ANALYSIS OF ELECTRON TRANSPORT THROUGH NOVEL NANOELECTRONIC AND SPINTRONIC DEVICES

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I would like to dedicate this work to my mother, Lori C. Cutright:
She inspired my sense of scientific curiosity at a young age,
and has unwaveringly supported the entirety of my academic career.
ABSTRACT

Traditionally, computer components like transistors have been large enough that they obey classical physical law. Today, as computers continue to be miniaturized, traditional components no longer operate correctly because their dimensions are close to, or on, the atomic scale. Quantum physics takes over in this regime, so new components and computing techniques must be devised.

Two such new sets of devices and techniques are nanoelectronics and spintronics. Nanoelectronics are very similar to current microelectronics, but their size constraints force them to operate in the quantum mechanical regime. Spintronics is a field whereby the intrinsic fermion spin of the electron is used to represent binary bits. In my work we propose new device schemes with applications in both nanoelectronics and spintronics.

In the nanoelectronic realm we propose that a series of Aharonov-Bohm Rings, with quantum dots in each arm of the rings, can be linked via intermediate quantum dots. Applying an external magnetic field to this system proves interesting, since the system can be made to change its overall conductivity via this tunable, external magnetic field. Typical Single Electron Transistors (SET) operate by employing the Coulomb Blockade Effect and Voltage Biasing to manipulate the conductivity of a nanostructure. The proposed device would, in principle, perform the same task, but the novel approach may have certain advantages over the SET.

In the field of spintronics we propose a simple, spin-polarizing device. Typically, any current used by a computer has electrons with randomly oriented spin-states. This is okay, however, because the system ignores these states. A spintronic device, however,
would need an input current with a precise spin orientation, so that the spin-states of the electrons could be accurately manipulated. This means a current that will be fed into a spintronic device needs to be filtered first, to ensure that the device has a base current to work with. While spin-state filtering has been researched and achieved experimentally it is inefficient, often only reaching thirty or forty percent polarization. Other techniques have been developed that do reach up to full spin-filtering of a current, but these are expensive and time consuming since they generally require extensive lithographic work and high grade graphene sheets or carbon nanotubes. We endeavor to show that a simple series of QDs can potentially be used to efficiently spin-polarize a current, with the added bonus that current-day techniques which are well understood could be used to construct such a device.

Each system will be attached to input and output nanowires in which the g-factor is close to zero, so that any external magnetic field penetrating the device will not affect the output in the transmission lines themselves. Each system is then modeled with the Tight Binding Approximation (TBA) to the Schrödinger Equation. Mathematica is then used to solve the systems of equations generated with TBA, so that the transmission of the system can be plotted as a function of electron energy and external magnetic field. It is found that a series of Aharonov-Bohm rings in series may be useful as a spin-polarizer, and potentially as a single electron transistor. The quantum dot spin-polarizer may also be used to spin-polarize currents, but in combination with multiple Aharonov-Bohm rings, a stronger spin-polarized current may be produced.
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Chapter 1: Introduction

1.1. Spintronics

Spintronics is a portmanteau of “Spin Electronics”, and is the study of active control and manipulation of spin degrees of freedom in solid state systems for use in computation or study [1]. The typical circuit element in a modern computer specifically takes advantage of the “charge degree of freedom” of the electron [2]. This means that a bit of information is represented by the presence or absence of charge in a solid state system, like a MOSFET. Spintronic systems would take advantage, instead, of the spin degrees of freedom of the electron.

The primary impetus behind spintronic research is Moore’s Law (Fig. 1.1.1). Moore’s law states that microprocessor computing power will double every 18 months, as silicon chips become smaller [3,4].
Figure 1.1.1: A graph showing Moore's Law. Every 18 months the processing power of computers doubles as chips shrink[4].

This law, however, does not take into account the fact that once the silicon devices we use today are on the size scale of atoms, they cease to function. Even worse, these same silicon devices experience problems with leakage and heat dissipation long before they get so small. This means that the devices will have difficulty confining the electrons they need to do calculations and the heat generated by the devices will be great enough to damage the unit.

Current silicon-based chips have already hit this size-limiting problem; many people are trying to design novel devices that can perform computations which are so small that they operate at the atomic level, or the nanometer scale. The single electron transistor is one way around this problem, and is discussed later. It operates using electron charge, like a traditional microelectronic device, but also incorporates quantum
theory, so that it can function at the nanometer scale. Even so, spintronic devices may provide an equally good or better solution, and there are certainly advantages to spintronics.

Spintronics has a few advantages that seem to make it a favorable solution for making even smaller transistors [1]. First, is the enormous amount of information that could be theoretically held and processed by spin-states, through the use of qubits and the quantum entanglement of qubits.

Another big advantage to spintronics is the ability to control spin with magnetic and electric fields. Spin-states can be controlled by magnetic fields since spin is just a manifestation of a magnetic dipole moment. Electric fields can also be used to control a spin-state through things like the Rashba field effect [5], where the spin-state is made to flip because of an external electric field. Even though we can use both magnetic and electric fields to exert control over the electron’s spin-degrees of freedom, we will concentrate on how the magnetic control can be of use.

Still another advantage of spintronics over traditional electronics is spin-coherence. The spin-states of an electron have a very long relaxation time [1]. It is also difficult to destroy a spin-state with impurities in the transmitting medium or electron-electron interactions. This means that spin-states of electrons provide a very robust method for handling information.

The last reason that spintronics have gained so much interest is centered on Shor’s and Grover’s algorithms [3]. These algorithms perform basic functions; factorization of large prime numbers and the inversion of a function, respectively. Quantum computing
has the potential to increase the processing speed of these two important functions dramatically, making computers not only smaller, but even faster than previously thought.

Overall, the advantages of the spintronic quantum computer are quite impressive. Despite some of the shortcomings, like measuring the spin-states, many devices are being designed that take advantage of spin, and some are even already on the market.

**Spintronic Devices**

Many of the current spintronic devices depend on two phenomena; giant magnetoresistivity [6, 7] and electron transport through quantum dots [8]. Many other phenomena have been championed as well, but GMR is quite prevalent as it is already used in modern hard drives, and quantum dot structures hold promise as they may be easily integrated into current computing devices. Both GMR and electron transport through QDs take advantage of the fact that the two spin-states of an electron will react to potential barriers or material interfaces in different ways. Our work is centered on the transport through quantum dots and how it can be potentially used to create a spin-transistor and a spin-polarizer.

The main goal behind most spintronic research is to create spintronic analogs to current digital devices. In Fig. 1.1.2 is a short outline of the standard electronic devices and the spintronic analogs that we are trying to, or have already, created. Notice that standard electronic devices have been “unified”. This means that they all work on the same principle; all of them are made of semiconducting materials, and employ some sort
of junction to process a current or voltage. This unification also makes standard electronic devices easy to mass produce and to integrate with one another, since they all function on the same basic principles. Spintronics are not unified, as they employ many phenomena, since we are still trying to develop the basic devices. Below are descriptions of two spintronic devices that have already been built and tested.

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Figure 1.1.2: Electronics devices and their spintronic analogs.

Spin-Filters

A spin-filter is used to take a spin-unpolarized current and remove one spin-state, so that only one remains. This is often accomplished by splitting the energy levels in a QD and then somehow isolating one of the resonant Zeeman split energy levels. In Fig.
1.1.3 is a circuit that is designed to take advantage of the resonant energies of a Zeeman split QD.

Figure 1.1.3: Experimental setup of a proposed spin filter, where the space next to “E” is a quantum dot cut out of the 2DEG by the confining gate voltages. [9].

The unfortunate aspect to this particular spin-filter is that it can reach only 70% spin-polarization, at maximum. Typically only about 50% is actually achieved [9]. Currently, other spin-polarizers that have been demonstrated do not polarize a current to a very high degree either. This is quite bad for spintronics, since all computational devices require that the baseline current going into the system be very homogenous. For an electronic circuit this means rectifying alternating current into a usable direct current, and for a spintronic device rectifying a direct current further into a spin-polarized current.
Later, a potential design schematic for a simple spin-polarizer is suggested and subsequent simulation results are shown which provide a basic proof of principle.

Overview

To date, one of the biggest areas of research in spintronics is the production of spin-polarized current. While there are systems that are capable of producing this, the systems are still too large, and need to be further refined so that the overall spin-polarization of the generated current is purer. Spin-amplification is still a hot topic because a method for amplifying a spin-polarized current has yet to be rigorously demonstrated. Before any quantum computer can be built we still need to develop clever new algorithms that operate on quantum principles, since we have only Shor’s and Grover’s algorithms to work with. Graphene spintronics have recently shown a lot of promise and are being heavily researched [10, 11]. Whether or not this will provide anything useful is still up in the air. There have been some real triumphs, however, in memory. To date many computers now use spintronic-based hard drives that use GMR as the primary method of reading and writing information. These hard drives can store close to an order of magnitude more information than their counterparts. Along with this, some companies have also developed spintronic magnetic random access memory with read write times as fast as 50 nanoseconds; a significant improvement [12]. In the end, there is still a lot of work to be done before we can start to unify the methods for creating spintronic devices and then start building usable computers.
1.2. Semiconductors and the Formation of Nanoscale Devices

A semiconductor is a specific type of material that traditionally is crystalline in nature, like silicon, gallium arsenide, or germanium, all of which are very prevalent in modern micro and nanoelectronics. At absolute zero they have the property of being very good insulators, because their band structure has an intrinsic energy gap between the filled valence band and the empty conduction band (Fig. 1.2.1).

![Diagram of band structures in a semiconductor](image)

**Figure 1.2.1:** (a) Example curves of the conduction and valence bands in a semiconductor. (b) Energy versus wavevector plot for an electron in vacuum and GaAs [8].

This gap is often referred to as a forbidden zone, since an electron wave function cannot exist there. This means that electrons will tend to stay in the filled valence shells, unless they gain energy equal to or above this energy gap. By doping these materials with impurities, forming heterojunctions and structures with them, and applying external fields to them, we can exert a certain amount of control over the electrons at the valence band edge of the semiconductor structures. Under the right conditions, an electron can be given enough energy to jump past the forbidden zone and into the conduction band, so that we
can move the electron around in a predictable and useful way. Likewise, we can also simply leave the electron in the valance band. This level of control over the relative conductivity of the electrons in the structure makes these materials invaluable, as they can be used to create transistors, switches, diodes, photovoltaic cells, many kinds of detectors, and thermistors [13].

