could thus result in a net, finite value of spin polarization.

\[
\left[ \frac{k_1}{k_3} \right]^2 \frac{|E|}{A} = \frac{4k_1 k_3^2 k_3}{[k_3(k_1 + k_1) \cos k_2 L + \sigma(k_1 + k_1) \sin k_2 L]^2 + [(k_3^2 + k_3 k_3 - \sigma^2) \sin k_2 L - 2\sigma k_2 \cos k_2 L]^2}
\]  

(4)

It is also intuitive that the $P$ value of spin-polarized current should increase with the number of such symmetric barriers used. It has been mentioned in section 3.2.1 that, in our work, we will use a periodic system of double-pair magneto-electric barriers to generate spin-polarized current. It is thus important for us to first understand the polarization capability of one double-pair barriers, shown in Fig. 3.3. Below is the derivation of transmission probability for an anti-symmetric double-pair barrier.

\[
\begin{array}{cccc}
A,B & C,D & E,F & G,H & I,J \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\
k_1 & k_2 & k_1 & k_2 & k_1 \\
x=0 & L & g+L & g+2L
\end{array}
\]
Spin characteristics of electron transport in semiconductor

The transmission matrix for a double-pair barrier consist of two multiplicative matrices as shown in Eqs. (5) and Eqs. (6).

\[
\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix} ; \quad \begin{pmatrix} E \\ F \end{pmatrix} = \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} \begin{pmatrix} I \\ 0 \end{pmatrix}
\]

(5)

\[
\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} \begin{pmatrix} I \\ 0 \end{pmatrix} = \begin{pmatrix} a_1a_2 + b_1b_2 & a_1b_2 + b_1a_2 \\ c_1a_2 + d_1b_2 & c_1b_2 + d_1a_2 \end{pmatrix} \begin{pmatrix} I \\ 0 \end{pmatrix}
\]

(6)

The transmission probability is given by \( \left| \frac{A}{I} \right| = |a_1a_2 + b_1b_2| \). Detailed derivations are shown in Appendix I. The matrix components are shown below:

\[
a_2 = \left[ \frac{4k_1k_2 \cos k_z L - 2i(k_z^2 + k_i^2 + \sigma^2) \sin k_z L}{4k_1k_2} \right] e^{i\delta k_1} = a_1
\]

(7)

\[
b_1 = \left( \frac{(k_i^2 - k_z^2 - 2 \sigma \alpha \kappa_1) \sin k_z L}{2k_1k_2} \right) e^{-i\delta k_1}
\]

(8)

\[
c_2 = \left( \frac{(k_i^2 - k_z^2 + \sigma \alpha \kappa_1) \sin k_z L}{2k_1k_2} \right) e^{i(2L+\pi)\delta k_1}
\]

(9)

From Eqs. (8) and (9), we can derive for \( b_1c_2 \) as shown in Eq. (10) and Eq. (11) below:

\[
b_1c_2 = \left( \frac{(k_i^2 - k_z^2 - \sigma^2 \alpha \kappa_1) \sin k_z L}{2k_1k_2} \right) \left( \frac{(k_i^2 - k_z^2 + \sigma^2 \alpha \kappa_1) \sin k_z L}{2k_1k_2} \right) e^{i(2L+\pi)\delta k_1}
\]

(10)

\[
b_1c_2 = \left( \frac{(k_i^2 - k_z^2 + \sigma^2 \kappa_1^2) \sin^2 k_z L + 4\sigma^2 k_i^2 \sin^2 k_z L}{4k_1k_2^2} \right) e^{i(2L+\pi)\delta k_1}
\]

(11)

Eq. (11) shows that because of the \( \sigma^2 \) terms in \( a_1, a_2, \) and \( b_1c_2 \), the anti-symmetrical double-pair barriers also shows no spin-dependence. Symmetric barriers might thus be the preferred configurations to use to produce spin-polarized current. However, symmetric barriers are difficult to realize in practice compared to the anti-symmetric barriers if the longitudinal magnetization methods [6,7,8,9,10,11] were to be used. Symmetric barriers could, however, be more conveniently implemented if the ferromagnetic gates can be perpendicularly magnetized. Multiple symmetric barriers might result in low transmission or high resistance for the device charge current. We thus conjectured that the anti-symmetric barriers should still be used to induce spin
polarization, by either applying electrical potentials to regions II-IV, or using $B$ fields of different strengths within a double pair element.

### 3.2.2 Spin dependent conductance

Figure 3.1 shows that multiple anti-symmetric barriers can be implemented by selectively magnetizing the multiple ferromagnetic gate stripes on top of the heterostructure. The following sections would thus focus on modifying the anti-symmetric barriers to achieve spin polarization, and yet maintaining a reasonably high charge current conductance. The $T$ expressions that have been derived so far for the magnetic barriers shown in Eqs. (1)-(4) are for one conductance mode. Since the application of bias voltage to the system has minimal effect on the system’s conductance, spin-polarization of conductance would thus imply the spin-polarization of current. It thus makes sense that the spin polarization of conductance / current for one mode of electron transmission can be defined by Eq. (12)

$$p = \frac{T^+(E,k_x,B,U) - T^+(E,k_x,B,U)}{T^+(E,k_x,B,U) + T^+(E,k_x,B,U)}$$

(12)

Figure 3.4 shows the schematic illustrations of conductance derivations.

![Diagram](image)

**FIG. 3.4.** (a) Schematic illustration of the 2DEG system. (b) Fermi circle of the GaAs 2DEG shows conductance can be found by integrating the transmission probability of each mode over the right half of the Fermi circle.
Spin characteristics of electron transport in semiconductor

$L_y$ is the transverse length of the 2DEG, $\phi$ is the angle between any $k_F$ and the $x$ axis. The number of electrons over the right half Fermi surface is $\frac{\pi k_F}{2\pi / L_y}$. For a perfect transmission system, conductance of one electron mode is $\frac{2e^2}{h}$. Total conductance is thus:

$$G = T_{ave} \left( \frac{2e^2}{h} \frac{\pi k_F}{2\pi / L_y} \right)$$

$$= T_{ave} \left( \frac{2e^2}{h^2} m^* v_f L_y \pi \right)$$

(13)

where $v_f$ is the Fermi velocity. The average transmission probability over the Fermi surface for one electron is:

$$T_{ave} = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} T(E_F, k_x, k_y) \cos \phi d\phi$$

$$= \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} T(E_F, \sqrt{E_F} \sin \phi) \cos \phi d\phi$$

(14)

The term $\sin \phi$ is related to:

$$k_x^2 = k_y^2 \sin^2 \phi$$

$$k_y = \frac{1}{h} \sqrt{2mE_F} \sin \phi$$

(15)

The total conductance is thus obtained below as:

$$G^+ = \frac{2e^2}{h^2} m^* v_f L_y \int_{-\pi/2}^{\pi/2} T^+(E_F, \sqrt{E_F} \sin \phi) \cos \phi d\phi$$

(16)

If there is a difference of Fermi energies between two contacts, eg. in the metal-insulator-metal type of structure, conductance is:

$$G^z = \frac{2e^2}{h^2} m^* v_f L_z \int_{-\pi/2}^{\pi/2} T^+(E_F, \sqrt{E_F} \sin \phi) \cos \phi d\phi dE$$

(17)
3.3 Electron motion in delta magneto electric barriers

3.3.1 Minimal coupling and wave-vector filtering

This section provides the theoretical analysis of wave-vector filtering by the double-pair magneto-electric barrier element. For convenience, the notation \((B_1, B_2, B_3, B_4)\) is used to represent the magnetic barrier configuration, and \((U_1, U_2)\) represents the electric barrier configuration. Electron motion in the 2DEG can be described by a ground state (lowest sub-band) Fermi circle, with \(k_x\) and \(k_y\) denoting the in-plane wave-vectors. The minimal-coupling Hamiltonian that describes the influence of \(U\) and \(B\) barriers on the electron motion is

\[
H = \frac{p_x^2}{2m^*} + \frac{(p_x + (e/c)A_y(x))^2}{2m^*} + U(x) + \frac{eg^* \alpha \hbar}{2m_0} B_z(x)
\]

(18)

where \(m^*, m_0\) is the electron’s effective and real mass, respectively, \(g^*\) is the effective Lande factor, \(\sigma = +1/-1\) for spin up/down electrons, \(p_x\) and \(p_y\) are electron momentum in the \(x\) and \(y\) directions, respectively. Considering the translational symmetry in \(y\), the wave-function of electrons is given by \(\psi(x, y) = e^{ixy}(A e^{i\alpha y} + B e^{-i\alpha y})\). In classical motion, an electron with \(+p_y\) moving through \(B_z\) will experience a Lorentz force and hence deflection in \(-y\). Therefore an electron with \(-p_y\) gains kinetic energy. The system can be described by the Lagrangian for 1-degree of freedom \(L = 1/2m(\dot{x}^2) - (e/c)\dot{x}A_y\), where \(\dot{x}\) is velocity in \(y\). Performing Legendre transformation of the Lagrangian, \(H = \dot{x}p_y - L\) leads to the Hamiltonian in Eq. (18) with \(p_y + eA_y\). Equation (19) will be used to find the electron wave vectors as follows:

\[
\frac{d}{dx^2} \psi - [k_y + \frac{e}{\hbar} A_y]^2 \psi + \frac{2m^*}{\hbar^2} [E - U(x)] + \frac{eg^* \alpha \hbar}{2m_0} \frac{d}{dx} B_z(x) \psi = 0
\]

(19)

The eigenvalue equation can thus be found as below:

\[
k_y^2 + [k_y + \frac{e}{\hbar} A_y]^2 = \frac{2m^*}{\hbar^2} [E - U(x)]
\]

(20)

The 2DEG sub-band can be absorbed in \(U(x)\). However, for simplicity, \(U(x)\) is taken to represent the applied electric barrier only. For ease of calculation in later sections, all parameters are
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reduced to dimensionless units in the following manner: $x \rightarrow l_n x$, $E \rightarrow \hbar \omega_c E$, $l_n = \sqrt{\hbar/eB_0}$, $\omega_c = eB_0/m^*$. $B_0$ is some commonly achievable magnetic field. Equation (20) is thus reduced to a simpler form as shown below in Eqs. (21):

$$k_x^2 + \left[ k_y + \frac{e}{\hbar} A_y \right]^2 = \frac{2m^*}{\hbar^2} \hbar \omega_c [E - U(x)]$$

$$k_x^2 = \frac{2m^* eB_0}{\hbar} \frac{E - U}{m^*} - \left[ k_y + \frac{e}{\hbar} A_y \right]^2$$  \hspace{1cm} (21)

Further simplifications are shown in Eqs. (22):

$$\frac{1}{l_n^2} k_x^2 = \frac{2[E - U]}{l_n^2} - \left[ \frac{1}{l_n} k_y + \frac{e}{\hbar} A_y \right]^2$$

$$k_x^2 = 2(E - U) - \left[ k_y + \frac{e}{\hbar} B_0 l_n A_y \right]^2$$  \hspace{1cm} (22)

The final expression for the wave-vector in dimensionless units is shown in Eq. (23). $k_y$ is now expressed in the multiple of $1/l_n$; $E$ and $U$ are expressed in the multiple of $E_0$; $A_y$ is expressed in the multiple of $B_0 l_n$. Wave-vectors of Figs. 3.5 (a)-(g) are derived from Eq. (24) and shown in Fig. 3.5 (h) and 3.5 (i), respectively.

$$k_x = \sqrt{2(E - U) - [k_y + A_y]^2}$$  \hspace{1cm} (23)

where for $x=1$, Eq. (23) is reduced to Eq. (24):

$$k_x = \sqrt{2(E - U) - [k_y + B]^2}$$  \hspace{1cm} (24)

3.3.2 Concept of zero gauge

We conceived that using many double-pair barriers to increase spin polarization as has been analytically deduced in section 3.2.1 will lead to low $T$ value as the electron’s required transverse ($y$) kinetic energy increases with each barrier crossed. Such reasoning is supported by analyzing the wave-vector equations of Eq. (23) for an electron traveling in the $x$ direction of the device that shows the coupling of $B$ to the transverse wave-vector. We therefore conjectured that the magnetic
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bars that we use for the device must satisfy the requirement that the total available kinetic energy, $E - U_{eff}$ where $U_{eff}$ is the effective potential energy, is always sufficient to ensure that $k_x$ does not become evanescent. It is important to ensure that the transverse kinetic energy required by the electrons in tunneling through the barriers must be kept to the minimal [13,14,15,16]. In our design, each double-pair (Figs. 3.5 (a)-(f)) forms a repeating unit of the periodic system. The magnetic barrier height and orientation in each unit is designed to ensure that an electron passing through the barriers, in the Landau gauge $A = (0, A_y(x), 0)$ where $A_y$ is the magnetic vector potential of the system, will require zero transverse kinetic energy. This can be accomplished by ensuring in our barrier configuration that the discrete values of $A_y(x)$ on the right-end of a double-pair magnetic barrier is zero. Such magneto-electric double-pair is described as the “zero-gauge” double-pair in our work. In this way, multiple double-pairs can be used to increase $P$ without accumulating the discrete $A$ values and translating the $T$ curve to higher energy.

FIG. 3.5. (a) A double-pair, magneto-electric barrier unit used in a periodic series of $n$ such double-pairs; wave-vectors of this structure are denoted by $k_1, k_2, k_3, k_4, k_5$ in (i). Y-axis of each figure shows $A$ values; X-axis shows distance in $x$. (b)-(f) Other zero-gauge double-pairs. (g) Non-zero-energy double pair shows an accumulation of $A$ with $x$; wave-vectors of this structure are denoted by $k_1, k_2, k_3, k_4, k_5$ in (i).
3.4 Spin polarization effects

3.4.1 Zero-gauge magnetic barriers

Figures 3.5 (a)-(f) shows six possible zero-gauge double-pairs that can be used to form a periodic series of magneto-electric barriers consisting of “n” double-pairs. Figure 3.6 (a) shows that the transmission curve for Fig. 3.5 (g) translates significantly to the higher energy as n increases from 1 to 5. Similar energy-translation also occurs with higher barrier height from $B_0$ to $4B_0$ for $n=3$ double pairs as shown in Fig. 3.6 (b). Figures 3.6 (c) and (d) show a gradual shift in energy for increasing $n$, and increasing barrier height, respectively when the zero-A structure is used. As both high $n$ and $B$ are necessary for increasing $P$, our finding shows that Figs. 3.5 (a)-(f) are preferred to the non-zero-gauge structure of Fig. 3.5 (g).

FIG. 3.6. (a) Non-zero-gauge structure of Fig. 3.5 (g) shifts transmission curve toward higher energy as $n$ (1,2,3,4,5) increases. (b) Non-zero-gauge structure shifts transmission curve toward higher energy with larger barrier heights. (c) Zero-gauge structure does not shift toward higher energy when more double-pairs are used. (d) Zero-gauge structure shifts gradually toward higher energy when larger barrier heights are used. The energy x axis of the above figures are expressed in the multiple of $E_0$. 

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However, it’s important to ensure that increasing $n$ does not increase the electron path in $x$ beyond the electron mean free path (MFP). This can be achieved by using high quality GaAs 2DEG, where electron MFP is in the μm range [17, 18].

3.4.2 Magnetic barrier symmetry

Computation for $n=27$ (a sufficiently large number) double-pairs for field configuration of type Fig. 3.5 (a) where $(U_1, U_2)=(+3, -3)$, $(B_1, B_2, B_3, B_4)=(+2, +2, -2, -2)$, shows that $P$ reaches -100%, 75%, -75% at $E=2E_0$, $4E_0$, $8E_0$, respectively as shown in Fig. 3.7 (a). $P$ at −75% at $8E_0$ shows high transmission for up spin at probability 0.5. In standard 2DEG GaAs, material parameters are as follows: $m^*=0.067m_0$, $g^*=0.44$, $g=0.0295$; for $B_0=0.02T$, $l_B=182$nm, $E_0=0.34$meV.

FIG. 3.7. (a) Results for Fig. 3.5 (a) show $P=−75\%$ at $E=0.8E_F$. (b) Results for field configuration of types Fig. 3.5 (c) & (f) show $P=−75\%$ at $E=5E_0$ and $P=100\%$ at $E=8E_0$. (c) Results for field configuration of types Fig. 3.5 (b) & (e) show $P=−20\%$ at $E=6E_0$. (d) $P=0$ when $(U_1, U_2)=(0, 0)$.
In the above calculations, the energy $x$ axis of Figs. 3.7, 3.9, 3.10, 3.11, 3.12 are expressed in the multiple of $E_0$. Fermi energy is $E_F = 3.55 \text{meV}$ for $n_e = 10^{11} \text{cm}^{-2}$, thus $P = -75\%$ occurs at $0.8 \ E_F$.

Computation for field configuration of types Figs. 3.5 (c) and (f), the anti-symmetrical barriers, also shows high $P$ when $|B_2|, |B_3|$ are lower than their respective $|B_1|, |B_4|$. This is in line with our earlier expectation that using $B$ fields of different strength within a double-pair element could induce $P$ in an anti-symmetrical double-pair element. With the aid of electric barriers, $P$ increases significantly. Results in Fig. 3.7 (b) show $P = -75\%$ at $E = 5E_0$ and $100\%$ at $E = 8E_0$ for $(U_1, U_2) = (+3, -3), (B_1, B_2, B_3, B_4) = (4, -2, +2, -4)$. This also confirms our thought that applying electrical potentials to regions II and IV could induce $P$ in an anti-symmetrical double-pair element. In comparison, computation for field configuration of types Figs. 3.5 (b) and (e) show a moderate $P$. Results in Fig. 3.6 (c) show $P = -20\%$ for $(U_1, U_2) = (+0.5, -0.5), (B_1, B_2, B_3, B_4) = (+5, -5, -5, +5)$ or $(-5, +5, +5, -5)$ at $E = 6E_0$. The results of Figs. 3.6 (b) and (c) show that $P$ can be improved when the degree of symmetry in magnetic barriers configuration is further reduced by choosing $|B_2| = |B_3| < |B_1| = |B_4|$.

### 3.4.3 Electric barrier symmetry

It has been observed in section 3.4.2 that electrical potentials are required to induce $P$ in an anti-symmetrical double-pair element. Figure 3.6 (d) shows that $P$ has no net value when electrical potentials are not applied to region II and IV of a double-pair barrier. This is in line with the finding of earlier papers [8,9] that also reported zero $P$ values for the single-pair anti-symmetrical barriers, i.e. spin-polarized current cannot be generated by the anti-symmetrical barriers. We had also shown in Eqs. (7)-(11) that $T$ of the anti-symmetrical barriers shows no spin dependence. This is because the anti-symmetrical double-pair element is also characterized by a symmetrical distribution of discrete $A$ values across the double-pair as shown in Fig. 3.8 below.
The anti-symmetrical double-pair element is also characterized by symmetrical A distribution across a double-pair element. Breaking this symmetry could induce spin-polarized current across the barriers.

The application of electric potential in these regions in the form of positive potential to region II and negative potential to region IV, could result in the breaking of this symmetry. This causes current transmitting through these barriers to acquire a net $P$ value. This finding suggests the potential usefulness of this device as an electronic switch. As electric barriers are necessary to “turn on” the polarization capability of these barriers, the anti-symmetrical double-pairs exhibit behavior suitable for switching devices. However, electric barrier value should not exceed $E_F$ of the 2DEG system as this would shift the $T$ curve out of the Fermi circle.

### 3.4.4 Number of zero-gauge magneto-electric barriers

Since the use of zero-gauge type of double-pair barriers ensures high electron transmission, it is anticipated that by increasing the number of double-pair elements, higher spin-polarized current of higher $P$ can be generated. The type of magneto-electric barriers used here is that of Fig. 3.5 (a). The effect of the number of double-pair ($n$) on $P$ value can be seen by inspecting the results of Fig. 3.9 and Fig. 3.10. Figure 3.9 shows that for $n=1$, spin-polarized current has low average $P$ value of less than 1% over electrical potential range of 0.17 mV to 6.8 mV applied to regions II and IV of the double-pair element as positive and negative potential, respectively. However, when $n$ is
increased to a moderately higher value of 27, Fig. 3.10 shows relatively higher average $P$ value for spin-polarized current over the same electrical voltage range of 0.17 mV to 6.8 mV.

FIG. 3.9. Results show spin polarization (red) and transmission probability (green) for $n=1$ double-pair, and anti-symmetrical magnetic barriers configuration of $B=(+2,+2,-2,-2)B_0$. It is worth noting that the positive and negative potentials applied to regions II, IV, respectively are required to induce a net $P$ value.

FIG. 3.10. Results show spin polarization (red) and transmission probability (green) for $n=27$ double-pairs, and anti-symmetrical magnetic barriers configuration of $B=(+2,+2,-2,-2)B_0$. It is worth noting that the positive and negative potentials applied to regions II, IV, respectively are required to induce a net $P$ value.
3.4.5 Magnetic barrier strength

The effect of magnetic barrier strength on spin polarization can be observed by comparing Fig. 3.9 to Fig. 3.11, and Fig. 3.10 to Fig. 3.12. Figures 3.9 and 3.11 show results for \( n=1 \) double-pair barriers of anti-symmetrical configuration, over the same electrical potential range but of different field strengths. Figure 3.9 shows results for field strength of \( B=(+2,+2,-2,-2)B_0 \) while Fig. 3.11 shows results for field strength of \( B=(+5,+5,-5,-5)B_0 \). The same applies to Figs. 3.10 and 3.12, except that in this case, \( n=27 \). Figure 3.11 shows higher average value of spin polarization than Fig. 3.9, while Fig. 3.12 shows higher spin polarization than Fig. 3.10. Thus, higher magnetic barrier strength generally produces larger spin polarization. However, the difference of polarization values between Fig. 3.12 and Fig. 3.10 is greater than the difference between Fig. 3.11 and Fig. 3.9. This shows that the effect of magnetic barrier height on \( P \) value is especially significant when the number of barriers is large. This also means that large \( n \) increases the device sensitivity to \( B \) variations.

![Graphs showing spin polarization and transmission probability](image)

FIG. 3.11. Results show spin polarization (red) and transmission probability (green) for \( n=1 \) double-pair, and anti-symmetrical magnetic barriers configuration of \( B=(+5,+5,-5,-5)B_0 \). It is worth noting that the positive and negative potentials applied to regions II, IV, respectively are required to induce a net \( P \) value.
We have shown in previous sections that in general $P$, close to maximum can be achieved with a periodic series of zero-gauge, magneto-electric, double-pair barriers. $P$ increases with the number of double-pairs while $T$ is high and kept at energy levels within the Fermi circles, when the zero-gauge double-pairs are used. The anti-symmetrical double-pairs have not been able to induce spin-polarized current. However, with intervention like applying electrical potentials, or using $B$ fields of different strength within a double-pair element, the symmetrical $A$ distribution could be broken and spin-polarized current can be induced. As high electrical barriers shift transmission curve to higher energies, gate voltage should be optimized depending on material types and doping density, to ensure transmission threshold is well within $E_F$. Anti-symmetrical double-pair could thus behave like a switch as they show $P$ only when electrical voltages are applied and such behavior is suitable for devices. It is worth noting that in the context of a transistor like device,
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electron mean free path (MFP) could be a cause for concern as high $n$ and $l_B$ may be required for enhancing spin polarization and this implies longer device length. It would thus be important to consider implement the field configurations in high quality 2DEG that can be obtained from molecular beam epitaxial fabrication of III-V semiconductor. Electron MFP in high quality GaAs 2DEG has been found to be as high as 120 μm.

3.6 Device tunneling time

In this section, we will study the time required for an electron to tunnel through the barrier. This is important because the tunneling time might have an effect on the total device response time if these magneto-electric barriers were to be adapted for device use. This switching occupies finite time duration for coherent rotation of the magnetization for the new barrier configuration to be constructed, and the switching time is labeled $T_s$ here. In this work, we conjectured that even after the new barrier are reconstructed as a result of switching, it does not imply a steady current is readily measurable. This is because electrons take a finite value of time $T_d$ to tunnel through the barriers. We therefore deduced that the total device response time would be $T=T_s+T_d$ i.e. after switching, the device would wait a time $T_d$ before the current or voltage through it can stabilize. In our estimation of tunneling time, we used the device of Fig. 3.13 that shows a single-pair of magnetic barriers only. Figure 3.13 also shows the schematic illustration of device response time. The dotted line is not a computed graph, it is for illustrating the transient state of electron transmission. The steady state transmission probability (achieved after $T=T_s+T_d$) is a computed value.
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FIG. 3.13. The total device response time is illustrated above as the time taken for the transmission probability of electrons or the current to reach its steady value right after a remagnetization of the ferromagnetic gate.

