Quantum dot quantum computation in III-V type semiconductor

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Quantum Dot Quantum Computation in III-V type Semiconductor

by

Sanjay Kumar Prabhakar

A Dissertation submitted to the University at Albany, State University of New York in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy

College of Nanoscale Science and Engineering
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Abstract
Among recent proposals for next-generation, non-charge-based logic is the notion that a single electron can be trapped and spin of the electron can be manipulated through the application of gate potentials. In the thesis, there are two major contributions of the manipulation of electron spin. In regard to the first contribution, we present numerical simulations of such a spin in single electron devices for realistic asymmetric potentials in electrostatically confined quantum dot. Using analytical and numerical techniques we show that breaking in-plane rotational symmetry of the confining potential by applied gate voltage leads to a significant effect on the tuning of the electron g-factor. In particular, we find that anisotropy extends the tunability to larger quantum dots in the GaAs case. Although the same extension of tunability exists in the InAs quantum dot case, we find a new effect in the InAs case. The new discovery is that broken in-plane rotational symmetry due to the Rashba spin-orbit coupling in an asymmetric potential results in a significant reverse effect in the tuning of the electron g-factor. This effect can not be observed in symmetric case. The derivative of the g-factor with respect to the electric field has the opposite sign in the above two potentials.

The manipulation of Berry phases of spin in nano-scale devices is a topic that has received recent attention as a promising candidate for solid state quantum computation and non-charge-based logic devices. A single electron in an electrostatically defined quantum dot located in a 2 dimensional electron gas (2DEG), for example, can be trapped and the spin can be manipulated by simply moving the center of mass of the quantum dot adiabatically along a closed loop in the 2D plane via the application of gate potentials. In relation to the second contribution, we present numerical simulations and analytical expressions for the spin-dependent electron propagator (a matrix-valued function of position) for an electron trapped in a quantum dot, while the center of mass of the quantum dot is adiabatically moved in the 2D plane in the presence of the Rashba and Dresselhaus spin-orbit interactions. We apply the Feynman disentangling technique to determine the non-abelian matrix Berry phase, we find exact analytical expression for the propagator in three cases: (a) pure Rashba coupling; (b) pure Dresselhaus coupling; and (c) a combination of equally strong Rashba and Dresselhaus couplings. For other cases of interest where the solution of the propagator can not be found analytically, we present results obtained by numerically solving the Riccati equation resulting from the disentangling procedure. We also find that the presence of both spin-orbit couplings leads to a larger spin-flip probability than what would result from either mechanism considered separately.
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List of Publications:

[1] Sanjay Prabhakar and James E Raynolds
   Gate Control of a QD single electron-spin in realistic confining potentials: anisotropic effects

   Manipulation of single electron spin in a GaAs quantum dot through the application of geometric phases: the Feynman disentangling technique
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   Manipulation of the Lande g-factor in InAs Quantum Dots through application of anisotropic gate potentials
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   Gate Control of a quantum dot single-electron spin through Geometric Phases: Feynman Dis-entangling method

[5] Sanjay Prabhakar and James E Raynolds
   Gate control of a single electron spins in realistic asymmetric confining potentials in III-V semiconductor quantum dot
   MRS symposium Boston 2007

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   Gate control of single-electron spins in GaAs/AlGaAs semiconductor quantum dot
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[7] Sanjay Prabhakar and James E Raynolds
Gate control of single electron spins: a multi-scale numerical simulation approach
American Physical Society, 2008 APS March Meeting, March 10-14, 2008

[8] Sanjay Prabhakar and James E Raynolds
Gate control of single electron spins through Berry Phase in a realistic asymmetric confining potentials in III-V semiconductor quantum dots American Physical Society, 2009 APS March Meeting, March 16-20, 2009

[9] Sanjay Prabhakar, James E Raynolds and Akira inomata
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Chapter 1

Introduction and Background

Electrons confined at the interface of an AlGaAs/GaAs heterojunction due to different band offset with the help of gate potentials form a 2 Dimensional Electron Gas (2DEG). This offers a promising system in the low dimensional semiconductor nanostructures (LD-SNs) such as quantum dots, wires, and even wells in the potential applications of light emitting diodes, logic devices, for example, OR gates, AND gates, quantum dot quantum computation and quantum information processing and others. An electron in a 2DEG allowed to move in the z direction is a quantum dot. Quantum dots have been studied in order to find physical realizations of qubits, fundamental to quantum computation.

The continuous research efforts in both the semiconductor industry and in academics have made it possible to design systems on the size of the Bohr atomic radius in manipulating the quantum nature of quantum dots. The spin degree of freedom in GaAs quantum dots has attracted attention for many reasons but two of them are important. First, electron spin in a quantum dot provides a natural quantum two level system which is suitable for data storage and encoding information as a qubit. Second, the spin in this type of system is weakly coupled to the environment due to electron orbital degree of freedom which provides longer coherent time than decoherent time. This is a very important property of electrons in a quantum dot for quantum processors in a quantum computer, in order to keep information encoded for a longer period of time.

Even though the best experimental data shows that we can control and manipulate electron spin in a quantum dot as a qubit in a quantum computer, it is still far away from mass production in the semiconductor industry. However, the spin in a quantum dot is strongly decoupled from the environment and thereby from leakage of information to the external world. Information can be stored in a semiconductor dot as electron spin direction values which should be decoupled from environmental fluctuations. The orbital degree of freedom of such spin is used for spin manipulation for data storage purposes.

Such spin manipulation is possible due to two different types of spin-orbit interactions in a GaAs quantum dot. One kind of spin-orbit interaction is due to structural inversion symmetry, refereed to as Rashba coupling. The other kind of spin orbit interaction is due
to Bulk inversion asymmetry, which is referred to as Dresselhaus coupling. The strength of these two couplings depends on the electric field of a gate potential. Manipulation of electron spin with the help of these electric fields is described in more detail in Chapters 4 and 5.

The goal of the present work is to utilize state-of-the-art numerical techniques based on the Finite Element Method to study electrostatically defined quantum dots, and to explore the fundamental physics of single-electron spin to provide realistic information for the practical design of such systems. A key result of the present work is the discovery that spatial symmetry breaking resulting from the anisotropy of realistic confining potentials offers an enhancement of the electric-field tunability of the electron g-factor over that found for symmetric potentials for dots larger than roughly 65 nm.

Indeed, symmetry plays a key role in spin-orbit interactions in systems such as the one considered in this work. The Dresselhaus and Rashba coupling terms are manifestations of spin-orbit interaction arising due to bulk inversion asymmetry and quantum well confining potential asymmetry respectively. The forms of these interactions are well established and have been used in many studies [5, 7]. It is also generally understood that the Zeeman splitting depends on the direction of an applied magnetic field and is thus described by a g-factor tensor. Some authors have also explored the effects of asymmetry of quantum dot confining potentials in coupled quantum dot systems [4, 9]. But a subject that seems to have received little attention is the question of anisotropy effects in a single dot, which is the subject of the present investigation.

Cyclic variation of external parameters often leads to a net evolution involving a phase depending only on the geometry of the path traversed in parameter space. We provide numerical and analytical expressions of the transition probability of electron spin of a quantum dot moving under the influence of spin-orbit interaction. The physical movement of a quantum dot adiabatically in the plane of 2DEG in a closed loop is a topological effect. We also discuss the exact analytical expressions of the propagator of the electron moving under the influence of spin orbit interaction. A key result of Chapter 5 is the discovery that one can enhance the transition probability of electron spin over pure Rashba or pure Dresselhaus cases considered separately. More specifically, by the application of in-plane gate potentials, one can manipulate electron spin in a quantum dot which moves adiabatically along a closed loop under the influence of spin orbit interaction.

1.1 2DEG in III-V Type Semiconductor

In Fig. 1.1 the presence of electric fields due to material mismatch in III-V type semiconductor creates the band-bending expected at the AlGaAs/GaAs interfaces. We know that electrons accumulate at the corners of the quantum well due to band bending at the heterojunction. In fact, only one heterojunction is required to trap electrons as shown in Fig. 1.1. Generally, the donors in the AlGaAs layer are purposely separated from the
Figure 1.1: Electrons in the donor-doped AlGaAs fall into the GaAs potential well and become trapped. As a result, the undoped GaAs becomes n-type, without the scattering of the ionized donors which is typical of bulk n-type material. The thin sheet of charge due to free electrons at the interface forms a 2DEG.

interface by around 100Å. Using this configuration, we can achieve a high electron concentration in the channel while retaining high mobility, since the GaAs channel region is spatially separated from the ionized impurities which provide the free carriers [1, 6, 10–12].

Mobile electrons generated by the donors in the AlGaAs diffuse into the small band gap GaAs layer, and they are prevented from returning to the AlGaAs by the potential barrier at the AlGaAs/GaAs interface. The electrons in the almost triangular well form a two-dimensional electron gas (2DEG). Sheet carrier densities as high as \(10^{12} \, cm^{-2}\) can be obtained at a single interface such as that shown in Fig. 1.1. Ionized impurity scattering is greatly reduced simply by separating the electrons from the donors. Also screening effects due to the extremely high density of the 2DEG can reduce ionized impurity scattering further. In properly designed structures, the electron transport approaches that of bulk GaAs with no impurities and mobility is limited by lattice scattering.

1.2 Single Charge Tunneling via Ultra Small Tunnel Junctions

With the advance in recent years of fabrication process techniques such as electron beam lithography and optical lithography, it is now possible to design tunnel junctions of increasingly smaller dimensions to the size of the atomic Bohr radius, thereby decreasing the capacitance \(C\). Suppose the charging energy of tunnel junctions is \(E_c = e^2/2C\). If it becomes larger than the thermal energy \(k_B T\) then it is important to study experimentally
and theoretically the I-V characteristics of such junctions for the application of CMOS technology [8].

It is possible to design such tunnel junctions in the plane of 2DEG formed by semiconductor heterostructures. Metal-insulator-metal tunnel junctions produced by electron beam lithographic techniques are widely studied. The general setup consists of two pieces of metals separated by a thin insulating barrier where one can inject and detect electron spins. The working principle of such devices is explained in more detail in the following sections. The metal may be either normal ferromagnetic materials or super conducting materials at low temperatures.

Classically, there is no electrical transport through the barrier and the junction will act like a simple capacitor of capacitance C. The junction may be charged by connecting it to the external circuit. The charge at the junction can be written as $Q = CV$ where $V$ is the voltage across the junction. A very small shift of the electrons by a tunneling process to the quantum dot formed in the plane of 2DEG from the two leads will cause a small change in $Q$. In contrast to the charge motion in the electrodes, this type of transport process gives the charging energy $E_C = e^2/2C$.

Suppose the charge $Q$ on the junction is controlled by the external circuit of current $I$. At zero temperature, a tunneling process between the two leads, from the charge $Q$ to $Q - e$ through the junction, is possible only if

$$
\Delta E = \frac{Q^2}{2C} - \frac{(Q - e)^2}{2C} > 0.
$$

(1.1)

The above condition is satisfied only if $Q > e/2$ or if the voltage across the tunnel junction $U > U_c = e/2C$. Suppose the charge $|Q|$ is less than $e/2$ in an ideal current biased junction. In this case, the junction is charged by the external current. When the charge $Q$ at the junction is greater than $e/2$ then one electron may tunnel into the available states in the quantum dot and thereby decrease the charge on the junction below the threshold $e/2$. The above process starts again. The process where the frequency $f = I/e$ is determined by the external bias current $I$ is called Single Electron Transistor (SET) oscillations.

The argument as mentioned above, there will be no current if the external voltage is smaller than $e/2C$. Greater than this voltage, one finds that the average current is determined by an ohmic-current voltage characteristic with tunneling resistance $R_T$ shifted the voltage by $e/2C$ at zero temperature. This type of shift is called the Coulomb gap and the phenomenon of suppression of the current below $U_c$ is referred to as Coulomb Blockade.

The detailed working principle and control of electron spin in a single electron transistor through gate potentials are described in Chapter 4 and 5.
1.3 Berry Phase with GaAs Quantum Dot

The time evolution of a quantum system is fully described by the time dependent Schrödinger equation. We would like to see the eigenvalues and wave functions of such Hamiltonian by changing some parameter adiabatically. In such cases, the understanding of the time evolution operator will become important. The surprising discovery by Berry in 1984 found that a quantum state has an extra in addition to the familiar dynamical phase if the quantum state moves adiabatically in a closed loop [3]. The extra phase factor and its generalizations became known as the “Berry Phase”. The Berry Phase was first observed by Pancharatnam in 1986 by the rotation of polarization of a classical light field in a twisted fibre bundle [2]. In Chapter 5, I will discuss in more detail realization of the Berry Phase for both degenerate and non degenerate systems in the cyclic rotations of a quantum dot in the presence of spin orbit interactions.

Two concepts are important in order to understand the evolution of the Berry Phase in a quantum system. They are “Anholonomy” and “Adiabaticity”.

Anholonomy is a geometrical phenomenon in which non-integrability of the quantum state alters some variables in the system so that the system returns to the original state by an extra geometric phase [14]. The simplest examples of anholonomy are the parallel transport of vectors, change in the direction of swing of a Foucault pendulum after one complete rotation of the earth, and change in the direction of the linear polarization of light in a coiled optical fibre. The anholonomy described here is a quantum mechanical effect where the phase of a state is parallel transported around a closed loop.

The meaning of adiabaticity in quantum and in classical mechanics is slow change, and therefore denotes the working principle of any system at the border between dynamics and statics. The variables in the Hamiltonian can be choosen to move the quantum state in a closed cycle. If the motion of the state is slow then the adiabatic theorem guarantees that the quantum state will return to its original state with a nontrivial geometric phase called the Berry Phase which is the manifestation of anholonomy. This is the study of our interest.

1.4 Overview of the Thesis

In chapter 2, we give an overview of the literature about suitable candidates for quantum computation.

Chapter 3 presents a brief review of density-functional theory that can be used to find the conduction band diagram of an AlGaAs/GaAs heterojunction. The computational solution of the eigenvalues and wave functions of the ground and first excited states is reviewed, followed by a discussion of the AlGaAs/GaAs conduction band. We utilize a multiscale multiphysics simulation strategy based on the finite element method to provide a realistic description of the physics of single-spin devices in three dimensional geometries.
The gate-induced electrostatic potentials that cause the formation of a quantum dot in the plane of a two dimensional electron gas (2DEG) at the AlGaAs/GaAs heterojunction can be used to manipulate the electron spin in a single electron transistor.

Chapter 4 presents the key results of the thesis. When additional gates provide the lateral confinement, a single electron can be trapped in a GaAs quantum dot whose orbital states in an external magnetic field perpendicular to the 2DEG are well known Fock-Darwin states. We consider the effect of Rashba and Dresselhaus spin orbit interactions in the Fock-Darwin spin doublet ground state in a quantum dot. Using the effective mass approximation and a numerical approach based on the Finite Element Method, we show that the tunability of the electron g-value extends to a large quantum dot radius through the application of electric and magnetic fields in anisotropic realistic confining potentials.

Chapter 5 presents an additional mechanism of controlling the electron spin through geometric phases with the application of gate potentials. The Hamiltonian of the quantum dot in the plane of 2DEG is exactly diagonalized for a case of anisotropic confining potentials in the presence of external electric and magnetic fields. Analytical expression of the Berry Phase for a distortion confining potential for non degenerate case has been discussed. With the help of the Feynman disentangling method, the analytical solutions of the propagator of the Hamiltonian of a quantum dot in the presence of spin orbit interaction is found for three different cases: (a) Pure Rashba; (b) Pure Dresselhaus; and (c) equal strength of Rashba and Dresselhaus coupling. For the general case, when the solution becomes non-trivial, numerical solutions of such a propagator is carried out for several values of the radius of the closed orbit where the quantum dot moves adiabatically.

Chapter 6 presents the results of our calculations. Breaking the in-plane rotational symmetry of the confining potentials leads to a significant effect on the tunability of
the electron g-value with applied gate potentials. In particular, anisotropy extends the
tunability to larger quantum dot radii. One can switch the electron spin in several times
by revolving the quantum dot adiabatically in a closed loop.
Chapter 2

Quantum Computers Reviewed

In this chapter, we review the principles of quantum computation and some of the quantum computers presently available.

2.1 Quantum Computation

2.1.1 Principles

Moore’s law, describing a long term trend in the development of computing hardware, states that the number of transistors in an integrated circuit doubles in nearly every 18 - 24 months. The exponential increase of the number has not yet reached its saturation level. However, as Gershenfeld [47] pointed out, if we make the transistors smaller and smaller, then the width of the node in a transistor that stores a bit of information becomes comparable to the size of the atomic Bohr radius in next two decades. In such a scale the rules of classical physics are no longer applicable. Quantum effects will dominate.

As is well-known, a bit (binary digit) is the basic unit of information in classical devices, whereas a qubit (quantum bit) is the basis of quantum information. Classical bits are manipulated through Boolean logic gates. In contrast, quantum gates correspond to unitary transformations on quantum states. A quantum computer consists of many qubits whose time-evolutions are controllable by unitary operators. In 1982, Richard Feynman [42] suggested that the quantum computer is most suitable for simulation of a quantum mechanical system. In 1985, David Deutsch laid out for the first time a mathematical foundation for quantum computer and quantum circuits.

In classical computing, a bit of information, defined as a variable that can take only two values, either 0 or 1, is prepared and stored by a digital device or by a physical two-state system. The qubit, the quantum counterpart of the classical bit, also can have two possible values, 0 and 1, here corresponding to two quantum states, $|0\rangle$ and $|1\rangle$, respectively. In general, a qubit is represented as a linear combination of $|0\rangle$ and $|1\rangle$,

$$|\Psi\rangle = a|0\rangle + b|1\rangle,$$

(2.1)
where $a$ and $b$ are complex numbers satisfying the normalization condition,

$$|a|^2 + |b|^2 = 1.$$ 

The normalization condition is needed in order to interpret the state vector $|\Psi\rangle$ as the probability amplitude. Thus the qubit is characterized by two complex numbers subjected to the normalization condition (i.e., three real numbers). This means that a qubit can contain more information than a classical bit.