The band gap of a semiconductor is defined as the energy difference between the lowest point in the conduction band, or the conduction band edge, and the highest point in the valence band, or the valence band edge. At absolute zero, the thermal energy of the electrons is not high enough to excite electrons into the conduction band, and the material is an insulator. If the material is at room temperature, then some of the electrons may be energetic enough to jump across the band gap. When this happens, however, the valance orbital of one of the atoms in the material is now left unfilled. This electrical hole left in the orbital can be treated as a particle with charge equal to the absolute value of the electron charge. This vacant part of an orbital will react like a particle in all ways; it will respond to electric and magnetic fields; its overall wave vector will cancel out that of the electron that has been excited, meaning there will be no net change in the wave vector of the system, which is good because momentum is conserved (Fig. 1.2.2).
Figure 1.2.2: Sample band diagrams of Silicon and GaAs, showing where the electrons and their holes tend to arrange themselves [14].

Different semiconducting materials will have different band gaps relative to each other. The Fermi energy, $E_F$, of a semiconductor is related to its band gap, and a material with a large band gap will have a higher $E_F$ than that of one with a smaller band gap. This property is useful, since it is what allows us to create heterojunctions (Fig. 1.2.3).

Figure 1.2.3: A heterojunction formed by two dissimilar semiconductors. The $E$ vs $k$ plots show that the electron motion is limited to one direction [15].

A heterojunction is formed when two different semiconductors are layered one on top of the other. Layering even more semiconductors onto a system creates a
heterostructure. The difficulty in creating these systems, however, is that at the boundary between two dissimilar semiconductors a discontinuity is formed in either the valence or conduction band. This discontinuity creates a structural strain on the device. This is why certain heterojunctions are more prevalent than others. The best types of semiconductors for forming these junctions are III-V, and their solid solution counterparts. A good example of this is the Al\text{GaAs}/GaAs/Al\text{GaAs} heterostructure, where Al\text{GaAs} is a solid solution of GaAs. The lattice constant of GaAs is 5.6533 Å, and that of the ternary compound Al\text{$_x$Ga$_{1-x}$As} can have a lattice mismatch of less than 0.1% [14]. This means that the Al\text{GaAs}/GaAs/Al\text{GaAs} heterostructure has an approximately constant lattice constant [8], making the material more stable, and thus suitable for device construction.

At the boundary of dissimilar semiconductors another interesting effect takes hold, if we use modulation doping to add impurities to one of the materials. The Al\text{GaAs} layer in Fig. 1.2.4 has been doped such that it is now an n-type semiconductor, meaning that it has extra donor electrons that it can lose, without sacrificing the completeness of its electron orbitals.

![Image: Diagrams showing how the donor electrons are redistributed when two dissimilar semiconductors form a heterojunction, and the subsequent potential well created. The new potential well confines the donor electrons in a 2DEG.]
The $E_F$ of the AlGaAs is higher than that of the GaAs layer. Looking to lower their energy, the donor electrons will tend to migrate from the higher energy state, to the GaAs layer. This in turn lowers the $E_F$ of the AlGaAs layer, and raises the $E_F$ of the GaAs layer until they are equal to each other. At the boundary, however, the mismatch in energy will remain, even as the overall $E_F$ equalizes. This means that as the electrons migrate to the GaAs they will be unable to return to their donors, even after the $E_F$ have equalized. Furthermore, the donor electrons lost energy $\Delta E_C$, while the $E_F$ of the GaAs has increased. By rearranging these conduction bands a triangular potential well is formed and a large number of electrons at the barrier, forming a 2D electron gas (2DEG). For this reason we refer to the heterojunction as a low-dimensional system, since the electrons can’t move in all three directions. The carrier concentration in this region will be quite high, meaning that the electrons are highly mobile. Overall, confining the electrons and making a 2DEG makes the electron quite easy to manipulate via external fields, making heterojunctions excellent for device fabrication.

When building devices, it is often more useful to confine the electrons in a thin layer of GaAs that is sandwiched between two thicker layers of AlGaAs. This structure effectively forms a potential well barrier in the GaAs layer, and forces the electrons to travel only in the plane of the GaAs layer (Fig. 1.2.5). This high level of confinement induces electron energy quantization, and allows us to build structures that can manipulate electrons at the nanoscale in predictable and useful ways, such as quantum dots and quantum wires.
Using lithographic techniques quantum dots (QD) and quantum wires can be formed in heterostructures. One such method uses quantum point contacts (QPC) to apply an electric field perpendicular to the 2DEG (Fig. 1.2.6). This cuts the 2DEG into shapes that are then useable, and can be used to further confine electrons into even smaller regions.

Figure 1.2.5: Formation of an AlGaAs/GaAs/AlGaAs heterostructure [8].

Figure 1.2.6: A quantum dot formed by quantum point contacts emitting an electric field into the 2DEG, providing further confinement [15].
In one case we can confine the electrons to move in only one direction, creating a quantum wire. By further confining the electrons we create a quantum dot. These structures are small enough that they have a discrete, measurable energy spectrum, like an atom. For this reason we often refer to QDs as artificial atoms, and arrays of them as artificial molecules. We can also build QDs by growing them directly on the substrate, where the substrate has been chemically etched to force the growth of the QDs in only certain regions (Fig. 1.2.7). This method is also useful for building quantum wires (Fig. 1.2.8), but it is often difficult to control precisely, and requires great knowledge about the growth processes of these complex materials, as well as how the electrons are transported in them. Overall, by building systems of quantum wires and dots we can begin to build devices, such as transistors, out of them, but on the nanoscale. This has many technological implications, since the potential to scale our computational devices down by factors of 100 or more means much greater processing power than is currently available [16].

Figure 1.2.7: A quantum dot formed by confining the electron to a small area in a semiconducting heterostructure [8].
Figure 1.2.8: A quantum wire formed from a thin heterostructure. The extra confinement in the $x$ direction forces the electron to travel only in the $y$ direction [8].

1.3. Zeeman Splitting

The Zeeman Effect is a phenomenon whereby the application of an external magnetic field to a particular electron energy level causes that energy level to split into two distinct states [5]. Electrons with differing quantum numbers, $n$, $l$, and $m$, may in fact have the same overall energy. When this happens we say that the electron wave functions at this energy are degenerate. The electron, being a fermion, has an intrinsic magnetic dipole moment, $\mu_j$. This magnetic moment can align or anti-align with an external magnetic field. Electrons with the same energy, but different quantum numbers, tend to react to an external perturbation, like a magnetic field, differently, such that the degeneracy in the system is lifted. In general, an electron energy level will have pairs of electrons, and with the application of an external magnetic field one of the electrons will be polarized spin up and the other spin down. Whenever we apply an external magnetic field, the electrons in these pairs will tend to be energetically split. Typically, the spin up
electron will gain energy and the spin down will lose, although this is not the case in every material.

The total angular momentum of an electron can be written as,

$$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S,$$

(1.3.1)

where the total angular momentum, $\vec{\mu}$, is simply the combination of the total orbital angular momentum, $\vec{\mu}_L$, and the spin orbital angular momentum, $\vec{\mu}_S$, also referred to as the magnetic moment of the electron [5]. Historically, the orbital angular momentum was first recognized and manipulated with external fields. Later, via the Stern-Gerlach experiment it was found that electrons also possess an intrinsic spin. The effect that magnetic fields can have on these spin states was not well understood at first, so it is referred to as the anomalous Zeeman Effect [17]. In general, this work focuses on the anomalous Zeeman Effect, since the orbital angular momentum of an electron entering a quantum dot is not affected by the application of an external magnetic field [18]. This occurs because the electrons are being confined to a 2DEG. An electron will feel the magnetic field via the Lorentz force,

$$\vec{F} = q\vec{v} \times \vec{B}.$$  

(1.3.2)

Typically the magnetic field in the simulations, however, will be parallel to the heterostructures forming the substrate for the quantum dots. This means that the force felt by the electrons will tend to push them against the barrier that they are being confined with, so their orbital degrees of freedom are limited in the QD. This simplifies things greatly, since we can focus only on the splitting of the spin-states of the electrons, and
effectively ignore the orbital motions of the electrons. This means that the total angular momentum is $\vec{\mu}_s$.

The magnetic moment, $\vec{\mu}_s$, of an electron, or any charged particle, in free space is defined as:

$$\vec{\mu}_s = \gamma \hbar \vec{f}, \quad (1.3.3)$$

where $\vec{f}$ is the total angular momentum of the particle, and $\gamma$ is the “gyromagnetic ratio” or “magnetogyric ratio”; the ratio of the magnetic moment of the particle to its angular momentum [13]. It is useful to define another quantity, the $g$-factor, as well, which is a dimensionless constant that describes the charge to mass distribution of an electron:

$$g\mu_B \equiv -\gamma \hbar, \quad (1.3.4)$$

where $\mu_B \equiv 5.788 \times 10^{-5} \text{eV} / T$ is the Bohr Magneton. Any electron in an external magnetic field, then, when it aligns or anti-aligns with the field it will have energy:

$$U = -\vec{\mu}_s \cdot \vec{B}. \quad (1.3.5)$$

In terms of the $g$-factor this energy is:

$$U = \varepsilon_z = m_j g\mu_B B, \quad (1.3.6)$$

where $m_j$ is the azimuthal quantum number. In this case, however, since we can neglect the orbital angular momentum, $m_j = \pm \frac{1}{2}$. The $g$-factor of an electron plays a large role in how the two potential spin orientations will align with the magnetic field. For a free electron, $g$ is 2.0023, which we usually just approximate as 2 [13]. In these systems, however, the electrons are confined to a 2DEG. A common material that is used to build
semiconducting heterostructures is GaAs and the $g$-factor of this material is -0.44 [19]. If the $g$-factor of a material is below zero then the spin up electrons in the material will tend to align parallel to an external magnetic field (Fig. 1.3.1).

![Diagram showing spin up and spin down electrons under an external magnetic field](image)

**Figure 1.3.1:** The spin magnetic moment of the electron orienting itself to an external magnetic field where the $g$-factor is below zero.

In the simulation data shown later the $g$-factor is not a huge concern. The simulations incorporate the Zeeman Effect more directly, by allowing the user to simply control the amount of Zeeman Splitting that the user wants in the system. This technique is used to show the general operation of the devices.

**Effect of Resonant Transmission Through Quantum Dots**

In order to implement the Zeeman Effect in the simulations we need to know how an external magnetic field will change the energy levels of a quantum dot. In these simulations a quantum dot is modeled as being a simple double potential barrier (Fig. 1.3.2).
A QD will have an intrinsic resonant energy level, in which electrons can exist in a quasi-bound state. Electrons transmitting through a QD structure will tend to be transmitted only around the resonant energy of the QD [8]. Using the tight binding equation, one can build a model of a QD to look at how it transports electrons. In Fig. 1.3.3 is a diagram of a QD with energy $\varepsilon_{\text{qd}} = 0$. Notice, that when electrons are transmitted through the device they are indeed moving through the device at an energy that centers on the resonant energy of the QD (Fig. 1.3.4).
Figure 1.3.4: Plot of $T$ vs. electron $E$ through a single QD. The QD energy is set at 0, and the energy window is centered on the Fermi energy of the system.