Various methods have been proposed to calculate the tunneling time [19,20,21,22]. In this thesis, we will use the phase delay method [21,22]. The transmission and reflection probabilities are shown below in Eqs. (25).

\[
|T(k)|^2 = \frac{k}{k_1} \left| \frac{1}{a} \right|^2 \quad \quad \quad |R(k)|^2 = 1 - |T(k)|^2
\]  

(25)

The phase of \( R \) and \( T \) are given by Eqs. (26):

\[
\delta(E) = \tan^{-1} \frac{\text{Im}[R]}{\text{Re}[R]} \quad \quad \text{and} \quad \quad \eta(E) = \tan^{-1} \frac{\text{Im}[T]}{\text{Re}[T]}
\]  

(26)

The total tunneling time is given by \( T_d = \tau_d + \tau_0 \) where \( \tau_d \) is the time delay due to the barrier and \( \tau_0 \) is the free particle tunneling time. Their expressions are shown in Eqs. (27).

\[
\tau_d = |R(k)| \frac{d\delta}{dE} + |T'(k)| \frac{d\eta}{dE} \quad \quad \tau_0 = \frac{mL}{\sqrt{2mE}}
\]  

(27)

Figure 3.14 shows the simulation results of tunneling time vs. electron energy for a magneto-electric barrier configuration. It can be seen that tunneling time decreases with increasing electron energy. This is because higher kinetic energies also imply higher electron velocities, which suggests shorter electron traveling time through a distance.
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Figure 3.14 (a) shows that higher electrical potential barrier increases tunneling time. This is in line with quantum mechanical prediction that infinitely high potential barriers reflects electron wave completely. Figure 3.14 (b) shows that higher magnetic barrier also increases tunneling time. The above analysis were conducted irrespective of electron spin. Simulations were also carried out to examine the effects of increasing potential barriers on tunneling time. Figure 3.15 shows that tunneling time increases gradually with $U$ at low potential value. When $U$ reaches approximately 6 $U_0$, tunneling time increases exponentially. To investigate the effects of magnetic barriers on tunneling time, we computed tunneling time for increasing magnetic barrier height. Results in Figure 3.16 shows that electron tunneling time increases smoothly with increasing magnetic barrier heights at low $B$ values. Tunneling time increases sharply when $B$ value reaches about 1.8 $B_0$. It is also seen that for a fixed $B$ value, tunneling time is shorter for lower potential barrier.
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FIG. 3.15. Tunneling time increases with increasing potential barriers.

FIG. 3.16. Tunneling time increases smoothly with increasing magnetic barrier heights at low $B$ values.
Thus, in general, the tunneling time $T_d$ increases with the height of the magnetic and electrical potential barriers. A steep increase in $T_d$ occurs in the tunneling regime, i.e. when the heights of the magnetic and electrical barriers exceed the kinetic energy of the electrons. $T_d$ is of the order of picoseconds, and about a thousand times faster than the conventional coherent switching duration of the ferromagnetic gates (of the order of a few nanoseconds). However, in future devices, these gates may be switched by precessional switching in order to increase its response speed. $T_d$ will then be a significant component of the total time delay since the timescale of precessional switching is also on the order of picoseconds [23, 24].

### 3.7 Conclusion

We have proposed the magneto-electric field configurations that produce a “zero-gauge” type of tunneling barriers which polarizes the spin of electron passing through the barriers. As there is no net change in the magnetic vector potential across the conduction path, we conjectured and proved that the zero-gauge barriers can be used to induce high spin filtering without suppressing electron current. With our theoretical models, we have performed simple simulation to evaluate spin transport in a 2DEG type of transistor devices, which consist of the ferromagnetic type of gate stripes. We have shown that the ferromagnetic gates can be magnetized in different configurations to implement spatially-discrete or “delta” magnetic fields, and net magnetic vector potential change across the current conduction path of the 2DEG.

### REFERENCES


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Chapter 4

Spintronics devices for logic and memory

4.1 Spintronics devices and functions

4.1.1 Development of spintronics devices

Spintronics devices refer to a class of devices that rely on the effects of molecular magnetic fields arising from orbital or spin moments, nuclear field, effective magnetic field arising from spin orbit coupling, or externally applied magnetic-electric fields, on the momentum of conduction electron to achieve electrical conductance modulation. The physics of magneto-transport is thus central to the working principles of these devices. In the ballistic transport regime, the wave-vector of conduction electron is coupled to the magnetic fields and device conductance can thus be controlled by manipulating these fields. Spin polarization can thus be studied in the ballistic regime for each single conductance mode. Prior to the surge of interest in semiconductor spintronic, magneto-transport devices i.e. the spin valve recording heads and the MRAM [1,2] have already been developed for recording and storage purposes. The success of these metal-based spintronics devices provides the necessary motivation for scientists to conceive realizing magneto-transport in semiconductor devices, or the spinFET. However, semiconductor materials are non-magnetic, and recent efforts to epitaxially fabricate magnetic semiconductor [3,4] has not been successful. It has thus been discussed in chapter 2 that spin injection is the most natural way of realizing magneto-transport in semiconductor devices. It was also discussed that the spin injection spinFET faces the problems of conductivity mismatch and various methods have been proposed to overcome it. In 1989, Datta and Das [5] proposed that the conduction band spin orbit coupling effects inherent in III-V semiconductor materials could be used to induce spin-polarized current in
the ferromagnetic drain-source, high electron mobility (HEMT) type of transistors. Since then, there has been many experiments and theoretical studies on transistor devices [5,6,7,8,9] that use various effects including the spin orbit coupling to generate spin-polarized current. In the mid 90s, Alam Majumdar and others [10,11,12,13,14,15,16,17] proposed the use of external fields to induce spin-polarized current in the ferromagnetic gate, HEMT type of spinFET.

4.1.2 Ballistic magneto-electric device

In this chapter, we will design more complex devices based on the basic ballistic magneto electric spinFET of chapter 3 and attempt to implement the functions of logic and memory. The basic device permits conductance modulation with both electric and magnetic fields applied perpendicular to its current conduction channel as described in chapter 3. Fields are applied through the ferromagnetic gates deposited on top of a HEMT heterostructure that contains a 2DEG for current conduction. The minimal-coupling Hamiltonian with spatially uniform electrical potentials, and delta Zeeman splitting is solved in the weak coupling limit for which the Rashba and the Dresselhaus spin orbit coupling is not considered. In this section, we conceived that the manipulation of the double-pair magnetic barriers’ geometrical symmetry and configurations could lead to device functionalities of digital logic operations (section 4.2) and non-volatile storage (section 4.3).

4.2 Spin logic devices

Spin logic represents one of the most promising areas in which spintronic devices exhibit superiority over conventional devices. In current digital electronics, the functions of logic gates (such as OR, AND, NOR, NAND gates, and flip-flop) are realized by using the charge property of electron. The transport of electron charges from one location to another, and the detection for their presence are the basic principle to realize the many functions of today’s logic gates. In this project
the “spin” instead of the charge property will be manipulated to realize logic functions. By using spin property, magneto-electric type spinFET could replace conventional MOSFET logic gates.

Figures 4.1 (a) and (b) show a device with four ferromagnetic (FM) gate stripes on the heterostructure. FM gates 1 and 3 have fixed magnetizations of (+B,+B), while gates 2 and 4 have variable magnetization, which form the two inputs of a conventional digital logic gates like AND, NAND, etc. The free gates of 2 and 4 can be magnetized in four different combinations: (+B,-B), (-B,-B), (-B,+B), (+B,+B), corresponding to digital logic inputs of (1,0), (0,0), (0,1), (1,1), respectively. The last configuration of (+B,+B) forms an all-parallel, magnetic field configuration of (+B,+B,+B,+B) that constitutes the largest resultant barrier to electron motion. Figure 4.2 shows that in an all-parallel configuration, $|E_{th}|$ is shifted to 18 $E_0$ or clearly above the Fermi energy of 10 $E_0$. Whereas, in the other three configurations, the thresholds $|E_{th}|$ are appreciably smaller at 6-8 $E_0$. Therefore a low resistance state is resulted from the first three configurations, while a high resistance state is resulted from the last configuration. Figure 4.1 (a) therefore shows a device that replicates the Boolean algebra operation of the AND gate of (1+0=0, 0+1=0, 0+0=0, 1+1=1). The FM gates of 1 and 3 can be reversed. By similar reasoning and reinspecting the logic truth table, it can be found that Fig. 4.1 (b) now shows a device that replicates the Boolean operation of the NAND gate. It is thus clear that the spinFET can function as a programmable spin logic. The ability of the spinFET to simulate Boolean algebra operation implies that a spin-FET can form the basic unit of logic gates, and can be combined to form more complex digital logic devices e.g. decoders, encoders, etc.

It can be deduced that spinFET logic gates have three distinct advantages compared to conventional FET-based logic gates. Firstly, spinFET-based logic gates are programmable, the magnetization of the fixed gates can be re-set in a different configuration, to yield an NAND function instead of an AND function. With adaptations, it might be possible that an AND gate can
be converted to a NAND gate by just applying voltage. Secondly, spinFETs operate at a higher speed since magnetization flipping can be achieved at a faster rate than the depletion of an inversion layer or transporting of charges to capacitances, which occur in conventional devices. Thirdly, conventional digital logic gates can only be constructed with multiple MOSFET devices. The spinFET-based digital logic gates can be implemented with just one spinFET as shown in Fig. 4.1. It can therefore be smaller, and consume less power.

The term “spinFET” is used to describe the basic units of our devices as a matter of convenience because not all devices in this chapter require spin-polarized current. In spin logic devices, and the perpendicular magnetization non-volatile memory, conductance modulation is achieved by shifting electron transmission thresholds.

FIG. 4.1. Programmable AND/ NAND gate can be realized with just a single spinFET by re-magnetizing FM gates 1&3 of the device. FM gates 2 and 4 are two input to the logic gate. (a) shows the design of an And gate, (b) shows the design of an NAND gate.
Figure 4.2 shows our computation results of a spinFET functioning as a AND gate when the inputs of FM 2 and 4 receive the various inputs of (0,0), (0,1), (1,0), (1,1).

![Computation results of device conductance resulting from the input conditions of the FM 2 and 4.](image)

FIG. 4.2. Computation results of device conductance resulting from the input conditions of the FM 2 and 4.

It is important to note that in our work in this section, we have focused only on the device concept of using transconductance modulation via FM and NM gates to program desired logic functions. However, for logic devices to be fully functional, characteristics such as logic margin, fan-out, threshold, propagation delay, slew rate, bandwidth, etc. have to be well-established. For instance, detailed study on tunneling time and magnetic switching time is required to establish propagation delay, slew rate, and bandwidth required, while that on demagnetizing fields and spin transfer switching modes, device source and input impedances are required for determining logic margin, fan-out, and threshold parameters.

### 4.3 Non-volatile memory

To realize non-volatile storage, periodic gate elements [10,11,12] can be magnetized in-plane (Fig. 4.3) or perpendicular-to-plane (Fig. 4.5) to implement the suitable barrier configuration. By changing the magnetization direction of the gate stripes, the spinFET can be switched between the
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symmetry and asymmetry configurations or between the zero-gauge and the non-zero-gauge configuration. The former modulates the conductance (i.e. creating high and low resistance states in the device) mainly by modulating $P$, while the latter relies primarily on the shift in the transmission threshold $|E_{\text{thr}}|$. When the gate stripe is magnetized in the in-plane direction, the drain’s magnetization is set in the $z$ direction, and is thus able to convert $P$ modulation into conductance modulation. When the gate stripe is magnetized in the perpendicular direction, the drain is made non-magnetic. The modulation in $|E_{\text{thr}}|$ is then translated into conductance modulation by the application of a bias voltage. In both adaptations, the source is magnetized in the horizontal $x$ direction. Magnetization in an axis orthogonal to $z$ shows that incident electron wave to the barrier array has equal components polarized in the $\pm z$ directions, as indicated by Eqs. (1) and (2).

$$\left| \frac{1}{2} \right> = \frac{1}{\sqrt{2}} \left| 1 \right> - \frac{1}{\sqrt{2}} \left| 0 \right>$$  \hspace{2cm} (1)

$$\langle \sigma_z \rangle = \frac{1}{2\hbar} \langle \chi | \sigma_z | \chi \rangle = \frac{1}{2\hbar} (c_1 \epsilon^* - c_2 \epsilon^* ) = 0$$  \hspace{2cm} (2)

where $c_1 = 1/\sqrt{2}$, $c_2 = -1/\sqrt{2}$ if $|\chi\rangle = |+1/2\rangle_z$. In GaAs 2DEG, the material parameters are: $m^* = 0.067m_0$, $g^* = 0.0295$; for $B_0 = 0.2\text{T}$, $l_B = 57\text{nm}$, $E_0 = 0.34\text{meV}$. Fermi energy is $E_F = 3.55\text{meV} \sim 10 E_0$ for electron density, assuming free electron model, $n_e = 10^{11}\text{cm}^{-2}$. $E_F$ can be varied about 3.5 meV by changing doping concentration of the AlGaAs layer.

4.3.1 Symmetry and asymmetry configuration

Figure 4.3 shows an in-plane adaptation where high/low resistance states are toggled by constructing / removing the symmetric configuration of the magnetic fields emanating from the FM gates. In a heterostructure where two gate electrodes are deposited adjacent to each other, the left gate is permanently magnetized to induce the first magnetic field pair of (+1,-1). The adjacent right gate is then magnetized in either direction to induce (+1,-1) or (-1,+1). Thus the resultant
magnetic field from the two gate electrodes switches between the symmetric (+1,-1,-1,+1) and the asymmetric (+1,-1,+1,-1) configurations. The applied electrical voltages are (10, 10). Only the symmetric configuration can induce a net finite $P$ because the symmetric configuration provides an asymmetric $A$ field distribution across the conduction path of the electrons. Figure 4.4 (a) shows results for a symmetric $B$ field but asymmetric $A$ field configuration in which $P$ is induced for $U=20$. Figure 4.4 (b) shows results for an asymmetric $B$ but symmetric $A$ configuration in which $P$ is zero unless electrical barriers are applied to the non-magnetic gates to break the symmetry of $A$ distribution. Figure 4.4 (c) shows results for a lower $U$ of 10. Therefore, by switching between the symmetric and asymmetric zero-gauge units, $P$ can be modulated from zero to an arbitrary value, and this translates to a modulation of the conductance. The distance between two barriers, $L$ is set at $2l_B$ or 104 nm, which ensures that electron mean free path [18,19] exceeds the electron transmission path, i.e. transport is ballistic. A small $L$ is important to minimize spin depolarization due to the D’yakonov [20] mechanism.

FIG. 4.3. The spinFETs can be adapted to function as a single-transistor non-volatile memory cell, by constructing and removing the symmetrical configuration of discrete magnetic vector potential values within a double-pair element.

To obtain a sizable $P$, more barriers are used. Figure 4.4 also shows the variation in $P$ with electron energy for up to $n=10$ double-pair barriers. $P$ rises to 0.05, 0.1, 0.2 at energies 0.7 $E_F$, 1.4 $E_F$, 1.9 $E_F$, respectively. These finite $P$ values correspond to the LOW resistance memory states. In the asymmetric field configuration, $P$ falls to zero and this yields a HIGH resistance memory state.
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These devices may rely either on current-induced magnetization switching (CIMS) [21, 22] of the FM gates, or field-induced switching via the write line method used in MRAM to switch the magnetization of the ferromagnetic gates.

FIG. 4.4. Results shows the high and low resistance states of the spinFETs when it is toggled between the asymmetrical and symmetrical A configuration. (a)-(b) shows resistance states under the electrical potential of $U=20E_0$. (c)-(d) shows resistance states under the electrical potential of $U=10E_0$.

4.3.2 Zero-gauge and non-zero-gauge configuration

Figure 4.5 shows an adaptation of the spinFET which utilizes a perpendicular gate magnetization, so that a high / low resistance state is created by toggling between the zero-gauge and non-zero-gauge configurations of the magnetic field profile, as shown in Fig. 4.5 (a) and (b), respectively. Fig. 4.6 (a) shows that for the zero-gauge configuration, $|E_{thr}|$ is $10E_0$ ($\approx E_F$), thus allowing electron transmission and creating a low resistance state. In the non-zero-gauge or all-parallel
configuration of Fig. 4.5 (b), calculation in Fig. 4.6 (b) shows that $|E_{\text{thr}}|$ for $n=2$ double-pairs has been shifted to way beyond $E_F$ to about $100E_0$ or $10E_F$. Since conductance is dominated by electrons at the Fermi level, this essentially cuts off electron flow from the source to drain electrodes, thus creating a very high resistance state. This ability of the perpendicular magnetization adaptation to switch between very high/low resistance states suggests an advantage over the in-plane magnetization adaptation.

FIG. 4.5 The spinFETs can be adapted to function as a single-transistor non-volatile memory cell, by constructing and removing the zero-gauge and non-zero gauge configuration within a double-pair element.

FIG. 4.6. Results show the high and low resistance states of the spinFETs when it is toggled between the zero-gauge and non-zero-gauge configuration. Results in (b) show that in the non-zero-gauge configuration, resistance increases significantly with increasing number of barriers used.
4.4 Linear modulation of spin-polarized current polarization

Field-induced spinFET has been studied for its polarization capability, but the variation of $P$ with the size of the electrical barriers applied to the gates has not been discussed in details. In this section, we investigated the sensitivity of $P$ to the electrical barrier height $U$, which is an important property for the spinFET to function as a signal amplification device. It was found that $P$ induced by multiple zero-gauge magnetic field elements is highly sensitive to the change of $U$. Figure 4.7 (a) shows that $P$ modulation by $U$ displays two regions of sensitivity on the dotted curve. In region I, $P$ increases from 0 to -50% for $U$ changes from 5-9 $E_0$ (over just 1 mV). In region II, $P$ changes from -50% to 0 for $U$ changes from 9-30 $E_0$ (over 7 mV). It is clear from Fig. 4.7 (a) that region II of the dotted curve (at 1 $E_F$) is a preferred region for signal modulation.

To further investigate $P$ with respect to both the incident electron energy $E$ and electrical barrier height $U$, a 3D-plot of $P$ versus both $E$ and $U$ is shown in Fig. 4.7 (b). It can be seen that a reasonably large, monotonic modulation of $P$ by $U$ can be achieved at selected range of electron energies. The $B$ barrier height and the number of gate stripes provide the additional tuning parameters to shift monotonic $P$ zone to the vicinity of $E_F$. Therefore, the application of $U$ can modulate the ballistic conductance of electrons in the 2DEG in the linear operating regime if the pre-determined biasing conditions are correctly tuned. The spinFET is thus potentially capable of functioning as a very low signal amplification device.
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FIG. 4.7  (a) $P$ modulation can be achieved by varying the electrical potential.  (b) Large, monotonic modulation of $P$ by $U$ can be achieved at selected range of electron energies.

4.5 Multiple programmable logic functions

Following adaptations in section 4.2 for spin logic operation, careful optimization of device parameters could lead to the design of spinFET for multiple programmable logic functions again, all within a single spinFET. The adapted device for multiple programmable logic consists of a set of four ferromagnetic (FM 1-4) gates and two non-magnetic (NM 1-2) gates on the heterostructure of Fig. 4.8. Gates (NM a,b,c) are required for multi-bit storage but not for logic functions. The device can be programmed to perform up to seven different logic functions i.e. two-input AND, OR, NAND, NOR, and XOR, and single-input NOT, and YES, according to the fixed gate settings, i.e. the magnetization directions of FM 1 and FM 3, and the application of $U$ on NM1 and NM 2. The variable gate settings, i.e. magnetization directions of FM 2 and FM 4 function as the two inputs to the logic gate, where $\pm 1.5B_0$ (i.e. along $\pm z$ axis) represents 1/0, respectively.
The pre-determined gate values of (FM 1, FM 3, NM 1, NM 2) for AND gate is given in row 1 of Table 4.I. Similarly, by selecting appropriate gate values, the other six logic functions can be achieved. To facilitate the logic function selection, we set gates of (FM 1, FM 3, NM 1, NM 2) to $(B_1, B_2, 0, 0)$ and consider a plot of $T$ in $(B_1, B_2)$ space under all four possible inputs of (FM 2, FM 4)= (0,0), (0,1), (1,1), (1,0), as shown in Fig. 4.9, clockwise from upper left. By appropriate selection of points on Fig. 4.9, e.g. for (FM 1, FM 3)=(0,0) marked by “star”, (0,1) marked by “triangle”, (1,0) marked by “square”, and (1,1) marked by “diamond”, the device can be made to perform logic functions of AND, OR, NAND, NOR, respectively. In a similar fashion, by having the gate settings at (FM 1, FM 3, NM 1, NM 2)= (1, 0, $U_1$, $U_2$) we consider a contour plot (not shown) of $T$ in $(U_1, U_2)$ space that yields other logic functions of XOR, NAND. Table 4..I summarizes the fixed gate configurations, the resulting outputs $T$ for all four inputs, the corresponding logic functions, and clearly shows that programmable logic functions can be achieved in a single multi-gate transistor.
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TABLE 4.1. Summary of 7 different logic functions deduced from their electron transmission curves.

<table>
<thead>
<tr>
<th>2 Input Logic gates</th>
<th>Selection at (FM1, FM3, NM1, NM2) of (B1, B2, U1, U2)</th>
<th>Transmission Probability, $T$ for Inputs (In1,In2)</th>
<th>Function Realized</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(-1.5 , -1.5, 0, 0)</td>
<td>(0, 0)</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(-1.5, +1.5, 0, 0)</td>
<td>0.0973</td>
<td>0.9887</td>
</tr>
<tr>
<td></td>
<td>(+1.5, -1.5, 0, 0)</td>
<td>0.8134</td>
<td>0.9948</td>
</tr>
<tr>
<td></td>
<td>(+1.5, +1.5, 0, 0)</td>
<td>0.9373</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(+1.5, -1.5, +6, +6)</td>
<td>0.0415</td>
<td>0.7329</td>
</tr>
<tr>
<td>1 Input Logic gates</td>
<td>(B1, B2, IN1, U1, U2)</td>
<td>In2 = (0)</td>
<td>In2 = (1)</td>
</tr>
<tr>
<td></td>
<td>(+1.5, +1.5, -1, 0, 0)</td>
<td>0.9373</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(-1.5, +1.5, -1, 0, 0)</td>
<td>0.0973</td>
<td>0.9887</td>
</tr>
</tbody>
</table>

4.6 Multi-bit storage

The device of Fig. 4.8 can be adapted to function as a multi-level memory device, by employing a “weighted” gate concept as shown in Fig. 4.10. This differentiates the FM gates such that the left (right)-most magnetic gate corresponds to the lowest (highest) binary digit. The weight accorded to each magnetic gate can be manipulated by varying the FM gate dimension, geometry, or material composition, in order to modify the total magnetic moment of each gate and hence the strength of the delta-$B$ field generated by it. For illustration, we devise a 3-bit memory element (shown in Fig. 4.10) which produces $2^3 = 8$ distinct output levels that can be detected in the current or voltage detection mode. FM 4, 3, 2 are now the bit storage elements in descending binary order.

To assign the correct weights to the three FM gates, the delta-$B$ field strengths for gates (FM 1, 2, 3, 4) are set to $(1.5B_1, 0.2B_2, 0.35B_3$ and $0.6B_4)B_0$, respectively while $U$ for gates (NM 1, a, 2, b, c) are set to $(-0.65, -0.92, -1.45, +5, -3)E_0$, respectively.
FIG. 4.9. Plots of $T$ curves for different combination of $(B_1, B_2)$. The four plots correspond to different input combinations (IN1,IN2) as stated at the bottom of each graph. The magnetic $B$ and electric barrier $U$ are in units of 0.2 T and 0.35 meV, respectively. The device can be programmed to function like the AND gate (star), OR gate (triangle), NAND gate (square), and NOR gate (diamond).