For example, the spin states of a spin 1/2 particle may be used as a foundation of qubit values\cite{62}. The spin-up state and the spin-down state are usually identified with $|0\rangle$ and $|1\rangle$, respectively. Then a particular qubit value is given by a spin state pointing in a particular direction, which is indeed described by a superposition of the up and down states. Two real numbers are the angles specifying the direction of spin, while the remaining real number contributes as an unimportant phase of the state.

The basic principles in quantum mechanics are assumed to be valid in quantum computation.

(a) **Superposition principle**: If $|\alpha\rangle$ and $|\beta\rangle$ are possible states, a linear combination of the two, $a|\alpha\rangle + b|\beta\rangle$, is also a possible state. Here $a$ and $b$ are complex numbers satisfying the condition, $|a|^2 + |b|^2 = 1$.

(b) **Schrödinger equation**: The quantum state $|\psi(t)\rangle$ of a quantum system characterized by the Hamiltonian $H$ evolves with time by obeying the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H|\psi(t)\rangle$$ 

as

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$$

where $U(t, t_0)$ is the unitary operator given by

$$U(t, t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}.$$ 

(c) **Probability interpretation**: Suppose $|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of a physical observable $Q$ belonging to eigenvalues $a$ and $b$ respectively. Suppose the system is in a superposition state $a|\alpha\rangle + b|\beta\rangle$. If $Q$ is observed, then the superposed state collapses to either $|\alpha\rangle$ with probability $|a|^2$ or $|\beta\rangle$ with probability $|b|^2$.

A quantum computer is a collection of a finite number of qubits, i.e., a quantum computer consisting of $N$ qubits may be considered a quantum register of size $N$. If we prepare $N$ qubits, then we can realize a superposition of $2^N$ states. The base states in binary form are defined by a direct product of $N$ single binary states. For instance, if
$N = 2,$

$$|00\rangle = |0\rangle \otimes |0\rangle, \ |01\rangle = |0\rangle \otimes |1\rangle, \ |10\rangle = |1\rangle \otimes |0\rangle, \ |11\rangle = |1\rangle \otimes |1\rangle.$$  

An arbitrary state of the $N$ qubit quantum computer is given by a superposition

$$|\Psi\rangle = \sum_{i=0}^{2N-1} c_i |i\rangle$$

where

$$\sum_{i=0}^{2N-1} |c_i|^2 = 1.$$  

This can also be expressed in terms of the binary states $|0\rangle$ and $|1\rangle$ as

$$|\Psi\rangle = \sum_{a_1=0}^{1} \sum_{a_2=0}^{1} \cdots \sum_{a_N=0}^{1} c_{1,2,\ldots,N} |a_1\rangle \otimes |a_2\rangle \otimes \cdots \otimes |a_N\rangle.$$  

The state of the quantum computer is characterized by $2(2^N - 1)$ independent real parameters (disregarding the unimportant global phase). While the memory in a classical computer is proportional to the number of bits, the memory of a quantum computer increases as an exponential function of the number of qubits.  

For example, a general state of a 2 qubit computer is

$$|\Psi\rangle = c_0|0\rangle + c_1|1\rangle + c_2|2\rangle + c_3|3\rangle$$

or

$$|\Psi\rangle = c_{00}|00\rangle \otimes |0\rangle + c_{01}|00\rangle \otimes |1\rangle + c_{10}|10\rangle \otimes |0\rangle + c_{11}|11\rangle \otimes |1\rangle$$

or, in short

$$|\Psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle.$$  

with

$$|c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c_{11}|^2 = 1.$$  

Evidently the two qubit state involves 4 arbitrary complex numbers (i.e., 8 real numbers) which is constrained by the normalization condition. If a global phase containing a real parameter is ignored, then the state depends on $8 - 2 = 6$ or $2(2^2 - 1) = 6$ real parameters.  

Quantum gates are constructed by unitary transformations. Single qubit gates include the Hadamard gate and the phase-shift gate, both of which are represented by 2-dimensional unitary matrices. The former acts as

$$U_H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad U_H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle),$$

with

$$|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad \overline{|0\rangle} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).$$

$$\overline{|0\rangle} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).$$
and the latter acts as

\[ U_\delta |0\rangle = |0\rangle, \quad U_\delta |1\rangle = e^{i\delta} |1\rangle. \]

The most important 2 qubit gate is the controlled NOT gate, which works like the classical XOR (exclusive or) gate, namely,

\[ CNOT(|x\rangle \otimes |y\rangle) = |x\rangle \otimes |x \oplus y\rangle \]

where \( x \oplus y = x + y \mod 2 \). It can be expressed by a \( 2 \times 2 \) unitary matrix. In general, an arbitrary \( 2^N \) dimensional unitary operator acting on \( N \) qubit states can be decomposed into the one-qubit gates and the two-qubit CNOT gate. Quantum computation can be performed by a \( 2^N \) dimensional unitary transformation in combination with the gate operations. Such a unitary transformation converts \( 2^N \) states simultaneously, and enables carrying out \( 2^N \) parallel computations. This is the unique feature of a quantum computer that makes quantum computation much faster than classical calculation.

### 2.1.2 Entangled Quantum States

Another important feature of quantum states is what is called entanglement [38, 51, 66]. The quantum state of a quantum computer is not necessarily factorizable in the form

\[ |\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle. \]

A state which cannot be factorized is called ‘entangled.’ The Bell base states for a two qubit state are the entangled states,

\[ |\Phi_1\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \]

\[ |\Phi_2\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) \]

\[ |\Phi_3\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \]

\[ |\Phi_4\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) \]

which can be generated from \( |00\rangle, |10\rangle, |01\rangle \) and \( |11\rangle \), respectively, by the Control NOT gate. Such an entangled state has a remarkable property.

Let us take the entangled state \( |\Phi_3\rangle \). Let the first entry of the state be the control bit and the second be the target bit. Then the entangled state shows that if the control qubit is in \( |0\rangle \) the target qubit is in \( |1\rangle \) and that if the control qubit is in \( |1\rangle \) the target qubit is in \( |0\rangle \). That is, once the first state is observed the second is uniquely determined. The entangled
state is precisely the one used in the Einstein-Podolsky-Rosen (EPR) paradox [38]. As predicted by Bell’s theoretical study [21] and confirmed by the experiment by Aspect et al [16], there can be, via an entangled state, strong nonlocal correlations between two events separated by a macroscopic distance. Entanglement is a key element of quantum teleportation.

### 2.1.3 Quantum Decoherence

In quantum computing, it is important to perform unitary transformations while the state is coherent. To build a quantum computer, the injected coherent state should be isolated from the environment. In practice, however, interaction between the quantum computer and the environment is inevitable, and decoherence will always occur. But the superposition principle does not work if the states are not coherent. This means that error in quantum computation increases with time.

The main issue for the design of a quantum computer is to maintain a low decoherence time [15]. For quantum computing, it is desirable that $\tau_{\text{dec}} \gg \hbar/\Delta E$ where $\tau_{\text{dec}}$ is the decoherence time and $\Delta E$ is typical energy splitting in a two level system. The coherent time $\tau_c$ should be sufficiently longer than the running time of computation. Let $\tau_s = \hbar/\Delta E$ be the minimum time required to execute one quantum gate operation. In principle, the larger the ratio $m = \tau_c/\tau_s$ is, the smaller the computational error becomes. Below is the road map for the characteristic time in seconds for the solid state quantum computer of different materials [44].

<table>
<thead>
<tr>
<th>Possible candidate for qubit</th>
<th>$\tau_s$</th>
<th>$\tau_c$</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trapped ions</td>
<td>$10^{-14}$</td>
<td>$10^{-1}$</td>
<td>$10^{13}$</td>
</tr>
<tr>
<td>Nuclear spin</td>
<td>$10^{-3}$</td>
<td>$10^{4}$</td>
<td>$10^{7}$</td>
</tr>
<tr>
<td>Electron quantum dot</td>
<td>$10^{-6}$</td>
<td>$10^{-3}$</td>
<td>$10^{3}$</td>
</tr>
<tr>
<td>Electron spin</td>
<td>$10^{-3}$</td>
<td>$10^{4}$</td>
<td>$10^{7}$</td>
</tr>
</tbody>
</table>

### 2.1.4 Quantum Error Correction

A quantum computer should be able to maintain coherence during the process of computation on a macroscopic scale. To accomplish this, it must be protected from decoherence due to various environmental disturbances. And hardware improvements can help maximize this protection. It is also desirable to make error corrections at the software level. It may appear that such error correction in a quantum computer cannot be done in principle. As soon as an error is detected, the wave packet must collapse into a particular state and coherence will be lost. Furthermore, according to the no-cloning theorem, it is not possible to duplicate any state in a quantum computer.

Peter Shor and others [22, 63] discovered a remarkable algorithm that can make error corrections without losing quantum coherence issue. The quantum error correction code
they proposed is a quantum generalization of the classical error-correction code. It works by encoding this information of one qubit as a highly entangled state of nine qubits. The basic idea for quantum error correction is to control several quantum systems which are initially prepared in the same state. If the quantum states are each completely isolated then there should be no errors due to decoherence, and each quantum system will act independently. Suppose one state in the group acts differently due to decoherence or noise. This breaks the symmetry and produces errors in the system. This type of error in the state can be corrected with the help of the correction code. The quantum error correction code which can help to protect quantum information against errors due to decoherence or noise.

2.2 Quantum Computers

Possible Candidates for Quantum Computation

1. Ion-Trapped Quantum Computer.
4. Quantum Dots Quantum Computer.
5. Superconductor Quantum Computer.

2.2.1 Ion-Trapped Quantum Computer

A number of cold ions interacting with laser light and moving in a linear trap provides a realistic physical system to implement a quantum computer. The distinctive features of this system are: (a) it allows the implementation of n-bit quantum gates between any set of ions; (b) decoherence can be made negligible during the whole computation; and (c) the final read out can be performed with unit efficiency [30, 68]. The ions can be linearly trapped and their eigenstates can be manipulated with high efficiency by using the method of quantum jumps. Their decoherence time can be made negligible. In this system, all cold ions in the linear trap have the same charge. These charges repel each other by the coulomb repulsive force so that motion of any single ion can be transferred to its neighboring ions. A single ion can be brought in motion by directing a laser pulse to that particular ion. Since the inter-ion separation is much larger than the the wavelength of the laser pulse, no other ions in the linear trap are affected, and further, decoherence time can be made negligible. This result is a realistic physical system to implement a quantum computer. This idea was first proposed by Cirac and Zoller [30].

Different laser beams in a standing wave configuration are brought in contact with N laser cooled ions confined in a linear trap. The motion of the ions along all three directions
can be described in terms of normal modes of anisotropic potentials of frequencies $v_x << v_y, v_z$. These frequencies are greater than the photon recoiling frequency corresponding to the transition used for laser cooling. The coulomb repulsive force between the charged ions provides a physical mechanism of controlling a NOT-gate between ground and first excited state of the ions. Finally, quantum data is transferred between different ions by utilizing a particular quantized mode of the phonon [24, 29].

This idea has been successfully implemented experimentally in controlled NOT-gate operation of a linearly trapped ion by using a single mode trapped Beryllium ion and two of the ion’s internal hyperfine structure states [36]. Tunable spin -spin interactions have been experimentally realized by simultaneous coupling of ground and first excited states of two and three linearly trapped $^{171}\text{Yb}^+$ ions along the closely spaced transverse modes of motion. An optical-spin-dependent force is applied on such modes, and Bell state entanglement fidelities of greater than 96% are found [43, 54, 67, 74, 85]. Another group claimed that Bell state entanglement fidelities of $(89 \pm 2)\%$ can be achieved for two ytterbium ions confined in two independent traps separated by 1 meter. The qubits in this system are encoded between the long-lived hyperfine “clock” states, and mediated photons carrying frequency can be implemented [61, 64].

There is another proposal for the manipulation of qubits in linearly trapped ions for quantum computation. In this case, the linearly trapped ions act as a quantum dot and one can move that quantum dot adiabatically in a closed loop with the help of laser beams. This type of idea is called geometric manipulation of trapped ions for quantum computation [37, 65, 84]

### 2.2.2 Nuclear Magnetic Resonance Quantum Computer

Direct manipulation and detection of nuclear spin states of an atomic nucleus in a magnetic field with the help of radio frequency electromagnetic waves is a well-developed field known as Nuclear Magnetic Resonance (NMR). The NMR signal from a single molecule is very weak and its quantum state is completely impossible to detect for large number of logic operations for quantum computing. To avoid this difficulty, one needs to use a large number of identical copies of the molecule to amplify the signal for qubit operations. This can be easily achieved because a few milligrams of a chemical compound will contain the required number of molecules. However, keeping the same coherent states of the molecules in the device during the entire computational work is another challenge for the design of a quantum computer and logic devices [33, 34, 46, 52, 53, 76, 79]

The Hamiltonian of a spin $-1/2$ particle in a static magnetic field $B_0$ along the $\hat{z}$ direction is

$$H_0 = -\hbar \gamma B_0 I_z = -\hbar \omega_0 I_z = \begin{bmatrix} -\hbar \omega_0 / 2 & 0 \\ 0 & \hbar \omega_0 / 2 \end{bmatrix}$$

where $\gamma$ is the gyromagnetic ratio of the nucleus and $I_z$ is the angular momentum operator
along the z direction. Here $\hbar \omega_0$ is the energy difference between the eigen value of spin up and down and is called the Zeeman splitting.

For nuclear spins in molecules like $^1\text{H}, ^{13}\text{C}, ^{19}\text{F}$, there are more than one spin present and all have 1/2 nuclear spins. Nature provides two different dominant mechanisms for the interaction of these spins: (a) direct-dipole coupling and (b) indirect through-bond electron-mediated interactions.

The Hamiltonian of the nuclear spins interacting through dipole coupling is given by

$$H_{1,2}^D = \frac{\gamma_1 \gamma_2 \hbar}{4r^3} \left[ (\vec{\sigma}_1 \cdot \vec{\sigma}_2) - 3 (\vec{\sigma}_1 \cdot \hat{n}) (\vec{\sigma}_2 \cdot \hat{n}) \right]$$

(2.3)

where $\hat{n}$ is the unit vector along a line joining the two nuclei and $\sigma$ is the magnetic moment vector.

The second interaction between nuclear spins is also called J-coupling or indirect coupling or scalar coupling. The interaction mechanism in this coupling is mediated by electrons shared through a chemical bond; and the state of the electronic cloud is perturbed by the internal magnetic field seen in the nucleus. These perturbed states interact with another nucleus through the overlap of the electronic wave function. The Hamiltonian of the coupling in this case can be written as

$$H_{1,2}^J = \frac{\hbar J}{4} Z_1 Z_2 + \frac{\hbar J}{8} [\sigma_+ \sigma_- + \sigma_- \sigma_+]$$

(2.4)

where J is the coupling strength between two nuclear spins. In liquid, interacting nuclear species may have vastly different precession frequencies and the J value may be very weak. In this case, the second term in Eq. (2.4) becomes very small. So the Hamiltonian takes the form

$$H_{1,2}^J \approx \frac{\hbar J}{4} Z_1 Z_2$$

(2.5)

The state of a spin 1/2 particle can be manipulated also by applying an electromagnetic field $\vec{B}_1(t)$ which rotates in the $\hat{x}-\hat{y}$ plane with frequency $\omega_{rf}$ at or near the spin precession frequency $\omega_0$. The single-spin Hamiltonian corresponding to a radio frequency (RF) field is given by

$$H_{rf} = -\hbar \gamma B_1 \left[ \cos (\omega_{rf} t + \phi) \sigma_x - \sin (\omega_{rf} t + \phi) \sigma_y \right]$$

(2.6)

where $\phi$ is the phase of the RF field and $B_1$ is the amplitude.

In practice, an oscillating magnetic field is applied in a direction perpendicular to the static magnetic field $B_0$ along a fixed axis in the laboratory frame. This oscillating field splits into two counter-rotating fields. The first component of the field rotates at $\omega_{rf}$ in the direction of spin so as to set on or near resonance with that spin. The other component of the magnetic field rotates in the direction opposite to that of the spin so as to set very far off-resonance (by about $2\omega_0$) [17, 28, 48].
2.2.3 Cavity Quantum Electrodynamics Quantum Computer

In Cavity Quantum Electrodynamics (QED), atoms are placed in cavities of very high Q and if the wavelength of light is equal to the dimensions of the cavity then the optical modes can be used to encode or process quantum information. There are only one or two optical modes available in the cavity. The electric fields in the cavity are very high and the dipole coupling between the atom and such electromagnetic fields is very strong. Because of high Q, photons in the cavity will get a chance to interact many times with the atoms before escaping from the cavity. This unique property opens the doors to new and exciting phenomena which manifestly rely on the quantum nature of the atom-field interaction for the design of single or double qubit quantum computers [26, 63]. The process of trapping atoms, ions, or molecules in the cavity can be explained by the working principle of Fabry-Perot cavity QED.

A Fabry-Perot cavity is made from two plane parallel mirrors of very high reflectivities. The light incident normally on the mirror from outside enters and goes multiple reflection before escaping from the cavity. The atoms and the light in the cavity will interact through dipole interaction \( \vec{d} \cdot \vec{E} \) where \( \vec{d} \) is the dipole moment and \( \vec{E} \) is the electric field. The electric field of the mode inside the cavity is given by

\[
\vec{E} = i \vec{e} E_0 \left[ a e^{ikr} - a^\dagger e^{-ikr} \right]
\]

(2.7)

where \( k = \omega/c \) is the wave vector, \( E_0 \) is the field strength, \( \epsilon \) is the polarization of the light, and \( r \) is the position where the field is measured. \( a \) and \( a^\dagger \) are the raising and lowering operators of the photons in the cavity mode. The Hamiltonian of the photons in the cavity can be written as

\[
H_{\text{field}} = \hbar \omega a^\dagger a
\]

(2.8)

where \( \hbar \omega = E_2 - E_1 \). \( E_2 \) and \( E_1 \) are the two eigen energies of the atom in the cavity. The transition between these two eigen states produces photons which can be used to perform quantum computation in two different ways. In one approach, a quantum bit can be encoded by photon states, using cavities with atoms to provide nonlinear interactions.

In the second approach, qubits can be encoded by atomic states by using photons to communicate between the atoms. The final state can be read out by using a photomultiplier tube, enabling application in quantum computation or logic devices.