If we apply an external magnetic field, however, to the system then the energy level will be Zeeman split by some amount $\pm \varepsilon_z$ (Eq. 1.3.1) [19]. The electrons that encounter this system will tend to either align or anti-align with the magnetic field, so they will either be spin up or down. Remember, however, that the energy of a spin up electron is lower than that of a spin down. This means that the spin up electrons will tend to be transmitted through the lower energy level, and the downs through the higher, assuming a $g$-factor that is negative (Fig. 1.3.5).

Figure 1.3.5: The resonant transmission through a quantum dot after its energy level has been spin-split by an external magnetic field.
1.4. System Designs

In this thesis we study three systems of QDs; multiple Aharonov-Bohm Rings (AB Rings) put in series with one another, where intermediate QDs separate the rings, and an external magnetic field applied to the system in the plane of the rings spin-splits all the QD energy levels (Fig. 1.4.1, 1.4.2); the multi-AB Ring system, but with spin-split intermediate QDs (Fig. 1.4.3); a spin-polarizer made of QDs in series with one another, where one of the dots has had its energy level split with an external magnetic field (Fig. 1.4.4).

In each of the ring systems it is assumed that every ring has a QD in each of its arms, and that these QDs have been created in a layer of bulk GaAs (Fig 1.4.1). This material has a $g$-factor of -0.44 [20], which means that the application of an external magnetic field produces a measurable change in the Zeeman Splitting Energy ($ZSE$) of the QDs. The nanowires comprising the input and outputs leads are also made of a periodic lattice of QDs, but they have been created in a layer of material that has a $g$-factor close to zero, so that they are approximately spin-neutral. A good example of a material that could be used for the leads is InAs [21]. This allows us to spin-split the energy states in the rings QDs, and examine how this affects the transmission, without having to worry about the contribution of the leads themselves. The reason for having the two different materials is that, in practice, the external magnetic field will be difficult to confine solely to the length of the ring. This makes the possibility of physically creating a system that reacts as the simulations predict more feasible. Each of the QDs in the ring is also assumed to have an energy level, $\mathcal{E}$, that can be controlled via Quantum Point
Contacts (QPC) acting as voltage gates (Fig. 1.4.1, 1.4.2) There are also QPC which act to form the QDs and are represented as the potentials between QDs, $V$ (Fig. 1.4.1, 1.4.2). It is assumed that we can control these as well. In the nanowires leading into and out of the system the energy of each QD and the coupling between each site, $V_o$, are not controllable, but are intrinsic to the material used. Fig. 1.4.2 shows how a physical AB ring might be constructed, and the QPC used to control the device.

Figure 1.4.1: A single AB Ring with input and output nanoleads and an external magnetic field parallel to the plane of the ring.

Figure 1.4.2: Construction of a physical AB Ring with quantum dots embedded in each arm of the ring [22].
In the multi-ring systems (Fig. 1.4.3, 1.4.4) we build the QDs in the same way as the single ring structure, except that we now have rings in series with one another. In the first case that we treat the intermediate dots are not affected by the application of the external magnetic field. This could be accomplished with the low $g$-factor material again. While these results prove interesting, the system itself may prove to quite impractical to build. Nevertheless, analysis of the system gives answers which explain some of the workings of the multi-ring system where the intermediate dots are made from the bulk GaAs, like the ring QDs. The splitting of the intermediate dots also makes it possible to calculate the differential spin-polarization for the multi-ring system; something not possible when they are not split. An important note about the multi-ring system with the spin-split intermediate dots: when all the QDs in the system have been spin-split, only the upper levels are connected to each other, and likewise for the lower levels, when the Tight-Binding Approximation is applied to the system. This means that an electron that is spin up will not actually have the chance to interact with a spin down electron until it either reaches the output lead or is reflected back to the input lead.

Figure 1.4.3: Multiple AB Rings in Series with one another. Notice in this diagram that the intermediate dot is not spin-split.
The final system analyzed is a series of quantum dots, where the first quantum dot is again made out of GaAs, so that its energy level can be spin-split, and the following ones are made out of something with a $g$-factor close to zero (Fig. 1.4.5). Two cases are studied; one where following the spin-split QD there is one QD with an energy level that can be tuned, $E_{qd}$, which then leads to the output of the system; a second where there are two tunable QDs after the spin-split one, and then the output lead. As before, the input and output leads are made of a material with a $g$-factor close to zero. The potentials between the controllable QDs are all set to the same value, $V$, also under our control (Fig. 1.4.5). Fig. 1.4.6 shows how a device comprised of QDs in series might be physically constructed.
Figure 1.4.6: Physical construction of quantum dots in series with one another. The leads forming the QDs are QPC formed with lithography techniques [25].
Chapter 2: Methods of Analysis

2.1. Energy Scales

In order to link the simulations to experimental work the parameters of the system are set based on typical voltages, currents, etc. found in the literature. To start, it is assumed that all of the quantum dots are built in bulk GaAs, which has a $g$-factor of -0.44 [20]. It is also assumed that the input and output leads of the system are built out of a substance that has a $g$-factor relatively close to zero, so that they are spin-neutral and don’t effect the overall spin-transmission [24,25]. One such material that can accomplish this is InAs [21]. In general we ignore the effects of the AlGaAs/InAs junctions, but further work may need to be done in order to take these effects into account. We will also say that the typical quantum dot energies in the system are around 100 $\mu$eV [19]. From the dispersion relation of the nanowires we know that the energy window of the system is $-2 \, \mu$eV $< E < 2 \, \mu$eV (Sec. 2.2). From this we can normalize the energies in the plots to the potentials in the nanowires, $V_o$, which is set to 1 $\mu$eV. Finally, we can now define the Zeeman energy scales. From (Eq. 1.3.6) we can calculate that:

$$\Delta e_z = m_i g_i \mu_B B = (-12.78 \, \mu$eV/T)$B \quad (2.1.1)$$
This allows us to also calculate the relative magnetic field needed to produce the results in the simulations. Using the dispersion relation:

\[ B = \frac{2 \mu eV}{12.78 \mu eV/T} = 0.157 \text{ T.} \tag{2.1.2} \]

This means that whenever we want to use the maximum amount of Zeeman spitting energy available we must use a magnetic field with strength 0.157 T. If the magnetic field exceeds this value the simulations cease to be realistic.

2.2. The Tight-Binding Approximation

The Tight-Binding Approximation is a single electron approximation to the Schrödinger Equation. By applying it to a 2D QD system we can calculate the electron transmission and reflection of the system as a whole. The general form of this time independent approximation is:

\[ -\sum_{m} V_{n,m} \Psi_{m} + \epsilon_{n} \Psi_{n} = E \Psi_{n}, \tag{2.2.1} \]

where \( V_{n,m} \) is the overlap integral of the potential at site \( n \) with the wave at site \( m \), and is referred to as the coupling of that site; \( \Psi_{n} \) is the electron wave function at site \( n \), and correspondingly for site \( m \); and \( \epsilon_{n} \) is the energy of the QD at site \( n \) [13, 26]. When applying this approximation it is important to choose the number of neighbors to include for each equation, since each QD will get a different equation from the others. In the simulations, we chose to use the nearest neighbor approximation, which means that when trying to figure out how the wavefunction at a particular site overlaps with those at other
sites the approximation only looks to the wavefunctions at the closest sites. In general it is possible to include second nearest, third nearest, etc., but for this work the nearest neighbor approximation should be sufficient, since it is assumed that the individual sites are far enough apart that only the nearest neighbor contribution is great enough to consider.

In principle, the Tight-Binding Approximation is an application of Bloch’s Theorem from quantum mechanics [13]. A line of quantum dots, all with the same confining potentials and site energies, will constitute a linear, periodic lattice. The potential of this structure is referred to as the “Dirac Comb” (Fig. 2.2.1).

![Figure 2.2.1: Plot of a periodic potential created by a lattice of atoms. Referred to as the "Dirac Comb" [13].](image)

When trying to solve the Schrödinger Equation for this system we can take the solution to satisfy the condition:

\[ \Psi(x + a) = A e^{iKan} \Psi(x) = A e^{i\theta n} \Psi(x), \]  

(2.2.2)

where \( \theta = Ka \), \( A \) is a periodic Bloch function that has the same periodicity as the potential, and \( e^{i\theta n} \) describes the electron as a plane wave moving through the system. By using Eq. 2.2.2 as the form of our wavefunction we can build a system of equations using
the Tight-Binding Approximation. Applying this to the nanowires that are acting as the source and drain in the systems we can calculate the dispersion relation [27] for the leads:

\[ E = -2V_o \cos \theta + \varepsilon_n. \]  

(2.2.3)

This relation is quite important, as it allows us to simplify any expression that involves the input or output leads, and it indicates that the allowed spread of electron energy levels is \(4V_o\).

Finally, in order to incorporate the Zeeman Effect into the simulation, it is necessary to treat the Zeeman-split energy levels as two separate energy levels in the Tight Binding Approximation (Fig. 1.4.1). We generally refer to these as \(\varepsilon_{up}\) and \(\varepsilon_{down}\). This means that each individual QD will actually have two separate equations describing the electron transport though the QD, one for each energy level. Correspondingly, each one of these levels will also have its own associated wavefunction in the Tight-Binding equations. This is what allows for the spin-polarization of the electrons as they traverse the device, when an external magnetic field is applied. It is important to note that this does change the simulation slightly, since each QD in the ring structure will now be coupled to the sites on either side of the ring twice. This actually increases the coupling to the adjacent sites, in relation to a ring that has no Zeeman Splitting included in it. This is accounted for by multiplying the couplings in the Zeeman split ring by \(\sqrt{2}\). This is only necessary, however, if you wish to compare the output of two systems where one incorporates the Zeeman Effect, and the other does not.

Finally, once we have the system of equations we can solve it quite readily, since the system can be represented in matrix form:
\[ \vec{M} \cdot \vec{v} = \vec{c}, \]  

(2.2.4)

where \( \vec{M} \) is the matrix formed by the equations, \( \vec{c} \) is the vector of constants associated with \( \vec{M} \), and \( \vec{v} \) is the solution vector, which holds all of the unknowns in the system of equations. Via Mathematica we can invert \( \vec{M} \) and dot \( \vec{c} \) into it, which allow us to solve for \( \vec{v} \). Once this is done we simply select the part of \( \vec{v} \) which represents the wavefunction of the site we are interested in. Taking the absolute value of that wavefunction squared allows us to then plot that wavefunction as a function of the electron energy. Typically we plot the \( T = |t|^2 \) and \( R = |r|^2 \), since the transmission tells me what output to expect from one of the novel devices [13]. In this case \( t \) and \( r \) are the coefficients of the wavefunctions at the input and output of the system. The reflection is useful since plotting the sum of the transmission and reflection tells me whether or not the simulation is functioning correctly, since that quantity should always be unity.