The resultant weighted sum of $1.15B_1$ to $0.6B_4$ accumulates as the net change in $A_y$ in region V. It is thus necessary to negate the influence of $A_y$ on $k_x$ in the intervening regions II, III, IV. The choice of $(-0.65, -0.92, -1.45)E_0$ is motivated by the need to keep the net $A_y$ in these regions to be close to zero. The large positive $B_1$ value is to ensure a net positive $A_y$ in region V. This is necessary because the $(A_y)^2$ dependence of the effective barrier in region IV means that $\pm A_y$ will yield the same $T$. We have simplified our analysis by restricting $k_y$ to 0. This is a reasonable
assumption given that the $B$ values considered are such that $(A_y)^2 = (eB_yx/\hbar)^2$, and is significantly larger than $k_y^2 + 2k_y(e/\hbar)B_x$, so that $k_y$ and hence $T$ is independent of $k_y$, i.e.

$$k_y = \sqrt{\frac{2m}{\hbar^2}(E-U) - \left(k_y^2 + 2k_y\frac{e}{\hbar}B_x + \left(\frac{e}{\hbar}B_x\right)^2\right)} = \sqrt{\frac{2m}{\hbar^2}(E-U) - \left(\frac{e}{\hbar}B_x\right)^2}$$  (3)

Finally, a large positive $U_4$ is required to maintain a tunnel barrier in region V for all 8 levels, which is found to improve the linearity of the output. With these gate settings, the $A_y = B_x$ value and hence the $k_y$ wave vector in region V reflects the binary combinations ‘000’, ‘001’, … to ‘111’ of ‘FM 4, 3, 2’. This then translates into a monotonic shift of the $T$ threshold corresponding to states ‘000’ to ‘111’ as shown in Fig. 4.11. Current detection of the 8 levels can be achieved by setting the Fermi level ($E_F$) of 10 $E_0$=3.5meV, which yields eight distinct levels of $T$ corresponding to the binary states. However, due to the oscillatory form of the $T$ curves, it may be difficult to perform current detection for a larger number of binary states. To perform voltage detection, an extra voltage $\Delta U_4$ is applied to NMb and varied such that a constant current corresponding to $T=0.3$ (say) is obtained. Figure 4.11 shows that $\Delta U_4$ causes curves 1-8 to be shifted to point $P (T = 0.3, E_F=90E_0)$. The inset of Fig. 4.11 plots the $\Delta U_4$ values for the 8 binary states, and reveals a monotonic and reasonably linear response.

![Figure 4.10](image_url)

FIG. 4.10 The magneto-electric device can be adapted by employing the “weighted” gate concept to perform the function of multi-bit memory within a single transistor.
It can be seen that this device can potentially perform a digital-to-analog conversion, in which case, the 3-bit binary digital inputs gives rise to either an 8-level transmitted current, or 8-level voltage change at NM b, depending on the mode of detection. However, linear signal output is essential in digital to analog conversion. The inset of Fig. 4.11 shows a rather monotonic change of $\Delta U_d$ with the 8 digital input conditions from (000) to (111). However, it is not a straight line as would be required by precise conversion of digital input to analog output. Further optimization of the gate settings would thus be required to improve the linearity. The use of the single transistor device as a digital to analog converter would mark a significant saving in terms of the number of transistors as well as current digital analog converter uses the operational amplifier and a ladder of resistor network.

**FIG. 4.11.** $T$ curves correspond to the eight binary states of the multi-bit memory device. The vertical (horizontal) dotted line depicts current (voltage) detection modes. In the inset, the x axis shows the eight curves of the main graph, each corresponding to a binary input configuration of FM 4,3,2 of (000)-(111).
4.7 Device design and conductance detection

4.7.1 Device material, geometry, practical concerns

Figure 4.12 schematically shows the general layout of a magneto-electric barrier spinFET which comprises a substrate consisting of GaAs or other suitable semiconductor materials such as GaSb, InAs, InSb, or Si. The source is adapted to inject spin-polarized current into the HEMT like channel region. The source can be made of a NM material, a FM material, a half metal, or a magnetic semiconductor and is magnetized in the $x$-direction. The drain can be made of a FM material, a half metal, or a magnetic semiconductor or combinations thereof. Further, the drain is adapted to detect spin polarized electrons, in particular the drain is adapted to detect electrons polarized in the $z$-direction.

FIG. 4.12. The magneto-electric transistor can be realistically fabricated with the above dimensions, as well as material choices.

The channel region which produces the 2DEG, comprises three sub layers. The first sub layer deposited on the substrate consists of GaAs and acts as a buffer layer. The second sub layer deposited on the first sub layer, consists of AlGaAs and acts as a spacer layer. The third sub layer, which consists of $n^+$ acts as a donor layer. Further, the spinFET comprises a gate comprising
magnetic double pair elements patterned on top of the third sub layer. Each magnetic double pair element can be realized by two permanent magnets of CoCrPt, FePt, FeCo, CoPd. The non-magnetic metallic element acts as a spacer to separate the magnetic regions from each other so that the perpendicular field can approach the ideal profile of two well separated square barriers.

However, for these devices to be fully functional, it’s important to consider other practical parameters like the logic margin, fan-out, threshold, propagation delay, slew rate, bandwidth etc., as in the case of present CMOS logic devices. For instance, a detailed study on tunneling time and magnetic switching time is required to establish the propagation delay, slew rate, and bandwidth, while investigations on demagnetizing fields and spin transfer switching modes, and device source and input impedances are required for determining logic margin, fan-out, and threshold parameters. These detailed studies are beyond the scope of the thesis, but should be considered in the experimental device design.

4.7.2 Temperature

We have taken note of the effect of temperature on the ballisticity of the device, i.e. for the GaAs-based HEMT device to operate in the ballistic regime at room temperature, its gate length has to be shortened to the range of 200 nm. This is because in present high-quality 2DEGs of e.g. GaAs/AlGaAs or InAs/AlSb HEMT devices, electron mean free path could reach 100-200 nm at room temperature. Some engineering challenges may be faced in implementing the requisite magneto-electric field distribution within this gate length. However, this problem can be mitigated by optimizing the ferromagnetic gate size and geometry, as well as material composition of the 2DEG heterostructure. We have also considered the effect of temperature on spin relaxation. Zeeman energy of 1 meV (achievable with a B field of 1 T in III-V materials) is lower than the temperature effect of 25meV. However, phonon cannot flip spin without the necessary spin orbit
coupling or magnetic field effects. This explains why electron spin resonance experiments can be carried out at room temperature despite the small splitting energies of 1meV. Therefore it is possible to ensure minimal spin flip due to temperature, if high quality material for spin-polarized current conduction can be fabricated.

4.8 Conclusion

We have used the magneto-electric barriers that we conceptualized in chapter 3 to realize some logic and memory functions. Using different ferromagnetic gate configurations, we have also shown that it is possible to realize more complex logic and memory functions. We have demonstrated theoretically that a single transistor, programmable logic device capable of up to six different logic functions can be realized using our device. We have also shown the implementation of a multi-level non-volatile memory storage, which can also be optimized to function as a analog-to-digital converter. Our main contribution here is that we have proposed a way of using single-transistor with multiple gates to realize logic / memory functions that currently can only be implemented with many transistors.

REFERENCES


Spin characteristics of electron transport in semiconductor


Chapter 5

Effect of bulk crystal and nuclear field on electron transport in semiconductor

5.1 Spin orbit coupling

5.1.1 Spin relaxation

It is well known that in III-V semiconductor materials, spin relaxation can be attributed to three mechanisms i.e. Dy’akonov Perel (DP) [1], Bir Aronov Pikus (BAP) [2], and Elliot Yafet (EY) [3], of which the DP effect arises from the conduction band spin orbit coupling first described by Dresselhaus [4] in 1955. The Dresselhaus effect describes the lack of inversion center in bulk III-V materials as the cause of spin-splitting in conduction band electron. It is a form of spin orbit coupling effect that occurs in the non-relativistic limit as can be predicted from Dirac’s equation, minimally coupled to external E and B fields. Thus, in these materials, electron experiences an effective magnetic field perpendicular to the direction of its motion. The DP effect is thus dominant in zinc-blende crystals (eg. GaAs) without inversion center. The DP mechanism describes that the Dresselhaus spin orbit coupling effect is thus equivalent to an effective magnetic field that leads to the precessing of electron spin around the direction $x$ with frequency $\Omega(k)$. Spin splitting is proportional near the $\Gamma$ point to the cube of the electron momentum as shown in Eq. (1)

$$\hbar\Omega(k) = \alpha \left(2m_e^*E_g\right)^{1/2}x$$

where $x_x = p_y(p_y^2 - p_z^2), x_y = p_y(p_y^2 - p_z^2), x_z = p_y(p_y^2 - p_z^2), \alpha = \frac{4\Delta}{\left(E_g + \Delta\left(3E_g + 2\Delta\right)\right)^{1/2}m_e}$,

where $m_e$ is a constant. At low temperature, momentum scattering is minimal, and $\Omega \tau_p > 1$. 


where $\tau_p$ is the momentum scattering time. Spin relaxation is thus described by $1/\tau_s = 1/\tau_p$, where $\tau_s$ is the spin relaxation time. For thermalized electrons, electron-electron scattering cannot be neglected, and $\Omega \tau_p < 1$ because of high momentum scattering rate. The mean square angle covered by a precessing electron in time $t$ is given by $\langle \theta^2 \rangle = \langle (\Omega \tau_p)^2 \rangle (t / \tau_p)$, where $(t / \tau_p)$ is the number of effective field axis change within time $t$. Spin relaxation is given by $1/\tau_s \propto \langle (\Omega \tau_p)^2 \rangle$, the rate at which the mean square angle value reaches 1. The mean square angle here is averaged over temperature and energy as shown in Eq. (2):

\[
\langle (\Omega^2 \tau_p) \rangle = \frac{\sum_m \left[ \sum_{i=1}^n \Omega_i^2 \tau_{p_i} \right] / n}{m}
\] (2)

where $n$ is the number of temperature terms to be taken, and $m$ is the number of energy eigenvalues to be taken for the averaging. The phenomenological equation is given by Eq. (3)

\[
1/\tau_s = q \alpha^2 \frac{T^3}{h^2 E_g} \tau_p
\] (3)

where $T$ is the temperature and $E_g$ is the semiconductor bandgap. The BAP and the EY mechanism will only be briefly discussed here as these two effects are not related to spin orbit coupling. The BAP mechanism arises from the scattering of electron spin with simultaneous spin flip by holes. The probability of these processes is determined by the exchange interaction of the electron and holes as shown in the Hamiltonian of Eq. (4)

\[
H = D(J \sigma) \delta(R), \delta(p, p')
\] (4)

where $J$ is the orbital angular momentum of the hole, $D$ is the exchange interaction, $R$ is the distance between the electron and the hole, $p$ and $p'$ are the momentum of the electron and the hole, respectively. The EY mechanism is due to the valence band spin orbit coupling that results in the overlap of the conduction and valence band wave functions.
5.1.2 Spin polarization

Spin orbit coupling has been described by DP as the dominant form of spin relaxation mechanism in zinc-blende materials at low electron momentum and high temperature. However, recently the spin orbit coupling effect has also been conceived as a means of inducing spin polarization of electron current in transistor-like devices [5,6,7]. Bulk Dresselhaus spin orbit coupling (DSOC) modifies the Hamiltonian of electron transport in the conduction band, such that at a particular energy level, electron wave vectors show dependence on their spin. If potential barriers are established in the electron conduction path, a spin dependent transmission through the barriers can be obtained. Figure 5.1 shows a schematic design of a device that could utilize the DSOC effect to induce the spin polarization of current. Electrons traveling vertically down might have to transmit through interfacial potential barriers. The DSOC effect causes electron transmission to be spin dependent, resulting in the generation of spin polarized current.

![Figure 5.1. Schematic structure of a III-V semiconductor materials that generate spin polarization.](image)

Figure 5.2 shows that spin polarization of current is obtained for electron tunneling through a potential barrier in a III-V material of Fig. 5.1. Spin-polarized current is induced by the Dresselhaus spin orbit coupling effects. Electrical potential can be established across L and R contacts.
FIG. 5.2. Computation shows spin polarization can be achieved when electron tunnels through a delta-like potential barriers in a III-V bulk semiconductor materials.

5.2 Magneto-electronic device

5.2.1 Spin-polarized current induced by Dresselhaus effect

The device of Fig. 5.1 is not practical, nor is it typical of transistor-based devices in which current conducts through channel from source to drain. Figure 5.1, however, shows a perpendicular-to-plane device that might be suitable for the CPP type of recording device. In this section we will focus on utilizing the DSOC effect to generate spin-polarized current in a transistor device [5,6,7]. As we know, the bulk inversion asymmetry of zinc blende crystal structure causes a traveling electron to be coupled relativistically to the inherent electric field within the crystal lattice. The effective magnetic field causes the electron spin to precess about the field axis, and eventually align parallel to it. Since the effective field axis is dependent on the electron’s wave vector
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[1,4,7,8] the random motion of the electron randomizes its own spin state. It is therefore instructive that electron spin coherence can be preserved by constraining the electrons’ random motion.

To achieve this, we propose a field-effect transistor type of device [6] as shown in Fig. 5.3, in which electron motion is predominantly in the longitudinal $z$ direction, and its transverse wave vector ($k_x$) can be constrained [6] by some means. The semiconductor substrate of the device is selected with its $c$-axis [001] aligned with the $z$-direction, i.e. the electron conduction path from the source of the transistor device to its drain. The constraint on $k_x$ and the crystalline axis alignment cause the DSOC [1,4,5] effect to essentially couple the electron spin to the perpendicular direction ($y$) with respect to the substrate surface. The DSOC thus acts as a perturbation to the effective mass Hamiltonian, and the perturbed Hamiltonian can then be diagonalized to give the energy eigenvalue equations. The energy equation shows that electrons of opposite spins of the same energy level can be differentiated by their wave-vectors. By applying periodic, delta magnetic barriers [9,10,11,12,13] perpendicular to the substrate surface, the difference in the electron wave vector is translated to a difference in the transmission probability ($T$) for the two spin directions defined along the $y$-axis, giving rise to a finite spin polarization ($P$).

We showed that $P$ induced by DSOC can be increased by having a periodic system of magneto-electric barriers that constitute a net “zero-gauge” periodic unit [14,15,16], as described in greater details in Ref. 14 and chapter 3. However, it is important to note that the main studies in this section are magneto-transport utilizing the Dresselhaus spin orbit coupling effect and external fields. The utilization of “zero-gauge” periodic magneto-electric barriers is only an added feature and is not crucial to producing spin-polarized current in our device. Spin-polarized current can be produced in this device regardless of the types of magneto-electric barrier configurations.
In this chapter, the notation \((B_1, B_2, B_3, B_4)\) denotes the magnetic barrier configuration of one periodic unit, while \((U_1, U_2)\) represent the electric barriers within that unit. Our study focuses on achieving a high \(P\) by spin filtering electrons that travel across the magneto-electric barriers within the semiconductor only. We have neglected spin-polarized tunneling of electron from the ferromagnetic electrode into semiconductor, and vice-versa, since the process is subject to interfacial effects that are not easily controllable.

![Diagram of Magneto-electronic device](image)

**FIG. 5.3.** Magneto-electronic device that utilizes the Dresselhaus spin orbit coupling to produce spin-polarized current. Current flows from left electrode to right electrode and becomes spin polarized in the \(y\) axis as it travels through the bulk.

Table 5.I summarizes the parameters of the III-V materials which are use for calculating spin-polarized current through device of Fig. 5.3.

<table>
<thead>
<tr>
<th>Material</th>
<th>(\eta_D) (eV A(^3))</th>
<th>(m_r/m_0)</th>
<th>(\rho=\eta_D m_r)</th>
<th>(g) factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaSb</td>
<td>187</td>
<td>0.041</td>
<td>7.667</td>
<td>8</td>
</tr>
<tr>
<td>InAs</td>
<td>130</td>
<td>0.023</td>
<td>2.99</td>
<td>0.44</td>
</tr>
<tr>
<td>GaAs</td>
<td>24</td>
<td>0.067</td>
<td>1.608</td>
<td>-50</td>
</tr>
<tr>
<td>InP</td>
<td>8</td>
<td>0.081</td>
<td>0.648</td>
<td></td>
</tr>
<tr>
<td>InSb</td>
<td>220</td>
<td>0.013</td>
<td>2.86</td>
<td></td>
</tr>
</tbody>
</table>
5.2.2 Theoretical descriptions

The Hamiltonian that describes electron transport subject to the DSOC, but in the absence of magneto-electric barriers, is given by

\[
H = H_0 + H_D = \frac{p_x^2}{2m} + \eta_D [k_x (k_x^2 - k_y^2) \sigma_x + k_y (k_y^2 - k_z^2) \sigma_y + k_z (k_z^2 - k_x^2) \sigma_z]
\]  

(5)

where \( (\sigma_x, \sigma_y, \sigma_z) \) are the Pauli spin matrices, \( \eta_D \) is the Dresselhaus constant (the unit of \( \eta_D \) is \( eV m^3 \)), and \( (k_x, k_y, k_z) \) are the electron wave vectors. \( k_z \) is elevated to operator as electron travels across magneto electric barriers from source to drain across \( z \). Translational symmetry is assumed in \( x \) and \( y \) directions, and \( k_y \) assumes continuous values along the substrate thickness. The Hamiltonian of Eq. (5) can then be simplified to:

\[
H = \frac{p_x^2}{2m} - \eta_D [k_x \sigma_x - k_y \sigma_y] \frac{\partial^2}{\partial z^2}
\]  

(6)

The above Hamiltonian can be diagonalized by its eigenspinors. To find the eigenspinor, we proceed as shown in Eq. (7):

\[
\begin{pmatrix}
\frac{\hbar^2 k_x^2}{2m} & -\alpha k_y - \alpha k_z \\
\alpha k_y + \alpha k_z & \frac{\hbar^2 k_y^2}{2m}
\end{pmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix}
= \xi
\begin{bmatrix}
a \\
b
\end{bmatrix}
\]

(7)

where \( \alpha = \eta_D k_z^2 \)

Expanding the matrix equation above results in two simultaneous equations shown in Eq. (8) and Eq. (9):

\[
\frac{\hbar^2 k_x^2}{2m} a - \alpha (k_x + k_y) b = E a
\]  

(8)

\[
\frac{\hbar^2 k_y^2}{2m} b + \alpha (k_y - k_z) a = E b
\]  

(9)

After simplification, Eq. (8) leads to a series of derivations denoted by Eqs. (10):
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\[
\frac{\hbar^2k^2}{2m}ab - \alpha(b_{k_x} + k_x)p_1 = \frac{\hbar^2k^2}{2m}ba + \alpha(b_{k_y} - k_y)p_2
\]

\[
-\alpha(b_{k_x} + k_x)p_2 = \alpha(b_{k_y} - k_y)p_1
\]

\[
a = \pm \frac{k_x + ik_y}{\sqrt{k_x^2 + k_y^2}} = \pm \frac{k_x + ik_y}{k_y}
\]

and +/- signs denote spin up/down components, respectively. After normalization which requires that \(|a|^2 + |b|^2 = 1\), and making use of the last of Eqs. (11),

\[
\frac{a}{b} = \frac{k_x + ik_y}{\sqrt{k_x^2 + k_y^2}}
\]

\[
|a|^2 = \frac{k_x^2 + k_y^2}{\sqrt{k_x^2 + k_y^2}} = 1
\]

we obtained the values for \(2|\psi|^2 = 1\), and \(|\psi| = \frac{1}{\sqrt{2}}; |\psi| = \frac{1}{\sqrt{2}}\). The eigenvector can therefore be written in Eq. (12) as:

\[
\chi^s = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \frac{k_x + ik_y}{k_y} \\ 1 \end{array} \right)
\]

The eigenvector shows that the spin points in the y direction when \(k_y\) is zero and the x direction when \(k_y\) is zero. The spin orientations around the \(k_y-k_x\) diagram are shown in Fig. 5.4 below.

FIG. 5.4. This diagram shows the orientation of electron spin for the (+) branch, i.e. s=+1 with respect to different electron wave vector orientation.
Spin characteristics of electron transport in semiconductor

Having found the eigenspinors, we will now proceed to find the eigenvalue equations. Considering spin up (+) only, we write Eqs. (13) in the form of eigenfunction solutions, such that solving the left hand side of Eqs. (13) allows the finding of the eigenenergies \( E \).

\[
\begin{align*}
\left[ \frac{\hbar^2 k_z^2}{2m} - \alpha k_y - \alpha k_x \right] \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right) & = E \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right) \\
\alpha k_y - \alpha k_x \left[ \frac{\hbar^2 k_z^2}{2m} \right] \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right) & = E \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right)
\end{align*}
\]

(13)

where \( \alpha = \eta_D k_z^2 \). Proceeding from Eqs. (13), we could find the eigenenergies by comparing \( E \) on the right hand side of Eqs. (14) to the corresponding terms on the left hand side.

\[
\begin{align*}
\frac{1}{\sqrt{2}} \left[ \frac{\hbar^2 k_z^2}{2m} \frac{k_y + ik_x}{k_\|} - \eta_D \frac{k_y + ik_x}{k_\|} \frac{1}{\sqrt{2}} \right] & = E \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right) \\
\frac{1}{\sqrt{2}} \left[ \frac{\hbar^2 k_z^2}{2m} \frac{k_y + ik_x}{k_\|} - \eta_D \frac{k_y + ik_x}{k_\|} \frac{1}{\sqrt{2}} \right] & = E \frac{1}{\sqrt{2}} \left( + \frac{k_y + ik_x}{k_\|} \right)
\end{align*}
\]

(14)

Taking the general approach where \( s \) represents spin up or down, the energy eigenvalue equations can be found in a similar way through Eqs. (15) and (16):
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\[
\begin{bmatrix}
\frac{\hbar^2 k^2}{2m} & -\alpha k_x - \alpha k_y \\
\alpha k_y - \alpha k_x & \frac{\hbar^2 k^2}{2m}
\end{bmatrix}
\frac{1}{\sqrt{2}} \begin{bmatrix} k_x + ik_y \\
-k_y
\end{bmatrix} = E \frac{1}{\sqrt{2}} \begin{bmatrix} k_x + ik_y \\
-k_y
\end{bmatrix}
\]

where \( \alpha = \eta dk_z^2 \)

\[
\frac{1}{\sqrt{2}} \begin{bmatrix}
\frac{\hbar^2 k^2}{2m} k_x + ik_y + s \eta_{\nu} k_{\mu} (ik_x + k_y) k_z^2 \\
s \eta_{\nu} k_z^2 (ik_y - k_x) + \frac{\hbar^2 k^2}{2m}
\end{bmatrix} = E \frac{1}{\sqrt{2}} \begin{bmatrix} k_x + ik_y \\
-k_y
\end{bmatrix}
\]

\[
\frac{1}{\sqrt{2}} \begin{bmatrix}
\frac{\hbar^2 k^2}{2m} k_x + ik_y - s \eta_{\nu} k_{\mu} (ik_x + k_y) k_z^2 \\
-s \eta_{\nu} k_z^2 k_y + \frac{\hbar^2 k^2}{2m}
\end{bmatrix} = E \frac{1}{\sqrt{2}} \begin{bmatrix} k_x + ik_y \\
-k_y
\end{bmatrix}
\]

\[
\frac{1}{\sqrt{2}} \begin{bmatrix}
\frac{\hbar^2 k^2}{2m} - s \eta_{\nu} k_z^2 k_y \\
\frac{\hbar^2 k^2}{2m} - s \eta_{\nu} k_z^2 k_y
\end{bmatrix} = E \frac{1}{\sqrt{2}} \begin{bmatrix} k_x + ik_y \\
-k_y
\end{bmatrix}
\]

where \( s \) represents the spin up/down states in this basis, respectively; \( k_y \) lies along the \( x-y \) plane, perpendicular to the electron’s traveling direction (\( z \)) i.e. \( |k_y| = \sqrt{k_x^2 + k_y^2} \). By constraining \( k_x \) to 0, the eigenspinor in Eq. (12) becomes

\[
\chi^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm i \\ 1 \end{pmatrix}
\]

Electron spin is thus orientated in the same direction as the delta magneto-electric fields that were applied perpendicular (\( y \)) to the substrate surface. Assuming an eigenstate of the form

\[
\psi^\pm = u^\pm (x, y, z) \chi^\pm = e^{i(k_x x + k_y y)} (A e^{i k_z z} + B e^{-i k_z z})
\]

results in the following eigenvalue solutions obtained from Eq. (16):

\[
\left[ \frac{\hbar^2 (k_x^2 + k_y^2)}{2m} - s \eta_{\nu} k_z^2 k_y \right] \chi' u' = E' \chi' u' \Rightarrow E' = E_o - s \Delta E
\]
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For ease of calculation, all parameters are reduced to dimensionless units (refer chapter 3). In the presence of magneto-electric barriers, \( H_0 \) in Eq. (5) is transformed to \( H_B \):

\[
H_0 \rightarrow H_B = \left( \frac{p_x + eA_z}{2m^*} \right)^2 + \left( \frac{p_y}{2m^*} \right)^2 + U(x) + \frac{e \varepsilon}{2m_0} sB_z(x)
\]  

(19)

where \( m^*, m_0 \) is the electron’s effective and real mass, respectively, \( g \) is the Lande factor, and \( p_x \) and \( p_y \) are electron momentum in the \( x \) and \( y \) directions, respectively. Note that we have chosen the Landau gauge \( A=(A_x,0,0) \) in the above. Thus, in the presence of a magnetic field \( B_y \), the system can be described by a Lagrangian with one degree of freedom: \( L = \frac{1}{2m(v_x)^2} - \epsilon e/\hbar A_x \). Legendre transformation of the Lagrangian \( H = v_x p_x - L \) leads to the Hamiltonian of Eq. (20). Since \([H_B, H_D]=0\), the energy equation is

\[
E = \left( \frac{p_x + eA_z}{2m^*} \right)^2 + \left( \frac{p_y}{2m^*} \right)^2 + U(x) + \frac{e \varepsilon}{2m_0} sB_z(x) - s\eta k_z^2
\]  

(20)

From Eq. (20), we obtained the wave-vectors through the following simplification process:

\[
k_z^R = \frac{2m^*}{\hbar} (E^* - U) - (k_z + eA_z)^2 - k_z^2 \quad \text{and} \quad k_z^L = -\frac{2m^*}{\hbar} (E^* - U) - (k_z + eA_z)^2 - k_z^2
\]  

(21)

for right-moving \( (k_z^R) \) and left-moving \( (k_z^L) \) wave functions, respectively. The corresponding wave amplitudes are determined by amplitude matching and ensuring flux continuity across the delta-function magnetic barriers. The flux-matching yields the following relation:

\[
\left[ \int_{-\frac{\hbar}{2m^*}}^{\frac{\hbar}{2m^*}} \nabla^2 + s\Lambda \delta dx - s\eta k_z \right] \psi(x) = \int_{-\frac{\hbar}{2m^*}}^{\frac{\hbar}{2m^*}} E^* \psi(x) dx
\]  

(22)

where, \( \Lambda = \frac{e \varepsilon}{2m_0} B_y \), \( \varepsilon \) is the small energy change. Continuity equation at the first \( B \) barrier is given by:

\[
\frac{\hbar}{2m^*} i(k_z^R \Lambda + k_z^L B) = \frac{\hbar}{2m^*} i(k_z^R C + k_z^L D) - \frac{\Lambda}{\hbar} (C + D)
\]  

(23)
where $A$ and $B$ are the $z$-traveling wave function amplitudes in region I, associated with $k_{1R}$ and $k_{1L}$, respectively. $C$ and $D$ are the corresponding wave amplitudes in region II. Transmission through multiple ($n$) double-pair barriers can be obtained by repeated transfer matrix multiplication, i.e.

$$
\begin{bmatrix}
A_1 \\
B_1 
\end{bmatrix} =
\begin{bmatrix}
a_1 & a_2 \\
a_3 & a_4 
\end{bmatrix}
\begin{bmatrix}
e^{-ik_{1R}g} & 0 \\
0 & e^{-ik_{1L}g} 
\end{bmatrix}
\begin{bmatrix}
b_1 & b_2 \\
b_3 & b_4 
\end{bmatrix}
C_2
$$

(24)

where $(a_1, a_2, a_3, a_4)$ and $(b_1, b_2, b_3, b_4)$ are the matrix components corresponding to the first and second pair of magnetic delta-function barriers of Fig. 5.3, respectively. $A_1, B_1, C_2, D_2$ are the wave-function amplitudes at the different locations of the delta barriers as shown in Fig. 5.5 below.