2.2.4 Superconductor Quantum Computer

Accordingly, one of the most attractive approaches for the building blocks of quantum computing and logic devices is a Josephson Junction devices in superconductive technology because it offers devices with little dissipation, ultrasensitive magnetometers, electrometers for state readout, large-scale-integration, and a family of classical electronics that could be used for quantum bit control. The qubits in this system are superconduct-
ing circuits made of Josephson junctions and operating at very low temperatures such as in the millikelvin range. Information is stored in either the charge on a nanoscale superconducting island, the flux or phase drop in a circulating current, or in the energy levels in a single junction [18, 23, 59].

Recent progress in the fabrication of high quality superconducting materials such as Josephson Junction devices offers an attractive possibility for the realization of qubits for quantum computation and quantum information processing. A Josephson Junction is formed by two semiconductor electrodes separated by a thin dielectric barrier where tunneling of charges can be brought about with the help of either gate potentials or external magnetic fields. Different kinds of quantum effects such as quantum tunneling, coherent oscillations of flux between two different degenerate eigen states, and entanglement of superconducting qubits, have been observed in Josephson Junction type devices, by several groups [56, 60, 71, 77, 81]. Quantum bits can be controlled for the realization of quantum logic gates in suitable Josephson Junction devices. These superconducting devices have been fabricated by well advanced lithographic techniques [18, 25, 75].

Two different possibilities of the realization of superconductor quantum bits have been proposed for mass production in the semiconductor industry. The first kind of device is a low capacitance superconducting Josephson-Junction where charge can be manipulated as a qubit with basis states differing by one cooper pair in an electron box. The tunneling of charges in an electron box can be manipulated by an applied gate potential [18, 58, 75]. On the other hand, flux can be manipulated as a qubit near a degenerate eigen state in a Josephson Junction ring type of geometry with the help of external magnetic fields. In this case, flux qubits are the superpositions of coherent oscillations of flux eigen states between degenerate levels [50, 62, 81].

**Josephson Junction Charge Qubit**

A schematic diagram of a Josephson Junction charge qubit is shown in Fig. 2.1(a). A small superconducting island is connected to a superconducting reservoir by a Josephson tunnel junction of capacitance $C_J$ and Josephson coupling energy $E_J$. The island or electron box has $n$ excess cooper pairs relative to some neutral reference state. A gate voltage $V_G$ is applied to one end of the reservoir of capacitance $C_G$. Here $C_G \leq 10^{-15} F$ and gate capacitances can be chosen smaller than $C_G$. It means, the charging energy is always the dominating parameter over the Josephson energy, i.e. $E_c \gg E_J$. The charge on superconducting islands is referred to as the quantum degree of freedom. The Hamiltonian for coherent single cooper-pair tunneling in the Josephson superconducting junction is given by

$$H = 4E_c(n - n_G)^2 + E_J \cos \phi$$

(2.9)

Here $E_G = \frac{e^2}{2(C_G + C_J)}$ is the single electron charging energy. $\phi$ is phase of the supercon-
Figure 2.1: (a) Superconducting Josephson Junction charge qubit is formed in a superconducting electron box which is separated by a Josephson tunnel junction from a superconducting reservoir. (b) The charging energy of the superconducting tunnel junction is plotted against the normalized gate charge $n_G$ for different numbers of extra Cooper pairs [59].

The working principle of the above device is same as a quantum dot formed in a single electron transistor. When $n_G$ is approximately equal to a half-integer and the charging energies of two adjacent states (i.e. $V_G = \frac{C_G V_0}{2\pi}$) are close to each other, then the Josephson tunneling states mixes strongly as shown in Fig. 2.1(b). The voltage in the gate can be applied near a degenerate state where only two charge states $|0\rangle$ and $|1\rangle$ play a role in the tunneling process. In this case, the superconducting charge box starts working as a qubit.

Finally, the quantum state must be read out for the data transfer. This can be done by coupling Josephson charge qubit to the single electron transistor. In this case, the transistor has weak coupling to the qubit for turned off voltage. On the other hand, the dissipative current through the single electron transistor destroys the phase coherence of the qubit within a short time of turn on voltage.

**Josephson Junction Flux Qubit**

The schematic diagram of a Josephson Junction flux qubit in a superconducting quantum interference device is shown in Fig. 2.2.4(a). It consists of a superconducting ring geometry followed by one or several Josephson Junctions where flux is always the dominating
parameter, i.e. $E_J >> E_C$. The flux is referred to as quantum degree of freedom. If the magnetic flux bias is equal to $\Phi_0/2$ where $\Phi_0 = \pi \hbar/e = 2.07 \times 10^{-15} \text{Wb}$, then its potential energy has two symmetric minima and the flux can tunnel between these two symmetric minima as shown in Fig 2.2.4(b). It means degenerate ground state energy is split into two parts, the superconducting energy difference $\Delta E$, and the mixed energy states which have two quantum flux states. Therefore, if we maintain decoherence time in the system low enough then the magnetic flux will oscillate back and forth between these two symmetric quantum flux states at the frequency $\Delta E / 2\pi \hbar$ [27, 31, 56, 60, 71, 77, 78, 81]. The Hamiltonian of a single Josephson Junction can be written as

$$H = -E_J \cos \left( \frac{2\pi \Phi}{\Phi_0} \right) + \frac{(\Phi - \Phi_x)^2}{2L} + \frac{Q^2}{2C}$$

(2.11)

where $\Phi$ is the magnetic flux, $\Phi_x$ is the externally applied magnetic flux, and $L$ is the self-inductance of the superconducting loop. The first two terms in the Hamiltonian forms the double quantum well near $\Phi = \Phi_0/2$ shown in Fig (b). Finally, the quantum flux qubit can be read out by the external control parameter of the magnetic field in the superconducting quantum interference device (SQUID).

### 2.2.5 Quantum Dot Quantum Computer

Quantum dot single electron spin in a single electron transistor is another research proposal within existing semiconductor technology for the next generation of solid state quantum computing and non-charge-based logic devices [19, 20, 32, 39, 57]. Electric fields generated by gate potentials can be used to manipulate single electron spin in a III-V type
semiconductor quantum dot device formed in a single electron transistor [35, 55, 69, 70].

The understanding and manipulation of topological phases in a single electron transistor through active modification of spin-orbit interaction in a quantum dot formed in the plane of a two dimensional electron gas offers an attractive option for the design of solid state quantum computing and non-charge-based logic devices [40, 45, 49, 82, 83]. Accomplishing gate control of single electron spin in a quantum dot through geometric phases can extend the possibilities of next generation spintronics logic devices. Adiabatic control of electron spin in a degenerate eigen state provides a new mechanism for manipulating such spins via non-abelian matrix Berry phase [41, 72, 73, 80].

A schematic diagram of the working principle of a single electron transistor based qubit is shown in Fig. 2.3. The electrons are injected into the ground state of the semiconductor layer from a ferromagnetic material and the injected electron is spin split because of the Rashba interaction. This electron spin can be trapped in the quantum dot by coulomb blockade energy. The spin-splitting energy can be varied with the help of gate potentials externally applied to the dot. Its spin orientation encodes a qubit. Arbitrary qubit rotations can be brought in resonance or out of resonance to the global ac magnetic field via appropriate variation of amplitude and duration of the gate potentials applied to the dot. Finally, the current induced between the two ferromagnetic layers under an applied gate potential can be measured with existing semiconductor technology. Thereby, a qubit spin orientation can read out in a single electron transistor. The ferromagnetic layer for spin injection is known a polarizer and spin detection is known an analyzer.

A Single Electron Transistor consists of two tunnel junctions sharing by a common electrode of low capacitance known as the island. The electrical potential of the island can be tuned via the variation of a gate potential which is capacitively connected to the island. When a positive voltage is applied to the gate, the energy level of the island is lowered and one electron from the left lead tunnels into the vacant energy level of the island and finally tunnels from there to the right lead [20].
Figure 2.3: Schematic diagram of a prototype single-electron-transistor.
Chapter 3

Numerical Calculations of AlGaAs/GaAs Band Diagram

To understand the band structure of AlGaAs/GaAs, it is necessary to deal with the many-electron problem. Here we start with reviewing standard approximation methods for a many-electron system, which include the Hartree method, the Hartree-Fock method with electron exchange effects, and the Hohenberg-Kohn-Sham density functional theory with exchange and correlation effects. Common to these approaches is to solve a coupled single-electron equations self-consistently. Then we report our numerical calculations for the AlGaAs/GaAs band diagram. We solve the single-electron wave equations coupled with the electrostatic Poisson equation self-consistently to determine an asymmetric triangular quantum well, the energy eigenvalues and the corresponding wave functions for the ground and first excited states of electrons in the AlGaAs/GaAs heterojunction. We also obtain numerically the wave functions for a quantum dot of radius 20 nm confined in an assumed potential with a characteristic parameter $l_0 \approx 20$ nm.

3.1 Self-Consistent Single Electron Equations

Hartree introduced the self-consistent single-electron equation, the so-called Hartree equation, which contains the effects of the atomic Coulomb interaction and the electron-electron repulsive interaction. Taking Pauli’s exclusion principle into consideration, Fock modified the Hartree equation by antisymmetrizing the $N$-electron wave function. The modified equation, called the Hartree-Fock equation, involves the electron exchange effects in addition to the interaction potentials possessed by the Hartree equation. Using the second quantization method, Hoehberg, Kohn and Sham derived self-consistent equations including exchange and correlation effects, which are applicable to inhomogeneous electron gas.
3.1.1 The Hatree Method

The Hamiltonian for an atom of \( N \) electrons is written as

\[
H = \sum_{i=1}^{N} H_i
\]  

(3.1)

where

\[
H_i = -\frac{\hbar^2}{2m} \nabla_i^2 + U_i(r_i).
\]  

(3.2)

The potential term consists of two parts,

\[
U(r_i) = U^{\text{ion}}(r_i) + U^{\text{el}}(r_i)
\]  

(3.3)

where the first term is the Coulomb potential on the \( i \)th electron due to bare nuclei fixed to points \( \mathbf{R} \) of the Bravais lattice,

\[
U^{\text{ion}}(r_i) = \sum_{\mathbf{R}} \frac{Ze^2}{|r_i - \mathbf{R}|},
\]  

(3.4)

and the second term represents interelectronic interactions,

\[
U^{\text{el}}(r_i) = \sum_{j \neq i} \frac{e^2}{|r_i - r_j|},
\]  

(3.5)

the summation being over all values of \( j = 1, 2, ..., N \) except for \( j = i \).

The wave function for a system of \( N \) electrons may be expressed as a function of the coordinates of electrons; namely, \( \Psi(r_1, r_2, \ldots, r_N) \). In the so-called Hartree approximation, the wave function is assumed to be a product of \( N \) single electron wave functions, that is,

\[
\Psi(r_1, r_2, \ldots, r_N) = \psi_1(r_1)\psi_2(r_2)\cdots\psi_N(r_N),
\]  

(3.6)

where \( \psi_i(r_i) \) is the normalized wave function of the \( i \)th electron located at position \( r_i \). Furthermore it is assumed that the wave function obeys the energy eigen-equation,

\[
H\Psi = E\Psi.
\]  

(3.7)

The goal is to find the one-electron wave functions \( \psi_i \) from (3.7).

The electron interaction potentials depend not only on the position \( r_i \) of the \( i \)th electron but also coordinates \( r_j \) of other electrons. Therefore the Schrödinger-like eigen-equation (3.7) is not separable to a collection of single-electron Schrödinger equations. Since there are more than \( 10^{11} \) electrons in the AlGaAs/GaAs channel, it is hopeless to solve the equation of type (3.7), even numerically. To simplify the interaction potentials (3.5), the electrons surrounding the \( i \)th electron are altogether treated as a smooth distribu-
tion of negative charge with charge density \( \rho(r) \). Then the interaction potentials can be expressed as

\[
U_{i}^{el}(r_i) = - \int dr' \rho(r') \frac{e}{|r_i - r'|}.
\]  

(3.8)

The charge density due to the surrounding electrons is given by

\[
\rho(r) = -e \sum_{j \neq i} |\psi_j(r)|^2.
\]

(3.9)

Since \( \psi_j(r) \) is normalized, it is obvious that

\[
\int \rho(r) \, d^3r = -(N - 1)e
\]

(3.10)

which is the total electronic charge interacting with the \( i \)th electron. Substitution (3.9) into (5.68) yields

\[
U_{i}^{el}(r_i) = \sum_{j \neq i} \int d^3r' |\psi_j(r')|^2 \frac{e^2}{|r_i - r'|}.
\]

(3.11)

which is a function of \( r_i \). With the potentials (3.4) and (5.70), the \( N \) particle wave equation (3.7) can be separated into the one-electron Schrödinger equations,

\[
\left[ -\frac{\hbar^2}{2m} \nabla_i^2 + U_{i}^{ion}(r_i) + U_{i}^{el}(r_i) \right] \psi_i(r_i) = \varepsilon_i \psi_i(r_i),
\]

(3.12)

where \( E = \sum_i \varepsilon_i \). This is usually referred to as the Hartree equation \[89\].

It is possible to derive the Hartree equation by the variational method from (3.7) with the trial function (3.6). The energy expectation value of the \( N \) electron system is given by

\[
\langle \Psi | H | \Psi \rangle = \sum_i \int \psi_i^*(r_i) \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + U_{i}^{ion}(r_i) \right] \psi_i(r_i) \, d^3r_i
\]

\[
+ \frac{1}{2} \sum_i \sum_{j \neq i} \int \psi_i^*(r_i) \psi_j^*(r_j) \frac{e^2}{|r_i - r_j|} \psi_i(r_i) \psi_j(r_j) \, d^3r_i \, d^3r_j.
\]

(3.13)

Note that \( \Psi \) is normalized since all \( \psi_i \) are normalized.

The optimum \( \Psi \) can be obtained by varying each of \( \psi_i \) independently to minimize (3.14). Namely

\[
\frac{\delta \langle \Psi | H | \Psi \rangle}{\delta \psi_i^*} = 0
\]

(3.14)

leads to the equation,

\[
H_i \psi_i = \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + U_{i}^{ion}(r_i) + \sum_{j \neq i} \int |\psi_j(r_j)|^2 \frac{e^2}{|r_i - r_j|} \, d^3r_j \right] \psi_i(r_i) = \varepsilon_i \psi_i(r_i)
\]

(3.15)
where \( \varepsilon_i \) is the lowest eigenvalue belonging to an eigenfunction of the one-electron Hamiltonian \( H_i \). This is indeed the Hartree equation (3.12).

In practice, the Hartree equation (3.12) is solved by iteration. The interelectronic potential \( U_i^{el} \) is first approximated by an appropriately chosen form \( V(1) \) to determine a set of approximate solutions \( \{ \psi_i^{(1)}(r) \} \). Then (3.5) is calculated with the resulting wave functions. Again with a newly formed potential \( V_i^{(2)} \), the Hartree equation is solved for a newer wave function \( \psi_i^{(2)} \). This iteration process is repeated until the set of wave functions \( \{ \psi_i^{(n-1)}(r) \} \) used for calculating \( V_i^{(n)} \) converges to a set of \( \{ \psi_i^{(n)}(r) \} \) obtained from the wave equations with \( V_i^{(n)} \), which is called Hartree’s self-consistent method.

### 3.1.2 The Hartree-Fock Method

In the Hartree approximation, the \( N \) electron wave function is given as a simple product of single-electron wave functions, so that the electron correlations are ignored. According to Pauli’s exclusion principle, the total wave function should be antisymmetric under the interchange of every pair of electrons. Fock [92] modified the Hartree equation by taking the exchange effect into consideration.

First we define the \( N \) electron wave function as a function of collective variables \( q_i = (r_i, s_i) \) representing spin degrees \( s_i \) as well as coordinates \( r_i \); namely, \( \Psi(q_1, q_2, \ldots, q_N) \). Then we express the wave function in terms of one-electron wave functions by the Slater determinant [99]

\[
\Psi(q_1, q_2, \ldots, q_N) = \begin{vmatrix}
\psi_1(q_1) & \psi_1(q_2) & \cdots & \psi_1(q_N) \\
\psi_2(q_1) & \psi_2(q_2) & \cdots & \psi_2(q_N) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_N(q_1) & \psi_N(q_2) & \cdots & \psi_N(q_N)
\end{vmatrix},
\]

(3.16)

which is completely antisymmetrized. The energy expectation value (3.14) with the antisymmetrized wave function (3.16) takes the form,

\[
\langle \Psi | H | \Psi \rangle = \sum_i \int d^3r \, \psi_i^*(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U^{ion} \right] \psi_i(r) + \frac{1}{2} \sum_i \sum_{j \neq i} \int \int d^3r \, d^3r' \left| \psi_i(r) \right|^2 \frac{e^2}{|r - r'|} \left| \psi_j(r') \right|^2 \\
- \frac{1}{2} \sum_i \sum_{j \neq i} \int \int d^3r \, d^3r' \, \psi_i^*(r) \psi_j^*(r') \frac{e^2}{|r - r'|} \delta_{s_is_j} \, \psi_j(r) \psi_i(r').
\]

(3.17)

In the above, the orthonormality relation \( \langle s_i | s_j \rangle = \delta_{ij} \) of spin states has been used.
Minimizing (3.18) with respect to \( \psi_i^* \) yields the equation of the form,

\[
\left[-\frac{\hbar^2}{2m} \nabla_i^2 + U_i^{\text{ion}}(r) + U_i^{\text{el}}(r) \right] \psi_i(r) - \sum_{j \neq i} \int d^3r' \frac{\varepsilon_j^2}{|r - r'|} \psi_j(r) \psi_i(r') = \varepsilon_i \psi_i(r)
\]  

(3.18)

where \( U_i^{\text{el}} \) is the interelectronic potential defined by (5.70). This equation is known as the Hartree-Fock equation, which is a generalized form of the Hartree equation (3.12). The last term on the left hand side of (5.67) is due to the exchange interaction which is the very effect of antisymmetrization.

### 3.1.3 Density Functional Theory

In application to the AlGaAs/GaAs band structure, we have to include applied fields in the single-electron equation. Hohenberg-Kohn-Sham density functional theory is powerful for treating electrons in an inhomogeneous electron gas [90, 91, 95, 96, 98]. The Hohenberg-Kohn formulation is based on the second-quantization procedure. However, without resorting to second quantization, it is possible to derive a single-electron Schrödinger equation for an inhomogeneous electron gas [96].