2.3. Weighted Spin-Polarization

The weighted spin-polarization of the transmission of one of the devices is a mathematical technique whereby the degree to which the transmission has been spin-polarized can be readily represented. It is useful to represent the transmission in this way, because it allows us to find useful regions of parameter space; those that switch the spin-polarization with only a small change in the parameters of the system; those which create a maximal spin-polarized transmission, while reducing the other significantly; those which create a spin-polarized transmission that, experimentally, would be easy to
measure or manipulate. In order to calculate the spin-polarization we first calculate the transmission of a system through only the spin up states, and then through the spin down states, i.e. we must calculate the transmission twice. Then, we can find the spin-polarization term, \[ \frac{T_{up} - T_{down}}{T_{up} + T_{down}} \], which is useful because even if the transmissions are small, the ratio may still approach unity. This helps to extract the degree of spin-polarization, even when the transmission peaks are quite narrow. When the spin-polarization term is multiplied by the transmission of one of the states, we find the degree of spin-polarization:

\[ Pol_{up} = \frac{T_{up} - T_{down}}{T_{up} + T_{down}} T_{up}, \]  
\[ Pol_{down} = \frac{T_{up} - T_{down}}{T_{up} + T_{down}} T_{down}. \]  

The polarizations of the energy state, once calculated, can also be used to find the differential spin-polarization of the system:

\[ \Delta Pol = Pol_{up} - Pol_{down}. \]  

This tells us the change in the weighted spin-polarization, and also makes finding the degree of spin-polarization produced much easier to visualize, since all spin up states will have positive values, and spin down states will have negative values, or vice versa depending on the sign of the g-factor of the material used.
2.4. Calculation of IV Curves

In order to calculate the overall theoretical current that is passing through one of the devices, the electron transmission of the system must first be found. Each system has input and output leads which correspond to the source and drain. In an experimental set-up these two contacts will be kept at different voltages, which will force the source and drain to have different electrochemical potentials. The applied voltage bias across the system can be defined as:

\[ -qV = \mu_2 - \mu_1, \tag{2.4.1} \]

where \( V \) is the applied voltage, \( q \) is the electron charge, and \( \mu_1 \) and \( \mu_2 \) are the electrochemical potentials of the source and drain respectively [28]. The source and drain will locally be in equilibrium, since we are providing a constant voltage source. This means that both the source and drain will have their own, constant, Fermi functions:

\[ f_1(E) \equiv \frac{1}{e^{\frac{E-\mu_1}{k_BT}} + 1}, \tag{2.4.2} \]
\[ f_2(E) \equiv \frac{1}{e^{\frac{E-\mu_2}{k_BT}} + 1}. \tag{2.4.3} \]

where \( E \) is the energy of an electron in the system, \( k_B \) is Boltzmann’s constant, and \( T \) is the temperature of the system [28]. The source would like the number of electrons at its Fermi energy to be \( f_1(E) \), while the drain would prefer \( f_2(E) \). This means that the drain will try to reduce the Fermi energy of the source by pulling electrons away from it and then sending them back to the power supply. The source, however, will replace those electrons with those coming from the source. In this way a steady state number of
electrons, N, somewhere between \( f_1(E) \) and \( f_2(E) \) will arise in the system, as well as a steady current. Using the Fermi functions of the source and drain, as well as the electron transmission through the system we can now calculate the current of the overall device:

\[
I = \frac{q}{h} \int_{-\infty}^{\infty} dE \ T(E) \ (f_1(E) - f_2(E)),
\]

(2.4.3)

where \( h \) is Planck’s constant [28]. This calculation is generally correct; however it is important to remember that we are assuming, by using this formula, that the current is a coherent stream of electrons. This means that none of the electrons undergo phase-breaking scattering processes that cause a change of state in an external object. More succinctly, this means that when an electron scatters off part of the lattice that it is confined in we assume that the lattice does not vibrate, or at least not very much.
Chapter 3: The Aharonov-Bohm Ring

3.1. Simulation Parameters

In the simulations of this chapter the site energies for the nanoleads, $E_{\text{site}}$, are set to 0.0, as well as the site energies of all the intermediate QDs, $E_o$ (Fig. 3.1.1). The coupling parameters between sites in the nanoleads, $V_o$, are set to 1, and this value is used as a unit of energy through the discussion. Each one of the rings has an asymmetric configuration, meaning that the site energy of the lower dot is equal in magnitude to that of the other, but always opposite in sign (i.e. odd QDs have $E = 0.1$ and even have $E = -0.1$). Any coupling constant leading to a QD in the system is set to 0.1. The external magnetic field being applied to the system is parallel to the plane of the ring structure, so that no flux is present. The limit to the external magnetic field is 0.157 T, which translates to a Zeeman Splitting energy of $ez = \pm 2 \, \mu eV$. This keeps the system within the energy window as prescribed by the dispersion relationship (Sec. 2.1). The number of rings in the system, the electron energy, and the amount of ZSE are the varied parameters.
3.2. The Multi-AB Ring System

The single AB ring (Fig. 1.4.1) is a well-studied system, in which the Zeeman Effect and the Aharanov-Bohm Effect have been used to characterize the system in great detail [26]. Further work with this system has also shown that, under certain conditions, the AB ring can spin-polarize an electron transmitted through the system. In this work we endeavor to further characterize the AB ring by linking a multitude of them in series with one another and by utilizing the Zeeman Effect to spin-split the energy levels in the systems QDs. The main objective in doing this is to generate a system which can spin-polarize a current efficiently. The results show that a series of these rings does not immediately lend itself well to being used as a spin-polarizer, but may be of use as a single electron transistor (SET), a nanoelectronic device [29,30].

A single QD will transmit electrons that are at or near the quasi-bound energy state of the QD (Fig. 1.3.4). The peak in Fig. 1.3.2 can be moved along the x-axis of the
system by simply changing the energy of its resonant energy level, which would represent higher energy electrons transmitting through the QD if you increase the QD site energy. The width of the peak can also be manipulated by increasing the couplings around the QD, which increases the width of the peak, and vice versa. In this way we can directly control the output transmission of the system. By applying an external magnetic field we can spin-split the energy level of the QD, and in this case resonance peaks will form around these two new energy levels (Fig. 1.3.5). These basic techniques for manipulating the transmission of a QD apply to a system of QDs as well (Sec 1.3).

In the case of the asymmetric AB ring we have two QDs, each with an independent energy level, through which the electrons can travel. As such the transmission will look quite similar to that of the single Zeeman split QD, but the current produced by the system will have no spin-polarized elements (Fig. 3.2.1). Applying an external magnetic field spin-splits both of the AB ring’s QDs, giving the electrons four potential paths to traverse (Fig. 3.2.2). This, however, means that the energy levels interlace with each other, requiring a greater magnetic field to separate the spin-states energetically.
Figure 3.2.1: Transmission vs. electron energy through a single AB ring without an applied external magnetic field. Electron transmission is occurring at the quasi-bound energy state of each of the QDs, where $\mathcal{E}_{QD} = \pm 0.1$.

Figure 3.2.2: Transmission vs. electron energy through a single AB ring with Zeeman splitting energy of 0.1.

The interesting phenomenon of this system arises with the addition of rings to the system. In Fig. 3.2.3 is a set of transmission results for the multi-ring system, where the intermediate dots are not spin-split (Fig. 1.4.3).
Figure 3.2.3: Transmission through the unsplit intermediate dot multi-ring system for two (a-c), five (d-f), ten (g-i), and twenty (j-l) ring structures. The leftmost graphs show no ZSE. The central graphs are for a ZSE of 0.05, and the rightmost 0.1.

With every additional ring added to the first an additional pair of peaks is added to the transmission. These extra resonances always have a higher magnitude energy than the peaks corresponding to the quasi-bound energy state that the QDs have been set at. As the ring number increases the number of these resonant peaks increases, but the energy range in which they appear stays constant, $-0.4 < E < 0.0$ for the peaks corresponding to the lower QDs’ energy levels, and $0.0 < E < 0.4$ for the upper QDs’. Notice that the edges
of the band gaps are at a slightly higher energy than that of the QDs. This effect is magnified as the site energies are set farther away from 0, the Fermi energy of the system. At high ring number, the peaks narrow and begin to form a continuum. Two conduction bands, separated by a band gap that is approximately $2\epsilon_{qd}$, form, as rings are added, so the system resembles a semiconductor (Fig. 3.2.3). By adjusting the QD site energies in the system the conduction bands can be manipulated, creating a smaller or larger band gap. This is done in real life by adjusting a gate voltage that is not used to confine the electrons (Fig. 1.1.4). This is quite interesting, since the band gap of a typical semiconductor cannot be controlled, but is an intrinsic property of the material. Unfortunately for this particular set up, the application of an external magnetic field produces rather strange results. The outer peaks, formed by the addition of extra rings beyond the first, are not spin-split by the magnetic field. This is unrealistic, since any electron energy state in a magnetic field will split into two states. The reason this occurs is the physical construction of AB rings would prevent us from allowing the intermediate QD between the rings to remain unaffected by Zeeman splitting. This manifests itself in the program first, by not spin-splitting the outer peaks, but also in the strange form of the resonances created when the external field is added (Fig. 3.2.4, 3.2.5).
Figure 3.2.4: Plot of transmission vs. Zeeman splitting energy and electron energy for the multi-ring system. Notice that the outer peaks do not split like the central ones.

Figure 3.2.5: Further transmission plots for the multi-ring system, showing the transmission at $ZSE$ of 0.2, 0.3, and 0.4, from left to right (Fig. 3.2.4).
Even though the simulation may not be very realistic, the data produced are still very instructive when trying to understand the outer peaks in the transmission at zero external magnetic field. First, the outer peaks are always present at energies higher in magnitude than that of the QD site energy associated with the conduction band in question. This is also true when the central peaks have been spin-split; the outer peaks increase in energy in order to remain at an energy that is higher than its peak in magnitude (Fig. 3.2.4, 3.2.5).