In the device of Fig. 5.3., the left electrode is magnetized in the $z$ axis, so that the resulting spin-polarized current has equal polarization in $+y$ and $-y$. Similar to the device in chapter 4, the device in Fig. 5.3 relies on the magnetized stripes patterned on top of the heterostructure to produce delta $B_y$ which vertically penetrates the substrate surface. These magnetized stripes can be made from materials like FeCo, CoCrPt, CoPd, FePt.
5.2.3 Spin-polarized current for GaAs, GaSb, InAs, and InSb

Based on the spin dependent wave vectors derived in Eqs. (21) and following the transmission procedures, we simulated spin-polarized current for device made from bulk GaAs, GaSb, InSb. At room temperature, the energy spread of electrons above the conduction band for GaAs, GaSb, InSb ranges between 0-20 meV (30-60 $E_0$) at carrier density $10^{16}$-$10^{17}\text{cm}^{-3}$. We thus optimized the device to obtain transmission and spin polarization in this energy range. Figure 5.4 shows the $P$ curves of the GaAs ($n=1$) device for different electron energies $E$ in the multiple of $E_0$. Computation results show that the resulting $P$ due to the DSOC effect alone (dark $P$ curve) was < 1%.

The following magneto-electric fields were then applied: $B= (+4, +4, -4, -4)B_0$ and $U=(80, 80)E_0$. It is worth noting that the application of these fields results in a vector potential $A$ profile which is symmetric across regions I-V. It has been shown that such fields will not be able to induce any $P$ in the absence of the SOC effects, as has been previously discussed in chapter 3 and 4. However, our results in Fig. 5.6 shows that in the presence of these fields and the DSOC effects, $P$ increases significantly to an average of 2% over 0-30 meV (grey $P$ curve) peaking at 6% at 10 meV. Between 8-15 meV, spin-polarized current polarization fluctuates rather severely from +6% to -6%. The calculation was then repeated for $n=3$ double-pairs and this yields a slight increase in $P$ to 3% average over 0-30 meV, peaking at 10% at 10 meV (not shown).
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FIG. 5.6. Computation results are shown for $T$ and $P$ curves of the device of GaAs materials. External fields were applied in the form of $n=1$ zero-gauge double-pair gates. Grey curve shows average $P$ of 2% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero, peak $P$ less than 1%.

The same calculations were repeated for GaSb ($n=1$) and similar effects were manifested in the resonance peaks and troughs of the $T$ and $P$ curves for increasing electron energies. Figure 5.7 shows that the application of a perpendicular magnetic field causes $P$ to increase from 2% average to 5% average over 0-30 meV, peaking at 10%, 25% at 10 meV, 15 meV, respectively.

FIG. 5.7. Computation results are shown for $T$ and $P$ curves of the device of GaSb materials. External fields were applied in the form of $n=1$ zero-A double-pair gates. Grey curve shows average $P$ of 5% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero peak $P$ around 2%.
Spin characteristics of electron transport in semiconductor

For larger number of double-pair elements, eg. \( n=5 \), Fig. 5.8 shows that spin polarization of current increases significantly to an average of about 10\% over the 10-30 meV range. Spin polarization reaches 60\% at about 12 meV, and -60\% at about 15 meV.

![Graph showing T and P curves for GaSb materials](image)

**FIG. 5.8.** Computation results are shown for \( T \) and \( P \) curves of the device of GaSb materials. External fields were applied in the form of \( n=5 \) zero-gauge double-pair gates.

Similar calculations were performed for the high-mobility, high \( g \) factor InSb for \( n=5 \) double pairs. Figure 5.9 shows an average \( P \) of 10\% over 0-30 meV, peaking at 23\%, 80\% at 10 meV, 15 meV, respectively. Results in Fig. 5.9 clearly show that \( P \) of this device can be further increased if longer conduction path length can be tolerated (eg. InSb with long mean free path) as more zero-gauge double-pair barriers can be added. Meanwhile the larger increase in \( P \) as a result of applying external fields in the case of GaSb and compared to GaAs, is primarily due to the larger \( g \) factor of GaSb. Larger \( g \) factor results in a larger Zeeman splitting at the delta-function magnetic barriers.
Spin characteristics of electron transport in semiconductor

FIG. 5.9. Computation results are shown for $T$ and $P$ curves of the device of InSb materials. External fields were applied in the form of $n=5$ zero-gauge double-pair gates. Grey curve shows average $P$ of 10% near the conduction band (0-30 meV). Dark curve shows average $P$ close to zero, peak $P$ around 3-4%.

It is also observed in the presence of the DSOC effect alone (i.e. without applying external field), that $P$ is only marginally larger in GaSb than GaAs (3% against 2%) despite the significantly larger $\rho$ of GaSb (7.6 c.f. 1.6). It’s worth noting that numerical simulations were only performed for specific device parameters to illustrate spin-polarized current generation utilizing the Dresselhaus and field-enhancement effects. The device can be further optimized to obtain more favorable results, depending on specific tolerances, and requirements.

We also performed simulations for the materials of InAs for $n=1$. Since InAs does not have large $g$ the effect of magneto-electric barriers on spin polarization is minimal as shown in Fig. 5.10 (a).

Since InAs also has low $\rho$ of 2.99 compared to 7.6 for GaSb, we would expect that spin polarization due to the Dresselhaus effect only is substantially lower for InAs compared to GaSb as shown in Fig. 5.10 (b). However, Fig. 5.10 (c) shows that spin polarization increases to a discernible average of approximately 5%, peaking at 10% at 15 meV. This clearly shows that combined effect of Dresselhaus and field-barriers enhances spin polarization significantly. Such
enhancements could not be achieved by utilizing either the Dresselhaus or the field effect only. Fig. 5.10 (d) shows magnified spin polarization curves of Fig. 5.10 (c).

FIG. 5.10. Computation results are shown for $T$ and $P$ curves of the device of InAs materials. External fields were applied in the form of $n=1$ zero-gauge double-pair gates.

5.3 Nuclear field for spin polarization

The effect of nuclear field on conduction electron will only be discussed analytically in this section. Derivations will be provided to illustrate the effects of electron interaction with nuclear field on the electron wave vectors. The dependence of wave vector on spin indicates the possibility of harnessing these effects to generate spin polarized current. The interaction of electron with atomic nuclear field of III-V semiconductors results in the hyperfine interaction [17,18,19,20] that can potentially be used to induce the polarization of spin-polarized current.

The hyperfine interaction consists of the following contributions: 1. Electron spin interacting with the nuclear dipole (real magnetic field), 2. Electron spin interacting with nuclear magnetic moment
or spin (Fermi contact), 3. Electron spin interacting with the effective nuclear field that arises from
the orbital motion of the electron around the nucleus. Fermi contact is most dominant among the
three interaction. The Hamiltonian that describes the hyperfine interaction is therefore given by:

\[ H = H_0 + g\mu_B B_z \sigma_z + \sum_j a_j A_j \langle P_j \rangle \sigma_z \]  

(25)

where \( g \) is the Lande g factor, \( H_0 = g\mu_B B_z \sigma_z + \sum_j a_j A_j \langle P_j \rangle \sigma_z \) is the Bohr magnetron, \( \langle P_j \rangle \) is the
spin polarization of different nuclear isotopes, \( a_j \) indicates the number of nuclear isotopes of type \( j \).

The hyperfine coupling constant \( A_j \) is given by:

\[ A_j = \frac{8\pi \mu_0}{3} \frac{\eta_j}{4\pi} g\mu_B \hbar \gamma \langle \psi_j(0) \rangle \]  

(26)

where \( \gamma_j \) is the gyromagnetic ratio and \( \langle \psi_j(0) \rangle \) is the probability density of conduction electron
found in site \( j \) of nucleus type \( j \). The hyperfine interaction is equivalent to electron spin (note only
spin) interaction with an effective field of \( B_{HF} \) which contains the effects of Fermi contact and
nuclear spin orbit coupling although the latter effect is only a small fraction of the former. The
Hamiltonian can thus be written as:

\[ H = g\mu_B (B_z + B_{HF}) \sigma_z \]  

(27)

The eigenspinors for spin up \( \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) and spin down \( \begin{pmatrix} 0 \\ 1 \end{pmatrix} \) represent up and down in the direction along
which the isotope polarization is defined. The energy eigenvalue equations are:

\[ E^\pm = E_k + U \pm g\mu_B(B_z + B_{HF}) \]  

(28)

where \( \pm = \pm 1 \) denote spin up/ down, respectively, \( E_k \) is the kinetic energy and \( U \) is the potential
energy of the electron. The spin-dependent wave vectors would thus be given by:

\[ k^\pm = \sqrt{\frac{2m^*}{\hbar^2} \left( E^\pm - U \pm g\mu_B(B_z + B_{HF}) \right) - k^2_j - k^2_i} \]  

(29)
Following the standard procedures of computing transmission probability for electrons through a potential barrier, Eq. (29) would thus result in spin-dependence conductance, similar to what we have observed for spin-polarized current in the magneto-electronic devices.

5.4 Conclusion

We have shown that the strength of the bulk DSOC effect in III-V semiconductors alone is not sufficient for it to act as an efficient source of $P$ on its own. This is despite having an optimal device geometry to constrain the transverse wave vector of the conduction electrons, thus preventing spin relaxation. The field enhancement of $P$ also implies the presence of additional control parameters ($B$ and $U$) that can be used to modulate and optimize $P$ near the conduction band. The combined effect of DSOC and magneto-electric barriers also results in a significant value of $P$ even for a small number of periodic units of double-pair gate elements ($n$=1-5). Hence in such device, much fewer gate elements (and thus smaller device length) are required compared to devices which rely only on external fields but do not utilize any SOC effects. It is feasible that these devices (esp. InSb) generate significant spin-polarized current and operate in the ballistic regime.

REFERENCES

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Chapter 6

Rashba spin orbit coupling induced magneto-transport

6.1 Structural inversion asymmetry

It has been described in chapter 3 that the coherent transport of electron in III-V semiconductor 2DEG can be manipulated by the application of external magnetic and electric field [1,2,3,4,5,6]. The high mobility of electron in high-quality semiconductor 2DEG eg. GaAs-InGaAs ensures minimal extrinsic scattering of electrons, hence ballistic transport in the 2DEG channel. In this regime, electron conductance in respective individual mode is studied for their magnitude and spin dependence. In chapter 5, the bulk crystal effective field [7, 8, 9] as well as the nuclear fields cum spin-spin [10,11] interaction were studied for their ability to induce spin transport carried by conduction electrons. In the 2DEG, the non-uniform vertical distribution of confining potential results in the structural inversion asymmetry that also gives rise to spin orbit coupling that could induce magneto-transport. Similar to the DSOC effect described in chapter 5, this is a relativistic effect in the non-relativistic limit. The effective magnetic field experienced by electron in the two-dimensional system will be utilized here to induce spin polarization of current. This effect is known as the Rashba spin orbit coupling (RSOC) effect. The RSOC effect has been keenly studied ever since the Datta and Das proposal [12] of utilizing this effect in a HEMT type spintronic device. The RSOC effect [13,14,15,16,17,18,19] has then been widely researched for their ability to induce spin-polarized current in various ways and devices.
6.2 Magneto-electronic device

It is therefore widely known that the conduction band spin orbit coupling effects of Rashba (RSOC) and Dresselhaus (DSOC), the nuclear fields, as well as the external magneto-electric fields can each be utilized to induce spin-polarized current in magneto-electronic device. In this chapter, we will study the combined effects of magneto-electric barriers and the RSOC on spin polarization of current in a HEMT structure reminiscent of the Datta and Das device, in which current flows within a 2DEG under the influence of delta magnetic fields applied through the ferromagnetic gates as shown in Fig. 6.1. The harnessing of the RSOC effects in the presence of in-plane delta magnetic fields specifically has not been previously analyzed. The combined effects of RSOC and in-plane fields have especially not been studied in the context of a transistor device, and for their ability to produce spin-polarized current. Previous works have largely focused on perpendicular delta fields and have not considered the spin scattering effects caused by the effective magnetic fields of the RSOC.

(a)                                                                                  (b)

FIG. 6.1. (a) Device with delta $B$ field oriented in y direction in the 2DEG. (b) Device with delta $B$ field oriented in the z direction in the 2DEG. The former can utilize RSOC to enhance spin polarization of current. In the latter device, spin polarization could be mitigated by the in-plane RSOC effects.
The devices of Fig. 6.1 bear close similarity to those used in chapter 4 (not chapter 5) except that here magnetic fields are applied in-plane as shown in Fig. 6.1 (a). Figure 6.1 (b) shows the perpendicular field magneto-electronic device for comparison. Similar to the chapter 3 device, it consists of the ferromagnetic gate stripes, patterned on top of the multilayer heterostructure. The magnetic field from the gate which can be approximated as a delta function of strength $B_y$, aligned electron spin parallel to the effective field axis. Thus an effective field axis is resulted from the effect of RSOC and the $B_y$ field. We showed, in this section that the in-plane field has significant advantages over the perpendicular field in generating spin-polarized current with net polarization $(P)$ value, especially when large fields or multiple barriers are required to generate high $P$. The RSOC effect is also discussed for their effects on reinforcing the external fields to generate spin-polarized current as well as its adverse effects on scattering spin-polarized current generated by the external field. The application of $B_y$ field shifts the effective magnetic field axis closer to the $y$ axis, thus increasing the projection of $P$ onto the $y$ axis. This is equivalent to modulating spin-polarized current polarization in the $y$ axis or $P_y$ by controlling the strength of $B_y$ field. We confined our model to studying the spin-dependent tunneling effect across in the semiconductor 2DEG only as shown in Fig. 6.2. Electron transport from ferromagnet to semiconductor and then to ferromagnet is not considered here as more refined models would be required to take into account interfacial effects. Narrow-gap semiconductors are preferred materials as they form a natural 2DEG and forms good Ohmic contact with the ferromagnet.

FIG. 6.2. Electron tunnels through the barriers from region I on the left to region V on the right. $A-J$ are wave-function amplitude in different regions. $A_1$-$D_2$ are wave-function amplitudes at the delta barriers.
6.3 Theory

6.3.1 Spin operator and symmetry

Spin can be detected with certainty in the direction where magnetic field has been applied. Electron precesses around the $B$ field axis as the spin vector rotates around it. The direction of the $B$ field is conventionally taken as $z$. As is known and implicitly used without discussion in chapter 5, the equations of (1) & (2) describe the system with a $z$-spin operator acting on a $z$-vector, giving rise to an angular momentum eigenvalue of $\frac{h}{2}$.

$$S_z \varphi_s = \frac{1}{2} \hbar \varphi_s$$

(1)

$$S_z \varphi_s = \frac{1}{2} \hbar \left( \begin{array} { c c c } { 1 } & { 0 } & { 1 } \\ { 0 } & { 1 } & { 0 } \end{array} \right) \varphi_s = \frac{1}{2} \hbar \left( \begin{array} { c } { 1 } \\ { 0 } \end{array} \right) \varphi_s = \frac{1}{2} \hbar \varphi_s$$

(2)

Spin transformation comprises the transformation of the spin operator as well as the spin state vector, e.g. applying a 90-rotation matrix rotates the spin vector to the $x$-axis. The rotated vector represents a state in which the spin angular momentum is oriented in $x$ and can be detected with certainty in $x$ with a value of $\frac{h}{2}$. The mathematical representation of state transformation is given by Eq. (3). We know from experiments that this can only be achieved when the magnetic field points in the direction of $x$. Therefore the above transformation represents a situation in which the magnetic field is rotated from $z$ to the $x$ axis. The transformed spin vector (spinor) should be an eigenstate of the transformed operator which is mathematically derived in Eq. (4).

$$|\varphi_s \rangle_z \rightarrow U|\varphi_s \rangle_z = |\varphi_s \rangle_x$$

(3)

$$USU^* = S_z$$

(4)

The transformed system can be described as follows: the state in which the spin angular momentum points to $x$ can be measured with certainty when the $B$ field is applied in the $x$ direction. The post-transformed state ($x$, in this case) shares the same eigenvalue as the pre-
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Equation (5) describes the symmetry property of spin transformation, in which the eigenvalue of $\hbar/2$ is preserved throughout.

\[ S_z |\phi_z\rangle = US_z U^* |\phi_z\rangle = U \frac{1}{2} \hbar |\phi_z\rangle = \frac{1}{2} \hbar |\phi_z\rangle \]

(5)

6.3.2 Energy and wave-vector analysis

The minimal-coupling Hamiltonian that describes electron energy in a 2DEG in the presence of Rashba spin-orbit coupling, delta in-plane field in the delta field region is given by:

\[ H = H_0 + H_s + H_R + H_Z = \frac{p_z^2}{2m} + \left( \frac{p_x + eA_y}{2m} + e\xi F_x + \eta_R (k_x \sigma_x - k_y \sigma_y) - \sigma_y \right) \left( \frac{eg*\hbar}{4m_0} \right) B_y \]

(6)

where $H_0$, $H_s$, $H_R$, and $H_Z$ correspond to the kinetic energy, sub-band energy, the Rashba effect, and the Zeeman effect, respectively; $x=0$ is where the delta $B_y$ field is applied. The Rashba effect is quantified by a parameter $\eta_R = \alpha F_z$ ($F_z$ being the intrinsic electric field perpendicular to the 2DEG plane), and arises from space inversion asymmetry in the 2DEG. In solving $H$, the eigenspinors are obtained by solving the 2x2 matrix equation of:

\[
\begin{bmatrix}
H_0 + H_s + U & \eta_R k_x + i \eta_R (k_y + (\Lambda/\eta_R)) \\
\eta_R k_y - i \eta_R (k_x + (\Lambda/\eta_R)) & H_0 + H_s + U
\end{bmatrix} \chi^z = E^z \chi^z
\]

(7)

where $\Lambda = \frac{eg*\hbar}{4m_0} B_y$. The eigenspinors are obtained by solving Eq. (7):

\[ \chi^z = \frac{\pm k_y + i(k_x + (\Lambda/\eta_R))}{\sqrt{k_y^2 + (k_x + (\Lambda/\eta_R))^2}} \]

(8)

The spin dependent eigenenergies are $E^z = \pm \eta_R \gamma$ where $\gamma = \sqrt{k_y^2 + (k_x + (\Lambda/\eta_R))^2}$. When $k_x = 0$, effective field is aligned with the $y$ axis, the eigenspinor thus corresponds to spin quantization in $y$.

To simplify wave function matching, the Cartesian frame is now rotated such that the $z$ axis coincides with a particular effective field axis that corresponds to a particular set of values for $(B_y, \eta_R, k_y, k_x)$. Such rotation can be accomplished by transforming Eqs. (7) and (8) with a unitary
matrix, $U(\theta = \pi/2, \phi)$. Because of symmetry, the spin dependent energy eigenvalues obtained in the rotated frame are the same as that obtained in the original frame. In the newly rotated frame (where $z$ is in-plane and coincides with the effective field axis), the one-dimensional wave functions in $x$ in regions I, II are given by:

$$\psi_1(x) = A^+ e^{ik_1x} + B^+ e^{-iq_1x} + A^- e^{iq_1x} + B^- e^{-ik_1x}$$

$$\psi_2(x) = C^+ e^{ik_2x} + D^+ e^{-iq_2x} + C^- e^{iq_2x} + D^- e^{-ik_2x}$$

where $(+k_1, -k_1, +q_1, -q_1)$ and $(+k_2, -k_2, +q_2, -q_2)$ are the wave vectors of the four degenerate eigenfunctions in region I and II, respectively. To find the wave vectors in regions I, II, we take a digression back to the original frame again. Wave function in $y$ is given by $\phi(y) = e^{ik_2y}$, due to translation invariance in $y$. Wave function in $z$ is given by the Airy function of $\phi(z)$. The total wave function of the system in region I can thus be expressed in the spinor form of:

$$\psi(x, y, z) = e^{ik_1y} \phi(z) \begin{pmatrix} A^+ e^{ik_1x} + B^+ e^{-iq_1x} \\ A^- e^{iq_1x} + B^- e^{-ik_1x} \end{pmatrix}$$

It can be seen in Eq. (11) that the wave function is separated into two independent branches, each spin branch obeying its own continuity of wave / flux amplitude in space. Solving the Hamiltonian in the original frame in region I or II gives:

$$H \psi(x, y, z) = \left( -\frac{\hbar^2}{2m^*} \phi''(z) - \frac{ie\hbar\Lambda}{m^*} \phi(z) + \left( \frac{p_\parallel^2}{2m^*} + U + H_z + \frac{e^2A_z^2}{2m^*} \right) \phi(z) + e\zeta F, \phi(z) \right) \phi(x, y)$$

where $m^*$ ($m_0$) is the electron’s effective (real) mass, $g^*$ the Lande factor, and $p_\parallel$ the in-plane electron momentum, $s=+1/-1$ denote spin up/down, respectively. The wave function confined in the original $z$ axis is:

$$\phi(z) = e^{z\eta_1} \text{AiryA} \left[ \frac{b^2 + 4ac - 4aE_z + 4adz}{4a^{4/3}d^{1/3}} \right]_1 + e^{z\eta_2} \text{AiryB} \left[ \frac{b^2 + 4ac - 4aE_z + 4adz}{4a^{4/3}d^{1/3}} \right]_2$$
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where $a = \hbar^2 / 2m^*$, $b = ieA_z / m^*$, $d = eF_z$, $c = p_\mu^2 / 2m^* + U + H_R + e^2A_z^2 / 2m^*$, $c_1$, $c_2$ are constants in which $c_2$ is 0 such that $\phi(z)$ is a well-behaved function. Taking the boundary condition of $\phi(z = 0) = 0$, where $z = 0$ is referenced to the lowest point of the 2DEG in the $z$ axis. To find the roots for $\phi(z) = e^{-\frac{\hbar v}{2m^*}} AiryAi\left[\frac{b^2 + 4ac - 4aE_R + 4adz}{4a^{2/3}d^{2/3}}\right]c_1$, we used the Mathematica software that numerically calculated the roots to be -2.338, -4.088, and so on. Taking the root of -2.338 for the ground state energy, it is found that $E_\phi = (b^2 / 4a) + c + 2.338a^{1/3}d^{2/3}$. Substituting for $a, b, c$ into the ground state energy, it is straightforward to obtain the energy equation of:

$$E_\phi = \frac{p_\mu^2}{2m^*} + U + H_R + 2.338\left(\frac{(eF_z \hbar)^2}{2m^*}\right)^{1/3} = \frac{p_\mu^2}{2m^*} + U_{eff} + H_R$$  \hspace{1cm} (14)

It is interesting to note that the gauge $A_z$ has not entered the energy equation of Eq. (14). The 2DEG sub-band wave-vector ($k_\mu$) has thus been able to preserve its original form, i.e. it is not minimally-coupled to the magnetic vector potential. The original form refers to the sub-band energy equation form which was due solely to the 2DEG-typical triangular barrier confinement only. Since the sub-band energy is a constant (independent of $B_y$ strength), it can be absorbed in $U_{eff}$. In region I, II, the eigenspinor is $\chi^\mu = \left(\pm \frac{k_\mu + ik_\nu}{\sqrt{k_\mu^2 + k_\nu^2}}, 1\right)$, and the spin dependent eigenenergies are: $E^\mu = \pm \eta_k k_\mu$ . Elevating Eq. (12) to its operator form and solving for $\varphi(x)$, the in-plane wave-vector can be obtained as below:

$$k_\nu^2 + s\eta_k \frac{2m}{h^2} k_\nu - \frac{2m}{h^2}(E - U_{eff}) = 0$$  \hspace{1cm} (15)

The solutions to (15) are Eqs. (16) and (17):

$$k_\nu = -s\eta_k \frac{m}{h^2} \pm \sqrt{\left(\eta_k \frac{m}{h^2}\right)^2 + \frac{2m}{h^2}(E - U_{eff})}$$  \hspace{1cm} (16)
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\[ k_x^2 = -s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2 \]  \hspace{1cm} (17)

Equation (17) yields four in-plane wave vector solutions at Fermi energy level \((E_F)\). It is obvious that \(k_x\) can be expressed in the forms shown by Table 6.I (a) and (b) for the Northern Hemisphere and Southern Hemisphere, respectively of Fig. 6.3.