The ground state energy of an interacting inhomogeneous gas in a static potential \( v(r) \) has been given in the form,

\[
E = \int v(r)n(r) d^3r + \frac{1}{2} \int \int \frac{n(r)n(r')}{|r - r'|} d^3r d^3r' + G[n] 
\]  

(3.19)

where \( n(r) \) is the electronic density in the ground state of the electron gas, and \( G[n] \) is a universal functional of \( n(r) \), valid for any number of electrons and any external potential. Of course, the total number \( N \) of electrons in the gas is

\[
N = \int n(r) d^3r. 
\]  

(3.20)

In order to obtain a self-consistent equation analogous to Hartree’s, the universal functional is assumed to be of the form,

\[
G[n] = T[n] + E_{xc}[n],
\]  

(3.21)

where \( T[n] \) is the kinetic energy of a noninteracting electron gas with density \( nr \), and \( E_{xc}[n] \) is the exchange and correlation energy of an interacting gas with density \( nr \). The unique feature of the present approach is to include via \( E_{xc}[n] \) the two-particle correlation function defined in terms of the one- and two-particle density matrices as

\[
C(r, r') = n_2(r, r'; r, r') - n(r) n(r').
\]  

(3.22)
If the density function \( n(r) \) is sufficiently slowly varying, \( E_{xc}[n] \) may be approximated by

\[
E_{xc}[n] = \int n(r) \epsilon_{xc}(n(r)) \, d^3r
\]

(3.23)

where \( \epsilon_{xc}(n(r)) \) is the exchange and correlation energy per electron of a uniform non-interacting homogeneous electron gas of density \( n \), and is assumed to be known from theories of the homogeneous electron gas.

As before, let us apply the variational principle. Since in the density functional theory the density \( n(r) \) plays a role of a basic variable. Thus we optimize the total energy (3.19) with respect to \( n(r) \) under the condition that the number (3.20) of electrons is preserved, i.e.,

\[
\frac{\delta E}{\delta n} = 0,
\]

(3.24)

under the condition,

\[
\int \delta n(r) \, d^3r = 0.
\]

(3.25)

As a result of this stationary property, we obtain

\[
\int \delta n(r) \left\{ \varphi(r) + \frac{\delta T[n]}{\delta n(r)} + \mu_{xc}(n(r)) \right\} \, d^3r = 0.
\]

(3.26)

Here

\[
\varphi(r) = v(r) + \int \frac{n(r')}{|r - r'|} \, d^3r'
\]

(3.27)

and

\[
\mu_{xc}(n) = \frac{d(n \epsilon_{xc}(n))}{dn}
\]

(3.28)

which is the exchange and correlation contribution to the chemical potential of a uniform gas of density \( n \). Now we set

\[
n(r) = \sum_{i=1}^{N} |\psi_i(r)|^2,
\]

(3.29)

to express

\[
\delta n = \sum_{i=1}^{N} \{ \delta \psi_i^*(r) \psi_i(r) + \psi_i^*(r) \delta \psi_i(r) \}.
\]

(3.30)

As in the Hartree-Fock case, the variation with respect to \( \psi_i^*(r) \) in (3.26) leads to the single-electron Schrödinger equations

\[
\left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + [\phi_i(r) + \mu_{xc}(n(r))] \right\} \psi_i(r) = \epsilon_i \psi_i(r)
\]

(3.31)

which have to be solved self-consistently. The results are similar to the Hartree-Fock equations. The difference is that the new equations include the correlation effects as well as the exchange effects. The density functional theory has been widely used in various
fields in physics. In the present thesis, we are interested in the single-electron wave equations for an inhomogeneous electron gas subjected to additional potentials.

3.2 Computations for the AlGaAs/GaAs Band Diagram

The band offset at the interface of AlGaAs/GaAs heterojunction can be approximated by an asymmetric triangular quantum well along the growth direction (say, the z-direction). Since the motion of electrons is constrained to the z-direction, we consider the one-electron Schrödinger equation in one dimension. An effective potential that influences an electron moving in the z-direction has been given by [87, 100, 101]

$$V(z) = -e\phi(z) + V_h(z) + V_{ex}(z).$$  \hspace{1cm} (3.32)

Here $\phi(z)$ is the electrostatic potential and is evaluated numerically by solving the Poisson equation, $V_h(z)$ is the potential energy associated with the band discontinuity of the heterojunction, and $V_{ex}(z)$ is the local exchange-correlation potential of the electron present in the channel, which was for the first time introduced by Kohn and Sham [96].

The electron wave function $\psi_i(z)$ in the $i$th sub-band of the quantum well obeys the slightly modified one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left( \frac{1}{m(z)} \frac{d\psi_i(z)}{dz} \right) + V(z)\psi_i(z) = E_i\psi_i(z)$$  \hspace{1cm} (3.33)

where $m(z)$ is the effective mass whose value changes with position, and $E_i$ is the energy of the electron in the $i$th sub-band. The electrostatic potential $\phi(z)$ in (3.32) is obtained by solving the modified Poisson equation

$$\frac{d}{dz} \left( \epsilon_0\kappa(z) \frac{d\phi(z)}{dz} \right) = e \sum_i N_i|\psi_i(z)|^2 - \rho_I(z)$$  \hspace{1cm} (3.34)

where $N_i$ is the number of electrons per unit area in the $i$th sub-band, and $\kappa(z)$ is the position dependent dielectric constant. The conduction band in the AlGaAs region will bend in the presence of applied gate potentials, which is difficult to handle mathematically. To circumvent this problem [101], we choose the following different forms of the potential $V_h(z)$,

$$V_h(z) = \epsilon_h[1 - G(z)],$$  \hspace{1cm} (3.35)
with

\[ G(z) = \begin{cases} 
(z + z_h)/z_t, & 0 < z < z_h - a_t, \\
z + 3z_h - a_t + (2a_t/\pi) \cos[\pi(z - z_h)/2a_t]/(2a_t), & z_h = a_t < z < z_h + a_t, \\
1, & z > z_h + a_t, \\
1 - G(-z), & z < 0, 
\end{cases} \]

(3.36)

where \( V_h \) is the barrier height, \( z_t \) and \( a_t \) are the parameters that characterize the transition layer \( z_t \geq 2a_t > 0 \) and \( z_h = z_t/2 \). Also \( z_t + a_t \) nominal thickness of the transition layer.

The exchange correlation potential may be approximated with the help of the Kohn-Sham local density function theory for a homogeneous electron gas. For our calculation, we use the simple analytical expression for the exchange correlation potential suggested by other authors [93, 94, 101],

\[ V_{ex}(z) = - \left[ 1 + 0.7734\xi \ln \left( 1 + \frac{1}{\xi} \right) \right] \left( \frac{2}{21\pi\alpha\xi} \right) R^*_y \]  

(3.37)

where \( \alpha = (4/9\pi)^{1/3}, \xi(z) = r_s(z)/21, \) and

\[ r_s(z) = \left[ \frac{4}{3\pi\alpha^3 n(z)} \right]^{-1/3} \]

(3.38)

with an effective Bohr radius,

\[ a^* = \frac{4\pi\epsilon_0 h^2}{m^*e^2} \]

(3.39)

and the corresponding Rydberg constant,

\[ R^*_y = \frac{e^2}{8\pi\epsilon_0 ka^*}. \]

(3.40)

### 3.3 Numerical Presentations of Wave Functions

Now we wish to calculate numerically the energy eigenvalues and the wave functions of the ground and first excited states of the electron in the AlGaAs/GaAs heterojunction.

We introduce several scaling factors to express positions in nanometers (nm) and energy in electron volts (eV). Accordingly, eqs. (3.33), (3.34), and (3.37) are written, respectively, as

\[ \frac{0.03808 \frac{d^2\psi}{dz^2}}{m^*} + V(\tilde{z})\psi = E\psi, \]

(3.41)

\[ -\frac{d^2(\kappa\phi)}{d\tilde{z}^2} = 18.07(N_d - n), \]

(3.42)

\[ V_{ex} = -0.1045\frac{\kappa}{m^*}n^{1/3}(z) \left\{ 1 + 0.430\frac{m^*}{\kappa}n^{-1/3}(z) \ln \left[ 1 + 1.79607\frac{\kappa}{m^*}n^{1/3}(z) \right] \right\} R^*_y. \]

(3.43)
where $\tilde{z}$ is a rescaled variable.

Other parameters used for our numerical simulations are as follows.

\begin{align*}
\xi &= 0.3, & V_b &= 0.3\text{eV} \\
m^*_\text{GaAs} &= 0.07, & m^*_{\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}} &= 0.088 \\
\kappa_{\text{GaAs}} &= 13.0, & \kappa_{\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}} &= 12.1 \\
z_t &= 0.4\text{nm}, & a_t &= 0.1\text{nm} \\
\text{channel electrons} &= 5 \times 10^{11}\text{cm}^{-2}, & \\
\text{accepted doping} &= 3 \times 10^{14}\text{electrons cm}^{-3},
\end{align*}

Quantum well: Using the above numerical data and with the help of COMSOL multi-scale multi-physics simulation strategy based on the finite element method [86], we solve (3.41)-(3.43) self-consistently to give the exact conducting band diagram of GaAs/Al$_{0.7}$Ga$_{0.3}$As heterojunction on one dimension where the Fermi level is set to be zero [88, 97, 102]. As a result, we obtain numerically the normalized wave functions of the ground and first excited states for electrons in the triangular quantum well [97]. We use the Neumann boundary condition at the interface, that is, we make the wave functions whose derivatives are continuous at the boundary. This is because the effective masses of GaAs and Al$_{0.7}$Ga$_{0.3}$As materials are different. On the other hand, we use the Dirichlet boundary condition at both ends of the heterojunction where the wave functions are to vanish.

Quantum dot: Next we consider the formation of an electrically defined quantum dot by applying a symmetric confining potential in the plane of the 2-dimensional electron gas as illustrated in Fig. 3.2. We use the confining potential of the harmonic oscillator type,

$$
V(x) = \frac{1}{2}m^*\omega_0^2x^2
$$

with the coupling strength converted to the dimension of length

$$
l_0 = \sqrt{\frac{\hbar}{m^*\omega_0}}.
$$

which we add to the potential (3.32). Again we solve (3.41)-(3.43) self-consistently on the two-dimensional $x - z$ plane. Fig. 3.2 clearly shows the formation of a quantum dot of radius 20nm in the potential well of the 2DEG as expected.
Figure 3.1: Heterojunction self-consistent potential (upper panel) and lowest two wave functions (lower panel) of the 2DEG. These results demonstrate consistency of our results with other published work [97].
Figure 3.2: Quantum dot wave function plotted in the x-z plane formed by applying a quadratic confining potential in the plane (i.e. along the $x$ axis). This potential is characterized by the parameter $\ell_o = 20$ nm [97].
Chapter 4

Spins in a GaAs Quantum Dot

In this chapter, we first study the energy spectrum of a single electron spin in a quantum dot in presence of a magnetic field along z-direction. We first introduce the effective mass approximation that will allow us to define the single-particle approximation of all the channel electrons present at the interface of III-V type heterojunction such as AlGaAs/GaAs and GaAs/InAs. We will comment on the origin of spin orbit interactions which plays a very important role for spin flipping in a quantum dot formed at the interface of these heterojunction. Taking a 3-Dimensional Finite Element modeling approach for the investigation of realistic potential of the realistic device, we will first review the most interesting results of other authors and after that we present our contributions in the calculation of electron g-value. We first study the energy spectrum of a quantum dot in the presence of symmetric and asymmetric confining potentials. Here we focus on the calculation of electron g-values for several different type of confining potentials.

The notion of using single-electron spins for quantum computing and next-generation logic is an attractive idea that has received considerable attention in recent years [114, 123, 138]. In order to integrate new concepts with existing semiconductor technology, a number of researchers have recently explored the possibility of using electric fields generated by imposed gate potentials to manipulate single-electron spins in quantum dot devices [117, 144, 145].

The goal of the present work is to utilize state-of-the-art numerical techniques to explore the fundamental physics of single-electron spin devices and to provide realistic information for the practical design of such systems. We utilize a finite-element based numerical technique to study electrostatically defined quantum dots that is similar to other recently published work [109]. A key result of the present work is the discovery that spatial symmetry breaking [118, 134, 135] resulting from the anisotropy of realistic confining potentials results in an enhancement of the electric-field tunability of the electron g-factor over that found for symmetric potentials for dots larger than roughly 65 nm.

Indeed, symmetry plays a key role in spin-orbit interactions in systems such as the one considered in this work. The Dresselhaus [120] and Rashba [112]coupling terms (dis-
cussed in detail below) are manifestations of the spin-orbit interaction arising due to bulk inversion asymmetry and the quantum well confining potential asymmetry respectively. The forms of these interactions, given in Eqs. 4.38, 4.39, and 4.40 are well established and have been used in many studies [117, 122, 134, 144].

It is also generally understood that the Zeeman splitting depends on the direction of an applied field and is thus described by a $g$-factor tensor [118, 131, 142]. Some authors have also explored the effects of asymmetry of the quantum dot confining potential in coupled quantum dot systems [104, 135, 146, 152]. A subject that seems to have received little attention is the question of anisotropy effects in a single dot and is the subject of the present investigation.

Our approach is most closely related to that of Ref. [117] but differs in that we take a numerical approach based on the finite element method [103] whereas the authors of Ref. [117] use perturbation theory and direct diagonalization techniques and didn’t consider anisotropy effects. Another recent work, similar to ours, employing real-space numerical (finite-difference) methods has also appeared [109]. This work was concerned with the determination of realistic self-consistent potentials, electron-electron interaction effects, and interaction with quantum point contacts.

### 4.1 $k \cdot p$ Band Structure Calculation for Zinc Blend Structure

Energy levels and wave functions of electrons can be approximately calculated with the help of $k \cdot p$ perturbation theory. The Bloch form of the electron wave function is chosen in this approach and was adopted for special purposes in the first generation calculation of the semiconductor band theory [159]. For example, Seitz adopted this $k \cdot p$ band structure calculation method to derive the expression for the effective mass [148]. Schockley derived more complicated form of the effective mass equations for degenerate sub bands [150].

Dresselhaus et al has an important contribution on deriving the semiconductor band on the basis of $k \cdot p$ method. The concept of spin orbit interactions have been adopted in his derivation and appear in their original classic paper on cyclotron resonance [121].

The Bloch functions $u_{nk}(r)$ form a complete set. It means, if we know the momentum and energy matrix elements of any bands in $k \cdot p$ space then we can easily calculate the other energies in other bands. The approach fully adopted in this process is called $k \cdot p$ representation. The $k \cdot p$ results are derived on the basis of a one-electron Hartree Hamiltonian.
4.2 The \( k \cdot p \) Representation

Let us consider a semiconductor with an electron which is free to move in a crystal lattice. One can make the assumption that the crystal potentials can be disturbed by the atoms in the lattice and other electrons that present in the crystal lattice [157]. The wave function of the moving electrons is then given by the Bloch form. The exact form of Bloch wave functions have been calculated by several band structural calculations. Suppose the moving electrons in a crystal is confined from all three directions by an additional potential then the cluster of these electrons will form the quantum dot which has potential application in semiconductor industry. The additional potentials have various origins such as metallic gate potentials, charged impurity bonding of the electron, and different material composition in the confinement region. The Schrödinger equation for an electron moving in a periodic potential \( V(r) \) in the crystal lattice is given by

\[
H\psi = \left\{ \frac{P^2}{2m} + V(r) \right\} \psi = E\psi
\]  \( (4.1) \)

The electron wave function \( \psi \) can be written in terms of Bloch wave function \( u_{nk} \) in the crystal lattice as,

\[
\psi = e^{ikr}u_{nk}(r)
\]  \( (4.2) \)

Where \( u_{nk}(r) \) has the periodicity of the crystal lattice in the potential \( V(r) \). \( k \) lies in the first Brillouin zone and the band index \( n \) runs over a complete set of bands. Substituting Eq. \((4.2)\) in Eq. \((4.1)\), we get

\[
\left\{ \frac{P^2}{2m} + \frac{\hbar}{m}k \cdot p + \frac{\hbar^2k^2}{2m} + V(r) \right\} u_{nk}(r) = E_{nk}u_{nk}
\]  \( (4.3) \)

At \( k_0 = (0, 0, 0) \), Eq. \(( 4.3)\) reduces to

\[
H\psi = \left\{ \frac{P^2}{2m} + V(r) \right\} u_{n0} = E_{n0}u_{n0}
\]  \( (4.4) \)

The eigenvalue \( E_{n0} \) and and wave function \( u_{n0} \) are found from Eq. \((4.4)\) either by Hartree-Fock or Kohn-Sham density functional theory approach. Then we can treat the terms \( \hbar k \cdot p/m \) and \( \hbar^2k^2/(2m) \) as perturbations part in Eq. \((4.3)\) and the eigenvalue and the wave functions in Eq. \((4.3)\) can be fully calculated by either degenerate or nondegenerate perturbation theory. This method for calculating the band dispersion relation is called the \( k \cdot p \) method [159].

Let the system appearing in Eq. \((4.4)\) and Eq. \((4.3)\) are non-degenerate. Then the first order correction in energy and wave function for non-degenerate case can be written as
\[ u_{nk} = u_{n0} + \frac{\hbar}{m} \sum_{n' \neq n} \frac{\langle u_{n0} | k.p | u_{n'0} \rangle}{E_{n0} - E_{n'0}} u_{n'0}. \]  \hspace{1cm} (4.5)

and

\[ E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n' \neq n} \frac{|\langle u_{n0} | k.p | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}}. \]  \hspace{1cm} (4.6)

For small value of k, the Eq. (4.6) can be written as

\[ E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*} \]  \hspace{1cm} (4.7)

where \( m^* \) is the effective mass of the band. Comparing Eq. (4.6) and Eq. (4.7), we will have the expression for the effective mass of electron in the band as

\[ \frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2} \sum_{n' \neq n} \frac{|\langle u_{n0} | k.p | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}}. \]  \hspace{1cm} (4.8)

The expression in Eq. (4.8) shows that moving electron in a crystal lattice has different mass than that of a free electron. This is because the electron in the band has an interaction with the other bands and their states have been coupled with other electronic states in different bands via the \( k \cdot p \) term.