In order to produce more realistic results, the intermediate QDs are now spin-split in the simulation. From Fig. 3.2.6 it is evident that as we apply an external magnetic field to the system all of the resonant peaks become spin-split, which is what we would expect (Fig. 3.2.3 3.2.6). This is good, since the fact that all the peaks become spin-split only when the intermediate quantum dots (IQD) are as well demonstrates that in the previous simulation the transmission was limited by the unchanging IQD site energy. In effect, that site energy not being affected by the magnetic field demonstrates a few things when compared to the spin-split IQDs; the outer peaks are indeed caused by the addition of the rings; the transmission through multiple rings is highly dependent on the IQD; spin-polarized transmission through unsplit IQDs becomes “bottlenecked” at the unsplit IQD, effectively creating a system of individual rings that transmit electrons to each other, rather than a system comprised of many rings in series.
Figure 3.2.6: Transmission through multi-ring systems for two (a-c), five (d-f), then (g-i), and twenty (j-l) ring structures. The leftmost graphs show no applied external magnetic field. The central graphs show a ZSE of 0.05, and the right most 0.1.
To further understand the multi-ring system, the external magnetic field is applied in order to study the effect it has on the transmission (Fig. 1.4.4). At 0.0 Zeeman splitting energy (ZSE) the transmission is identical in form to that of the unsplit IQD system. The band gap is still slightly wider than $2\mathcal{E}_{qd}$, and the conduction bands are now confined to the energy ranges $-0.3V_o < E < -\mathcal{E}_{qd}$ and $\mathcal{E}_{qd} < E < 0.3V_o$. Like the unsplit IQD simulations, adding rings to the system causes the conduction bands to become better defined, as the transmission peaks become sharper and closer together. The application of an external magnetic field now splits all of these resonant peaks, causing the conduction bands to become even more of a continuum. Increasing the ZSE further causes the spin-polarized bands to start crossing over one another, reducing the band gap to zero when the ZSE is on the order of the QD energy levels (Fig. 3.2.6). Increasing the ZSE past three times that of the QD site energies causes the spin-polarized conduction bands to separate again, forming three individual band gaps in the transmission (Fig. 3.2.7).
Figure 3.2.7: Plot of the five ring system with varied ZSE.

Figure 3.2.8: Transmission results for the 5 ring system with spin-split intermediate dots. The amount of ZSE is (a) 0.2, (b) 0.3, and (c) 0.4, from left to right (Fig. 3.2.7).
One way we can further characterize this system, and to evaluate its potential as a nanoelectronics/spintronics device, is by calculating the tunneling current through the system (Sec. 2.4) and plotting the I-V curve of the system. In these calculations we assume that the leads are symmetric, \( \mu_L = \frac{eV_{sd}}{2} \), where \( V_{sd} \) is the applied source-drain voltage, and that the Fermi energy, \( E_F = 0.0 \). This source drain voltage will be varied, allowing us to characterize the tunneling current over the whole energy window of the transmission \( T \). Since the energies of the QDs are controllable, the band gap can be manipulated easily. Fig. 3.2.9 contains I-V plots corresponding to the transmission plots in Fig. 3.2.6.

When no external magnetic field is present the systems I-V characteristics resemble that of a semiconductor [30] (Fig. 3.2.9 a, d, g, j). Increasing the ZSE to the order of the QD site energy (\( E_{qd} = 0.1 \)) produces a linear I-V curve that resembles a conductor (Fig. 3.2.9 c, f, i, l). By increasing the ZSE further, band gaps form in the system for energies \( E_{qd} > 0.3 \) and the system returns to semiconductor I-V characteristics, but now with multiple band gaps (Fig. 3.2.6). Notice that the system’s I-V characteristics start to saturate after 5 rings have been included, meaning that past this number the I-V curves change to a lesser degree with the addition of more rings. For this reason the five ring structure is studied further, since it can provide a great deal of information about the system without sacrificing simulation time.
Figure 3.2.9: I-V Plots for the multi ring structure. The plots are arranged in similar fashion to those in Fig. 3.2.6, and each I-V plot is associated with the same transmission plot. Adding more rings makes the system more distinctly a semiconductor, until five. With more than five the system saturates and further change in the conductance is not plainly seen.
The relative spin-polarization of the five ring structure is also important to the discussion, and in Fig. 3.2.10 the contour plot shows how the differential spin-polarization (Sec. 2.3) of the multi-ring system evolves, with added ZSE. Fig. 3.2.11 contains sample differential spin-polarization plots to better illustrate the spin-polarization of the system. A majority of the time, with the application of the ZSE, the system is in a spin-mixed state. In other words, the spin-polarized transmission peaks have not been differentiated from one another in energy. At \( ZSE = 0.4 \) the system becomes fully spin-polarized, as both of the spin-states have been completely energetically separated from one another. The system presents an interesting quality then, since in previous work [26] the single AB ring was quite capable of producing similar spin-polarization, but only with a few resonant peaks for each state. Experimentally this would be difficult to measure, since the narrow resonant transmission peaks only allow a few electrons with a small energy window through the system. In this case, the conduction bands allow for a broader energy spectrum of electrons to be transmitted, meaning the spin-polarized currents produced will be stronger, and therefore easier to measure. In all the plots shown, the inter-dot coupling integrals were set to \( V_n = 0.1 \). If we increase these couplings, the resonant peaks in these conduction bands will broaden, generating a larger area of spin-polarization in the system (Fig. 3.2.12, 3.2.13, 3.2.14) [26]. In this way, the multi-ring system is acting as an even better spin-polarizer. In both cases, however, the spin-polarized currents are not physically separated at the output of the device, so a way to isolate the currents needs to be found.
Figure 3.2.10: Plot of the differential spin-polarization for the 5 ring system with varied amount of ZSE.

Figure 3.2.11: Plots of the 5 ring structure’s ΔPol with changing amounts of ZSE. The first plot, a, shows $EZ=0.0$, b $EZ=0.1$, c $EZ=0.2$, d $EZ=0.3$, e $EZ=0.4$, and f $EZ=0.5$ (Fig 3.2.10).
Figure 3.2.12: The transmission of the five ring system with varied ZSE. In this case the coupling has been increased from $V = 0.1$ to $V = 0.3$.

Figure 3.2.13: Transmission plots accompanying the contour plot above. The first plot shows (a) $EZ = 0.0$, and this value increases with each graph by 0.1, until (e), which is $EZ = 0.4$ (Fig. 3.2.12).
Figure 3.2.14: Contour plot showing the differential spin-polarization vs. $EZ$ and $E$. This is the relative spin-polarization for the system in Fig. 3.2.13. Notice that wide, spin-polarized conduction bands have been generated by the system.

3.3. Applications

From the I-V characteristics, we propose that the multi-ring system may be useful as a nanoelectronic device, the single electron transistor (SET). The typical SET operates using a gate voltage to control the tunneling current through the Coulomb Island in the device [29, 30]. The multi-ring system may serve the same function, except the external magnetic field manipulates the overall I-V characteristics. An incident electron, close to
the Fermi energy of the system, would effectively be blocked by the free standing semiconductor configuration, where ZSE = 0.0, but be allowed to pass if the system is switched to a conductor in that energy range.

In the realm of spintronics, this device may prove quite useful as either a spin-transistor or spin-polarizer. The ability of the system to create a wide energy range spin-polarized current will potentially give experimentalists the ability to generate a spin-polarized current large enough, and refined enough, to be useful as a power supply. The problem remains, however, that the system is not able to physically separate the two currents.

The device may also be useful as a spin-transistor. We have already seen its potential as a SET, but if the system is made able to physically differentiate between the spin-states, by effectively filtering the other out, then it could produce a current that uses the spin-states as signal, switching between transmitting one state or the other. Notice, however, that we need a way to physically separate the spin-polarized currents in order for this, or the spin-polarizer to work. This issue is addressed in a simple model of the spin-polarizer.
Chapter 4: The Quantum Dot Spin-Polarizer

4.1. Simulation Parameters for the Quantum Dot Spin-Polarizer

In the simulations of this chapter, the site energies for the nanoleads are set to $E_o = 0.0$. The coupling parameters between sites in the nanoleads, $V_o$, are set to 1, and this value is used as a unit of energy through the discussion (Fig. 4.1.1). The site energies for the two quantum dots will be equal, unless otherwise noted. Only the first QD will be affected by the Zeeman Effect, and it will have a site energy of $E_{qd} = 1.0$. The inter-dot coupling integrals of any path leading to a QD are set to $V = 0.2$. The limit to the external magnetic field is 0.157 T, which translates to a Zeeman Splitting energy of $EZ = \pm 2 \mu eV$. This keeps the system within the energy window as prescribed by the dispersion relationship (Sec. 1.3). The couplings between dots and the energy levels of the dots, and the ZSE are the varied parameters.
4.2. The Double Quantum Dot System

The difficulty of physically separating the spin-states of a current which has energetically separated spin-polarized currents is now addressed. To start, the system’s reaction to an external field when the filtering quantum dot (FQD) has a site energy of zero is exactly that of the single Zeeman split QD attached to input and output nanoleads (Sec. 1.3). When the FQD’s site energy is increased, the Zeeman split energy level that is closest in energy to the FQD tends to be favored over the other (Fig. 4.2.1). When the energy of the FQD equals that of one of the Zeeman split levels, that level will transmit at a significantly higher energy than the other, but only if the ZSE is high (Fig. 4.2.1, 4.2.2). If we increase the FQD site energy past that of the favored Zeeman split energy level then its transmission begins to be filtered as well, but not to the extent of the other, which will be reduced even further (Fig. 4.2.1). To optimize the spin-polarization of the system we add enough ZSE to push the resonant peaks to the edges of the energy window (Fig. 4.2.3). Tuning the FQD to one of the energy levels we can achieve a moderately spin-polarized current, where the electrons with energy equal to the favored site energy are transmitted at 100%, and those of the other peak only a little under 40% (Fig. 4.2.3).
Figure 4.2.1: Transmission plots for the DQDS. In each plot the vertical red line is at the site energy of the FQD. The two vertical black lines are at the site energies of the Zeeman split energy levels.
Figure 4.2.2: Transmission plot from the table above, where the site energy of the FQD equals that of the higher energy Zeeman split state.

Figure 4.2.3: The basic optimized DQDS. The amount of Zeeman splitting energy is increased to 1.9, and the FQD’s energy level is changed to match the upper peak. Notice that the transmission of the peak furthest from that of the site energy of the FQD is reduced by a little over 60%, a good start to producing a spin-polarized current.
4.3. The Triple Quantum Dot System

The triple quantum dot system (TQDS) produces the same results as the double quantum dot system (DQDS) when the site energy of the two FQDs are centered in the energy window (Fig. 4.3.1).