TABLE 6.I. (a) Electron wave-vectors traveling in \(x\) and \(-x\), at a particular energy level \(E\) in the Northern Hemisphere of Fig. 6.3. i.e. for \(+k_y\) values.

<table>
<thead>
<tr>
<th>(s)</th>
<th>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</th>
<th>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (+k_y)^2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(s=-1)</td>
<td>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</td>
<td>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (+k_y)^2} )</td>
</tr>
<tr>
<td>(s=+1)</td>
<td>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</td>
<td>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (+k_y)^2} )</td>
</tr>
</tbody>
</table>

TABLE 6.I. (b) Electron wave-vectors traveling in \(x\) and \(-x\), at a particular energy level \(E\) in the Southern Hemisphere of Fig. 6.3. i.e. for \(-k_y\) values.

<table>
<thead>
<tr>
<th>(s)</th>
<th>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</th>
<th>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (-k_y)^2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(s=-1)</td>
<td>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</td>
<td>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (-k_y)^2} )</td>
</tr>
<tr>
<td>(s=+1)</td>
<td>(k_x = - \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - k_y^2} )</td>
<td>(k_y = + \sqrt{-s \eta R \frac{m}{\hbar^2} \pm \left( \eta R \frac{m}{\hbar^2} \right)^2 + \frac{2m}{\hbar^2} (E - U_{eff}) - (-k_y)^2} )</td>
</tr>
</tbody>
</table>

The assignment of spin value \((s=+1\) or \(-1)\) to the wave-vectors for each hemisphere follows the prescriptions applied when \(k_x=0\). The wave vectors for the Northern Hemisphere can therefore be simplified by representative notations in region I of Fig. 6.2 in Eqs. (18) & (19) as follows:
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\[ + k_i = \sqrt{a + \sqrt{b}} \hat{e}_i^2 - k_i^2, \quad - k_i = \sqrt{a - \sqrt{b}} \hat{e}_i^2 - k_i^2 \]  

(18)

\[ + q_i = \sqrt{a + \sqrt{c}} \hat{e}_i^2 - k_i^2, \quad - q_i = \sqrt{a - \sqrt{c}} \hat{e}_i^2 - k_i^2 \]  

(19)

FIG. 6.3. Wave vector diagram in a RSOC semiconductor. 1,2,3,4,5,6,7,8 denote the degenerate wave vectors for one energy level.

Similarly, the wave-vectors for the Northern Hemisphere can be simplified by representative notations in Eqs. (20) and (21) for region II of Fig. 6.2, as follows:

\[ + k_2 = \sqrt{a + \sqrt{c}} \hat{e}_2^2 - k_2^2, \quad - k_2 = \sqrt{a - \sqrt{c}} \hat{e}_2^2 - k_2^2 \]  

(20)

\[ + q_2 = \sqrt{a + \sqrt{c}} \hat{e}_2^2 - k_2^2, \quad - q_2 = \sqrt{a - \sqrt{c}} \hat{e}_2^2 - k_2^2 \]  

(21)

where \( a = \eta_m \frac{m}{\hbar^2}, \quad \sqrt{b} = \sqrt{\left(\frac{\eta_m}{\hbar^2}\right)^2 + \frac{2m}{\hbar^2}(E - U_{\text{eff}})} \), \( \sqrt{c} = \sqrt{\left(\frac{\eta_m}{\hbar^2}\right)^2 + \frac{2m}{\hbar^2}(E - U_{\text{eff}})} \). To solve for the electron wave function, we need to i) match the amplitude of the wave function and ii) ensure flux continuity at the delta boundary, \( x=0 \) as shown in Fig. 6.2. Equation (22) shows the matching amplitudes.

\[
\begin{pmatrix}
A^+ + B^+ \\
A^- + B^-
\end{pmatrix} = \begin{pmatrix}
A^+ + B^+ \\
C^- + D^-
\end{pmatrix}
\]  

(22)
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It is important to note here that waivfunction matching is carried out at \( k_y = 0 \) or small \( k_y \) values only compared to \( k_x \). To derive the flux continuity relation for each spin across a boundary, we integrate the time-independent 1-D (\( x \)) Schrödinger equation over a small range \([+\xi, -\xi]\) on either side of the boundary:

\[
\lim_{\xi \to 0} \left[ \int_{-\xi}^{\xi} \left( \frac{p_x^2}{2m^*} + \eta_y k_y \sigma_z \right) (\psi^+) \, dx \right] = \int_{-\xi}^{\xi} \mathcal{E} (\psi^-) \, dx
\]  

(23)

which leads to:

\[
\frac{\hbar}{2m^*} \psi^+(0) + \frac{i\lambda \eta}{2h} \psi(0) + \frac{U_n}{\hbar} \psi(0) = \frac{\hbar}{2m^*} \psi^+(0) + \frac{i\lambda \eta}{2h} \psi(0)
\]  

(24)

\[
\frac{\hbar}{2m^*} i(k_x C + k_y B) = \frac{\hbar}{2m^*} i(k_x C + k_y D) - \frac{U_n}{\hbar} (C + D)
\]  

(25)

\[
\frac{-i\hbar^2}{2m^*} \left[ \left( k_x C^* - q_x D^* \right) - \left( k_x A^* - q_x B^* \right) \right] + \eta_y \int_{-\xi}^{\xi} \left[ \frac{k_y^2 + (k_x - (\Lambda/\eta_y))^2}{k_y^2 + (k_x - (\Lambda/\eta_y))^2} \right] \psi^- \, dx = 0
\]  

(26)

Solving Eq. (26) explicitly results in the following relation in Eq. (27). This is because in the integration portion of Eq. (26) where integration is over a small region that approaches zero, the term \( \Lambda/\eta_y \) approaches infinity, making it the only finite term that still exists after the integration.

All the other terms in the integrand vanish, resulting in Eq. (27)

\[
\left( \frac{-i\hbar^2}{2m^*} \left[ \left( k_x C^* - q_x D^* \right) - \left( k_x A^* - q_x B^* \right) \right] + \left( \psi^+(0) \Lambda^2 \xi \right) \right) = 0
\]  

(27)

note that \( (\Lambda^2 \xi) \) is not 0 because \( B_y \) becomes infinitely large when the delta field is shrunk to a delta function. The wave function amplitude in region I / II are thus given by Eq. (28) and Eq. (29).

\[
\begin{bmatrix}
A^+ \\
B^+
\end{bmatrix} =
\begin{bmatrix}
q_1 + k_x + i\theta \\
k_1 + q_1 \\
k_1 - k_x - i\theta \\
k_1 + q_1
\end{bmatrix}
\begin{bmatrix}
C^+ \\
D^+
\end{bmatrix}
\]  

(28)

\[
\begin{bmatrix}
A^- \\
B^-
\end{bmatrix} =
\begin{bmatrix}
k_1 + q_1 \\
k_1 - k_x - i\theta \\
q_1 + k_x + i\theta \\
k_1 + q_1
\end{bmatrix}
\begin{bmatrix}
C^- \\
D^-
\end{bmatrix}
\]  

(29)
where $\vartheta = \left(\frac{m^*}{m_0}\right)^2 e^* g^* B_y \xi / \hbar$. Considering the transmitting wave has no reflection, the transmission probability through the delta barrier is given by:

$$T^+ = \frac{k_2}{k_1} \left| \frac{C^+}{A^+} \right|^2; T^- = \frac{q_2}{q_1} \left| \frac{C^-}{A^-} \right|^2$$  \hspace{1cm} (30)

$P$ can then be derived as follows:

$$P = \frac{T^+ - T^-}{T^+ + T^-} = \frac{q_1 k_2 |q_1 + q_2 - i\theta|^2 - k_1 q_2 |q_1 + k_2 + i\theta|^2}{q_1 k_2 |q_1 + q_2 - i\theta|^2 + k_1 q_2 |q_1 + k_2 + i\theta|^2}$$  \hspace{1cm} (31)

Inspection of Eq. (31) shows that $P$ is a function of the wave vectors, the strength of $B_y$ field, $U_{\text{eff}}$. This shows that spin-polarized current can be modulated in polarization by varying one of the above parameters. To focus on one transverse conductance mode i.e. $k_y=0$, the explicit expression for $P$ can be simplified to be:

$$P = \left( \frac{q_1 k_2 - k_1 q_2}{q_1 k_2 + k_1 q_2} \right) \left( \frac{1}{\sqrt{\eta s \frac{m^*}{\hbar^2}}} + \sqrt{\frac{E - U_{\text{eff}}}{\eta s \frac{m^*}{\hbar^2}}} \right) = \left( \frac{q_1 k_2 - k_1 q_2}{q_1 k_2 + k_1 q_2} \right) \left( \frac{1}{\sqrt{\eta s \frac{m^*}{\hbar^2}}} + \sqrt{\frac{E - U_{\text{eff}}}{\eta s \frac{m^*}{\hbar^2}}} \right)$$  \hspace{1cm} (32)

where $\sqrt{b} = \sqrt{\left(\eta s \frac{m^*}{\hbar^2}\right)^2 + \frac{2m}{\hbar^2}(E)}$, $\sqrt{c} = \sqrt{\left(\eta s \frac{m^*}{\hbar^2}\right)^2 + \frac{2m}{\hbar^2}(E - U_{\text{eff}})}$. Equation (32) shows that when $k_y=0$, $B_y$ field does not contribute to the strength of $P$ in any quantization axis (z in the corresponding new frame) for the spin-polarized current. However, for non-zero $k_y$, $B_y$ might have contribution to $P$. The important point here to note is that the application of $B_y$ plays the role of aligning the spin quantization axis closer to the y axis in the original frame as can be deduced from the eigenspinor of Eq. (3). For quantization axis closer / farther to the original y axis, spin projection in the y axis $(P_y)$ increases / decreases accordingly, providing a means for spin-polarized current modulation in the y axis. Therefore, for zero or non-zero $k_y$, $B_y$ strength can be manipulated to control $P_y$. In this system, the switching of $B_y$ field also switches the $P$ of spin-polarized current in y, providing the required feature of nonvolatile memory.
6.3.3 Theoretical advantage

Our derivations reveal significant advantages for in-plane fields as opposed to the out-of-plane fields of Refs. 1-6. First of all, with the in-plane delta $B_y$ fields, applying multiple magnetic barriers or increasing the strength of $B_y$ increases the spin-polarized current in $y$ direction without lowering the probability of electron transmission across the barriers as had been previously discussed in Refs. 20, 21, 22, 23. This is because in the case of the in-plane field, the magnetic vector potentials of $A_z$ have been eliminated from the transmission energy equations of Eq. (12); whereas in the out-of-plane field, $A_z$ is coupled to $k_y$ in the energy equations, resulting in additional energy cost to the total available energy for electron transmission.

It has been suggested in chapters 3 and 4 that the zero-gauge [20,21,22,23] type of field configurations should be used in the case of perpendicular fields, which implies that to achieve a high net $P$ of spin-polarized current at reasonably high conductance, more barriers or $B_z$ of greater strength would be required. This would render the device less suitable for small cell, high density application like memory. In our work, the elimination of $A_z$ from the energy equation means that using higher $B_y$ fields or multiple delta field barriers with the strength of $B_y$ each to increase $P$ of spin-polarized current would thus not result in lower device conductance. Furthermore, since the device is ballistic, it is necessary to ensure that the electron path between source and drain is smaller than the spin relaxation length associated with the spin orbit mechanism. Previous works involving the vertical delta magnetic fields have not considered the Dy’akonov [24,25] source of spin relaxation, and may have overestimated $P$ that can be achieved. By contrast, if we use a delta-function $B_y$ field, the transformation of spin operator and its eigenspinor due to the in-plane spin orbit field only involves the azimuthal angle. The transformed spin state will still have a component in the $y$ direction. The Dy’akonov spin relaxation mechanism is thus greatly reduced.

The use of in-plane field generates spin-polarized current with a net $P$ value in the quantization
axis that is a function of the Rashba spin orbit effect, and the electric potential, but not the delta field strength (in the case of \(k_y=0\)). However, as delta B field aligns quantization axis across the azimuthal angle in the 2DEG plane, the delta field strength contributes to \(P\) value in the y or x axis of the original frame. The availability of more parameters for the manipulation of spin-polarized current implies that such system is suitable for device applications.

**6.4 Conclusion**

We have conceived and derived equations that describe spin-dependent transport within a 2DEG in the ballistic regime under the influence of in-plane magneto-electric barriers and conduction band spin orbit coupling. The use of in-plane fields eliminates the need for the zero-gauge barriers that requires many barriers to generate high \(P\) at high device conductance. The active device length can thus be greatly reduced, making it easier to achieve the ballistic condition assumed in the calculations. In contrast to electron transport across a 2DEG with an out-of-plane field \(B_z\) (original frame), in which the SOC coupling has a detrimental effect on the \(P\) value of spin-polarized current, we have theoretically shown that spin-polarized current induced by the in-plane field is resistant to the Dy’akonov scattering effects.

**REFERENCES**


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Chapter 7

Spin coupling to continuous magnetic field

7.1 Introduction

It has been discussed in chapter 3 that wave vector coupling to delta magneto-electric [1,2] barriers has been utilized to model ballistic, spin-polarized current across the 2DEG of a HEMT type device. In more realistic models, wave-vector coupling to both crystal fields (Dresselhaus or Rashba) and delta magneto-electric barriers have also been discussed in some parts of chapters 5 and 6 [3,4,5,6]. It has also been proposed that crystal fields can be tuned to resonantly enhance spin polarization of current in the transistor device [7,8]. However, delta magnetic field is an ideal conception that cannot be fully implemented. The periodic spacing of multiple barriers that has been proposed to increase spin polarization [9,10,11,12], including the zero-gauge type requires long device gate length. Simulation results in chapters 3, 5 have also shown that spin polarized current induced by this method vary in polarization strength with energy, i.e. polarization is not usually constant over a wide energy range. This implies that careful device optimization would be needed to ensure high spin-polarization occurs at and around the Fermi energy.

In this chapter, we conceive that it would be important to also analyze electron transport under the influence of continuously distributed magnetic fields [13,14,15,16] (non-delta) in which electron spin is coupled to both the crystal and the continuously-distributed, external magnetic fields applied perpendicular (z) to a 2DEG plane. The main difference here is that in continuous magnetic fields, electrons trace circular motions and form Landau levels. Analysis in this chapter is focused on spin-dependent conductance within the framework of combined Landau and spin
orbit coupling effects. Previous models of magneto-electron transport under the influence of continuously distributed perpendicular magnetic fields had not been discussed in the context of ballistic transport. It remains unclear if spin-polarized current can be generated in the ballistic regime as theoretical analysis shows that total current $j_x$, remains zero in the absence of cross electric field. The spin polarization of current in specific axis and its manipulation by electrical means has also not been discussed.

7.2 Theoretical model

7.2.1 Eigenfunctions

In our work, we derived a ballistic transport model that couples electron spin to the crystal field, magnetic field, and transverse (cross) electric field, $E_y$. Cross magnetic electric field is applied to a III-V semiconductor 2DEG system. The relativistic effects [17,18] of electron traveling in the crystal and external field give rise to the effect of spin orbit coupling in the conduction band as shown in the Dirac equation. This system can therefore be considered in the form of a Zeeman and Dirac-term perturbation to a minimal-coupling type of cross magneto-electric field system with the Landau eigenfunctions serving as the basis functions for the perturbed system. The wave functions of the perturbed system is therefore a linear combination of Hermite functions. The Dirac-term perturbation includes the Rashba, Dresselhaus and transverse E-field effects as shown in Eq. (1). The Zeeman perturbation is a constant independent of space-time dynamics. The Dirac spin orbit coupling effects can be described in a 2x2 Hamiltonian with the Pauli matrices serving as the basis matrices. Relativistic effect due to the external $E_y$ is only presented for reference as its effect on spin-polarized current generation is minimal.
The gauge modification of the momentum operator, $k$, is derived through a Legendre transformation of the Lagrangian similar to earlier discussions in chapter 3. The Landau gauge of $(A_y, 0, 0) = (-By, 0, 0)$ is used for the above derivations of Eq. (1):

$$\left[ H_L + eE_y + g\mu B + vE_y (k_y + \frac{e}{\hbar}A_y) - (\alpha + i\beta)k_y - (\beta - i\alpha)(k_y + \frac{e}{\hbar}A_y) \right] \sum_{n} \varphi_n a_n^+ = \xi_n \sum_{n} \varphi_n a_n^- $$

(1)

where $\alpha$ is the Rashba constant, $\beta$ is the Dresselhaus constant, $A_y$ is the magnetic vector potential, $k_y$ is the transverse wave vector, $B$ is the perpendicular magnetic field, $H_L$ is the Hamiltonian for electron in $B$ field, $\mu$ is the Bohr magnetron, $g$ is the $g$ factor, $v$ is the coefficient in the Dirac term. $a_n^+$ is the up/down spin component of the eigenspinor. The conduction band wave function of the cross magnetic-electric, spin orbit coupling system that corresponds to energy eigenvalue $\xi_n$ is:

$$\psi_n = \sum_{n} \varphi_n (y - y_0) \begin{pmatrix} a_n^+ \\ a_n^- \end{pmatrix} \varphi(x) $$

(2)

Equation (1) is simplified to produce Eqs. (3) and (4) as follows:

$$\left[ H_L + eE_y + g\mu B + vE_y (k_y + \frac{e}{\hbar}A_y) - \xi_n \right] \sum_{n} \varphi_n a_n^+ + \left[ - (\alpha + i\beta)k_y - (\beta - i\alpha)(k_y + \frac{e}{\hbar}A_y) \right] \sum_{n} \varphi_n a_n^- = 0 $$

(3)

$$\left[ i\alpha \left( \frac{\partial}{\partial y} + (k_y + \frac{e}{\hbar}A_y) \right) + \beta \left( \frac{\partial}{\partial y} - (k_y + \frac{e}{\hbar}A_y) \right) \right] \sum_{n} \varphi_n a_n^+ + \left[ H_L + eE_y + g\mu B + vE_y (k_y + \frac{e}{\hbar}A_y) - \xi_n \right] \sum_{n} \varphi_n a_n^- = 0 $$

(4)

Equation (4) can be simplified to Eq. (5), using the substitutions of: $k_y = y_0 / r^2$, $A_y = -By$, where $r^2 = \hbar / eB$, $y_0 = l_0 - eE_y / mw^2$, $w = eB / m$ is the cyclotron frequency, $y_0$ is the cyclotron center in the
Spin characteristics of electron transport in semiconductor presence of $E_y$. $l_0$ is the cyclotron center in the absence of $E_y$. The harmonic oscillator potential for $H_L$ is $U_L(x) = 1/2m\omega^2(x - l_0)^2$. In the presence of the cross electric field of $E_y$, the harmonic oscillator potential for $H_c = H_L + eE_y y$ is $U_c(x) = 1/2m\omega^2(x - y_0)^2$.

$$
\left[ H_L + eE_y + g\mu_B + uE_x, \left( \frac{y_0}{r} - \frac{eBy}{\hbar} \right) - \xi_n \right] \sum_n \varphi_n a_n^* + \left[ \frac{i\alpha}{\hbar} \frac{\partial}{\partial y} \left( \frac{y_0}{r} - \frac{eBy}{\hbar} \right) - \beta \left( \frac{\partial}{\partial y} + \left( \frac{y_0}{r} - \frac{eBy}{\hbar} \right) - \xi_n \right] \sum_n \varphi_n a_n^* = 0
$$

(5)

Here, we examine the cross electric magnetic Hamiltonian of $H_c \equiv H_c + eE_y y$ in Eq. (6) first without considering the spin orbit coupling terms. The purpose is to find the eigensolutions of $H_c$ so that we can use these solutions as basis solutions for the total Hamiltonian that comprises cross electric magnetic and spin orbit coupling terms.

$$
(H_c) \varphi(y) \varphi(x) \equiv \left( \frac{\hbar^2 (k_x^2 - e/h)By^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + eE_y y \right) \varphi(y) \varphi(x)
$$

(6)

Using $w = eB/m$, Eq. (6) can be expanded and then simplified as shown in Eq. (7)

$$
\left( -\frac{\hbar^2}{2m} \varphi''(y) + \left( \frac{\hbar^2 k_x^2}{2m} - \hbar w k_x y + \frac{1}{2}m\omega^2 y^2 + eE_y y \right) \varphi(y) \right) \varphi(x)
$$

$$
\equiv \left( \frac{-\hbar^2}{2m} \varphi''(y) + \frac{1}{2}m\omega^2 (y - l_0)^2 \varphi(y) + eE_y y \varphi(y) \right) \varphi(x)
$$

(7)

where $l_0 = \hbar k_\perp / eB$, $y_0 = l_0 - eE_x / m\omega^2$, $V(E_y) = 1/2m\omega^2(l_0 - y_0)^2$. The $n^{th}$ eigenvalue of Eq.(7) is $(n + 1/2)\hbar \omega$. Its $n^{th}$ eigenfunction is the usual harmonic oscillator function of degree $n$, which also represents a $n^{th}$ level Hermite function as shown explicitly in Eq. (8)
\[ \varphi_s(y - y_0) = \exp\left(-\frac{|y - y_0|^2}{2r^2}\right) \frac{H_s\left(\frac{y - y_0}{r}\right)}{\sqrt{\pi} 2^s s! r} \] (8)

The set \( \left\{ H_s\left(\frac{y - y_0}{r}\right) \right\} \) is mutually orthogonal [13] in a weighted Sobolev space, i.e.

\[ \int_{\Lambda} H_n(y) H_m(y) \exp(-x^2) dx = c_n \delta_{n,m} \] (9)

where \( \Lambda = \{ x | -\infty < x < \infty \} \), \( c_n = 2^n n! \sqrt{\pi} \). The oscillator Hermite function of degree \( n \) can also be defined by:

\[ \varphi_s(y - y_0) = \exp(-x^2/2) H_s(y - y_0) \] (10)

Considering the total Hamiltonian now, we rearranged Eq. (5) and obtained Eq. (11)

\[ \begin{align*}
\left[ H_L + eE_y y + g\mu_B y - vE_y \left(\frac{y - y_0}{r}\right) - \xi_n \right] \sum_{i} \varphi_n a_n^{+} &+ \left( i\alpha \left( \frac{\partial}{\partial y} + \frac{y - y_0}{r^2} \right) - \beta \left( \frac{\partial}{\partial y} - \frac{y - y_0}{r^2} \right) \right) \sum_{i} \varphi_n a_n^{-} \\
\left( i\alpha \frac{\partial}{\partial y} - \frac{y - y_0}{r^2} \right) + \left( \frac{\partial}{\partial y} + \frac{y - y_0}{r^2} \right) \sum_{i} \varphi_n a_n^{+} &+ \left[ H_L + eE_y y - g\mu_B + vE_y \left(\frac{y - y_0}{r^2}\right) - \xi_n \right] \sum_{i} \varphi_n a_n^{-} = 0
\end{align*} \] (11)

Equation (11) is further simplified by substituting \( H_c \equiv H_L + eE_y y \) and \( Y = (y - y_0)/r \) and we obtained Eq. (12)

\[ \begin{align*}
\left[ H_c + g\mu_B - \frac{vE_y}{r} Y - \xi_n \right] \sum_{i} \varphi_n a_n^{+} &+ \left( i\alpha \left( \frac{\partial}{\partial Y} + Y \right) - \beta \left( \frac{\partial}{\partial Y} - Y \right) \right) \sum_{i} \varphi_n a_n^{-} \\
\left( i\alpha \frac{\partial}{\partial Y} - Y \right) &+ \left( \frac{\partial}{\partial Y} + Y \right) \sum_{i} \varphi_n a_n^{+} + \left[ H_c - g\mu_B + \frac{vE_y}{r} Y - \xi_n \right] \sum_{i} \varphi_n a_n^{-} = 0
\end{align*} \] (12)

The Hermite spectral method [12, 19] is then used to transform Eq. (12) to a more solvable form. The Hermite spectral identity of

\[ 2x\varphi_n = -\varphi_{n+1} - 2n\varphi_{n-1} \] (13)
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results in

\[ \sum_{n=0}^{\infty} a_n (2n \varphi_n) = - \sum_{n=0}^{\infty} a_n (\varphi_{n+1} + 2n \varphi_{n-1}) \] which can also be written as

\[ P_{xv}(x) = - \{1/2 \sum_{n=0}^{\infty} a_n (\varphi_{n+1} + 2n \varphi_{n-1}) \}, \] where \( x \) is an arbitrary parameter, and \( P_{xv}(x) \equiv \sum_{n=0}^{\infty} a_n \varphi_n(x) \). Using

\[
\int_A \varphi_n(x) \varphi_n(x) dx = c_n \delta_{n,m}
\]

of Eq. (9), it follows that:

\[
\int_A \varphi_n (P_{xv}(x)) dx = - \int \varphi_n \sum_{n=0}^{\infty} \left( \frac{a_n}{2} \varphi_{n+1} + n a_n \varphi_{n-1} \right)
\]

\[
= - \frac{a_{n+1}}{2} - (n+1)a_{n+1}
\]

The other Hermite spectral identity of

\[ \partial_x \varphi_n = n \varphi_{n+1} - (1/2) \varphi_{n+1} \]

results in

\[ \partial_x P_{xv}(x) = \sum_{n=0}^{\infty} (n+1)a_{n+1} \varphi_n - (1/2) \sum_{n=1}^{\infty} a_{n-1} \varphi_n \].