There is a band offset along growth direction in III-V type semiconductor which gives an asymmetric triangular quantum well at the interface. This breaks the inversion symmetry in hetero-type devices. As a result, in III-V hetero-type devices, the momentum matrix element between the two nearest \( \Gamma_1 \) and \( \Gamma_4 \) conduction band will not vanish but is still much smaller than its momentum matrix element with top \( \Gamma_4 \) valence bands. The conduction band effective mass \( (m_{c*}) \) between the direct band gap \( E_0 \) of the \( \Gamma_1 \) conduction band and the \( \Gamma_4 \) valence band is approximated as

\[ \frac{1}{m_{c*}} = \frac{1}{m} + \frac{2}{m^2 E_0 k^2} \sum_{n' \neq n} |\langle u_{n0} | k.p | u_{n'0} \rangle|^2 \]  \hspace{1cm} (4.9)

Three \( \Gamma_4 \) wave functions can be represented by the state vectors \( |X>, |Y> \) and \( |Z> \). From the \( T_d \) symmetry operations in III-V type semiconductor, it can be easily shown that the only non zero elements of \( |\langle \Gamma_1c | k.p | \Gamma_4v \rangle| \) in \( k \cdot p \) representation in Eq. 4.9 are

\[ < X|p_x| \Gamma_1 >= < Y|p_y| \Gamma_1 >= < Z|p_z| \Gamma_1 >= iP \]  \hspace{1cm} (4.10)

From Eq. (4.9), we get

\[ \frac{m}{m_{c*}} \approx 1 + \frac{2P^2}{mE_0} \]  \hspace{1cm} (4.11)

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4.3 Realistic Potential for Realistic Device

We utilize a multi-scale, multi-physics simulation strategy based on the finite element method [103] to provide a realistic description of the physics of single-spin devices in three-dimensional geometries. The ideal is to solve self-consistently the Maxwell equations of electrostatics with the Schroedinger equation in three dimensional geometry. Unfortunately such a solution is not feasible given currently available techniques due to the disparity of length scales in the problem. We thus seek an approximate solution that is built up in stages [143].

In the first step of our approach, we construct a three-dimensional model of the device and calculate the gate-induced electrostatic potentials that cause the formation of a quantum dot in the two-dimensional electron gas (2DEG) at a AlGaAs/GaAs heterojunction as illustrated in Figs. 4.3, 4.4, and 4.5. This geometry corresponds to prototype devices that are under consideration by experimentalists at the University at Albany, State University of New York [143].

In order to obtain the electrostatic solution for the confining potential, we approximate the 2DEG as a classical perfect conductor and give it a finite width. The width \((\approx 0.05\mu m)\) is unrealistically large from a quantum perspective but is assumed to give a reasonable description of the spatial variation of the potential in the layer of the 2DEG. In a subsequent step we treat the 2DEG from a realistic quantum mechanical perspective [143, 151].

Figs. 4.4 and 4.5 are one-dimensional plots obtained from Fig. 4.3 by plotting the potential along a line in the 2DEG along high symmetry directions. These one-dimensional potentials are then fit to polynomial forms \(P_x(x)\) and \(P_y(y)\). These are then used as a potential of the form
\[
V_{\text{real}}(x, y) \approx P_x(x) + P_y(y)
\]
(4.12)
to approximate the confining potential of the electron in the Schroedinger equation. Before considering electron motion in the above potential, \(V_{\text{real}}\), we consider the simpler quadratic potential
\[
V_{\text{quad}} \equiv \frac{1}{2} m\omega_0^2 \left(\alpha^2 x^2 + \beta^2 y^2\right)
\]
(4.13)
that allows for systematic studies. For convenience we have written the strength of the potential in harmonic oscillator form by defining the prefactor \(\frac{1}{2} m\omega_0^2\). The potential of Eq. 4.13 is a paraboloid of revolution and is commonly employed in model studies of 2D quantum dots [147]. The separable form given in Eq. 4.12 is a generalization of Eq. 4.13 from quadratic to polynomial form and is an ansatz. It is assumed to give a good description of the system and the results of Figs. 4.6 and 4.11 support this hypothesis.

In the remainder of this chapter we focus our attention on motion in the plane of the 2DEG and contrast effects associated with quantum dots in symmetric and asymmetric confining potentials as illustrated in Figs. 4.6(a) and 4.6(b) respectively. These figures
were obtained using the quadratic model potential of Eq. 4.13 with \( \alpha = \beta = 1 \) for the symmetric case (Fig. 4.6(a)), and \( \alpha = 1, \beta^2 = 2.8 \) for the asymmetric case (Fig. 4.6(b)), in the Hamiltonian, \( H_{xy} \), describing motion in the two-dimensional plane of the 2DEG (i.e. \( x - y \) plane), to be discussed in the following. The quantum dot radius defined by:

\[
\ell_o \equiv \sqrt{\frac{\hbar}{m\omega_o}},
\]

was chosen to have the value \( \ell_o = 30 \text{nm} \).

The parameters of the asymmetric potential were chosen so as to mimic the realistic potential of Figs. 4.4 and 4.5. In other words, we obtain \( x_o \) and \( y_o \) as the solutions to the following equations:

\[
\epsilon_o = P_x(x_o),
\]

(4.15)

and,

\[
\epsilon_o = P_y(y_o),
\]

(4.16)

where \( \epsilon_o \) is the ground state eigenvalue in the realistic potential of Eq. 4.12. We then fix the three parameters \( \alpha, \beta, \) and \( \omega_o \) as follows. As there are three parameters and two equations, we can choose one at will. We therefore take \( \alpha = 1 \) throughout the rest of the computational work. The ratio of \( \alpha \) to \( \beta \) is then determined by taking the ratio of the following equations:

\[
\epsilon_o = \frac{1}{2} m\omega_o^2 \alpha^2 x_o^2,
\]

(4.17)

and,

\[
\epsilon_o = \frac{1}{2} m\omega_o^2 \beta^2 y_o^2,
\]

(4.18)

to give \( \beta^2 = x_o^2/y_o^2 \). Lastly we choose \( \omega_o \) as determined by the coefficient of the quadratic term in \( P_y(y) \) (plotted in Fig. 4.5) (the polynomial \( P_x(x) \) has no quadratic term). The resulting values are \( \beta^2 = 2.8 \) and the value of \( \omega_o \) is most conveniently expressed equivalently by \( \ell_o \approx 30 \text{ nm} \).

4.4 Fock-Darwin Energy Levels of a Quantum Dot

Our analytical expressions for the energy spectrum of realistic device in the absence of spin orbit interactions are referred to as Fock-Darwin energy spectrum. The motion of the channel electrons confined in a two dimensional parabolic well by gate potentials in an external perpendicular magnetic field without electron spin, in the effective mass approximation is described by the following Hamiltonian [107]:

\[
H = H_{xy} + H_z
\]

(4.19)

where \( H_z \) represents the motion of the electron along growth direction, and:
\[ H_{xy} = \frac{\vec{p}^2}{2m} + \frac{1}{2} m \omega_z^2 (x^2 + y^2), \]  

where the kinetic momentum operator \( \vec{p} \), canonical momentum operator \( \vec{p} \) and the vector potential \( \vec{A} \) can be written as

\[
\vec{p} \equiv \vec{p} + \frac{e}{c} \vec{A} \\
\vec{p} \equiv -i\hbar (\partial_x, \partial_y, 0) \\
\vec{A} \equiv B \left(-y, x, 0\right)
\]

(4.21)

The eigenstates of \( H_{xy} \) in Eq. 4.42 with \( \alpha = \beta \) are the well-known Fock-Darwin energy states [116, 124].

The analytical expression for the eigen states of above Hamiltonian is first described by Fock [124] and Darwin [116]. To find the energy spectrum, let us first introduce the complex variables

\[ z = x + iy, \quad z^* = x - iy, \]

(4.22)

and

\[ \partial_z = \frac{\partial_x - i \partial_y}{2}, \quad \partial_z^* = \frac{\partial_x + i \partial_y}{2}, \]

(4.23)

Creation and Annihilation operators can be defined by

\[ a = \frac{z^* / 2l_0 + 2l_0 \partial_z}{\sqrt{2}}, \quad a^\dagger = \frac{z / 2l_0 - 2l_0 \partial_z^*}{\sqrt{2}} \]

(4.24)

\[ b = \frac{z / 2l_0 + 2l_0 \partial_z^*}{\sqrt{2}}, \quad a^\dagger = \frac{z^* / 2l_0 - 2l_0 \partial_z}{\sqrt{2}} \]

(4.25)

Where \( l_0 = \frac{l_B}{\sqrt{1 + 4\omega_0^2 / \omega_z^2}^{1/2}} \) is the effective length scale and \( l_B = \sqrt{\frac{\hbar e}{m}} \). The above operators satisfy the commutation relations, \([a, a^\dagger] = [b, b^\dagger] = 1, [a, b] = [a, b^\dagger] = 0\). The Hamiltonian (4.42) can be written as

\[ H = \hbar \omega_+ \left( aa^\dagger + \frac{1}{2} \right) + \hbar \omega_- \left( bb^\dagger + \frac{1}{2} \right) \]

(4.26)

Where \( \omega_\pm = \sqrt{\omega_0^2 + \frac{1}{2} \omega_z^2 \pm \frac{1}{2} \omega_z} \). The eigen energies corresponding to the states \(|n_+ n_- >\) are referred to as Fock-Darwin energy levels and is given by

\[ \epsilon(n_+ n_-) = \hbar \omega_+ \left( n_+ + \frac{1}{2} \right) + \hbar \omega_- \left( n_- + \frac{1}{2} \right) \]

(4.27)

The Fock-Darwin energy spectrum becomes degenerate in the absence of external magnetic field where \( \omega_+ = \omega_- = \omega_0 \). When the magnetic field becomes very large such
that $\omega_c \gg \omega_0$ then the energy spectrum leads to the Landau energy levels which is then
separated by the cyclotron energy $\hbar \omega_+ \approx \hbar \omega_c$.

The electron wave function of the above Hamiltonian in polar coordinates can be written as

$$
\Psi_{nm} = \psi_m(\theta)R_{nm}(r)
$$

(4.28)

Where,

$$
\psi_m(\theta) = \frac{1}{\sqrt{2}} e^{im\theta}
$$

(4.29)

$$
R_{nm}(r) = \frac{\sqrt{2}}{r_0} \sqrt{ \left( \frac{r}{r_0} \right)^{|m|} \frac{n_r!}{(n_r + |m|)!} } \exp \left[ -r^2 \frac{|m|}{2r_0^2} \right] \frac{n_r! \left( \frac{r^2}{r_0^2} \right)^{|m|}}{(n_r + |m|)!}
$$

(4.30)

The Laguerre polynomials can be written as

$$
L_{nr}^{|m|}(z) = \frac{1}{m!} z^{-|m|} e^z \frac{d^n e}{dz^n} \left( (z^{|m|} e^{-z}) \right)
$$

(4.31)

where principal quantum numbers $n = 0, 1, \cdots$, azimuthal quantum number $m = -n, -n+2, \cdots, \ n - 2, n$ and radial component $n_r = (n - |m|)/2$.

The wave function of the $H_z$ part of the Hamiltonian in Eq. 4.19 can be written in
terms of Airy function and its numerical simulations are discussed in more details in the
previous chapter.

$$
\Psi_{0z}(z) = 1.4261 \kappa^{1/2} Ai (\kappa z + \zeta_1)
$$

(4.32)

where $\zeta_1 = -2.3381$ is the first zero of the Airy function $Ai$. Also $\kappa$ can be defined
in terms of the electric field associated with asymmetric triangular quantum well along
z-direction and can be written as

$$
\kappa = \left( \frac{2m^* e E}{\hbar^2} \right)^{1/3}
$$

(4.33)

Based on Finite Element Method, we carry out the exact numerical simulation of
the Hamiltonian of Eq. 4.19 to find the evolution of energy spectrum of Fock Darwin
energy states to conform our numerical method. In Fig. (4.1), we plot the Fock-Darwin
energy levels along y-axis and magnetic field along x-axis in the confining potential of
30 nm quantum dot radius. The figure clearly shows that the separation of the energy
eigenvalues of the adjacent levels are so close that one needs to consider the admixture of
electron spin for the design of the device.

Also, we consider the exact numerical simulation of the Hamiltonian of a asymmetric
confining potential to find the energy spectrum as shown in Fig. (4.2). Here we plotted
the energy levels along y-axis and magnetic field along x-axis in the confining potential of
30 nm quantum dot radius and we choose $\alpha = 1$ and $\beta^2 = 2.8$. This value of $\alpha$ and $\beta$ have been chosen to mimic the realistic asymmetric confining potential of the realistic device.
The figure clearly shows that the separation of the energy eigenvalues of the adjacent levels are even larger than the symmetric potential but still very close to each other. So one still needs to consider the admixture of electron spin for the design of the device.

4.5 Spin-Orbit Interactions

We investigate precisely the role of spin orbit interactions in the laterally confined GaAs quantum dot in the plane of 2 dimensional electron gas. This spin orbit interactions are represented by Rashba and Dresselhaus (both linear and cubic dependent on momenta) terms and discussed in more details in this chapter [112, 120]. To apply the \( k \cdot p \) method to calculate the band dispersion near a degenerate band extremum we consider the highest energy \( \Gamma_2 \Gamma(\Gamma_4) \) valence bands at the zone center of semiconductors with the diamond (zinc-blend) structure. The valence band wave functions are p-like, and they will be represented by the eigenstates \( |X>, |Y>, \text{and} |Z> \). In atomic physics, the electron spin spin can be coupled to the orbital angular momentum via the spin-orbit interaction [159]. The Hamiltonian for the spin-orbit interaction is given by

\[
H_{so} = \frac{\hbar}{4e^2m^2} (\nabla V \times P) \cdot \sigma,
\]

where the components of \( \sigma \) are the Pauli spin matrices:

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(4.35)

The spin-orbit interaction in atomic physics is usually expressed in terms of \( l \) and the spin \( s \) as

\[
H_{so} = \lambda l \cdot s.
\]

(4.36)

The constant \( \lambda \) is referred to as the spin-orbit coupling and the total angular momentum \( j=l+s \) where \( l \) is the orbital angular momentum and \( s \) is the spin angular momentum.

The electron has a spin angular momentum described by the Hamiltonian \( \frac{1}{2}g_\mu_B \sigma_z B \) where \( \sigma_z \) is the Pauli matrix along growth direction. The spin orbit interaction in a 2DEG takes the form:

\[
H_{so} = H_R + H_{D1} + H_{D2}
\]

(4.37)

where \( H_R \) is the Rashba interation and \( H_{D1} \) and \( H_{D2} \) are the Dresselhaus interaction terms.

The Rashba interaction is associated with structural inversion symmetry in zinc blend type structures. There is a lack of inversion symmetry according to \( T_d \) symmetry operation in III-V type semiconductor with the comparison of diamond structure. There is an asymmetric triangular quantum well formation at the interface along growth direction in III-V type semiconductor which has significant contribution in the spin orbit interaction.
known as Rashba term. The total Hamiltonian associated with this interaction can be written as [112]

\[ H_R = \frac{\alpha_R eE}{\hbar} \left( \sigma_x P_y - \sigma_y P_x \right). \] (4.38)

Notice that the electric field in Rashba interaction in Eq. 4.38 is a control parameter that can be easily changed with the application of gate potential. The strength of the electric field in the heterojunction is related to \( |E| = \partial V(z) / \partial z \) where \( V_z \) is the asymmetric triangular quantum well arises due to band off set in III-V type semiconductor along growth direction and was expressed in details in previous section.

The Hamiltonian associated with bulk inversion asymmetry [120]

\[ H_{D1} = \frac{0.7794 \gamma c k^2}{\hbar} \left( -\sigma_x P_x + \sigma_y P_y \right), \] (4.39)

\[ H_{D2} = \frac{\gamma c}{\hbar^2} \left( -\sigma_x P_x P_y - \sigma_y P_y P_x \right) + \text{h.c.}, \] (4.40)

\( h.c. \) represents the Hermitian conjugate [117].

### 4.6 Lande g-factor for III-V type Semiconductor

The notion of using single-electron spins for quantum computing and next-generation logic is an attractive idea that has received considerable attention in recent years [107, 108, 111, 113, 114, 123, 126, 127, 129, 138, 156, 158].

In order to integrate new concepts with existing semiconductor technology, a number of researchers have recently explored the possibility of using electric fields generated by imposed gate potentials to manipulate single-electron spins in quantum dot devices [105, 110, 117, 119, 122, 125, 128, 130, 132, 136, 137, 139–142, 144, 145, 149, 153–155].

The goal of the present work is to utilize state-of-the-art numerical techniques to explore the fundamental physics of single-electron spin devices and to provide realistic information for the practical design of such systems. We utilize a finite-element based numerical technique to study electrostatically defined quantum dots that is similar to other recently published work [109].

It is also generally understood that the Zeeman splitting depends on the direction of an applied field and is thus described by a g-factor tensor [106, 115, 118, 131, 142]. Some authors have also explored the effects of asymmetry of the quantum dot confining potential in coupled quantum dot systems [104, 135, 146, 152]. A subject that seems to have received little attention is the question of anisotropy effects in a single dot and is the subject of the present investigation.

The total Hamiltonian of an electron present in a quantum dot in the plane of 2DEG
at the interface between III-V type semiconductor in presence of magnetic field along growth direction can be written as [117]

\[ H = H_{xy} + H_z + H_{so} \]  \hspace{1cm} (4.41)

where \( H_z \) represents the motion of the electron along growth direction and \( H_{so} \) is the hamiltonian of an electron coming from spin-orbit interaction.

\[ H_{xy} = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega_r^2(\alpha^2 x^2 + \beta^2 y^2) + \frac{1}{2}g_o\mu_B\sigma_z B, \]  \hspace{1cm} (4.42)

where the kinetic momentum operator \( \vec{p} \), canonical momentum operator \( \vec{p} \) and the vector potential \( \vec{A} \) can be written as

\[ \vec{p} = \vec{p} + \frac{\hbar}{c} \vec{A} \]

\[ \vec{p} = -i\hbar(\partial_x, \partial_y, 0) \]

\[ \vec{A} = \frac{B}{2}(-y, x, 0) \]

The eigenstates of \( H_{xy} \) in Eq. 4.42 with \( \alpha = \beta \) are the well-known Fock-Darwin energy states [116, 124].