![Image of transmission plot]

**Figure 4.3.1:** TQDS transmission plot that corresponds to Fig. 4.1.1 for the DQDS (Fig. 4.2.1). The ZSE is 1.0 again.

In the identical case to that above, where the ZSE pushes the resonant peaks of the spin-split QD to the edge of the energy window, and the site energies of the FQDs match that of one of the spin-split energy states, the transmission of the favored resonant peak is at 100%. The transmission of the other peak, however, is reduced further when compared to the DQDS, so that it is nearly non-existent (Fig. 4.3.2, 4.3.3). Adding a second FQD, then, has produced an even more efficient spin-polarizer. Manipulating the couplings in the TQDS allows us to create transmission peaks which cover a wide energy range (Fig. 4.3.4, 4.3.5, 4.3.6). This provides an advantage, experimentally, since the wider energy
band will allow more electrons to tunnel through the system, creating a larger, more readily measured tunneling current. In this case there are multiple optimizations.

Figure 4.3.2: A table of transmission plots for the TQDS which corresponds to Fig. 4.2.1, so that the DQDS and TQDS can be compared.
Figure 4.3.3: The TQDS optimized, with the same parameters as those of the DQDS in Fig. 4.2.3 ($ZSE = 1.9$, $V = 0.1$, $\varepsilon_{QD} = 1.9$).

Figure 4.3.4: The optimization of the TQDS transmission, where the coupling between sites is $V = 1.3$, the $ZSE = 1.9$, and the site energy of the FQD is $\varepsilon_{FQD} = 1.9$. 
Figure 4.3.5: Contour Plot of the TQDSP, where $E_Z = 1.9$, the site energy of the FQD is $E_{FQD} = 1.9$, and the interdot coupling $V$ is varied to show how the width of the spin-polarized transmission peak changes.

Figure 4.3.6: Plots showing the $\Delta Pol$ of the transmission in Fig. 4.3.5 a) The differential spin-polarization of the TQDS when $V = 1.3$, b) $V = 0.55$. 
The difficulty with this system is that, while the transmission is covering a wide range of energies, the spin-polarization of the transmission is not immediately obvious. Notice in Fig. 3.4.6 (a) the spin-polarization at $V = 1.3$ is actually spin-mixed. In Fig. 3.4.6 (b) $V = 0.55$, and the system is spin-polarized. The disadvantage, then, is the transmission of spin-polarized electrons is only around 65% at maximum, but it still covers a wide energy range, making it feasible that the TQDS could be used to produce a spin-polarized tunneling current.

4.4. Applications of the Quantum Dot Spin-Polarizer

Both the DQDS and TQDS are relatively simple models, and both seem to spin-polarize the transmitted electrons quite well, with the TQDS achieving approximately 100% in some cases. While this simple device may potentially serve as a spin-polarizer quite well, it also demonstrates that the FQDs are capable of excluding one spin-state from being transmitted, while allowing the other to pass. This result is quite important; since in Sec. 3.3 it was noted that without a method for excluding one spin-state from the transmission, the device would only spin-polarize the current energetically. To this end, adding FQDs to the multi-ring system may prove very beneficial, in that it could become a true spin-polarizer.
Chapter 5: Future Work

The next step to be taken in this research, first, is to combine the multi-ring system with the FQD concept, so that simulation results can show if the system can be turned into a spin-polarizer that creates a wide spin-polarized conduction band.

In order to further characterize the AB ring, it is also important to note that no mention of the AB Effect is made when analyzing the multi-ring system. Additional programming is necessary to make it capable of calculating the electron transmission if magnetic flux penetrates each of the rings (Append. A). It will also be important to study how the AB Effect and the Zeeman Effect alter the multi-ring results when coupled together. It will also be important for us to further manipulate the site energies and couplings in the system.

Finally, at some point it will also be necessary to physically build the devices devised. Without experimental work the system can never be proven in real life. This is necessary if any of the units are to be made practical computing components.
Chapter 6: Summary

In this research we apply the Tight Binding Approximation to quantum dot systems and study the electron transmission produced at the output. The overarching goal of the work was to try to create a device schematic that could serve as a spin-polarizer, or as some other useful spintronic or nanoelectronic device. In spintronics the need for an efficient spin-polarizer is quite large, since without it we cannot generate a current usable by all other spintronic systems. Experimentally, many spin-polarizers have been generated, but their efficiency was too low to be promising as a spintronic power supply (Sec 1.1).

To this end, simulations using the Tight-Binding Approximation were used to model two systems, the Multi-Aharonov-Bohm Ring and the Quantum Dot Spin-Polarizer (Sec 1.4, Ch. 2). For the multi-AB ring system, the number of rings in the system was varied along with the strength of an external magnetic field. We find that the multi-ring system I-V characteristics are akin to those of a semiconductor, because of the band gap present in the transmission. With the application of an external magnetic field, the energy states of the system are spin-polarized, producing more resonant peaks and making the semiconductor qualities even better defined, when the magnetic field is small. As the field strength is increased, the band gap decreases and the system eventually
becomes a conductor. Further increasing the field strength causes the system to become a semiconductor again, but with three band gaps instead of the original one. At this point, when the system has become a semiconductor again, the spin-polarized states of the system have also been energetically isolated from one other, forming wide spin-polarized conduction bands. The switching from semiconductor to conductor makes the device potentially useful as either a single electron transistor, a nanoelectronic device, or a spin-transistor. The ability to produce wide spin-polarized conduction bands makes it a good candidate for a spin-polarizer as well. A problem arises, however, in that the system does not physically separate the spin-polarized currents it produces. This would be necessary if it were to function as either spin-polarizer or spin-transistor.

The quantum dot spin-polarizer is proposed first as a solution to the problem of producing spin-polarized currents for spintronic devices. It also is possible that the results from this device may be applicable to the multi-ring system, so that it can function as a spin-polarizer/transistor. Results are promising, in that the DQDS is able to reduce the transmission probability of one of the spin-states by 60%, while leaving the other relatively untouched. The TQDS goes even further, and reduces the other spin-state to almost 0% transmission, while allowing the other to pass, effectively generating a spin-polarized tunneling current. Manipulation of the couplings in the TQDS also provides interesting results, where increasing the coupling creates a spin-polarized conduction band that covers a large portion of the energy window. This is advantageous, since, should the device be built, the tunneling current would be large enough to be readily measured experimentally.
REFERENCES


Appendix A:
Master Program for the Multi-Ring System

Clear["Global`*"]
(*This program will generate a matrix of equations based on the tight binding approximation. The system being modeled is a series of Aharonov Bohm rings.*)

(*This part of the program defines a matrix of zeros, sized for the number of equations we want to solve. It defines a new matrix, square, sized for the number of quantum dot energies. The second matrix is parsed into the first. This gives the diagonal term of energies. After that a loop creates an array with all the QD energy levels (generates variables). After that it assigns a value to the upper dots(odd numbered) and to the lower dots(even numbered]*)

(*The variables defined allow the user to simply pick the number of rings in the system.*)
numring=n = 2;
umidot = m=n-1;
umlead=2;
numrdot = 4*n;
(*This number accounts for the number of zeeman split energy levels, not the original number before the addition of the magnetic field.*)

matdimension = d1=numidot+numrdot+numlead;
submatdimension =d2 = d1-2;

(*"main" is the primary matrix that we’re trying to build up. The matrix will be all zeroes and is the exact size needed to solve the system of equations generated for the multi-ring system.*)
main = Array[0&, {d1,d1}];
MatrixForm[main];

(*Generates a submatrix that is smaller in both dimensions than the main one by 2. The energy terms for all of the wavefuncions form a diagonal that does not sit on the main diagonal. I use "around" as an intermediate sub matrix that will be inserted into "main"*)
sub = Array[0&, {d2,d2}];
MatrixForm[sub];

(*Generates an array that holds all of the values for the onsite energies.*)
energy = Array[ε#&, {d2}];
MatrixForm[energy];

(*The loop goes through around and assignes values along it's diagonal. Note that I'm also including the fermi energy of the system, as prescribed by TBT.*)
Do[sub[[i,i]]=ε-energy[[i]],{i,d2}];
MatrixForm[main];
MatrixForm[sub];
(*Inserting around into the appropriate place inside of main, without disturbing any other part of main. It's important to do this part first. If you use this technique and start with other things, like coupling constants, you will inadvertently delete some things when you insert the energies.*)

main[[2;;d1-1,3;;d1]] = sub;
MatrixForm[main];

(*Everything above was symbolic. The two loops show how I could assign energies to, say, all the top and bottom quantum dots. You don't have to do it this way, but I want a periodic system, so I'll assume that the energies of the sites are, in some way, uniform.*)

(*Typical Bloodshed would define the energies here, but the differential spin polarization needs them defined in the last section of this program in the spin up and down modules.*)

Do[energy[[i]] = uu, {i, 1, d2 - m, 4}];
Do[energy[[i]] = ul, {i, 2, d2 - m, 4}];
Do[energy[[i]] = lu, {i, 3, d2 - m, 4}];
Do[energy[[i]] = ll, {i, 4, d2 - m, 4}];

(*The next line defines the energy level of the intermediate dots when they aren't being spin split. When they are I refer to a variable called "em"*)

Do[energy[[i]] = eem, {i, d2 - m + 1, d2, 1}];
MatrixForm[energy];

(*Inserting quantum dot energy values into the main matrix.*)

Do[sub[[i, i]] = e-energy[[i]], {i, d2}];
main[[2;;d1-1,3;;d1]] = sub;
MatrixForm[main];

(*Generate an array to hold all the values for the coupling constants. Assuming that these are also periodic, like the on site energies.*)

couple = Array[V# &, {4*n+1}, 0];
MatrixForm[couple];
couple[[1]] = 1.0;
Do[couple[[i]] = 0.1, {i, 2, 4*n + 1}];
MatrixForm[couple];

(*Generate another array that will hold the arrays of constants that will also be inserted into "main".*)

parts = Array[0 &, {n-1}];
MatrixForm[parts];

(*The coupling constants are inserted into arrays in a periodic way. Look at a matrix for two or three rings to see what this means.*)

Do[parts[[i]] = {{couple[[4*i]], couple[[4*i]]},
  couple[[4*i+1]], couple[[4*i+1]],
  couple[[4*i+2]], couple[[4*i+2]],
  couple[[4*i+3]], couple[[4*i+3]]},
  {i, n-1}];
(*The arrays of coupling constants are inserted into "main" as well as their transposes. The indecies for the insertion are easy to figure out, you just have to think about where the arrays need to be inserted (again, check out a tbt matrix for multiple rings. there is a pattern).*)

Do[main[[(numrdot+i+1);;(numrdot+i+1),3+4*(i-l);;10+4*(i-l)]] = parts[[(i,1)],(i,1-n,1)];