It follows that

\[
\int \varphi_n (\partial_x P_{xv}(x)) dx = \int \varphi_n \sum_{n=0}^{\infty} (n+1)a_{n+1} \varphi_n - (1/2) \sum_{n=1}^{\infty} a_{n-1} \varphi_n \] dx

\[
= (n+1)a_{n+1} - (1/2)a_{n+1}
\]

Combining Eq. (14) and Eq. (16) results in Eqs. (17) and (18), i.e.

\[
- \int \varphi_n (\partial_x P_{xv}(x)) dx - \int \varphi_n (P_{xv}(x)) dx = -2(n+1)a_{n+1}
\]

\[
- \int \varphi_n (\partial_x P_{xv}(x)) dx + \int \varphi_n (P_{xv}(x)) dx = -a_{n+1}
\]

Using Eqs. (17) and (18) and rule \( \int \varphi_n(x) \varphi_m(x) dx = c_n \delta_{n,m} \), Eq. (12) can be transformed to Eq. (19) below by performing \( \int \varphi_n(x) M dx \) where M is the single column matrice of Eq. (12).

\[
\begin{bmatrix}
\left( (n+\frac{1}{2}) \hbar \omega + V(E_i) + g \mu B - \xi \right) a_n^+ + \frac{\alpha}{r} E_i \left( a_n^+ + (n+1)a_{n+1}^+ \right) + \frac{2i \epsilon}{r} (n+1)a_{n+1}^+ - \frac{d}{r} a_{n+1}^+
\end{bmatrix} = 0
\]

\[\frac{i \alpha}{r} a_{n+1}^+ + \frac{2 \beta}{r} (n+1)a_{n+1}^+ + \left( (n+\frac{1}{2}) \hbar \omega + V(E_i) - g \mu B - \xi \right) a_n^+ - \frac{\alpha}{r} E_i \left( a_n^+ + (n+1)a_{n+1}^+ \right)\]
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In narrow-gap semiconductor, the Dresselhaus effect can be neglected \((\beta\sim 0)\) compared to the Rashba. The relativistic effect due to external \(E_y\) field is also negligible \((\nu\sim 0)\) compared to conduction band spin orbit coupling because of low \(E_y\) field. However, it’s possible to increase \(E_y\) field by applying large voltage across device with very small lateral thickness. In this analysis, we assume the existence of the Rashba spin orbit coupling only. The approximated form of Eq.(19) is:

\[
\left[ \left( n + \frac{1}{2} \right) \hbar \omega + V(E_x) + g \mu B - \xi_n \right] a_{n+1}^* + \frac{2i\alpha}{r} (n+1) a_{n+1}^- = 0
\]

\[
\frac{ia}{r} a_{n+1}^* + \left( n + \frac{1}{2} \right) \hbar \omega + V(E_x) - g \mu B - \xi_n \right] a_{n}^-
\]

Row 1 of Eq. (20) shows relationship type (1) between \(a_{n+1}^-\) and \(a_{n+1}^*\), while row 2 of Eq. (15) shows relationship type (2) between \(a_n^-\) and \(a_{n-1}^-\). (1) and (2) are two independent relationships. Therefore row 1 of Eq. (20) should also show relationship type (1) between \(a_n^-\) and \(a_{n-1}^-\). This essentially means that Eq. (20) can be transformed by substituting \(n\) with \(s-1\) for row 1 and \(n\) with \(s\) for row 2 as shown below. In summary, Eq. (20) only shows relationship between 2 neighboring terms, but it cannot tell which terms should exist for a particular energy level. Equation (21) is resulted from Eq.(20) after the following substitution:

\[
n \rightarrow s-1 \text{ row 1} \\
n \rightarrow s \text{ row 2}
\]

\[
\left[ \left( s - \frac{1}{2} \right) \hbar \omega + V(E_x) + g \mu B - \xi_s \right] a_s^* + \frac{2i\alpha}{r} (s) a_s^- = 0
\]

\[
\frac{ia}{r} a_s^* + \left( s + \frac{1}{2} \right) \hbar \omega + V(E_x) - g \mu B - \xi_s \right] a_s^-
\]

Solving the infinite sets of equations described in Eq. (21) is equivalent to solving the following eigenequation of Eq. (22):

\[
\begin{bmatrix}
\left( s - \frac{1}{2} \right) \hbar \omega + V(E_x) + g \mu B \\
\frac{ia}{r}
\end{bmatrix}
\begin{bmatrix}
\left( s + \frac{1}{2} \hbar \omega + V(E_x) - g \mu B \right) + \frac{2i\alpha}{r} (s)
\end{bmatrix}
\begin{bmatrix}
a_{s-1}^- \\
a_{s-1}^*
\end{bmatrix}
= \xi_s
\begin{bmatrix}
a_{s-1}^- \\
a_{s-1}^*
\end{bmatrix}
\]

\[
\begin{bmatrix}
a_{s-1}^- \\
a_{s-1}^*
\end{bmatrix}
= \left[ \frac{1}{2} \right] \begin{bmatrix}
\left( s - \frac{1}{2} \right) \hbar \omega + V(E_x) + g \mu B \\
\frac{ia}{r}
\end{bmatrix}
\begin{bmatrix}
\left( s + \frac{1}{2} \hbar \omega + V(E_x) - g \mu B \right) + \frac{2i\alpha}{r} (s)
\end{bmatrix}
\begin{bmatrix}
a_{s-1}^- \\
a_{s-1}^*
\end{bmatrix}
= \xi_s
\begin{bmatrix}
a_{s-1}^- \\
a_{s-1}^*
\end{bmatrix}
\]
Therefore, solving Eq. (1) is equivalent to solving Eq. (22). To determine arbitrary \( N \) with respect to \( s \), it is important to determine the first energy level \( (E_i) \) and the first sub-band wave function that corresponds to \( s=0 \), by inspecting Eq. (22) which leads to Eq. (23)

\[
\frac{(s - \frac{1}{2})\hbar \omega + V(E_i) + g \mu B - \xi_n}{i \alpha \over r} = \frac{-2i \alpha s}{r} - \left( (s + \frac{1}{2})\hbar \omega + V(E_i) - g \mu B - \xi_n \right)
\]

It is thus clear that Eq. (24) is resulted from choosing \( s=0 \), and \( a_{s+1}^* = 0 \).

\[
\left( \frac{1}{2} \hbar \omega + V(E_i) - g \mu B \right) a_s^* = \xi_s a_s \quad \text{or} \quad \xi_{s+1} = \left( \frac{1}{2} \hbar \omega + V(E_i) - g \mu B \right)
\]

Thus the sub-band wave function is \( \psi_s = \phi_0 \begin{bmatrix} 0 \\ a_s^* \end{bmatrix} \). For \( s=1,2,3,\ldots \), Eq.(23) leads to Eq. (25)

\[
\xi_s^* = \sqrt{s \hbar \omega + V(E_i) \pm \sqrt{\xi_o^2 + 2s \left( \frac{\alpha}{r} \right)^2}}
\]

where \( \xi_{s+1} = (\xi_o + V(E_i)) \) and \( \xi_s = \frac{1}{2} \hbar \omega - g \mu B \). It is worth noting that \( N=1 \) corresponds to \( s=0 \), and \( s=1,2,3,\ldots \) corresponds to \( N=2,3,4,\ldots \) respectively. Equation (22) shows that for each value of \( s \), there are two energy levels: the (+) branch and the (-) branch. The eigenfunctions can be found by substituting the eigenvalues into Eq. (22). The eigenfunctions are:

\[
\begin{bmatrix} a_{s+1}^* \\ a_s^* \end{bmatrix} \equiv N_i \begin{bmatrix} A_s^* \\ 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a_{s+1}^- \\ a_s^- \end{bmatrix} \equiv N_i \begin{bmatrix} 1 \\ A_s^- \end{bmatrix}
\]

This is derived from solving Eq. (22) explicitly, and choosing \( N_i \) for \( a_s^- \) and solving for \( a_{s+1}^* \) in the (+) branch case and choosing \( N_i \) for \( a_{s+1}^* \) and solving for \( a_s^- \) in the (-) branch case. \( A_s^* \) and \( A_s^- \) are given by Eq. (27).

\[
A_s^* = \frac{2i \alpha s / r}{\xi_s + \sqrt{\xi_s^2 + 2s \left( \frac{\alpha}{r} \right)^2}} = i M_s^*; \quad A_s^- = \frac{i \alpha / r}{\xi_s + \sqrt{\xi_s^2 + 2s \left( \frac{\alpha}{r} \right)^2}} = i M_s^-
\]

The final form of the wave function for the (+) / (-) branches are:
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\[
\psi_+^{(y-y_0)}(x-x_0) = e^{i\phi_{+}N_{+}} \left( A_+ \varphi_{+,+}(x-x_0) \right)
\]

\[
\psi_-^{(y-y_0)}(x-x_0) = e^{i\phi_{-}N_{-}} \left( A_- \varphi_{-,+}(x-x_0) \right)
\]

(28)

where \( N_{+}, N_{-} \) are the normalization constants for wave function branch (+), (−), respectively.

The normalization constants of \( N_{+} \) and \( N_{-} \) for wave functions (+) and (−) branches, respectively of Eq. (28) can be found in the following way:

\[
N_{+} = \left( A_{+} \varphi_{+,+} \right) \sqrt{\varphi_{+,+}^2 + \varphi_{-+}^2}
\]

(29)

\[
N_{-} = \left( \varphi_{-,+} \right) \sqrt{\varphi_{-,+}^2 + \varphi_{-,+}^2}
\]

(30)

7.2.2 Spin-polarized current

Current in a 2DEG system with Rashba spin orbit coupling in the absence of external magnetic-electric fields can be derived as below:

\[
j_s = \frac{1}{2} \left[ \psi^*(a^+ b^+) \psi(a b) - \psi(a b) \psi^*(a^+ b^+) \right]
\]

(31)

where \( v_s \) is the electron velocity that can be found using the Hamilton equation that provides the first momentum derivative of the Hamiltonian matrix, i.e. \( v_s = \partial H / \partial p_s \). Using the RSOC eigenspinor derived in chapter 6, and further simplifying Eq. (31) leads to the following:

\[
j_s = \frac{1}{2} \left[ \psi^*(a^+ b^+) \psi(a b) - \psi(a b) \psi^*(a^+ b^+) \right]
\]

(32)

\[
j_s = \frac{1}{2} \left[ \psi^*(a^+ b^+) \psi(a b) - \psi(a b) \psi^*(a^+ b^+) \right]
\]

(33)
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\[ j_x = \frac{1}{2\hbar} \begin{pmatrix} a^* & e^{i\alpha} \frac{h^2 k_x}{m} + i \frac{e d}{h}\frac{\hbar^2 k_x}{m} \gamma \end{pmatrix} - \begin{pmatrix} a & -e^{i\alpha} \frac{h^2 k_x}{m} \gamma \end{pmatrix} \psi^\dagger \psi \] \quad (34)

Expanding Eq. (34) leads to Eqs. (35)

\[ j_x = \frac{1}{2\hbar} \left( \frac{h^2 k_x}{m} \left| a \right|^2 + \left| b \right|^2 + i \frac{e d}{h} \frac{\hbar^2 k_x}{m} \gamma \right) \] \quad (35)

\[ j_x = \frac{1}{\hbar} \left( \frac{h^2 k_x}{m} \left| a \right|^2 + \left| b \right|^2 \right) + 2i e \text{Im}(a \gamma b) \]  
\[ j_x = \frac{\hbar k_x}{m} \left| a \right|^2 + \left| b \right|^2 \right) - \frac{2}{\hbar} e \text{Im}(a \gamma b) \]

Taking the RSOC eigenvectors of \( \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm k_y + ik_x \\ k \end{pmatrix} \) which has been found in chapter 5,6, the (+) and (−) current can be found. The (+) / (−) current are:

\[ j_x^+ = \frac{\hbar k_x}{m} + \frac{2}{\hbar} \frac{e}{k} \] \quad (36)

For \( k_y = 0 \) then the (+) / (−) current are:

\[ j_x^+ = \frac{\hbar k_x}{m} + \frac{2}{\hbar} \alpha \] \quad (37)

Equations (36) and (37) clearly show the polarization of current in a RSOC 2DEG system. It is important to note that it has been shown in standard derivations that in the presence of perpendicular magnetic field, in-plane current \( j_x \) has a zero average value because of the cyclotron motion of the electrons as illustrated by Eq. (38) below:

\[ j_x = -\frac{\hbar}{2m} \left( \psi_x^* \frac{\partial \psi_x}{\partial x} - \psi_x \frac{\partial \psi_x^*}{\partial x} \right) = w \gamma L \psi_x \psi_x^* \rightarrow \langle j_x \rangle = 0 \] \quad (38)

It would therefore be of interest to study the current and its spin polarization in a 2DEG system with RSOC and cross electric magnetic fields where current is:
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\[ j_z = \frac{1}{2\hbar} \begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} \frac{\hbar^2(k_x + \frac{e}{h} A_y)}{m} a + i\alpha b \\ -i\alpha a + \frac{\hbar^2(k_x + \frac{e}{h} A_y)}{m} b \end{pmatrix} - (a) \begin{pmatrix} \frac{\hbar^2(k_x + \frac{e}{h} A_y)}{m} a^* + i\alpha b^* \\ -i\alpha a^* + \frac{\hbar^2(k_x + \frac{e}{h} A_y)}{m} b^* \end{pmatrix} \]  

(39)

\[ j_z = \frac{1}{2h} \left[ \frac{h^2(k_x + \frac{e}{h} A_y)}{m} \left| \psi^2 \right|^2 - 4\alpha \text{Im}[a^* b] \right] \]

(40)

\[ j_z = \left[ \frac{h(k_x + \frac{e}{h} A_y)}{m} \left| \psi^2 \right|^2 - 2\frac{\hbar}{\alpha} \text{Im}[a^* b] \right] \]

(41)

Note that the choice of gauge might present slightly different results as there are two common gauges associated with a \( B_z \) field, i.e. \((-A_y, 0, 0)\) or \((0, A_y, 0)\). In this case the \((-A_y, 0, 0)\), or \((-By, 0, 0)\) is chosen. Remember that \( \lambda_0 = \frac{\hbar k_z}{eB} \) because of the gauge \((-By, 0, 0)\) whereas \( \gamma_0 = \lambda_0 - \frac{eE_y}{m\omega} \) for both gauges stated above. Therefore current is:

\[ j_z = \left[ w_{\lambda_0} - \frac{eB_y}{m} - \frac{2\hbar}{\alpha} \text{Im}[a^* b] \right] \]

\[ j_z = \left[ w(\gamma_0 + \frac{eE_y}{m\omega} - w) + \frac{2\hbar}{\alpha} \text{Im}[a^* b] \right] \]

\[ j_z = \left[ w\gamma_0 + \frac{eE_y}{m\omega} \right] - \frac{2\hbar}{\alpha} \text{Im}[a^* b] \]

\[ j_z = \left[ w(y - \gamma_0) - \frac{E_y}{B} + \frac{2\hbar}{\alpha} \text{Im}[a^* b] \right] \]

(42)

where \( a / b \) is the spin up/down component of the eigenspinor. In the presence of SOC, the (+) / (-) branch current can be obtained by substituting the eigenspinor components into Eq. (26) and Eq. (42). The (+) / (-) current is then shown in Eqs. (43) and (44).

\[ j_z^+ = \left[ w(y - \gamma_0) - \frac{E_y}{B} \right] + \frac{2\hbar}{\alpha} \text{Im} \left[ M_{\phi,\phi'}^* \phi_{\phi'} + \phi_{\phi'}^* \phi_{\phi'} \right] \]

(43)

\[ j_z^- = \left[ w(y - \gamma_0) - \frac{E_y}{B} \right] + \frac{2\hbar}{\alpha} \text{Im} \left[ M_{\phi,\phi'}^* \phi_{\phi'} + \phi_{\phi'}^* \phi_{\phi'} \right] \]

(44)
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Current in the presence of spin orbit coupling effects and $E_y$ field can be found by the flux equation of $j_z = 1/2\langle \psi | v_z | \psi \rangle$. As the average of $w(y-y_0)$ across the cyclotron radius is zero, the average $(+)$ / $(-)$ current is thus the base value of $(E_y/B)$ plus / minus an additional current term of $2\alpha N_{1,2} M_x \phi_{+1,1} \phi / h$ as shown in Eqs. (43) and (44), respectively. This results in spin polarization of current in the $(+)$ / $(-)$ quantization axis in which the eigenspinors of Eq. (27) (not $[1\ 0]$ and $[0\ 1]$) are the basis eigenspinors. It is worth noting that the application of $E_y$ is essential as it provides a base value for the average current in the form of $(E_y/B)$. This ensures that there would be an average current even when all the SOC effects are absent. We have thus shown analytically, in the RSOC 2DEG system with cross electric magnetic field that current is spin polarized. The application of $E_y$ provides an electrical means to manipulate the polarization ratio of the spin-polarized current.

7.2.3 Spin density matrix

In this section, we will describe briefly the concepts of polarization in spin theory. The density matrix method can be used to deduce the polarization of electron in $x$, $y$, or $z$, for the wave functions of $(+)$ and $(-)$ branches derived in Eq. (26). The density matrix is shown in Eq. (45):

\[
\rho(x) = |x\rangle\langle x| = |x\rangle
\]

where $|x\rangle = c_1|1\rangle + c_2|2\rangle$ is an arbitrary spin state expressed in the basis eigenspinors of $|1\rangle$ and $|2\rangle$ that represent up and down states, respectively. Using Eq. (45), it follows that $\rho(c_1|1\rangle + c_2|2\rangle) = |x\rangle$.

Base on this the following can be derived:

\[
\langle 1 | \phi_{+1,1} + \langle 1 | \phi_{+2,2} = \langle 1 | x\rangle = c_1
\]

\[
\langle 2 | \phi_{-1,1} + \langle 2 | \phi_{-2,2} = \langle 2 | x\rangle = c_2
\]

The matrix representation of the density operator is:
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\[
\begin{bmatrix}
\langle 1 | \rho | 1 \rangle & \langle 1 | \rho | 2 \rangle \\
\langle 2 | \rho | 1 \rangle & \langle 2 | \rho | 2 \rangle
\end{bmatrix}
= \begin{bmatrix}
c_1 \\
c_2
\end{bmatrix}
\]  
(48)

The density matrix can also be written in the following ways:

\[
\begin{bmatrix}
\langle 1 | \rho | 1 \rangle & \langle 1 | \rho | 2 \rangle \\
\langle 2 | \rho | 1 \rangle & \langle 2 | \rho | 2 \rangle
\end{bmatrix}
= \begin{bmatrix}
c_1 c_1^* & c_1 c_2^* \\
c_2 c_1^* & c_2 c_2^*
\end{bmatrix}
= \begin{bmatrix}
\rho_{11} & \rho_{12} \\
\rho_{21} & \rho_{22}
\end{bmatrix}
\]  
(49)

From the density matrix, we will proceed to find the spin polarization of an arbitrary spin state.