The eigenvalue can be found numerically with respect to several control parameters: electric fields, magnetic fields and quantum dot radius with the help of Schrodinger equation \( H |\psi> = \epsilon |\psi> \) where \( H \) is in the form of Eqs. 4.41. The numerically found eigenvalue defines the effective electron \( g \) factor as:

\[ \epsilon = \frac{1}{2}g\mu_B\sigma_z B \]  \hspace{1cm} (4.44)

where \( \epsilon = \epsilon_2 - \epsilon_1 \) is the energy difference between the two lowest energy eigenvalue of spin up and down states. So the Eq. 4.44 can be written as:

\[ g = \frac{(\epsilon_2 - \epsilon_1)}{\mu_B B}. \]  \hspace{1cm} (4.45)

We carry out the numerical simulations study of Lande g-factor for GaAs and InAs quantum dots with respect to several parameters \( E \), \( B \) and \( \ell_o \). The results are presented below. Our approach is most closely related to that of Ref. [117] but differs in that we take a numerical approach based on the finite element method [103] whereas the authors of Ref. [117] use perturbation theory and direct diagonalization techniques and didn’t consider anisotropy effects. Another recent work, similar to ours, employing real-space numerical (finite-difference) methods has also appeared [109]. This work was concerned with the determination of realistic self-consistent potentials, electron-electron interaction effects, and interaction with quantum point contacts. We now turn to a discussion of our
4.6.1 Lande g-fator for GaAs Quantum Dot

In our numerical results for the GaAs quantum dot, we use bulk GaAs material parameters: $m^* = 0.067m_e$, $g_0 = -0.44$, $\gamma_c = 26ev \AA^3$, $\alpha_R = 4.4 \AA^2$.

We now turn to a presentation of the key results of this work: the tunability of the electron $g$-factor through the application of electric and magnetic fields in a GaAs quantum dot. Figure 4.7 is consistent with previous published work [117] and illustrates the $g$-factor tunability vs. the strength of the applied electric field and confining potential (as parametrized by the quantum dot radius $\ell_o$) for fixed magnetic field ($B = 1T$) for the symmetric quantum dot in the quadratic potential of Eq. 4.13 with $\alpha = \beta = 1$. We express $g$ relative to its non-relativistic free-electron value $g_o = 2$.

Figure 4.8 is consistent with previous published work [117] and illustrates the $g$-factor tunability vs. the strength of the applied electric field and and magnetic field for fixed confining potential (parametrized by the quantum dot radius $\ell_o = 20$ nm). Upon introducing in-plane anisotropy to the confining potential we find significant changes in the electric-field induced $g$-factor tunability for GaAs quantum dots larger than roughly 65 nm as illustrated in Fig. 4.9. This figure was generated by choosing $\alpha = 1$, and four values of $\beta$, given by $\beta^2 = 20, 40, 60,$ and $80$ in Eq. 4.13. By comparison of Fig. 4.9 with Fig. 4.7 we see that the major effects of anisotropy are for dots roughly larger than 65 nm.

To quantify the effects of in-plane anisotropy, we have carried out a parameter study of the $g$-factor tunability vs. degree of anisotropy and the results are presented in Fig. 4.10. This figure was generated by fixing the quantum dot radius at $\ell_o = 120$ nm and holding $\alpha = 1$ while varying $\beta^2$ with $B = 1T$. Lastly we consider the results for $g$-factor tunability for GaAs quantum dots in the realistic potential of Figs. 4.4 and 4.5 and Eq. 4.12. Figure 4.11 illustrates the results for a quantum dot in the realistic potential in comparison with several model potentials. The lowest curve, indicated by filled black squares represents the symmetric model of Eq. 4.13 with $\alpha = \beta = 1$ and the other curves with filled symbols represent varying degrees of anisotropy as follows. The filled red circles represents $\beta^2 = 2.8$, while the filled green upward pointing triangles correspond to $\beta^2 = 5$ and the blue downward pointing triangles corresponds to $\beta^2 = 10$. In each case of the quadratic model we have chosen $\ell_o = 30$ nm. The results for the realistic potential of Eq. 4.12 and Figs. 4.4 and 4.5 are represented by the open symbols. We see that results for the realistic potential are well represented by the asymmetric model of Eq. 4.13 with $\alpha = 1$, $\beta = 2.8$ and $\ell_o = 30$ nm. The good agreement between the asymmetric model potential and the realistic potential in 4.11 is reflected visually in Fig. 4.6(b) and 4.6(c) although there are is a slight underestimate of the magnitude of the wave function in Fig. 4.6(b) in comparison with Fig. 4.6(c). Obviously, however, from Fig. 4.11 this slight difference has little effect on the $g$-factor tunability as evidenced by the close agreement between the filled and open
circles in Fig. 4.11. The quantum dots of Figs. 4.6(a) and 4.6(b) correspond to the filled squares and circles of Fig. 4.11 respectively, emphasizing the importance of anisotropy.

### 4.6.2 Lande g-factor for InAs Quantum Qot

In our numerical results for the InAs quantum dot, we use bulk InAs material parameters: 

\[ m^* = 0.0239 m_e, \ g_0 = -15, \ \gamma_c = 130 \text{ ev } \text{Å}^{-3}, \ \alpha_R = 110 \text{ Å}^2. \]

The main observation is: the in-plane symmetry breaking in an anisotropic potential (i.e., \( \alpha \neq \beta \)) gives rise to qualitatively different behavior for the tunability of the electron g-factor with the application of electric and magnetic fields as compared to a symmetric potential (i.e. \( \alpha = \beta = 1 \)) for InAs quantum dot due to Rashba spin orbit coupling.

We focus our attention on motion in the plane of the 2DEG and contrast the effects associated with the quantum dots in symmetric and asymmetric confining potentials for InAs quantum dot as illustrated in Figs. 4.12(a) and 4.3(b), respectively. These figures were obtained by using the quadratic model potentials with \( \alpha = \beta = 1 \) for the symmetric case as in Fig. 4.12(a) and \( \alpha^2 = 1 \) and \( \beta^2 = 80 \) for asymmetric case as in Fig. 4.12(b), in the Hamiltonian \( H_{xy} \), describing motion in the plane of 2DEG (i.e., x-y plane). The quantum dot radius was chosen to have the value \( \ell_0 = 30 \text{ nm} \).

Figure 4.13(a) is also consistent result found in the Ref. [117] and illustrates the g-factor tunability vs. the strength of the applied electric field and confining potential (as parametrized by the quantum dot radius \( \ell_0 \)) for fixed magnetic field \( (B = 1 \text{ T}) \) for the symmetric quantum dot in the quadratic potential of \( \alpha = \beta = 1 \). We found that there is an abrupt change in the g-value vs. quantum dot radius near 35 nm for the symmetric potential. This is due to level crossings (two eigen states have the same spin) in the quantum dot system, as considered in Eq. 4.45.

Figure 4.14(a) is also consistent to the Ref. [117] and illustrates the g-factor tunability vs. the strength of the applied electric and magnetic fields for fixed confining potential (parametrized by the quantum dot radius \( \ell_0 = 20 \text{ nm} \)). Again, we found a level crossing near 3 T for the asymmetric potential.

To quantify the effects of in-plane anisotropy, we have carried out a parameter study of the g-factor tunability vs. several variables in an anisotropic case such as quantum dot radius \( \ell_0 \) in Fig. 4.13, magnetic field \( B \) in Fig. 4.14, electric field in Fig. 4.15(a), and degree of anisotropy \( (\beta^2/\alpha^2) \) in Fig. 4.15(b).

First, we consider the results for g-factor tunability for InAs quantum dots in the asymmetric confining potential of Figs. 4.13(b) and 4.14(b). Figure 4.13 illustrates the tunability of the Lande g-factor vs. electric field and confining potential \( \ell_0 \) in the symmetric potential in comparison with the model potential with parameters \( \alpha^2 = 1 \) and \( \beta^2 = 80 \). The lowest curve in Fig. 4.13(a), indicated by filled black squares, represents the symmetric model potential of \( \alpha = \beta = 1 \) and the other curves with filled symbols represent varying electric fields of \( (2, 5, 7, 100) \times 10^3 \text{ V/cm} \). Similarly, the top curve in
Fig. 4.13(b), indicated by filled black squares represents the asymmetric model potential of \( \alpha^2 = 1, \beta^2 = 80 \) and the other curves with filled symbols represent varying electric fields of \((2, 5, 7, 100) \times 10^5 \) V/cm. In each case of the symmetric and asymmetric quadratic model potential, we have chosen \( B = 1 \) T. By introducing the in-plane asymmetric potential, we found that the tunability of the electron \( g \)-factor is extended to larger quantum dot radius (roughly 55 nm quantum dot radius).

Figure 4.14 illustrate the tunability of the Lande \( g \)-factor vs. magnetic field in the symmetric potential in comparison with the asymmetric potential characterized by parameters \( \alpha^2 = 1 \) and \( \beta^2 = 80 \). The lowest curve in Fig. 4.14(a), indicated by filled black squares represents the symmetric model potential of \( \alpha = \beta = 1 \) and the other curves with filled symbols represent varying electric fields of \((2, 5, 7, 100) \times 10^5 \) V/cm. Similarly, the lowest curve in Fig. 4.14(b), indicated by filled black squares represents the asymmetric model potential with \( \beta^2/\alpha^2 = 80 \) and the other curves with filled symbols represent varying electric fields of strength \((2, 5, 7, 100) \times 10^5 \) V/cm. In each case (symmetric and asymmetric model potential), we have chosen \( \ell_0 = 20 \) nm. Again, we found that the tunability of the electron \( g \)-factor increases with the larger magnetic field.

Figure 4.15(a) illustrates the \( g \)-factor tunability vs. electric field and degree of anisotropy both cases: symmetric and asymmetric model potentials. The top curve in Fig. 4.15(a), indicated by filled black squares represents the symmetric model potential of \( \alpha = \beta = 1 \) and the other curves with filled symbols represent varying anisotropic potentials from \( \beta^2/\alpha^2 = 40 \) and \( \beta^2/\alpha^2 = 80 \). As before, we choose, \( B = 1 \) T and \( \ell_0 = 30 \) nm.

Lastly, Figure 4.15(b) illustrates the tunability of the \( g \)-factor to the degree of anisotropy in the model potential. The lowest curve in Fig. 4.15(a), indicated by filled black squares represents the symmetric model potential of electric field \( E = 10^4 \) V/cm and the other curves with filled symbols represent varying electric fields \( 2 \times 10^5, 5 \times 10^5, 7 \times 10^5 \) and \( 10^6 \) V/cm. We choose, \( B = 1 \) T and \( \ell_0 = 30 \) nm.

Indeed, in Fig. 4.13(a) we see that all of the curves collapse onto a single curve for large quantum dots (i.e. starting around \( \ell_o = 35 \) nm) negating the switching effect. With anisotropy, however, the range of switchability is shifted to larger dots. In Fig. 4.13(a), the Lande \( g \)-factor increases from 0.98 to 1.2 at \( \ell_0 = 30 \) nm with the increase in the electric field for the symmetric potential (i.e., \( \alpha = \beta = 1 \)). However, in Fig. 4.13(b), the Lande \( g \)-factor decreases from 0.98 to 0.82 at \( \ell_0 = 30 \) nm with the increase in the electric field for asymmetric potential (i.e., \( \beta^2/\alpha^2 = 80 \)). In Fig. 4.15(a), we see that the \( g \)-factor increases with the increase in electric field (filled black squares) for the symmetric potential. However, \( g \)-factor decreases with the increase in electric field in an anisotropic potential (filled red circles \( \beta^2/\alpha^2 = 40 \) and filled green triangles pointing down, \( \beta^2/\alpha^2 = 80 \)).

Another result of this work is the variation in the Lande \( g \)-factor with respect to the magnetic field as well as electric field in both symmetric and asymmetric potentials for fixed quantum dot radius \( \ell_0 \) that was illustrated in Fig. 4.14(a) and Fig. 4.14(b). Here,
we quantify the Lande g-factor increases from 0.98 to 1.5 with the increase in electric field from $1 \times 10^4$ V/cm to $100 \times 10^4$ V/cm at the magnetic field of 2 T for the symmetric potential (i.e., $\alpha = \beta = 1$) as shown in Fig. 4.14(a). However, the Lande g-factor decreases from 0.98 to 0.90 with the increase in electric field from $1 \times 10^4$ V/cm to $100 \times 10^4$ V/cm at the magnetic field of 2 T for asymmetric potential (i.e., $\alpha \neq \beta$) as shown in Fig. 4.14(b).

Lastly, we see that the degree of anisotropy need not to be very large in order to obtain significant changes in the gate induced $g$-factor tunability, as illustrated in Fig. 4.15(b). We see that the $g$-factor increases with the increase in the electric field for the anisotropic ratio of up to $\beta^2/\alpha^2 = 25$. Above this value, the $g$-factor starts decreasing with the increase in electric field.

By employing a fully numerical approach, we have shown that breaking in-plane rotational symmetry in an asymmetric potential can lead to a significant change in the tunability of the electron $g$-factor over the symmetric model potential due to Rashba effect in InAs quantum dot.

### 4.7 g-value Calculation by Perturbation Method

The spin orbit interaction effect given by Rashba and Dresselhaus terms in Eqs. 4.38 and 4.39 can be written in terms of Fock-Darwin energy operators [117]

\[
H_{D1} + H_R = \hat{V} \sigma_+ + \hat{V}^\dagger \sigma_-
\]

\[
\hat{V} = -\alpha_- a_-^\dagger + \alpha_+ a_+ + i\beta_- a_- - i\beta_+ a_+^\dagger
\]

(4.46)

(4.47)

where different parameters are defined as follows:

\[
\sigma_{pm} = \frac{1}{2} (\sigma_x \pm i\sigma_y)
\]

(4.48)

\[
\alpha_{\pm} = \alpha_R e E \xi_{\pm}
\]

(4.49)

\[
\xi_{\pm} = \frac{1}{\ell} \pm \frac{eB\ell}{2\hbar c}
\]

(4.50)

From Eq. 4.47, we see that Rashba and Dresselhaus first term are coupled with a quantum number differing by one energy levels. One can treat $H_R$ and $H_{D1}$ as a perturbation term in the Hamiltonian $H_{xy}$ and find the two ground state energy eigen value with the help of first order energy correction by perturbation theory. Finally, electron g-value can be calculated numerically by employing the formula $g = \frac{\beta}{\mu_B \alpha}$. Since the electric field associated with applied gate potential and asymmetric triangular quantum well along $z$-direction are so strong that this method will only work for very small value of electric field roughly less than 10 V/cm. So we carry out the numerical simulation of the main Hamiltonian based on finite element method to see the exact numerical results for
the electron g-value variation with several parameters such as electric fields, quantum dot radius and magnetic field.

Eq. (4.47) can be treated as a perturbative part of the Fock-Darwin energy state. Up to second order correction by perturbative approach, the energy spectrum can be written as

$$\epsilon_{00} = \epsilon_{00}^0 + \langle 00 | H_{SO} | 00 \rangle + \sum_{n_+n_- \neq 00} \frac{\langle 00 | H_{SO} | n_+n_- \rangle < n_+n_- | H_{SO} | 00 \rangle}{\epsilon_{00}^0 - \epsilon_{00}^{n_+n_-}}$$

where $H_{SO} = H_R + H_{D1}$ (we neglect $H_{D2}$ through out the g-value calculation by perturbative approach). The first order correction term in Eq. (4.51) is zero and $\epsilon_{00}$ is given by the Fock-Darwin energy spectrum from Eq. (4.27). To get the analytical expression for the electron g-value by considering the spin orbit Hamiltonian as a perturbative term, we consider three eigenstates $|00 >, |01 >, |10 >$ as an interaction term. In that case, the second order correction term can be written as

$$\epsilon_{00}^2 = \frac{\langle 00 | H_{SO} | 10 \rangle < 10 | H_{SO} | 00 \rangle}{\epsilon_{00}^0 - \epsilon_{10}^0} + \frac{\langle 00 | H_{SO} | 01 \rangle < 01 | H_{SO} | 00 \rangle}{\epsilon_{00}^0 - \epsilon_{01}^0}$$

With the help of Eq. (4.47), the energy spectrum can be written as [133]

$$\epsilon_{00} \uparrow = \epsilon_{00}^0 \uparrow + \frac{\alpha_+^2}{\epsilon_{00}^0 \uparrow - \epsilon_{10}^0 \downarrow} + \frac{\beta_+^2}{\epsilon_{00}^0 \uparrow - \epsilon_{01}^0 \downarrow},$$

$$\epsilon_{00} \downarrow = \epsilon_{00}^0 \downarrow + \frac{\beta_+^2}{\epsilon_{00}^0 \downarrow - \epsilon_{10}^0 \uparrow} + \frac{\alpha_+^2}{\epsilon_{00}^0 \downarrow - \epsilon_{01}^0 \uparrow}.$$  

The above equation might be written as

$$\epsilon_{00} \uparrow = \epsilon_{00}^0 \uparrow - \frac{\alpha_+^2}{\hbar \omega_+ - g_0 \mu_B B} - \frac{\beta_+^2}{\hbar \omega_+ - g_0 \mu_B B}$$

$$\epsilon_{00} \downarrow = \epsilon_{00}^0 \downarrow - \frac{\beta_+^2}{\hbar \omega_+ + g_0 \mu_B B} - \frac{\alpha_+^2}{\hbar \omega_+ + g_0 \mu_B B}$$

The electron g-value can thus be defined by

$$g = \frac{\epsilon_{00} \uparrow - \epsilon_{00} \downarrow}{\mu_B B}$$

Substituting Eqs. (4.55) and (4.56) into Eq. (4.57), we will get the analytical expression for the effective electron g-value and can be written as [117]
\[
g = g_0 + 2 \frac{m_e m^*}{\hbar^4} \left[ 0.6 \gamma_e^2 \kappa^4 (1 - \delta) - \alpha_R^2 e^2 E^2 (1 + \delta) \right] l_0^2 \\
- \frac{1}{2} \frac{m_e m^*}{\hbar^6} \left[ 0.6 \gamma_e^2 \kappa^4 \left( \frac{1}{2} - \frac{1}{2} \delta + \delta^2 + \delta^3 \right) - \alpha_R^2 e^2 E^2 \left( \frac{1}{2} - \frac{1}{2} \delta + \delta^2 + \delta^3 \right) \right] \omega_c^2 l_0^6 \\
+ \frac{3}{64} \frac{m_e m^5}{\hbar^8} \left[ 0.6 \gamma_e^2 \kappa^4 (1 - \delta + \frac{4}{3} \delta^2 - 4 \delta^3 - 8 \delta^4 - 8 \delta^5) - \alpha_R^2 e^2 E^2 (1 + \delta + \frac{4}{3} \delta^2 + 4 \delta^3 - 8 \delta^4 + \frac{8}{3} \delta^5) \right] \omega_c^4 l_0^{10} \cdots (4.58)
\]

Where \( \delta = g_0 m^*/m_e \). The above expression is valid up to second order in \( \omega_c/\omega_0 \).