Do[main[[(2+4*(i-l));;(9+4*(i-l)),(numrdot+i+2);(numrdot+i+2)]] = Transpose[parts[[(i,1)]],(i,1-n,1)];

(*The equation for n=0 in my model always has the same form and number of elements, regardless of the size of the system. I'm going to manually write the arrays and simply insert them in the appropriate spots in "main". *)

n0 = { {-couple[[1]]*Exp[-I*],0,couple[[2]],couple[[2]],couple[[3]],couple[[3]]} }

MatrixForm[n0];

main[[1;;1,1;;6]] = n0;

nr = {{couple[[2]]},{couple[[2]]},{couple[[2]]},{couple[[2]]}};

MatrixForm(nr);

main[[2;;5,1;;1]] = nr;

MatrixForm[main];

(*This next array builder will generate the equation for n=1, in my numbering convention. Make sure to look at the convention I'm using to organize my matrix.*)

n1 = Array[0&, {1,d1}];

MatrixForm[n1];

MatrixForm[n1];

n1[[1,2]] = -couple[[1]];

MatrixForm[n1];

(*I'm Using n1 as an intermediate array to help construct n1. n12 will be used to construct the c column of the matrix.*)

n11 = {couple[[4+2n]],couple[[4+2n]],couple[[5+2n]],couple[[5+2n]]};

n12 = Exp[I*]*{couple[[4+2n]],couple[[4+2n]],couple[[5+2n]],couple[[5+2n]]};

MatrixForm[n11];

MatrixForm[n12];

n1[[1;;1,3+4*(n-1);;6+4*(n-1)]] = n11;

MatrixForm[n1];

main[[d1;;d1,1;;d1]] = n1;

main[[2+4*(n-1);;5+4*(n-1),2;;2]] = n12;

(*After this step the entire main matrix has been built.*)

MatrixForm[n12];

MatrixForm[main];
(*Generating an array that will hold the basic values needed to create the constants used in the matrix equation. In any system of rings the constants will always start with these five. After that, you just need the appropriate number of zeros to fill in the rest. This is easily done, since we already have a value for the main matrix dimensions.*)

constants = Array[0&,{d1,1}];
beginconstants={{couple[[1]]*Exp[I*ϕ]},{-couple[[2]]},{-couple[[2]]},{-couple[[3]]},{-couple[[3]]}};
MatrixForm[beginconstants];
constants[[1;;5]]=beginconstants;
MatrixForm[constants];
MatrixForm[main];

(*At this point the matrix and constant vector are complete, but without the intermediate dots having been spin split.*)
(*This part of the program will rework the matrix "main", so that the intermediate dots are spin split.*)
(*This part of the program will recalculate the size of the matrix. Spin splitting the intermediate dots means you need to add some extra rows and columns.*)

e=0;
gutdr=d1-m-1;
gutdc=d1-m;
diffd=d1+m;
MatrixForm[parts];

(*Define the new matrix that is "different" from "main", hence the name.*)
maindiff=Array[0&,{diffd,diffd}];
(*MatrixForm[maindiff]*)

(*Gut the old matrix "main", and put the useable bits into the new matrix.*)
maindiff[[1;;gutdr,1;;gutdc]]=main[[1;;gutdr,1;;gutdc]];
maindiff[[diffd;;diffd,1;;gutdc]]=main[[dl;;dl,1;;gutdc]];
MatrixForm[maindiff];
(*This defines a small array of coupling constants. In the tight binding there are zeros between the couplings in the portion of maindiff that characterizes the intermediate dots. In main there is no separation.*)

Do[parts[[i]] = {couple[[4*i]], 0,
           couple[[4*i+1]], 0,
           couple[[4*i+2]], 0,
           couple[[4*i+3]], 0},
   {i,n-1}];
MatrixForm[maindiff];

(*This generates a small tensor that holds two arrays to account for the splitting apart of the couplings for the intermediate dots. This does the columns. Subgen2 takes the transpose of these parts, manipulates them a little, and then does the rows. Once the appropriate arrays are built they are inserted into maindiff*)

subgen1=Array[0&, {2,9}];
gen1=Array[0&, {m}];
Do[gen1[[i]]=subgen1,{i,1,m}];
MatrixForm[gen1];
MatrixForm[gen1[[1]]];
Do[
   gen1[[i]][[1;;1,1;;8]]=parts[[i]];  
   gen1[[i]][[2;;2,2;;9]]=parts[[i]],
   {i,1,m,1}];
MatrixForm[gen1];
MatrixForm[gen1];

Do[maindiff[[gutdr+1]+2*(i-1);(gutdr+2)+2*(i-1),3+4*(i-1);11+4*(i-1)]=gen1[[i]],{i,1,m,1}];
MatrixForm[maindiff];

subgen2=Array[0&, {9,2}];
gen2=Array[0&, {m}];
Do[gen2[[i]]=subgen2,{i,1,m}]
MatrixForm[gen2];
MatrixForm[gen2[[1]]];
Do[
   gen2[[i]][[1;;8,1;;1]]=Transpose[parts[[i]]];  
   gen2[[i]][[2;;9,2;;2]]=Transpose[parts[[i]],
   {i,1,m,1}];
MatrixForm[gen2];
MatrixForm[gen2];

Do[maindiff[[2+4*(i-1);10+4*(i-1),(gutdc+1)+2*(i-1);(gutdc+2)+2*(i-1)]=gen2[[i]],{i,1,m,1}];
MatrixForm[maindiff];

(*This generates the array of spin split energy levels in the intermediate dot.*)

energyint=Array[0&, {2m}];
MatrixForm[energyint];
Do[energyint[[i]]=e-(em+ez),{i,1,2m,2}];
Do[energyint[[i]]=e-(em-ez),{i,2,2m,2}];
(*Inserting the new energies into maindiff.*)

MatrixForm[energyint];
Do[maindiff[[gutdr+i,gutdc+i]]=energyint[[i]],{i,1,2m,1}];
MatrixForm[maindiff];

(*The array of constants will be the same, but will have more zeros. This guts "constants", builds a new array of appropriate length for maindiff, and then inserts the constants into the appropriate spot in the array.*)

diffconstants = Array[0&,{diffd,1}];
diffconstants[[1;;5]] = beginconstants;
MatrixForm[diffconstants];

(*This part of the program will calculate the differential spin polarization.*)

mainup=Array[0&,{d1,d1}];
maindown=Array[0&,{d1,d1}];
mainup[[1;;d1,1;;d1]]=main[[1;;d1,1;;d1]];
maindown[[1;;d1,1;;d1]]=main[[1;;d1,1;;d1]];
MatrixForm[mainup];
MatrixForm[maindown];

(*Now that there are two matrices, one for spin up and one for spin down, we must calculate the transmission for each path seperately.*)

mc1:=Inverse[mainup];
mc2:=Inverse[maindown];
JBF1:=mc1.constants;
t1:=Part[JBF1,2];
JBF2:=mc2.constants;
t2:=Part[JBF2,2];

(*Calculation of transmission is typical, but I must define the QD energies in the modules, otherwise their values will interfere with each other.*)

tup[en_,eez_]:=Module[{},
e:=en;
eu=0.1;
el=-0.1;
ez:=eez;
eem:=ez;
uu=eu + ez;
ul=uu;
l=el+ez;
l1=1;
\[ \text{\( \theta := \text{ArcCos}\left(- \left(\frac{e}{2.0}\right)\right) \)}; \]

\[ \text{\( \text{Return}\left(\text{\( t1 \)}\right) \)}; \]

\[ \text{tdown}[\text{en}_\text{\( , \text{eez}_\text{\( ] \)} := \text{Module}[\{\}, \text{\( e := \text{en} \)}; \text{\( e_u := 0.1 \)}; \text{\( e_l := -0.1 \)}; \text{\( e_z := \text{eez} \)}; \text{\( e_{em} := e_z \)}; \text{\( u_l := e_u - e_z \)}; \text{\( u_l := uu \)}; \text{\( l_l := e_l - e_z \)}; \text{\( l_l := lu \)}; \text{\( \theta := \text{ArcCos}\left(- \left(\frac{e}{2.0}\right)\right) \)}; \text{\( \text{\( \text{Return}\left(\text{\( t1 \)}\right) \)}\];} \]

\[ \text{Manipulate}\left[\text{Plot}\left\{\text{Abs}\left[\text{tup}\left[\text{ee}, \text{eez}\right]\right]^2\right\}, \text{ee}, -0.5, 0.5\right\}; \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \{\text{eez}, 0, 1.0\} \]

\[ \text{Manipulate}\left[\text{Plot}\left\{\text{Abs}\left[\text{tdown}\left[\text{ee}, \text{eez}\right]\right]^2\right\}, \text{ee}, -0.5, 0.5\right\}; \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \{\text{eez}, 0, 1.0\} \]

("Below I define new functions that will eventually lead to "deltapol", which is the differential spin polarization for the system.*)

\[ \text{tup1}[\text{en}_\text{\( , \text{eez}_\text{\( ] \)} := \{\text{Abs}\left[\text{tup}\left[\text{en}, \text{eez}\right]\right]^2\}; \]

\[ \text{tdown1}[\text{en}_\text{\( , \text{eez}_\text{\( ] \)} := \{\text{Abs}\left[\text{tdown}\left[\text{en}, \text{eez}\right]\right]^2\}; \]

\[ \text{polgen}[\text{ee}_\text{\( , \text{eez}_\text{\( ] \)} := \text{Abs}\left(\text{tup1}\left[\text{ee}, \text{eez}\right] - \text{tdown1}\left[\text{ee}, \text{eez}\right]\right) / \left(\text{tup1}\left[\text{ee}, \text{eez}\right] + \text{tdown1}\left[\text{ee}, \text{eez}\right]\right)\}; \]

\[ \text{polup}[\text{ee}_\text{\( , \text{eez}_\text{\( ] \)} := \text{tup1}\left[\text{ee}, \text{eez}\right] \ast \text{polgen}\left[\text{ee}, \text{eez}\right]; \]

\[ \text{poldown}[\text{ee}_\text{\( , \text{eez}_\text{\( ] \)} := \text{tdown1}\left[\text{ee}, \text{eez}\right] \ast \text{polgen}\left[\text{ee}, \text{eez}\right]; \]

\[ \text{deltapol}[\text{ee}_\text{\( , \text{eez}_\text{\( ] \)} := \text{polup}\left[\text{ee}, \text{eez}\right] - \text{poldown}\left[\text{ee}, \text{eez}\right]; \]

\[ \text{Plot}\left[\text{polup}\left[\text{ee}\right], \{\text{ee}, -0.5, 0.5\}, \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \]

\[ \text{Plot}\left[\text{poldown}\left[\text{ee}\right], \{\text{ee}, -0.5, 0.5\}, \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \]

\[ \text{Plot}\left[\text{poldown}\left[\text{ee}\right], \{\text{ee}, -2.0, 2.0\}, \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \]

\[ \text{Manipulate}\left[\text{Plot}\left[\text{deltapol}\left[\text{ee}, \text{eez}\right], \{\text{ee}, -2.0, 2.0\}, \text{Axes} \rightarrow \text{False}, \text{Frame} \rightarrow \text{True}, \right. \right. \]

\[ \left. \left. \text{PlotRange} \rightarrow \{-1.2, 1.2\}, \text{PlotStyle} \rightarrow \{\text{AbsoluteThickness}\left[2.8\right]\}, \text{FrameLabel} \rightarrow \{"E","T"\}, \text{BaseStyle} \rightarrow \{"\text{Times}, 20\}\}; \text{ImageSize} \rightarrow \{500, 500\}\right]; \{\text{eez}, 0, 1.0\} \right. \right. \]
PlotRange → {-1.2, 1.2}, PlotStyle → {AbsoluteThickness[2.8]},
FrameLabel → {"E", "T"}, GridLines → {{}, {{-1.0, Dashed}, {1.0, Dashed}}},
BaseStyle → {"Times", 20}, ImageSize → {500, 500}, {ezz, 0, 1.0}]