The spin polarization in x, y, and z are given by the first three of Eqs. (50).

\[
P_x = \langle \chi | S_x | \chi \rangle = \frac{1}{2} \hbar (c_1 c_1^* - c_2 c_2^*) = \rho_{11} - \rho_{22}
\]

\[
P_y = \langle \chi | S_y | \chi \rangle = \frac{i}{2} \hbar (c_1 c_2^* - c_2 c_1^*) = i(\rho_{12} - \rho_{21})
\]

\[
P_z = \langle \chi | S_z | \chi \rangle = \frac{1}{2} \hbar (c_1 c_1^* + c_2 c_2^*) = \rho_{11} + \rho_{22}
\]  
(50)

The density matrix of Eq. (49) can also be written in the following way in Eq. (50)

\[
\rho = \begin{bmatrix}
c_1 c_1^* & c_1 c_2^* \\
c_2 c_1^* & c_2 c_2^*
\end{bmatrix}
= \begin{bmatrix}
\rho_{11} & \rho_{12} \\
\rho_{21} & \rho_{22}
\end{bmatrix}
= \frac{1}{2} \begin{bmatrix}
1 + P_x & P_x - iP_y \\
P_x + iP_y & 1 - P_x
\end{bmatrix}
\]  
(51)

Expanding Eq. (51) results in Eq. (52)

\[
\rho = \frac{1}{2} \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
+ \begin{bmatrix}
0 & P_x \\
P_x & 0
\end{bmatrix}
+ \begin{bmatrix}
0 & -iP_y \\
iP_x & 0
\end{bmatrix}
+ \begin{bmatrix}
P_z & 0 \\
0 & -P_z
\end{bmatrix}
\]  
(52)

The electron in this system can be in a mixed state of:

\[
| \Psi^+ \rangle \langle \Psi | = P_a | \Psi^{(+)} \rangle \langle \Psi^{(+)} | + P_b | \Psi^{(-)} \rangle \langle \Psi^{(-)} |
\]  
(53)

where $| \Psi^{(+)} \rangle$ is the (+) branch state and $| \Psi^{(-)} \rangle$ is the (-) branch state and $P_a$ and $P_b$ are the probability of electrons being in state $| \Psi^{(+)} \rangle$ and state $| \Psi^{(-)} \rangle$, respectively.
7.3 Transverse spin polarization and electric fields

In this section, we calculated $P_y$, $P_x$, and $P_z$ at a fixed $y$ location as $E_y$ increases even though increasing $E_y$ shifts the cyclotron center, $y_0$ increasingly in $y$. Therefore $P_y$, $P_x$, and $P_z$ are actually detected at different radial distance with respect to the cyclotron center. The wave functions of Eq. (28) can be written for the (+) branch in Eq. (53), and (-) branch in Eq. (54).

$$\psi_+(y-y_0) = e^{i\theta_+} \left( \frac{iM_y \varphi_{-1}}{\sqrt{(M_y \varphi_{-1})^2 + \varphi^2}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) + \frac{\varphi_z}{\sqrt{(M_z \varphi_{-1})^2 + \varphi_z^2}} \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \right)$$ (53)

$$\psi_-(y-y_0) = e^{i\theta_-} \left( \frac{\varphi_{-1}}{\sqrt{\varphi_{-1}^2 + (M_y \varphi_z)^2}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) + \frac{-iM_y \varphi_z}{\sqrt{(M_z \varphi_{-1})^2 + \varphi_z^2}} \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \right)$$ (54)

Figure 7.1 shows that $P_y$ variation with $E_y$ for the (+) wave function is the sign inverse of that for the (-) wave function. The two curves cancel one another resulting in a net small value of $P_y$. It is assumed here that electron has equal probability of assuming the (+) branch or the (-) branch.

$$P_y^+ = \frac{1}{2\hbar} \left( \frac{2i(M_y \varphi_{-1})\varphi_z}{(M_y \varphi_{-1})^2 + \varphi_z^2} \right)$$ (55)

$$P_y^- = \frac{1}{2\hbar} \left( \frac{-2i(M_y \varphi_z)\varphi_{-1}}{\varphi_{-1}^2 + (M_y \varphi_z)^2} \right)$$ (56)

In the case of $P_x$, its value is zero for both (+) or (-) wave function, the net effect is therefore also zero. However, calculations for $P_z$ in Fig.1. show that its variation for (+) / (-) wave functions have the same positive sign. $P_z$ due to the (+) branch adds to that of due to the (-) branch.

$$P_z^+ = \frac{1}{2\hbar} \left( M_z \varphi_{-1} \right)^2 - \left( \varphi_z \right)^2 \left( \varphi_{-1}^2 + \varphi_z^2 \right)$$ (57)

$$P_z^- = \frac{1}{2\hbar} \left( \varphi_{-1} \right)^2 - \left( M_z \varphi_z \right)^2 \left( \varphi_{-1}^2 + \varphi_z^2 \right)$$ (58)

It is thus possible to obtain a net $P_z$ effect. We have thus identified that $z$ is the spin quantization axis along which net spin polarization can be obtained in the Landau spin orbit system. This is important to device application as conversion of spin polarization to resistance or current requires
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detection to be performed along the axis which shows net spin polarization. Therefore in devices that consist of such systems, spin polarization detection should be captured in the $z$ spin quantization axis.

FIG. 7.1. $P_z$ due to the (+) branch replicate that due to the (−) branch; $P_y$ due to the (+) branch is the sign inverse of that due to the (−) branch.

The results of Fig. 7.1 also show that $E_y$ provides an electrical means to control the spin polarization of current at a particular transverse distance ($y$). The result of Fig. 7.1 is a consequence of the spatial shift of the cyclotron center as a result of changing $E_y$. Increasing $E_y$ decreases ($y-y_0$) because the cyclotron center moves closer to the point $y$ at which detection is performed. Therefore spin polarized current is increasingly being detected at the shorter part of the cyclotron radius or closer to the cyclotron center.

Figure 7.2 shows the variation of $P_z$ and $P_y$ for the (+) wave function with radial distance, clearly demonstrating that the Landau Rashba spin orbit system is capable of separating current of different spin polarization. This is analogous to the monochromatic action that spatially separates light of different frequency. In the plot of $P_y$, $P_z$, and $P_z$ variation across the cyclotron radius, Fig. 7.2. shows that $P_x$ is constantly zero, while $P_y$ and $P_z$ show significant spatial variation (0-100%)
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across the cyclotron orbital diameter in $y$. It is also found that the frequency of such variation increases for higher Landau levels. However, at the center of the cyclotron orbit, $P_y$ is constantly zero while $P_z$ is constantly 1. These results allow us to identify the spatial point at which $P$ in a particular axis has the largest net value. By placing a $z$ magnetized probe electrode at the center of the cyclotron center, the strongest magnetoresistive modulation can be detected when the probe switch magnetization.

![Diagram](image)

**FIG. 7.2.** $P_y$ and $P_z$ both show spatial variation across the cyclotron diameter divided into 100 parts. Figure 7.3 shows that the variation of $P_z$ with $E_y$ actually differs across the Landau levels.

At low Landau levels of $n=1$, $P_z$ varies in half of a repeating cycle over the $E_y$ range of 100 V/µm. At higher Landau levels of $n=15-20$, the repetition increases in frequency to one repeating cycle for the same $E_y$ range, showing much increased $P$ sensitivity to $E_y$ change. Thus at high Landau levels, the Landau spin orbit system would be suitable for devices that perform very low signal detection or amplification. This is because small variation of $E_y$ causes substantial change in spin polarization, which could be converted to significant change of conductance or resistance provided a spin analyzer device or function is established at one point along the current flow path, eg. in a transistor device, a magnetized drain contact could serve the spin analyzer function.
The above theoretical model can be conveniently implemented in various device models [20,21,22] that contain ferromagnetic gates deposited on top of the 2DEG HEMT heterostructure, similar to the spinFET device discussed in chapters 3,4,5,6. Results in Fig. 7.1 and 7.3 have shown the potential usefulness of the Landau spin-orbit system as a spinFET, in which the net polarization axis of $z$ has been identified and $P_z$ can be modulated by electrical means i.e. by changing $E_y$.

Finally we have shown in Eqs. (43) and (44) that spin polarization of current can be obtained in the (+) / (−) quantization axis with the application of $E_y$. In fact Eqs. (43) and (44) show that the spin polarization of current (not just the spin polarization of wave function as shown in Fig. 7.1. and Fig. 7.2) can also be manipulated by electrical means i.e. by changing $E_y$ fields. This shows that the Landau spin orbit system can be utilized in spintronic device especially in the ballistic regime where current is required in the absence of any form of scattering. It can be concluded that in our model, the application of source-drain bias voltage could thus create a condition of non-equilibrium, under which spin polarized current flows in the ballistic regime.

FIG. 7.3. $P_z$ decreases from 1 to −1 with increasing $E_y$ strength in a repetitive manner. For higher Landau levels, the repetition increases and variation also becomes smoother.
7.4 Conclusion

We have theoretically demonstrated here that the application of continuously distributed magnetic fields could give rise to electron cyclotron motion that mixed the up and down spin of different band. We have also developed a model that takes into consideration the effects of cross electric fields. The resulting spin-polarization of current shows a transverse spatial distribution across the in-plane dimensions of the 2DEG, similar to the spin Hall effects. We have also shown that the application of a cross electric field can be an additional external parameter which can be used to optimize the spin polarization of current.

REFERENCES

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Chapter 8

Spin transport and filtering in mesoscopic structures

8.1 Non-equilibrium current

The study of spin transport in mesoscopic structures require the use of the non-equilibrium Green’s function technique. The Green’s function approach is an advanced method that takes into consideration the effects of external perturbations eg. by device leads, and interaction processes within the central device, eg. electron-electron (e-e), electron-phonon (e-ph), and electron-photon (e-p) interactions, on electron current transport. However, the disadvantage of this method lies in its complexity and abstract nature. It is complicated to implement even for a simple transport system. Thus it should only be used where high accuracy is absolutely necessary and where electron interactions cannot be neglected. In this thesis, the system under consideration comprises a central device and two leads as shown in Fig. 8.1.

FIG. 8.1. A two-dimensional central device with left and right electrodes. The device is spanned by the horizontal and the vertical lattices.
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The effects of interaction processes can be derived from the interaction picture that leads to a perturbative series of Green’s functions in second quantized form [1,2,3]. The Green’s function contains all the general interaction terms in the system since interaction was assumed to be turned on a long time ago, i.e. \( t \to -\infty \). Interaction terms have to be separately derived, which depends on the specific physics underlying the interaction eg. e-e, e-ph, or e-p. Using Wick’s theorem and Feynman diagrams, the perturbative Green’s functions can be rearranged and simplified. Finally, with Dyson’s equations that describe a perturbed Green’s functions in terms of the unperturbed Green’s functions and the self-energies, the self-energies can be found. In our work, we will consider the self-energies arising from the interaction between the central device and the right and left leads. For simplicity, we will not consider other interaction processes of e-e, e-ph, or e-p within the central device. Our central device will also be defined in a discretized form [4, 5] whose dimensions depend on the specific structures like quantum dot, or nanowire.

8.2 Field equations

The field equation describes the continuous variation of a quantity or a classical field like the vibration of a particle across a rod, over a sphere, or the vibration of sound in space. In quantum field theory, the concept is applied to the wave-functions like the Schrödinger, Dirac, or Klein Gordon functions representing the fields. Each mode of the quantum field can be associated with a particle. In normal charge transport, the particles are fermionic electrons.

8.2.1 Lagrangian

To further develop the field, the use of Lagrangian density as an energy description of the system is necessary because it can lead to the derivation of the Hamiltonian density. Finding the Lagrangian associated with a classical field is straightforward because the classical field is merely a functional variation of an observable in space (eg. vibration); and an observable can be related to
the energy equation of the system, which comprises the space in which the field spans. But the Lagrangian of a quantum field cannot be found in a straightforward manner because the functional variation of the quantum field is not an observable.

This problem can, however, be solved by using Noether’s theorem, which states that a conserved quantity can always be associated with the symmetrical property of the system. We know that the wave-function is invariant with the change of its phase component. This is a manifestation of the time-evolution symmetry property of the system. It can be proven that the conserved quantity associated with this symmetry is current. (A digression here: using Lie’s algebra, a generator associated with the symmetry can be found. For the case of the time-evolution symmetry, the generator is the Hamiltonian. Taking the exponential of the generator leads to the unitary representation of the time-evolution operator.) Comparing current obtained from the wave function, with current obtained from the Lagrangian derivatives, the Lagrangian can be found. Once the Lagrangian has been derived, there is a direct mathematical method, known as the Legendre transformation, to transform it to the Hamiltonian.

It is interesting to note that the Hamiltonian here is derived from, and therefore expressed in terms of the field that spans the real space and contains all momentum in the Fourier space. As each particle in a system is associated with one momentum value, it can be understood that the total field must have been resulted from the presence of many particles in real space, and is a mathematical summation of all momentum in Fourier space. The Hamiltonian therefore represents the total energy of the system. Eqs. (1) summarize the above descriptions.

\[
L(q, q) \rightarrow H(q, p) = H(q, \frac{dL}{dq}) \leftrightarrow \text{classical field}
\]

\[
L(\phi, \dot{\phi}) \rightarrow H(\phi, \pi) = H(q, \frac{dL}{d\phi}) \leftrightarrow \text{quantum field}
\]
8.2.2 Second quantization

It has been discussed that the Fourier components of the continuous field can be found, and each Fourier component is associated with the energy distribution of one particle in space. It is interesting to note that in field theory, the Fourier component, also known as the oscillator can be shown to have a mathematical relationship with its own conjugate. This relationship is commonly expressed as a Poisson bracket. In addition, there is an interesting correspondence between the Poisson bracket relationship of the oscillator components and the well-known Heisenberg uncertainty relation. It therefore suggests that the oscillators can be quantized, i.e. they can be modified to act as an operator which gives rise to discrete eigenvalues instead of continuous variables. Since the Fourier components combine to form the field operator, there must exist a many-body state vector that can be acted upon by the Hamiltonian field operator to produce the total energy of the system.

Besides the Hamiltonian, the momentum, or spin operator can also be constructed and these operators all consist of their respective oscillators. The many-body state vectors exist in a mathematical space known as the Fock’s space and mathematically they are analogous to single-particle wave function in the Hilbert space. The theory of second quantization is necessary to support the Green’s function formalism.

8.3 Green function formalism

Understanding the concept of second quantization is important as the Green’s function is by definition the time-ordered expectation of the ground state wave function, i.e.

$$G(x,x') = -i\langle T \psi(x) \psi^*(x') \rangle$$  \hspace{1cm} (2)
In the following Green’s function formalism, current is expressed in second quantized operators that can be related by definitions of (2) and others to the Green’s function. There are two approaches to these formalism i.e. the space discretization approach and the momentum space approach.

### 8.3.1 The space discretization approach

The space discretization approach [6,7,8,9] has been widely used to simulate current distribution in a central device region. This method is useful for simulating current distribution in the central device in an interacting, or non-interacting environment. The solution of the Green’s functions in the central device requires solving a series of equations by means of a mathematical method known as renormalization. However, in our work we will focus on the momentum space approach and the quantum dot device.

### 8.3.2 The momentum space approach

The momentum space approach was presented in detail by Yigal Mier et al. and others [10,11,12,13] in the early 90s. This is a simple approach for the computation of current through a quantum dot. In this chapter, we will adapt this method to compute the spin-polarized current which passes through a quantum dot. The spin polarized current will be studied for their influences on spin injection from magnetized leads into semiconductor i.e. the quantum dot. The effect of magnetization angular change on spin injection, spin-polarized current, spin transfer torque will also be studied.
8.4 Spin-polarized current through the central device

The current in the central device from the right / left lead is given in Eq. (3), with the subscript $L$ (R) denoting the left (right) lead [10,11]. These equations are based on the second quantized form as described by Caroli et al.. The second quantized representation of current can be rewritten in the Green’s function form.

\[
J_L = \frac{ie}{\hbar} \sum_{n,m} \int dE \left[ f_L(G_{nm}^r - G_{nm}^a) + G_{nm}^c \rho_L^a(V_n^a) V_m^a \right] \chi_L^a \chi_L^a
\]

\[
J_R = -\frac{ie}{\hbar} \sum_{n,m} \int dE \left[ f_R(G_{nm}^r - G_{nm}^a) + G_{nm}^c \rho_R^a(V_n^a) V_m^a \right] \chi_R^a \chi_R^a
\]

where $\alpha$ denotes the channel (in our case, the two spin channels), $n$, $m$ denote momentum eigenstates in the central device region; the density of states $\rho_{L}^{a}$ and the wave function coupling term $V_{n}^{a}$ are grouped under an expression for the left and right leads.

\[
\Gamma_{L}^{a} = 2\pi \sum_{\alpha \in L} \rho_{L}^{a}(V_{n}^{a}) \langle V_{m}^{a} \rangle
\]

\[
\Gamma_{R}^{a} = 2\pi \sum_{\alpha \in L} \rho_{R}^{a}(V_{n}^{a}) \langle V_{m}^{a} \rangle
\]

In symmetrization, $J_L$ and $J_R$ are added and the total current is shown in Eq. (5)

\[
2J = J_L + J_R
\]

\[
J = \frac{ie}{2\hbar} \sum_{n,m} \int dE \left[ \Gamma_{L}^{a} f_{L} - \Gamma_{R}^{a} f_{R} (G_{nm}^{r} - G_{nm}^{a}) + \left( \Gamma_{L}^{a} - \Gamma_{R}^{a} \right) G_{nm}^{c} \right]
\]

The above is the Eq. (5) of Yigal et al. expressed in the series-summation form. It can also be expressed in the form of the trace of a series of matrix multiplications. This is the current for the interacting case, and can be simplified further for the non-interacting case. In our studies, we will focus on the interacting form only. The series summation in Eq. (5) is the direct result of the application of Dyson’s equation to relate the perturbed Green’s functions to the unperturbed Green’s functions of the leads and the interacting region, which are as follows:
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\[ G^\alpha_{k \alpha n} = \sum_m V_{k \alpha k' m} \left[ g^\alpha_{k \alpha} G^\alpha_{k' \alpha m} - g^\alpha_{k' \alpha} G^\alpha_{k \alpha m} \right] \quad (6) \]

\[ G^\alpha_{\alpha k n} = \sum_m V^\dagger_{k \alpha k' m} \left[ g^\alpha_{\alpha k} G^\alpha_{\alpha k' m} - g^\alpha_{k' \alpha} G^\alpha_{\alpha k m} \right] \quad (7) \]

In the case of a quantum dot (with a single discrete energy level or discretized spatial point), only the first term in the series is used. In matrix form, only the upper left-most term of the entire matrix is used. Thus for a quantum dot, Eq. (5) can be expressed as follows:

\[ J = \frac{ie}{2h} \sum_\alpha \int dE \left( f_L \Gamma^\alpha_L - f_R \Gamma^\alpha_R \right) \left( G^\alpha_{11} - G^\alpha_{11} \right) + \left( \Gamma^\alpha_L - \Gamma^\alpha_R \right) G^\alpha_{11} \quad (8) \]

Note that the summation is only over spin channel but not \( n \) or \( m \). Equation (8) can be simplified to Eq. (9):

\[ J = \frac{ie}{h} \sum_\alpha \int dE \left( f_L - f_R \right) \left( \frac{\Gamma^\alpha_L \Gamma^\alpha_R}{\Gamma^\alpha_L + \Gamma^\alpha_R} \right) \left( G^\alpha_{11} - G^\alpha_{11} \right) \quad (9) \]

To explicitly show the above simplification, we consider the two currents of Eq. (3) where

\[ J_L = \frac{ie}{h} \sum_\alpha \int dE \left[ f_L \left( G^\alpha - G^\alpha \right) + G^\alpha \right] \Gamma^\alpha_L \quad \text{and} \quad J_R = -\frac{ie}{h} \sum_\alpha \int dE \left[ f_R \left( G^\alpha - G^\alpha \right) + G^\alpha \right] \Gamma^\alpha_R \quad \text{separately.} \]

Simple mathematics leads to:

\[ \Gamma^\alpha_L J_L = \frac{ie}{h} \sum_\alpha \int dE \left[ f_L \left( G^\alpha - G^\alpha \right) + G^\alpha \right] \Gamma^\alpha_L \Gamma^\alpha_L \quad (10) \]

\[ \Gamma^\alpha_R J_R = -\frac{ie}{h} \sum_\alpha \int dE \left[ f_R \left( G^\alpha - G^\alpha \right) + G^\alpha \right] \Gamma^\alpha_R \Gamma^\alpha_L \]

Adding the two equations above and taking \( J_L = -J_R = J \) lead to the following expressions of Eqs. (11).
\[ \Gamma^a_L J_L + \Gamma^a_R J_R = \frac{ie}{\hbar} \sum_{a \alpha} \int dE \left[ (f_L - f_R)(G^\prime - G^a) \Gamma^a_L \Gamma^a_R \right] \]

\[ J(\Gamma^a_L + \Gamma^a_R) = \frac{ie}{\hbar} \sum_{a \alpha} \int dE \left[ f_L (G^\prime - G^a) \Gamma^a_L \Gamma^a_R \right] \quad (11) \]

\[ J = \frac{ie}{\hbar} \sum_{a \alpha} \int dE \left[ f_L (G^\prime - G^a) \frac{\Gamma^a_L \Gamma^a_R}{\Gamma^a_L + \Gamma^a_R} - \frac{1}{\pi} \text{Im}(G^\prime) \right] \quad (12) \]

Further simplification leads to Eq. (12) which will be used in our calculations to obtain the current through a quantum dot:

\[ J = \frac{e}{\hbar} \sum_{a \alpha} \int dE \left( f_L - f_R \right) \left( \frac{\Gamma^a_L \Gamma^a_R}{\Gamma^a_L + \Gamma^a_R} \right) \left( \frac{-1}{\pi} \right) \text{Im}(G^\prime) \]

where \( f_L = \frac{1}{\exp\left(\frac{E - \mu_L}{kT}\right) + 1} \) and \( f_R = \frac{1}{\exp\left(\frac{E - \mu_R}{kT}\right) + 1} \) are the Fermi occupation probabilities of the left and right leads.

### 8.5 Spin-polarized current through a quantum dot

In this section, we will study electron tunneling through a quantum dot device using the momentum space Green’s function method [14,15,16]. The approach discussed in this section can be used to calculate the spin injection effects of section 8.5.1. Equation (12) is used to calculate the current through the quantum dot. Typical parameter values are chosen, as shown in Table 8.I. Note that the main purpose here is to introduce the rigorous Green’s function momentum space approach to calculate spin-polarized current, spin injection and spin transfer through the quantum dot.
 TABLE 8.1. Parameter values that are used to calculate spin-polarized current through the quantum dot device.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Energy Values</th>
<th>Energy (Γ multiple)</th>
</tr>
</thead>
<tbody>
<tr>
<td>kT</td>
<td>0.01 meV</td>
<td>0.1</td>
</tr>
<tr>
<td>μL</td>
<td>0.2 meV</td>
<td>2</td>
</tr>
<tr>
<td>μR</td>
<td>-0.2 meV</td>
<td>-2</td>
</tr>
<tr>
<td>Ec</td>
<td>2 meV</td>
<td>20</td>
</tr>
<tr>
<td>εξ1</td>
<td>0 meV</td>
<td>0</td>
</tr>
<tr>
<td>ΓL</td>
<td>0.1 meV</td>
<td>1</td>
</tr>
<tr>
<td>ΓR</td>
<td>0.1 meV</td>
<td>1</td>
</tr>
</tbody>
</table>

In the table, Ec is the Coulomb interaction, kT is the thermal energy, μL,R is the electrochemical potential of the left/right lead, εξ1 is the quantum dot eigenenergy in the absence of Coulomb repulsion. The retarded Green's function for the interaction between the quantum dot and the leads can be derived from the Hamiltonian using the equation of motion method, and is given by [12,13,17]:

\[
G^r_\sigma = \frac{E - \epsilon_{d\sigma} - E_c (1 - n_{-\sigma})}{(E - \epsilon_{d\sigma})(E - \epsilon_{d\sigma} - E_c) - \Sigma^r_\sigma (E - \epsilon_{d\sigma} - E_c)(1 - n_{-\sigma})}
\]  

(13)

where \( \Sigma^r_\sigma = \left(-i/2\right)(\Gamma^r_\sigma + \Gamma^a_\sigma) \) and \( n_{-\sigma} \) is the electron occupation number for spin \( \sigma \). \( n_{-\sigma} \) is not an independent variable, since it itself is related to the retarded and advanced Green's functions as follows [14,15]:

\[
n_{\sigma} = \frac{1}{2\pi} \int dE \left( \frac{f^\sigma_\sigma \Gamma^a_\sigma + f^\sigma_\sigma \Gamma^r_\sigma}{\Gamma^a_\sigma + \Gamma^r_\sigma} G^a_\sigma - G^r_\sigma \right)
\]

(14)

where \( G^r_\sigma = (G^a_\sigma)^\dagger \). Hence, \( n_{\sigma} \) and \( n_{-\sigma} \) has to be determined self-consistently using Eq. (13) and Eq. (14) taking into account the spin direction. The self-consistency scheme is illustrated in Fig. 8.2 below:

FIG. 8.2. The self-consistent method to determine the value of \( n \) and \( G \) of the quantum dot.
The self-consistent looping is stopped once the successive values of $n_{\uparrow,i}$ and $n_{\uparrow,i+1}$ have converged. The band structure diagram of the quantum dot and leads device is shown in Fig. 8.3 below, which shows spin accumulation at both sides of the leads.

FIG. 8.3. Band structure diagram that shows electrochemical potentials on the left and right leads, and electrons tunneling through a quantum dot eigenstate from left to right. Electron at each energy level is doubly degenerate when there is no magnetic field applied to the quantum dot, and the quantum dot is non-magnetic.

### 8.5.1 Spin injection

To compute spin injection for a quantum dot device, the leads are magnetized parallel as shown in Fig. 8.4.

FIG. 8.4. Quantum dot device with parallel magnetized leads.

Current for parallel and anti-parallel configurations of the leads magnetization is shown in Eq. (15) and Eq. (16), respectively.
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\[ J_p = \frac{e}{\hbar} \left( \int dE(f_L - f_R) \left( \frac{\Gamma_L^+ \Gamma_R^-}{\Gamma_L^+ + \Gamma_R^-} \right) \frac{1}{\pi} \text{Im}(G'_i) \right) + \int dE(f_L - f_R) \left( \frac{\Gamma_L^+ \Gamma_R^-}{\Gamma_L^+ + \Gamma_R^-} \right) \frac{1}{\pi} \text{Im}(G'_i) \]  \tag{15}

\[ J_{\Delta \mu} = \frac{e}{\hbar} \left( \int dE(f_L - f_R) \left( \frac{\Gamma_L^+ \Gamma_R^-}{\Gamma_L^+ + \Gamma_R^-} \right) \frac{1}{\pi} \text{Im}(G'_i) \right) + \int dE(f_L - f_R) \left( \frac{\Gamma_L^+ \Gamma_R^-}{\Gamma_L^+ + \Gamma_R^-} \right) \frac{1}{\pi} \text{Im}(G'_i) \]  \tag{16}

The line width function for up-/down- magnetized state in the leads are given by \( \Gamma^{\pm1} = \Gamma \sqrt{1 \pm \frac{\Delta}{\xi}} \), where \( p = \Delta \xi \) can be taken as a polarization value between 0 and 1. To calculate for spin injection, only Eq. (15) will be used. To calculate spin injection accurately, it’s important to determine spin accumulation \( \Delta \mu \) at the lead-dot junction self-consistently with the current for a fixed lead conductivity. However, for simplicity, we will choose an arbitrary spin accumulation \( \Delta \mu \). The current can, however, be self-consistent with the conductivity of the leads. This method will allow us to study the effects and trends of spin injection but not its absolute value. This because the arbitrary choice of \( \Delta \mu \) has pre-determined spin injection value.