In Eq. (4.58), it clearly shows that effective \( g \)-value depends on electric fields, magnetic fields and quantum dot radius. One can vary the electric field and control the electron \( g \)-value very precisely for the purpose of a quantum logic operation. When \( g - g_0 \) becomes positive and proportional to \( E^{4/3} \) then we conclude that the Rashba spin orbit coupling parameters are dominating. For quantitative point of view, one can see in Figure 4.7 that Rashba term are dominating for the electric fields from \( 10^4 \) to \( 7 \times 10^5 \) v/cm for any size of quantum dot.

On the other hand, when \( g - g_0 \) becomes negative and proportional to \( E^2 \) then Dresselhaus spin orbit coupling parameters are dominating. Quantitatively, this is the case for electric fields between \( 8 \times 10^5 \) to \( 10^6 \) v/cm and quantum dot radius from approximately 35 to 95 nanometers as in Figure 4.7.

From Figs. 4.7, 4.8, 4.9, 4.10, 4.11, we can conclude from the analytical expression of Eq. (4.58) that the Rashba spin orbit terms are the dominating mechanisms for positive \( g \)-value whereas Dresselhaus spin orbit terms are dominating mechanisms for negative value of electron \( g \)-value.

### 4.8 Summary and Conclusion

We carried out a numerical simulation study of gate-induced tunability of the electron \( g \)-factor in a prototype single electron spintronic device in GaAs and InAs quantum dots. We considered a realistic three-dimensional geometry and employed a numerical approach based on the finite element method. The key results of this work are illustrated in Figs. 4.7, 4.9, 4.10 and 4.11 for GaAs quantum dot and Figs. 4.13, 4.14 and 4.13 for InAs quantum dot. Here anisotropic confining potential significantly extends the size range of quantum dots that exhibits electric-field-induced \( g \)-factor tunability. Indeed, in Figs. 4.7 and 4.13(a), we see that all of the curves collapse onto a single curve for large quantum dots (i.e. starting around \( \ell_o = 65 \) nm for GaAs quantum dot and starting around \( \ell_o = 35 \) nm for InAs quantum dot) negating the switching effect due to level crossings. With anisotropy, however, the switchability of the \( g \)-factor increases so that the radius of the quantum dot increases for both GaAs and InAs cases.

Another result of this work is the demonstration that the degree of anisotropy need not
Figure 4.1: Evolution of Fock-Darwin Energy Levels for 30 nm quantum dot radius in a symmetric confining potential. Here we choose $\alpha = 1$ and $\beta^2 = 2.8$ to mimic the exact realistic potential.

be very large in both GaAs and InAs quantum dots in order to obtain significant changes in the gate induced $g$-factor tunability, as illustrated in Figs. 4.10 and 4.15. We see that the maximum effect is obtained for dots in the range of $\beta^2/\alpha^2 \approx 15 \cdots 25$ and begins to decrease slightly as the shape-anisotropy ratio becomes larger in a GaAs quantum dot (Fig. 4.10). However, we get the reverse effect for InAs quantum dot as shown in Fig. 4.15(b) at around $\beta^2/\alpha^2 \approx 15$ The jumps in the value of the $g$-factor from positive to negative are indicative of level crossings (e.g. the relative ordering of spin up and down levels changes as a function of the anisotropy). Lastly we argued from Fig. 4.11 that results for quantum dots in realistic potentials can be well represented by the anisotropic model of Eq. 4.13 with $\alpha = 1$, $\beta^2 = 2.8$ and $\ell_o = 30$ nm. By employing non-perturbative, fully numerical methods and realistic geometries, our approach provided insights that might be difficult or impossible to obtain using analytical techniques alone.
Figure 4.2: Evolution of Fock-Darwin Energy Levels for 30 nm quantum dot radius in a asymmetric confining potential. Here we choose $\alpha = 1$ and $\beta^2 = 2.8$ to mimic the exact realistic potential.
Figure 4.3: Electrostatic potential for a prototype single-electron device plotted in the 2DEG layer. This figure illustrates a single-spin device consisting of two triangular gates above a 2DEG. The gates were held at 1V and the 2DEG was held at 0 V. For simplicity of the electrostatic calculation, the 2DEG was treated as a classical perfect conductor. The dimensions of the device in the $x$ and $y$ directions are 2.8 $\mu m$ and 1.8 $\mu m$ respectively and the thickness is 1 $\mu m$. 
Figure 4.4: Electrostatic confining potential in the 2DEG along the symmetry axis of a prototype single-electron device. This figure was made by plotting the potential of Fig. 4.3 along a line in the 2DEG through the symmetry axis of the device (the x-axis of Fig. 4.3, i.e. a line running from one gate to the other) intersecting with the central region.
Figure 4.5: Electrostatic confining potential in the 2DEG normal to the symmetry axis of a prototype single-electron device. This figure was made by plotting the potential of Fig. 4.3 along a line in the 2DEG normal to the symmetry axis of the device (the y-axis of Fig. 4.3) and intersecting the central region.

Figure 4.6: In-plane wave-function for quantum dots formed by three potentials: (a) the symmetric quadratic model of Eq. 4.13 with $\alpha = \beta = 1$ and $\ell_o = 30$ nm (see Eq. 4.14); (b) the asymmetric quadratic model of Eq. 4.13 with $\alpha = 1$, $\beta^2 = 2.8$ and $\ell_o = 30$ nm; and (c) the realistic potential of Eq. 4.12 and Figs. 4.4, and 4.5.
Figure 4.7: Electric field induced changes in the $g$-factor vs. quantum dot radius for various electric field strengths for a symmetric quantum dot in the quadratic potential of Eq. 4.13. From top to bottom, the curves represent increasing electric field strength as follows. The first curve corresponds to $1 \times 10^4$ V/cm, and the rest range from $1 \times 10^5$ V/cm through $1 \times 10^6$ V/cm in equal steps with $B = 1$ T. This results is consistent with Ref. [117]. The parameter $g$ is expressed relative to its non-relativistic free-electron value $g_o = 2$. 
Figure 4.8: Electric field induced changes in the $g$-factor vs. magnetic field for various electric field strengths for the symmetric quantum dot. From top to bottom, the curves represent increasing electric field strength as follows. The first curve corresponds to $1 \times 10^4$ V/cm, and the rest range from $1 \times 10^5$ V/cm through $1 \times 10^6$ V/cm in equal steps. For this calculation, the quantum dot radius was fixed at $\ell_o = 20$ nm. We express $g$ relative to its non-relativistic free-electron value $g_o = 2$. 


Figure 4.9: Electric field induced changes in the $g$-factor vs. quantum dot radius for various electric field strengths for an asymmetric quantum dot for the asymmetric model of Eq. 4.13 with $\alpha = 1$, and $\beta^2 = 20, 40, 60,$ and $80$. In each panel, from top to bottom, the curves represent increasing electric field strength as follows. The first curve corresponds to $1 \times 10^4$ V/cm, and the rest range from $1 \times 10^5$ V/cm through $1 \times 10^6$ V/cm in equal steps. Again we choose $B = 1$ T. We express $g$ relative to its non-relativistic free-electron value $g_o = 2$. 
Figure 4.10: Electric field induced changes in the $g$-factor vs. the degree of anisotropy of the quantum dot confinement potential for various electric field strengths. From top to bottom, the curves represent increasing electric field strength as follows. The first curve corresponds to $1 \times 10^4$ V/cm, and the rest range from $1 \times 10^5$ V/cm through $1 \times 10^6$ V/cm in equal steps. This figure assumes the quadratic model of Eq. 4.13 with $\alpha = 1$, $\ell_o = 120$ nm and $B = 1$ T. We express $g$ relative to its non-relativistic free-electron value $g_o = 2$. 

Figure 4.11: Changes in the $g$-factor vs. electric field for quantum dots in the realistic potential of Figs. 4.4 and 4.5 (using the form of Eq. 4.12) in comparison to results for symmetric and asymmetric model potentials. The black (lowest) curve corresponds to the symmetric model of Eq. 4.13 with $\alpha = \beta = 1$ while the rest of the curves with filed symbols correspond to $\beta^2 = 2.8$ (red circles), $\beta^2 = 5$ (green upward pointing triangles) and $\beta^2 = 10$ (blue downward pointing triangles). In each of these curves corresponding to Eq. 4.13 we have chosen $\ell_o = 30 \text{ nm}$. The results for the realistic potential are given by the open circles. We note excellent agreement between the $\beta^2 = 2.8$ result and that for the realistic potential. We express $g$ relative to its non-relativistic free-electron value $g_0 = 2$. 
\[ E_1 = 0.003857 \text{ eV} \]

\[ E_1 = 0.017352 \text{ eV} \]

**Figure 4.12:** In plane wave functions for quantum dots formed by (a) symmetric quadratic potential with \( \alpha = \beta = 1 \), and (b) asymmetric quadratic potential with \( \alpha^2 = 1, \beta^2 = 80 \). In both cases, we choose \( \ell_0 = 30 \text{ nm} \), electric field = \( 10^5 \text{ V/cm} \), and magnetic field = \( 1 \text{ T} \).  

**Figure 4.13:** Electric-field induced changes in the g-factor vs. quantum dot radius for symmetric and asymmetric model potentials with (a) \( \alpha = \beta = 1 \) and (b) \( \alpha^2 = 1, \beta^2 = 80 \). In Fig 4.4(a), from bottom to top, the curves represent increasing electric field strength as \( 1 \times 10^4, 2 \times 10^5, 5 \times 10^5, 7 \times 10^5 \) and \( 10^6 \text{ V/cm} \). In Fig 4.4(b), from top to bottom, the curves represent increasing electric field strength as \( 1 \times 10^4, 2 \times 10^5, 5 \times 10^5, 7 \times 10^5 \) and \( 10^6 \text{ V/cm} \). In both cases, We choose the magnetic field = \( 1 \text{ T} \). We express \( g \) relative to its nonrelativistic free electron value \( g_0 = 2 \). We find a level crossing near 35 nm quantum dot radius in Fig 4.4(a) and 55 nm quantum dot radius in Fig 4.4(b).
Figure 4.14: Electric-field induced changes in the g-factor vs. magnetic field for symmetric and asymmetric model potentials with (a) $\alpha = \beta = 1$ and (b) $\alpha^2 = 1, \beta^2 = 80$. In Fig. 4.5(a), from bottom to top, the curves represent increasing electric field strength as $1 \times 10^4, 2 \times 10^5, 5 \times 10^5, 7 \times 10^5$ and $10^6$ v/cm. In Fig. 4.5(b), from top to bottom, the curves represent increasing electric field strength as $1 \times 10^4, 2 \times 10^5, 5 \times 10^5, 7 \times 10^5$ and $10^6$ v/cm. In both cases, we choose $\ell_0 = 20$ nm. We express $g$ relative to its nonrelativistic free electron value $g_0 = 2$. We find a level crossing near 3 T in Fig 4.5(a) and its value extends to the larger magnetic field in Fig 4.4(b).

Figure 4.15: (a) Changes in the g-factor vs. electric filed for quantum dots in the model potential characterized by $\alpha = 1, \beta = 1$ (black), $\alpha = 1, \beta^2 = 40$ (red)$\alpha = 1, \beta^2 = 80$ (green). (b) Electric field induced changes in the g factor vs. the degree of anisotropy of the quantum dot confinement potential for various electric field strengths. In each plot, from bottom to to, the curves represent increasing electric field strength as $1 \times 10^4, 2 \times 10^5, 5 \times 10^5, 7 \times 10^5$ and $10^6$ v/cm. We choose $B=1$ T and $\ell_0 = 30$ nm in each plot. We express $g$ relative to its nonrelativistic free-electron value $g_0 = 2$. 
Chapter 5

Geometric Phase

Geometric phases (or Berry phases) abound in physics and their study has occupied the attention of many researchers in various fields since the seminal work of Berry [160, 179]. In recent years, a number of researchers have investigated the geometric phases in single- and few-spin systems by considering their possible applications in the field of quantum computing and non-charge based quantum logic [162, 165–168, 173–175, 178, 180–183]. In this Chapter, we explore the geometric phases associated with the electron spin in an GaAs quantum dot. We first present analytical expressions for the Berry phase for degenerate systems of GaAs quantum dots in the presence of spin-orbit interaction, and for the transition probabilities of spin by using Feynman’s entangling technique. We obtain exact analytical results for three cases: (a) the Rashba coupling, (b) the Dresselhaus coupling, and (c) the symmetric mixture of the Rashba and the Dresselhaus coupling with equal strength. We also obtained a formal expression for a general mixture of the two couplings, for which we performed numerical simulations.

5.1 Introduction

An interesting idea is that the spin of a single electron trapped in an electrically defined 2-dimensional quantum dot can be manipulated through the application of gate potentials by moving adiabatically the center of mass of the quantum dot along a closed loop. The adiabatic motion of the quantum dot induces a non-Abelian matrix Berry phase. It is also interesting that the Berry phase may be changed dramatically by applying an external voltage and its effect may be detected in an interference experiment [178].

The main focus of the present work is to explore fundamental physics of the electron propagator (a matrix valued function of initial and final spin states) for the adiabatic motion of a single electron spin contained in the quantum dot [173, 177, 178, 180–182]. The propagator is a matrix element of the evolution operator. Since the Hamiltonian contains non-commuting $SU(2)$ spin operators, the evolution operator is a non-Abelian unitary operator. The non-Abelian nature makes calculation of the propagator complicated, so
many authors evaluate it approximately by expanding it perturbatively. In the present thesis we use a novel technique, the Feynman disentangling technique, without resort to perturbation expansion [164, 169–171].

5.2 Classical Parallel Transport

It is convenient to begin by obtaining the statement of ordinary parallel transport of a vector over the surface of a sphere. Let the unit vector \( \hat{e} \) be transported in such a way that \( \hat{e} \cdot \hat{r} \) must remain zero and \( \hat{e} \) and \( \hat{r} \) must not twist i.e. \( \Omega \times \mathbf{r} = 0 \). Here \( \Omega \) is the angular velocity [179]. It means

\[
\dot{\hat{e}} = \Omega \times \mathbf{e} \quad \text{where} \quad \Omega = \mathbf{r} \times \dot{\mathbf{r}} \tag{5.1}
\]

This law is nonintegrable. When \( \mathbf{r} \) returns to its original direction after traveling the circuit “C” then \( \mathbf{e} \) does not return but has turned through an angle \( \alpha(C) \). Let us define \( \mathbf{e}' = \mathbf{r} \times \mathbf{e} \) and the complex unit vector \( \psi = (\mathbf{e} + i\mathbf{e}')/\sqrt{2} \) is in the plane perpendicular to \( \mathbf{r} \). Then according to the parallel transport law, we have

\[
\text{Im} \psi^* \cdot \dot{\psi} = 0, \quad \text{Im} \psi^* \cdot d\psi = 0. \tag{5.2}
\]

Where \( d\psi \) is the change in \( \psi \) due to change in \( \mathbf{r} \). To find \( \alpha(C) \), we choose the local basis on the sphere as

\[
\mathbf{\hat{u}} = (\sin \phi, \cos \phi, 0), \quad \mathbf{\hat{v}} = (-\cos \theta \cos \phi, -\cos \theta \sin \phi, \sin \theta). \tag{5.3}
\]

Which is equivalent to specifying the complex unit vector as

\[
\mathbf{\hat{u}}(\mathbf{r}) = \frac{(\mathbf{\hat{u}}(\mathbf{r}) + i \mathbf{\hat{v}}(\mathbf{r}))}{\sqrt{2}} \tag{5.4}
\]

Suppose the angle made by \( \mathbf{e} \) and \( \mathbf{\hat{u}} \) is \( \alpha(t) \), then we have

\[
\psi = \mathbf{\hat{u}} \exp(-i\alpha) \tag{5.5}
\]

The above equation can be written as

\[
\alpha(C) = \text{Im} \int \int dX_1 dX_2 (\partial_1 n^* \cdot \partial_2 n - \partial_2 n^* \cdot \partial_1 n) \tag{5.6}
\]

Where \( X_1 \) and \( X_2 \) are arbitrary parameters and its value depend in position \( \mathbf{r} \) on the sphere. \( \partial_j = \partial / \partial X_j \). The choice of \( X_1 = \theta, X_2 = \phi \) in the above integrand of \( d\theta d\phi \sin \theta \) is the area element on the sphere which means the anholonomy \( \alpha(C) \) is the solid angle subtended by \( C \) at the center of the sphere [179].
5.3 Quantum Parallel Transport

To make the classical parallel transport law consistent with quantum mechanics, one needs to replace the normalized quantum state $|\psi\rangle$ in the Hilbert space and the position vectors $X = (X_1, X_2 \cdots)$. Its physical system is represented by $|\psi\rangle$. In this case, Eq.(5.2) can be written as [179]

$$\text{Im} <\psi|d\psi> = 0. \quad (5.7)$$

This law is also non-integrable. When $X$ is taken round a closed loop $C$ then the state $|\psi\rangle$ is returned to its original state with an additional geometric phase $\gamma(C)$.

$$<\psi_{\text{initial}}|\psi_{\text{final}}> = \exp \{i\gamma(C)\} \quad (5.8)$$

Let $|\psi\rangle = |n(X)\rangle \exp(i\gamma)$ where $|n(X)\rangle$ is a single valued. Then the geometric phase can be written as

$$\gamma(C) = -\int \int V(X) \quad (5.9)$$

Where $V = \text{Im} \langle dn \times dn \rangle$ is the phase 2-form whose flux through $C$ gives the geometric phase. Here $V$ is invariant under the gauge transformation

$$|n(X)\rangle \rightarrow |n'(X)\rangle = |n(X)\rangle \exp \{i\mu(X)\} \quad (5.10)$$

The total geometric phase may be calculated by substituting the above equation in the time dependent Schrodinger equation

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \quad (5.11)$$

The eigenstate of the Hamiltonian can be slowly changed by changing the arbitrary parameter in the Hamiltonian. The adiabatic theorem guarantees that the total phase of the system can be written as the sum of a dynamical phase factor as well as a geometric phase factor. Thus

$$<\psi_{\text{initial}}|\psi_{\text{final}}> = \exp \{i(\gamma_d + \gamma(C))\} \quad (5.12)$$

Where $\gamma_d$ can be written as

$$\gamma_d = -\frac{1}{\hbar} \int_0^T dt E_n(X(t)) \quad (5.13)$$

The calculation of Berry phase for degenerate and non-degenerate cases will be discussed in more details.
5.4 Diagonalization of the Hamiltonian of a Quantum Dot

The Hamiltonian of a quantum dot in the plane of 2DEG in the presence of an asymmetric distorted potential is given by [176, 181]

\[ H_0 = \frac{1}{2m^*}P^2 + \frac{1}{2}m^*\omega_0^2(\delta_x^2x^2 + \delta_y^2y^2) + \rho_xx + \rho_yy. \]  

(5.14)

In the above \( P_\perp \) is the horizontal component of the total momentum in the presence of a uniform magnetic field \( \mathbf{B} = (0, 0, B) \), which satisfies

\[ P^2_\perp = \left( p_x + \frac{e}{c}A_x \right)^2 + \left( p_y + \frac{e}{c}A_y \right)^2. \]

(5.15)

For the vector potential \( \mathbf{A} \), we choose the gauge as

\[ \mathbf{A} = (-\xi By, \eta Bx, 0) \]

(5.16)

which yields \( \nabla \times \mathbf{A} = \mathbf{B} \) provided that

\[ \xi + \eta = 1. \]

(5.17)

The distortion of the system is characterized by parameters, \( \delta_x, \delta_y, \rho_x, \rho_y, \xi \) and \( \eta \).