Needs["PlotLegends"]
ShowLegend[ContourPlot[deltapol[ee, eez], {ee, -1.2, 1.2}, {ezz, 0, 0.6}, PlotPoints → 100, Contours → 15, PlotRange → {-1., 1.}, FrameTicks → {Automatic, Automatic, None, None}, ImageSize → {500, 500}, FrameLabel → {"E", "EZ"}, PlotLabel → "Transmission", BaseStyle → {"Times", 20}, {ColorData["LakeColors"][1 - #1] & /@ {10, 1}, LegendLabel → None, LegendShadow → None, LegendPosition → {1., -.7}}]
Appendix B:

Spin Polarizer with Two Quantum Dots

Clear["Global`*"

v0=1.0; v=0.2;

ea=1.5; eb=-ea; e1=ea;

M:={
-v0*Exp[-I*θ],0,v,v},
{v,v*Exp[I*θ],e-ea,0},
{v,v*Exp[I*θ],0,e-eb},
{0,(v0*Exp[2*I*θ]+(e-e1)*Exp[I*θ]),v,v}}

MatrixForm[M]

v0=1.0

MatrixForm[M]

Mc:=Inverse[M];
const:={v0*Exp[I*θ],-v,-v,0};

u:=Mc.const;

t1=Part[u,2];
rl=Part[u,1];

T1[en_]:=Module[{},
    e:=en;
    θ:=ArcCos[-(e/v0)/2.0];
    t:=t1;
    Return[(t)]
];

R1[en_]:=Module[{},
    e:=en;
    θ:=ArcCos[-(e/v0)/2.0];
    t:=r1;
    Return[(t)]
];

Plot[{Abs[T1[ee]]^2 },{ee,0-2.0,2.0},Axes->False,Frame->True,
PlotRange->0.0,1.2],PlotStyle->AbsoluteThickness[2.8]],
FrameLabel->{"E","T"},
BaseStyle->"Times",20]]

Plot[{Abs[R1[ee]]^2 },{ee,-2.,2.},Axes->False,Frame->True,
PlotRange->0.0,1.0],PlotStyle->AbsoluteThickness[2.8]],
FrameLabel->{"E","T"},
BaseStyle->"Times",20]]

Manipulate[Plot[{Abs[T1[ee,ee1,vv,eea]]^2 },{ee,-2.,2.},Axes->False,Frame->True,
PlotRange->0.0,1.2],PlotStyle->AbsoluteThickness[2.8]],
FrameLabel->{"E","T"},GridLines->{},
BaseStyle->"Times",20]
Appendix C:  
Spin Polarizer with Three Quantum Dots

Clear["Global`*"]

M:=\{-v0*Exp[-I*\[Theta]],0,v,0\},
{v,0,e-ea,0,v},
{v,0,0,e-eb,v},
{0,v0*Exp[2*I*\[Theta]],v,v,e-e1},
{0,(v0*Exp[3*I*\[Theta]]+(e-e2)*Exp[2*I*\[Theta]]),0,0,v0}\)

const:={v0*Exp[I*\[Theta]],-v,-v,0,0};
MatrixForm[M]
MatrixForm[const]
v0=1.0;v=0.2;
e1=1.5;e2=1.5;

Mc:=Inverse[M];
u:=Mc.const;
t1=Part[u,2];

tup[en_,eez_]:=Module[{},
e:=en;
ea=eb=eez;
\[Theta]:=ArcCos[-((e/v0)/2.0)];
t:=t1;
Return[(t1)]
];

tdown[en_,eez_]:=Module[{},
e:=en;
ea=eb=-eez;
\[Theta]:=ArcCos[-((e/v0)/2.0)];
t:=t1;
Return[(t)]
];

tup1[en_,eez_]:={Abs[tup[en,eez]]^2};
tdown1[en_,eez_]:={Abs[tdown[en,eez]]^2};

polgen[ee_,eez_]:=Abs[(tup1[ee,eez]-
tdown1[ee,eez])/(tup1[ee,eez]+tdown1[ee,eez])];

polup[ee_,eez_]:=tup1[ee,eez]*polgen[ee,eez];
poldown[ee_,eez_]:=tdown1[ee,eez]*polgen[ee,eez];

deltapol[ee_,eez_]:=polup[ee,eez]-poldown[ee,eez];

Manipulate[
Plot[deltapol[ee,eez],[ee,-2.0,2.0],Axes->False,Frame->True,
PlotRange->{-1.2,1.2},PlotStyle->{AbsoluteThickness[2.8]},
FrameLabel->{"E","T"},GridLines->{{},{{-1.0,Dashed},{1.0,Dashed}}},
BaseStyle->{"Times",20},ImageSize->{500,500},{eez,0,1.0}]}
Appendix D:

Program for a Single Aharonov-Bohm Ring

Clear["Global`*"]
e1=0.01; e2=-0.01; em=0.;
v0=1.0;
v1=0.1; v3=0.1; v4=0.1; v2=0.1
e1u:=e1+ez; e1d:=e1-ez;
e2u:=e2+ez; e2d:=e2-ez;

M:={{v0*Exp[-I*θ],0,v1,v1,v2,v2},{v1,v3*Exp[I*θ],e-e1u,0,0,0},{v1,v3*Exp[I*θ],0,e-e1d,0,0},{v2,v4*Exp[I*θ],0,0,0,e-e2u,0},{v2,v4*Exp[I*θ],0,0,0,0,e-e2d,0},{0,-v0,v3,v3,v4,v4}}

(*v0:=1.;
e:=2*v0*Cos[θ];*)
MatrixForm[M]

Mc:=Inverse[M];
const:={v0*Exp[I*θ],-v1,-v1,-v2,-v2,0};

u:=Mc.const;
t1=Part[u,2];
r1=Part[u,1];

T1[en_]:=Module[{},
e:=en;
ez:=0.08;
θ:=ArcCos[-((e/v0)/2.0)];
t:=t1;
Return[(t)]
];
R1[en_]:=Module[{},
e:=en;
θ:=ArcCos[-((e/v0)/2.0)];
t:=r1;
Return[(t)]
];

Plot[{Abs[T1[ee]]^2 },{ee,-2.,2.},Axes->False,Frame->True,
PlotRange->{0.0,1.0},PlotStyle->{AbsoluteThickness[2.8]},
FrameLabel->{"E","T"},
BaseStyle->{"Times",20}]

Plot[{Abs[R1[ee]]^2 },{ee,-2.,2.},Axes->False,Frame->True,
PlotRange->{0.0,1.0},PlotStyle->{AbsoluteThickness[2.8]},
FrameLabel->{"E","T"},
BaseStyle->{"Times",20}]

Plot[{Abs[T1[ee]]^2 +Abs[R1[ee]]^2 },{ee,-2.,2.},Axes->False,Frame->True,
PlotRange->{0.0,1.1},PlotStyle->{AbsoluteThickness[2.8]},
FrameLabel->{"E","T"},
BaseStyle->{"Times",20}]

Plot[{}]
Appendix E:

Routine for Calculating IV Curves of Nanodevices using Simpson’s Rule

(*This routine calculates the theoretical current for the devices. It uses Simpson’s rule to integrate the transmission of the system. It relates the Fermi energy of the system and its electron transmission to applied voltages, and finds the current from this integration [28]. Credit goes to Sadeq Malakooti for building this code.*)

(*The variables are defined as follows:
- $ef$ is the Fermi energy of the leads. These need to be set to zero, so that the dispersion relation holds for the transmission/reflection calculations.
- $k$ is Boltzman’s constant in ev/T.
- $q$ is the ambient temperature around the device in Kelvin.
- $\beta$ is just the inverse of boltzman’s constant times the temperature.
- $\kappa$ is a parameter which controls how the voltage is applied to the system. If the voltage is applied evenly to the system (half at one end, the rest at the other end), then it is equal to 0.5.
- $v$ is the voltage being applied across the system*)

```math
ef := 0.0;
k := 8.6174 \times 10^{-5};
q := 300;
\beta := 1/(k \times q);
\kappa := 1/2;
IV = Function[e, (Abs[T[e]]^2) \times (1/(Exp[\beta \times (e - ef - (1 - \kappa) \times v)]) + 1) - 1/(Exp[\beta \times (e - ef + (\kappa \times v)]) + 1)];
Simpson1[a0_, b0_, m0_] :=
Module[{a = N[a0], b = N[b0], m = m0, k},
  h = (b - a)/(2 \times m);
  SumEven = 0;
  For[k = 1, k < m - 1, k++,
    SumEven = SumEven + IV[a + h \times 2 \times k];
  ];
  SumOdd = 0;
  For[k = 1, k < m - 1, k++,
    SumOdd = SumOdd + IV[a + h \times (2 \times k - 1)];
  ];
  Return[h/3 \times (IV[a] + IV[b] + 2 \times SumEven + 4 \times SumOdd)];
];
current = Simpson1[-2.0, 2.0, 100];
```

Plot[current, {v, -5, 5}, Axes -> False, Frame -> True, FrameStyle -> Thick, FrameLabel -> {"$V_{sd}$ (Volts)" , "I (\mu A)"}, BaseStyle -> {"Helvetica", 22, Bold}, PlotStyle -> {AbsoluteThickness[3]}, PlotRange -> {{-1, 1}}, ImageSize -> {500, 500}]