**FIG. 8.5.** Spin injection increases with increasing \( p \) value of the lead magnetization, in line with earlier prediction using the drift-diffusion methods.

Figure 8.5 shows that spin injection increases with the \( p \) value of the lead magnetizations, according to expectation. The absolute strength of the spin injection depends on the arbitrary choice of spin accumulation.
8.5.2 Angular dependence of spin torque transfer

In this section, we will show analytically that magnetization switching of the quantum dot shows an angular dependence in respect of the amount of torque that can be transferred to the dot. Here it is important to assume \([18,19,20,21]\) that the device acts like a perfect filter that only allows the spin up current to tunnel through. This can be achieved by assuming that the quantum dot itself is a perfect filter. Current magnetized by the right lead can be represented by a wave function that is a combination of the up and down wave function, depending on the angle.

![Image of quantum dot device with both leads magnetized at specific angle with the vertical axis.](image)

FIG. 8.6. Quantum dot device with both leads magnetized at specific angle with the vertical axis.

The left lead magnetization has an angle \(\theta\) with the vertical axis (z). This means that the wave function has a net spin expectation value in the z axis, which can be written as:

\[
\psi_{\theta} = \psi_0 \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] + \psi_1 \left[ \begin{array}{c} 0 \\ 1 \end{array} \right] = \psi_0 \cos(\theta/2) \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] + \psi_0 \sin(\theta/2) \left[ \begin{array}{c} 0 \\ 1 \end{array} \right]
\]  

(18)

In Eq. (18), electron is 100% polarized in the angular direction giving rise to \(p=1\) in the arbitrary angular direction. The spin down component is completely filtered as previously assumed, only the spin up current can pass through the central device. It is intuitive that when the angle is 0, the spin up current that passes through the central region has the highest value, likewise when angle is 180, there is no spin up current, and total current through the system is 0. At smaller angle, the amount of current that can pass through the central device gets larger. Higher current density enables the switching of the magnetization of the central device. However, at smaller angle, the amount of torque that can be transferred to the central device magnetization gets smaller. There are two opposing forces that competes for strength. There is therefore an optimal angle at which the
amount of torque that can be transferred is largest. We therefore proposed that the spin torque experienced by the quantum dot or any central device is given by the following phenomenological equation of Eq. (19)

\[ T \propto J^\uparrow \langle S_x \rangle \]  

(19)

It has been shown that spin up current is given by the expression of Eq. (20).

\[ J^\uparrow = \frac{e}{\hbar} \int dE (f_L - f_R) \left( \frac{\Gamma_L^\uparrow \Gamma_R^\uparrow}{\Gamma_L^\uparrow + \Gamma_R^\uparrow} \right) \left( -\frac{1}{\pi} \right) \text{Im}(G_{\uparrow}) \]  

(20)

The density of states in an arbitrary angular direction is given by \( g^*_\theta = \langle \psi_\theta(x) \psi_\theta^*(x') \rangle \). Similarly, the density of states in the up direction is related to the density of states in the arbitrary angle direction by \( g^\uparrow = \langle \psi_\uparrow(x) \psi_\uparrow^*(x') \rangle \). Therefore density of states in the up direction is given by \( g^\uparrow = \langle \psi^* \cos^2 \theta/2 \rangle = g^'_\theta \cos^2 \theta/2 \). Similarly, \( g^\uparrow = g^' \sin^2 \theta/2 \). In this section, we only need to analyze the spin up current, as the purpose here is to study the effect of spin up current on the magnetization of the quantum dot. Spin up current can be derived from the following reasoning of \( J^\uparrow \propto g^\uparrow \propto \Gamma^\uparrow \). It can thus be deduced that spin up current due to an angled (\( \theta \)) magnetization polarized in two opposite directions by \( p \) along the line angled \( \theta \) with the vertical axis is given by Eq. (21)

\[ J^\uparrow \propto g^\uparrow \propto \cos^2 \theta/2 + g^\uparrow \sin^2 \theta/2 \]  

(21)

Equation (21) leads to Eq. (22):

\[ J^\uparrow \propto \Gamma^\theta \cos^2 \theta/2 + \Gamma^- \sin^2 \theta/2 \]  

\[ J^\uparrow \propto \Gamma \left( \sqrt{1 + p \cos^2 \theta/2} + \sqrt{1 - p \sin^2 \theta/2} \right) \]  

(22)

The spin up current shows angular as well as density of states dependence as shown in Eq. (23)

\[ J^\uparrow = \frac{e}{\hbar} \int dE (f_L - f_R) \left( \frac{\Gamma_L^\uparrow \Gamma_R^\uparrow}{\Gamma_L^\uparrow + \Gamma_R^\uparrow} \right) \left( -\frac{1}{\pi} \right) \text{Im}(G_{\uparrow}) \]  

(23)

The expectation value of spin in \( x \) is given by:
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\[
\langle S_r \rangle = \frac{1}{2} \hbar \langle \chi \sigma, \chi \rangle
\]

\[
= \frac{1}{2} \hbar (ab^* + ba^*) = \hbar ab
\]

\[
= \frac{1}{2} \hbar \sin \theta
\]

(24)

The torque equation therefore shows angular dependence as shown by Eq. (25)

\[
Torque \propto J^1 \left( \frac{1}{2} \hbar \sin \theta \right)
\]

(25)

It’s clear from Eq. (25) that spin torque transfer shows a complicated dependence on magnetization angle with vertical axis. Figure 8.6 shows the plot of spin torque transfer (arbitrary unit) with the variation of this angle.

FIG. 8.7. (a) Spin torque transfer shows variation with angular change of the leads magnetization with the vertical axis. (b) Spin torque transfer shows variation with the \( p \) value of lead magnetizations.

At zero angle, spin up current from the right lead that can pass through the device is the largest. However at zero angle, current would not exert torque on the vertical magnetization of the quantum dot, resulting in net zero torque transfer. As the angle increases, current with spin polarized at an angular direction produces increasingly higher torque on the quantum dot’s vertical magnetization. This results in increasing torque transfer as shown in the middle part of Fig. 8.6. Spin torque is the largest at angle 90 but current strength is midway between angle 0 and 180. The
net results are spin torque transfer is largest at between 90 and 110. As angle increases to 180, spin torque transfer drops to zero again because spin down current from the right lead cannot pass through the quantum dot. Spin down current also produces no torque with the vertical magnetization of the quantum dot.

8.6 Conclusion

We have used the non-equilibrium Keldysh technique to study spin polarized current transport in the mesoscopic two-terminal QD device with Coulomb blockade and lead perturbation. We have derived analytical expressions for spin-polarized current using a new approach which is based on the lead density of states. We used these models to perform simulation of current polarization, spin injection efficiency, and spin transfer torque in the QD device subject to perturbations. Our theoretical models have shown that spin injection efficiency through the QD is strongly influenced by angular orientation of the leads’ magnetization (M) as well as the leads’ intrinsic spin polarization.

REFERENCES

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Chapter 9

Conclusion

9.1 Conclusion

In conclusion, we have studied the various theoretical means to induce spin-polarized current and transport the current across transistor-like devices. We have found that the long-standing problem of spin injection into semiconductors can be mitigated by using a bilayer injector structure [1] consisting of a nanopillar ferromagnetic (FM) spin injector with a non-magnetic spacer insertion layer between the FM injector and the semiconductor layer. The nanopillar geometry constricts the current flow in the FM layer and increases the overall spin injection and MR ratio. The same current constriction method has also been adapted in an all-metal CPP-CCP spin valve structure [2,3]. Their experimental finding that the overall MR is increased by the constriction of current flow provides vindication to our model.

In our work of ferromagnetic spinFET transistors with multiple gates, we have shown that the magnetization of ferromagnetic gates can be configured to implement various (spatially-discrete or “delta”) distribution of magnetic fields, and net magnetic vector potential change across the current conduction path. By manipulating the magneto-electric field configurations applied to the gate, we can achieve e.g. the “zero-gauge” type [4,5] configuration where there is no net change in the magnetic vector potential across the conduction path. We propose this zero-gauge configuration as a means of achieving high spin polarization without suppressing the carrier transmission across the device. Using more elaborate gate configurations, we have also shown that it is possible to realize more complex logic and memory functions [6,7,8], e.g. a programmable
logic capable of up to six different logic functions, and a multi-level non-volatile memory storage, which can also be optimized to function as a analog-to-digital converter.

Our theoretical studies of the Rashba and Dresselhaus spin orbit coupling (SOC) led to conclusions that these spin-splitting effects due to magneto-electric barriers alone are not sufficient to induce significant spin-polarized current. We have found that using these SOC phenomena in conjunction with external delta magneto-electric fields, spin-polarized currents with significantly higher polarization can be achieved. However, to implement this in a practical device would require a careful optimization of device geometry, device and operating parameters, and specific considerations of crystal axis alignment with current conduction path so as to maximize spin polarization. We have proposed magneto-electronic devices [9] that utilize the Dresselhaus [10], as well as Rashba [11] effects to produce significantly higher spin-polarized current, which is resistant to spin relaxation.

In the earlier parts of the thesis, we have considered the spatially confined (delta) magnetic field configuration. As in previous works in the literature, we have considered this idealized configuration because of its theoretical and conceptual simplicity in explaining its spin-splitting effects. However in practice, magnetic fields have a spatial spread. We thus presented a theoretical analysis and model of a spinFET with a continuous spatial distribution of magnetic fields [12] and SOC effects within the 2DEG. This results in new effects e.g. the presence of Landau levels and cyclotron-like motion of carriers. The resulting spin-polarization of current has a spatial distribution across the in-plane dimensions of the 2DEG. We have also shown that the application of a cross electric field can be an additional external parameter which can be used to optimize the spin-polarized current polarization.
Finally, in our last chapter, we ventured beyond the single effective mass approximation and apply the more refined Keldysh non-equilibrium [13] technique to model the spin transport in a quantum dot (QD) device. We derive analytical expressions and numerically calculate the spin-polarized current polarization, injection efficiency, and spin transfer torque in the QD device. We have shown that spin injection efficiency through the QD is strongly influenced by angular orientation of the leads’ magnetization (M). The angular orientation of M also affects the strength of the spin torque transfer in a rather complicated way with peak torque transfer efficiency at specific orientation of M.

9.2 Further work and future outlook

Semiconductor spintronic remains a relatively new area of research. Specifically, our proposal for a nanopillar spin injection technique is a promising area in view of recent experimental success in increasing MR using the CPP-CCP spin valves [2,3] with nanopatterned spacers. Nanopatterning of CPP sensors are extensively studied as the next potential improvement of the read head for the industry. These experimental developments will require new applications and adaptations of the basic nanopillar injector structure. In addition a more refined modeling work should be carried out in the future to yield a more realistic prediction of device performance. For instance, for greater accuracy spin relaxation could also be included in our model, using the more refined Rashba-Van Son [14] model. The insertion of half-metallic layers, and the patterning of other layers like the Cu or the half-metallic instead of the ferromagnetic layer should also be considered in future modeling work, in view of the high spin polarization of half-metallic materials. The incorporation of the effect of spreading resistances in these models, which has been neglected in most previous works, could also bring new insights into the precise mechanism of enhancement of spin injection efficiency or MR with these patterned layers.
The use of delta magneto-electric fields provides flexibility and logic function programmability. However, the implementation of spinFETs with the required spatially-discrete distribution of delta magnetic fields could face engineering difficulty as magnetic fields are invariably characterized by Lorentzian spatial distribution. Future work should look into material choices for the ferromagnetic gates and source/drain electrodes. Thermal effects should also be taken into consideration e.g. in spreading out the carrier distribution above the Fermi level. Further optimization of device dimensions, geometries, physical parameters should also be performed, taking into consideration the interfacial effects e.g. spin loss between FM and 2DEG. A more holistic device modeling where output of one transistor drives another might need to consider the issues of error margin, driving power, impedance matching between devices, etc.

In the studies of the Rashba and Dresselhaus spin orbit coupling, future work should focus on calculating spin-polarized current under the simultaneous presence of both effects especially in the context of a device with the electric fields applied. To enhance the model, these spin orbit coupling effects can be written in the second quantized form. In that way, the more general non-equilibrium Keldysh technique could be employed to study these Rashba and Dresselhaus SOC effects and their influence on the spin-polarized current polarization.

The application of continuously distributed magnetic fields gives rise to cyclotron motions that complicate analysis of spin-polarized current transport. In our present model we have included the effects of cross electric fields. Future models should be refined to explicitly include the electrochemical potentials, which presently is only implicit in the arbitrary choice of wave function amplitude, i.e. the non-equilibrium effect is not explicitly linked to the application of electrochemical potentials. As for the SOC effects, presenting the model Hamiltonian wholly in second quantized form is also a subsequent step in our future work, which will allow the application of theoretical methods for a more rigorous mesoscopic spin transport modeling.
Finally, the Keldysh technique used to analyze the spin transport in the QD device has allowed us to analyze the effects of leads perturbation, temperature, electron correlations and Coulomb charging effects on spin-polarized current, spin injection, and spin torque transfer. However, our present model and also the models available in the literature, treat the spin accumulation in the QD as an independent parameter. For a more refined modeling of the QD device, it is necessary to introduce spin accumulation self-consistently with the spin and charge currents across the QD.

REFERENCES

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+ This article can also be found in the Virtual Journal of Nanoscale Science & Technology - Volume 11, Issue 21, May 30, 2005.

* This article can also be found in the Virtual Journal of Nanoscale Science & Technology - Volume 11, Issue 18, May 9, 2005.
Appendix I

Single anti-symmetric barriers

Derivation of transmission probability for a single antisymmetric magnetic barrier shows zero spin polarization.

The transmission matrix is shown below:

\[ \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \begin{bmatrix} E \end{bmatrix} \]  

(1)

\[ A = \frac{[i(k_1 + k_2) - Z][i(k_1 + k_2) + Z][e^{i(k_1 - k_2)} + [i(k_1 - k_2) - Z][e^{i(k_1 + k_2)}]}{(2ik_1)(2ik_2)} \]

\[ A = \frac{[(k_1 + k_2)^2 - Z^2][e^{i(k_1 - k_2)} + [(k_1 - k_2)^2 + Z^2][e^{i(k_1 + k_2)}]}{(-4k_1k_2)} \]

\[ a = \frac{4k_1k_2L - 2i(k_1^2 + k_2^2 + Z^2) \sin k_2L}{4k_1k_2e^{-i\theta_1}} \]

which results in \[ \frac{a}{E} = \frac{4k_1k_2 \cos k_2L - 2i(k_1^2 + k_2^2 + Z^2) \sin k_2L}{4k_1k_2e^{-i\theta_1}} \]

Transmission probability is given by:

\[ \frac{E}{A} = \frac{4k_1k_2}{\sqrt{16k_1^2k_2^2 \cos^2 k_2L + 4(k_1^2 + k_2^2 + Z^2)^2 \sin^2 k_2L}} \]  

(2)

\[ \frac{|E|^2}{A} = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 \cos^2 k_2L + (k_1^2 + k_2^2 + Z^2)^2 \sin^2 k_2L} \]  

(3)

Z shows dependence (+1/-1 indicates spin up/dn, respectively). The \( Z^2 \) term shows that it is always positive. The matrice components of b and c are also shown below although they are not used to calculate spin polarization.
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\[
b_1 = \frac{[i(k_1 + k_2) - Z]}{2ik_1} \left[ \frac{[i(k_1 - k_2) + Z]e^{-i(k_1 - k_2)L}}{2ik_2} \right] + \frac{[i(k_1 - k_2) - Z]}{2ik_1} \left[ \frac{[i(k_2 + k_1) - Z]e^{-i(k_2 - k_1)L}}{2ik_2} \right]
\]

\[
b_1 = \left( \frac{k_1^2 - k_2^2 - 2Zik_1 + Z^2}{4k_1k_2} \right) e^{-ik_1L} + \left( \frac{k_1^2 - k_2^2 + 2Zk_1 - Z^2}{4k_1k_2} \right) e^{ik_2L}
\]

\[
b_1 = \left( -\frac{k_1^2 + k_2^2 + 2Zik_1 - Z^2}{4k_1k_2} \right) (2i \sin k_1 L) e^{-ik_1L}
\]

\[
b_1 = \left( \frac{[i(k_2 - k_1)^2 - Z^2] - 2Zk_1 |\sin k_1 L|}{2k_1k_2} \right) e^{-ik_1L}
\]

\[
c_1 = \left( \frac{k_2^2 - k_1^2 + 2Zik_1 + Z^2}{4k_1k_2} \right) e^{ik_2L} + \left( \frac{k_2^2 - k_1^2 + 2Zik_1 - Z^2}{4k_1k_2} \right) e^{ik_2L}
\]

\[
c_1 = \left( \frac{k_2^2 + 2Zik_1 + Z^2}{4k_1k_2} \right) (e^{-ik_2L} - e^{ik_2L}) - k_1^2 (e^{-ik_2L} - e^{ik_2L})
\]

\[
c_1 = \left( \frac{k_2^2 - k_1^2 + 2Zik_1 - Z^2}{4k_1k_2} \right) (2i \sin k_1 L) e^{ik_2L}
\]

\[
c_1 = \left( \frac{k_2^2 - k_1^2 - Z^2}{2k_1k_2} \right) |\sin k_1 L| e^{ik_2L}
\]

**Single symmetric barriers**

Derivation of transmission probability for a single symmetric magnetic barrier shows a net finite spin polarization.

\[
A = \left[ \frac{[i(k_1 + k_2) - Z]}{2ik_1} \right] \left[ \frac{[i(k_1 + k_2) + Z]e^{i(k_1 - k_2)L}}{2ik_2} \right] E + \left[ \frac{[i(k_1 - k_2) - Z]}{2ik_1} \right] \left[ \frac{[i(k_2 + k_1) + Z]e^{i(k_2 - k_1)L}}{2ik_2} \right] E
\]

\[
A = \left[ \frac{[i(k_1 + k_2) - Z][i(k_1 + k_2) - Z]e^{i(k_1 - k_2)L}}{-4k_1k_2} \right] E + \left[ \frac{[i(k_1 - k_2) - Z][i(k_2 + k_1) + Z]e^{i(k_2 - k_1)L}}{-4k_1k_2} \right] E
\]
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\[
A = \frac{1}{E} \left( [i(k_1 + k_2) - Z][i(k_1 + k_2) - Z]e^{-ik_2z} + [i(k_1 - k_2) - Z][i(k_2 - k_1) + Z]e^{ik_1z} \right) e^{ik_1z}.
\]

\[
E = \frac{4k_1k_2}{A} \left( [(k_1k_2 + k_1k_3 + k_2k_3) + iZ(k_1 + 2k_2 + k_3) - Z^2]e^{-ik_2z} + [(k_1k_2 - k_2k_3 - k_1k_3) - iZ(k_1 - 2k_2 + k_3) + Z^2]e^{ik_1z} \right) e^{-ik_1z}.
\]

Transmission probability is given by:

\[
\left[ \begin{array}{c} \frac{k_1}{k_1} \\ \frac{k_2}{k_2} \end{array} \right] = \frac{4k_1k_2}{[k_2(k_1 + k_3) \cos k_2L + Z(k_1 + k_3) \sin k_2L]^2 + [k_2^2 + k_3^2 - Z^2] \sin k_2L - 2Zk_2 \cos k_2L]^2}
\]

Double anti-symmetric barriers

The transmission matrix for a double-pair barrier consist of two multiplicative matrices as shown in Eqs. (5)&(6).

\[
\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}, \quad \begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix}
\]

\[
\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix} = \begin{bmatrix} a_1a_2 + b_1c_2 & a_1b_2 + b_1d_2 \\ c_1a_2 + d_1c_2 & c_1b_2 + d_1d_2 \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix}
\]

The transmission probability is given by \( \left| \frac{A}{J} \right| = |a_1a_2 + b_1c_2| \). The individual matrices are shown below:
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\[
\begin{bmatrix}
A \\
B \\
C \\
D
\end{bmatrix} =
\begin{bmatrix}
\frac{[i(k_1 + k_2) - Z]}{2ik_1} & \frac{[i(k_1 - k_2) - Z]}{2ik_1} \\
\frac{[i(k_1 - k_2) + Z]}{2ik_1} & \frac{[i(k_1 + k_2) + Z]}{2ik_1}
\end{bmatrix}
\begin{bmatrix}
C \\
D
\end{bmatrix}
\]

\[
\begin{bmatrix}
E \\
F
\end{bmatrix} =
\begin{bmatrix}
\frac{[i(k_2 + k_1) + Z]e^{i(k_1 - k_2)L}}{2ik_2} & \frac{[i(k_2 - k_1) + Z]e^{-i(k_1 + k_2)L}}{2ik_2} \\
\frac{[i(k_2 - k_1) + Z]}{2ik_2} & \frac{[i(k_2 + k_1) + Z]e^{-(k_1 - k_2)L}}{2ik_2}
\end{bmatrix}
\begin{bmatrix}
E \\
F
\end{bmatrix}
\]

The derivations for the matrix components are shown below:

\[
a_1 = \left[\frac{4k_1k_2 \cos k_1L - 2i(k_1^2 + k_2^2 + Z^2) \sin k_1L}{4k_1k_2}\right] e^{ik_1x} = a_1
\]

\[
b_1 = \left(\frac{k_1^2 - k_2^2 - Z^2 i - 2Zk_2 \sin k_1L}{2k_1k_2}\right) e^{-ik_1x}
\]

\[
c_2 = \left(\frac{[i(k_1 - k_2) + Z]e^{i(k_1 - k_2)L}}{2ik_1} \right) \left(\frac{[i(k_1 + k_2) + Z]e^{i(k_1 + k_2)L}}{2ik_1} \right) + \left(\frac{[i(k_1 + k_2) + Z]e^{i(k_1 - k_2)L}}{2ik_1} \right) \left(\frac{[i(k_2 - k_1) - Z]e^{i(k_1 + k_2)L}}{2ik_1} \right)
\]

\[
d_2 = \left(\frac{[i(k_1 - k_2) + Z]}{2ik_1} \right) \left(\frac{[i(k_1 + k_2) + Z]}{2ik_1} \right) + \left(\frac{[i(k_1 + k_2) + Z]}{2ik_1} \right) \left(\frac{[i(k_2 - k_1) - Z]}{2ik_1} \right)
\]

\[
b_1c_2 = \left(\frac{k_1^2 - k_2^2 - Z^2 i - 2Zk_2 \sin k_1L}{2k_1k_2}\right) \left(\frac{k_1^2 - k_2^2 + Z^2 i - 2Zk_2 \sin k_1L}{2k_1k_2}\right) e^{i(k_1 + k_2)L}
\]

\[
h_2c_2 = \left(\frac{k_1^2 - k_2^2 - Z^2 i - 2Zk_2 \sin k_1L}{2k_1k_2}\right) \left(\frac{k_1^2 - k_2^2 + Z^2 i - 2Zk_2 \sin k_1L}{2k_1k_2}\right) e^{i(k_1 - k_2)L}
\]
Spin characteristics of electron transport in semiconductor

\[ b_{c_2} = \left( -\frac{(k_1^2 - k_2^2 - Z^2)(k_1^2 - k_3^2 - Z^2)}{4k_1^2 k_2^2} - 2Zk_3(k_1^2 - k_2^2 - Z^2 + k_3^2 - k_1^2 + Z^2) + 4Z^2 k_1^2 \right) \sin^2 k_1 L \left( e^{i(1-x)k_1} \right) \]

\[ b_{c_2} = \left( -\frac{(k_1^2 - k_2^2 - Z^2)(k_2^2 - k_3^2 - Z^2)}{4k_1^2 k_2^2} + 4Z^2 k_1^2 \right) \sin^2 k_2 L \]

\[ b_{c_2} = \left( \frac{(k_3^2 - k_1^2 + Z^2)^2 \sin^2 k_1 L + 4Z^2 k_1^2 \sin^2 k_1 L}{4k_1^2 k_2^2} \right) \left( e^{i(1-x)k_1} \right) \]