After some tedious calculation, we can reduce the Hamiltonian (5.14) to the form,

\[ H_0 = \frac{1}{2m^*} \left\{ (p_x + px_0)^2 + (p_y + py_0)^2 \right\} + \frac{1}{2}m^*\Omega_1^2\gamma^2(x + x_0)^2 + \frac{1}{2}m^*\Omega_2^2\gamma^2(y + y_0)^2 \]

\[ + \omega_c \left\{ \eta(x + x_0)(p_y + py_0) - \xi(y + y_0)(p_x + px_0) \right\} - G \]

(5.18)

where

\[ \Omega_1 = \omega_0\delta_x, \quad \Omega_2 = \omega_0\delta_y, \quad \omega_c = eB/(mc), \quad \gamma^2 = 1 + \frac{\omega_c}{(\Omega_1 + \Omega_2)}, \]

(5.19)

\[ x_0 = \frac{\rho_x}{m^*(\Omega_1^2\gamma^2 - \omega_c^2\eta^2)}, \quad y_0 = \frac{\rho_y}{m^*(\Omega_2^2\gamma^2 - \omega_c^2\xi^2)}, \]

(5.20)

\[ px_0 = \frac{\omega_c\xi\rho_y}{\Omega_2^2\xi^2 - \omega_c^2\xi^2}, \quad py_0 = -\frac{\omega_c\eta\rho_y}{\Omega_1^2\eta^2 - \omega_c^2\eta^2}, \]

(5.21)

and

\[ G = \frac{1}{2m^*} \left( px_0^2 + py_0^2 \right) + \frac{1}{2}m^*\omega^2 \left( \Omega_1^2x_0^2 + \Omega_2^2y_0^2 \right). \]

(5.22)

Now we apply canonical transformations,

\[ x_1 = \sqrt{\frac{\Omega_1}{\omega}}(x + x_0), \quad x_2 = \sqrt{\frac{\Omega_2}{\omega}}(y + y_0), \]

(5.23)
and
\[ p_1 = \sqrt{\frac{\omega}{\Omega_1}}(p_x + p_{x0}), \quad p_2 = \sqrt{\frac{\omega}{\Omega_2}}(p_y + p_{y0}). \quad (5.24) \]

Even though we have introduced an adjustable parameter \( \omega \) in the above, the commutation relations, \([x_i, p_j] = i\hbar \delta_{ij}\) and \([x_i, x_j] = [p_i, p_j] = 0\), remain invariant under the canonical transformations.

At this point, for convenience, we choose,
\[ \xi = \frac{\Omega_1}{\Omega_1 + \Omega_2}, \quad \eta = \frac{\Omega_2}{\Omega_1 + \Omega_2} \quad (5.25) \]
so that \( \xi + \eta = 1 \). In terms of new canonical variables, we can write (5.19) as
\[ H_0 + G = \frac{\Omega_1}{\omega} \left( \frac{1}{2m^*}p_1^2 + \frac{1}{2}m^*\omega^2\gamma^2x_1^2 \right) + \frac{\Omega_2}{\omega} \left( \frac{1}{2m^*}p_2^2 + \frac{1}{2}m^*\omega^2\gamma^2x_2^2 \right) + \omega c \sqrt{\frac{\Omega_1\Omega_2}{\Omega_1 + \Omega_2}}(x_1p_2 - x_2p_1). \quad (5.26) \]

If we select \( \omega \) such that \( m\omega\gamma = 1 \), then (5.26) may be reduced to a simple form,
\[ h = \frac{2}{\Omega_1\gamma}(H + G) = p_1^2 + x_1^2 + b(p_2^2 + x_2^2) + c(x_1p_2 - x_2p_1) \quad (5.27) \]
where
\[ b = \frac{\Omega_2}{\Omega_1}, \quad c = \frac{2\omega c\gamma\sqrt{\Omega_1\Omega_2}}{\Omega_1 + \Omega_2}. \quad (5.28) \]

The energy spectrum, i.e., the set of eigenvalues of the Hamiltonian, can be found in a way similar to Schuh’s [176]. First we notice that (5.27) can be expressed in the matrix form,
\[ h = \check{\mathbf{P}} \mathbf{M} \mathbf{P} \]
where
\[ \mathbf{P} = \begin{pmatrix} p_1 \\ p_2 \\ x_1 \\ x_2 \end{pmatrix}, \quad \mathbf{M} = \begin{pmatrix} 1 & 0 & 0 & -c/2 \\ 0 & b & c/2 & 0 \\ 0 & c/2 & 1 & 0 \\ -c/2 & 0 & 0 & b \end{pmatrix} \quad (5.30) \]
and \( \check{\mathbf{P}} \) is the transpose of \( \mathbf{P} \). The matrix \( \mathbf{M} \) is diagonalizable by an appropriate orthogonal transformation \( \mathbf{U} \) as
\[ \mathbf{M}_D = \mathbf{U} \mathbf{M} \mathbf{U}, \quad \check{\mathbf{U}} \mathbf{U} = 1, \quad (5.31) \]
so that
\[ h = \check{\mathbf{P}} \mathbf{U} \mathbf{M} \mathbf{U} \mathbf{P} = \check{\mathbf{P}} \mathbf{M}_D \mathbf{P} \quad (5.32) \]
with

\[ P' = UP = \begin{pmatrix} p_1' \\ p_2' \\ x_1' \\ x_2' \end{pmatrix}. \]  

(5.33)

The diagonalization of \( M \) itself is rather easily performed by evaluating the determinant,

\[ |M - \lambda I| = 0, \]

(5.34)

whose roots are the eigenvalues of \( M \),

\[ \lambda_1 = \lambda_3 = \frac{1}{2}(b + 1 + d), \quad \lambda_2 = \lambda_4 = \frac{1}{2}(b + 1 - d), \]  

(5.35)

where \( d = \sqrt{(b - 1)^2 + c^2} \). Thus the diagonalized matrix is

\[ M_D = \frac{1}{2} \begin{pmatrix} 1 + b + d & 0 & 0 & 0 \\ 0 & 1 + b - d & 0 & 0 \\ 0 & 0 & 1 + b + d & 0 \\ 0 & 0 & 0 & 1 + b - d \end{pmatrix} \]  

(5.36)

As a result of diagonalization, (5.27) takes a form,

\[ h = \frac{1}{2}(1 + b + d)(p_1'^2 + x_1'^2) + \frac{1}{2}(1 + b - d)(p_2'^2 + x_2'^2). \]  

(5.37)

As we have seen above, it is not necessary to use the orthogonal matrix \( U \) of (5.31) in diagonalizing the matrix \( M \). However, in order to determine the primed variables \((p_1', p_2', x_1', x_2')\) in terms of the unprimed variables \((p_1, p_2, x_1, x_2)\), we have to have an explicit form of \( U \). It can be confirmed that the orthogonal matrix,

\[ U = \frac{1}{(s_+ - s_-)} \begin{pmatrix} 1 & 1 & -s_- & -s_+ \\ 1 & -1 & s_+ & -s_- \\ s_- & s_+ & 1 & 1 \\ -s_+ & s_- & 1 & -1 \end{pmatrix} \]  

(5.38)

where we let \( cs_\pm + 2 = 1 \pm b \) with \( d^2 = (b - 1)^2 + c^2 \), diagonalizes the matrix \( M \) via (5.31), resulting in the exactly same form as that of (5.36). By the transformation
P' = UP, we obtain

\[
p'_1 = \frac{1}{(s_+ - s_-)}(p_1 + p_2 - s_- x_1 - s_+ x_2)
\]

\[
p'_2 = \frac{1}{(s_+ - s_-)}(p_1 + p_2 + s_+ x_1 - s_- x_2)
\]

\[
x'_1 = \frac{1}{(s_+ - s_-)}(s_- p_1 + s_+ p_2 + x_1 + x_2)
\]

\[
x'_2 = \frac{1}{(s_+ - s_-)}(-s_+ p_1 + s_- p_2 + x_1 - x_2).
\]

Since \((s_+ - s_-)^{-2} = (s^2_+ + s^2_- + 2) = c^2/(4d^2)\), we see that \([x_i, p_j] = i\hbar \delta_{ij}\) and \([x_i, x_j] = [p_i, p_j] = 0\) imply \([x'_i, p'_j] = i\hbar \delta_{ij}\) and \([x'_i, x'_j] = [p'_i, p'_j] = 0\).

Next we define the annihilation operators \(a_{\pm}\) and the creation operators \(a^\dagger_{\pm}\) by

\[
a_+ = \frac{1}{\sqrt{2\hbar}}(x'_1 + ip'_1), \quad a^\dagger_+ = \frac{1}{\sqrt{2\hbar}}(x'_1 - ip'_1),
\]

and

\[
a_- = \frac{1}{\sqrt{2\hbar}}(x'_2 + ip'_2), \quad a^\dagger_- = \frac{1}{\sqrt{2\hbar}}(x'_2 - ip'_2).
\]

In terms of the unprimed canonical variables, we have

\[
a_{\pm} = \frac{1}{(s_+ - s_-)} \left\{ \pm(s_+ \pm i)p_1 + (s_- \pm i)p_2 + (1 \mp is_\mp) x_1 \pm (1 \mp is_\pm) x_2 \right\} \quad (5.42)
\]

\[
a^\dagger_{\pm} = \frac{1}{(s_+ - s_-)} \left\{ \pm(s_- \mp i)p_1 + (s_+ \mp i)p_2 + (1 \pm is_\pm) x_1 \pm (1 \pm is_\pm) x_2 \right\}. \quad (5.43)
\]

It is easy to show that \([a_{\pm}, a^\dagger_{\pm}] = 1\). As is well-known, \(a^\dagger_{\pm}a_{\pm}\) behave like the number operators acting on the Fock space (or in the number representation) as

\[
a^\dagger_{\pm}a_{\pm}|n_{\pm}\rangle = n_{\pm}|n_{\pm}\rangle, \quad n_{\pm} = 0, 1, 2, .... \quad (5.44)
\]

These operators and the number representation will be utilized later in our calculation of the Berry phase.

With the help of the above operators, (5.37) can be expressed as

\[
h = \hbar \left\{ (1 + b + d)a^\dagger a_+ + (1 + b - d)a^\dagger a_- \right\}. \quad (5.45)
\]

Hence

\[
\text{Spec}[h] = \hbar \left\{ (1 + b + d)n_+ + (1 + b - d)n_- \right\}. \quad (5.46)
\]

Accordingly, the eigenvalues of the original Hamiltonian (5.14) is given by

\[
E_{n_+n_-} = \frac{\Omega_j \gamma \hbar}{2} \left\{ (1 + b + d)n_+ + (1 + b - d)n_- \right\} - G, \quad (5.47)
\]

68
where \( G \) is a constant given in (5.22) and \( n_\pm = 0, 1, 2, \ldots \)

### 5.5 Analytical Expressions for Berry Phase

Consider a quantum system of Hamiltonian \( \hat{H} \) is changed its position adiabatically in a closed loop in such a way that the eigen state of that Hamiltonian will returned to the original state with an additional phase factor called geometric or Berry phase [160].

In other words, suppose, a quantum system of eigen state is slowly transported in a closed loop \( C \) by changing variables \((q_x, q_y)\) in its Hamiltonian \( H(q_x, q_y) \). Then the state will acquire an additional phase factor \( \exp\{i\gamma(C)\} \) in addition to the familiar dynamical phase factor. The additional phase factor is called the Berry Phase or Geometric Phase.

Let the Hamiltonian \( \hat{H} \) is brought adiabatically in a closed loop by changing parameters \((q_x, q_y)\). Then the state of the quantum system can be transported in a closed path in a parameter space with Hamiltonian \( \hat{H}(q_x, q_y(t)) \) between times \( t = 0 \) and \( t = T \). According to time dependent Schrodinger equation, the wave function \(|\psi(t)\rangle >\) of that state can be written as

\[
\hat{H}((q_x, q_y)(t))|\psi(t)\rangle = i\hbar|\dot{\psi}(t)\rangle >
\]

At any instant, the eigen states \(|n(q_x, q_y)\rangle >\) of the Hamiltonian that appear in Eq. (5.48) for \((q_x, q_y) = (q_x, q_y)(t)\) can be written as

\[
\hat{H}(q_x, q_y)|n(q_x, q_y)\rangle = E_n(q_x, q_y)|n(q_x, q_y)\rangle >
\]

with energies \( E_n(q_x, q_y) \). This eigen value equation implies no relation between the phases of the eigen states \(|n(q_x, q_y)\rangle >\) at different \((q_x, q_y)\). For the present purposes any (differentiable) choice of phases can be made, provided \(|n((q_x, q_y)(t))\rangle >\) in a single valued in a parameter domain that includes the circuit \( C \).

Where \( E_n(q_x, q_y) \) is the eigen value of the above Hamiltonian. Adiabatically, a system can be prepared in any of these states \(|n(q_x, q_y(0))\rangle >\) of Hamiltonian \( \hat{H} \) at any instant of time \( 0 \) and then in another state \(|n(q_x, q_y(t))\rangle >\) at another instant of time \( t \). The wave function of Eq. (5.48) can be written as

\[
|\psi(t)\rangle = \exp \left\{ -\frac{i}{\hbar} \int_0^t dt' E_n((q_x, q_y)(t')) \right\} \exp(i\gamma_n(t))|n((q_x, q_y)(t))\rangle >
\]

The first exponential term in Eq. (5.50) is called the dynamical phase factor which is very familiar in quantum mechanics. The second exponential term in Eq. (5.50) is called the geometric phase or Berry phase factor. Here \( \gamma_n(t) \) is not integrable quantity and it does not have a single-valued function around a closed loop. In other words, \( \gamma_n(T) \neq \gamma_n(0) \).
The total phase change of $|\psi\rangle$ round C is given by

$$|\psi(T)\rangle = \exp(i\gamma_n(C))\exp\left\{\frac{-i}{\hbar} \int_0^T dtE_n((\vartheta_x, \vartheta_y)(t))\right\} |\psi(0)\rangle$$ (5.51)

Where the geometric phase change can be written as

$$\gamma_n(C) = i \int_C <n(\vartheta_x, \vartheta_y)|\nabla_{(\vartheta_x, \vartheta_y)}n((\vartheta_x, \vartheta_y)) > \cdot d(\vartheta_x, \vartheta_y)$$ (5.52)

Thus scalar Berry phase $\gamma_n(C)$ is expressed in terms of circuit integral in parameter space. The gradient of the state vector $|n\rangle$ is imaginary number which guarantees that the Berry phase is a real observable quantity. Also, the Berry Phase is independent of how the circuit is traversed. It is very difficult to control the electron wave function in quantum mechanics. Such type of difficulties can be avoided by changing the line integral into surface integral by applying Stoke’s theorem.

$$\gamma_n(C) = -i \int \int_C dS \cdot \sum_{m \neq n} <\nabla n|m \rangle \times m|\nabla n \rangle$$ (5.53)

where $dS$ is the surface area in parameter space. The off-diagonal element can be written as

$$<n|\nabla n \rangle = \frac{<m|\nabla \hat{H}|n \rangle}{(E_n - E_m)}; \quad m \neq n$$ (5.54)

Thus $\gamma_n$ from Eq. (5.53) can be expressed as

$$\gamma_n(C) = -i \int \int_C dS \sum_{m \neq n} <n(\vartheta_x, \vartheta_y)|\nabla_{(\vartheta_x, \vartheta_y)}\hat{H}|m(\vartheta_x, \vartheta_y) \rangle \times <m(\vartheta_x, \vartheta_y)|\nabla_{(\vartheta_x, \vartheta_y)}\hat{H}|n(\vartheta_x, \vartheta_y) \rangle \frac{(E_n - E_m)^2}{(E_n - E_m)^2}$$ (5.55)

### 5.6 Computational Method for Scalar Berry Phase

we calculated the Berry Phase for two lowest eigen states $|00\rangle$ and $|10\rangle$. We found that the system has no Berry Phase for the Hamiltonian appear in Eq. (5.14) with zero distortion potentials along x and y directions. However, one can calculate the net Berry Phase for the Hamiltonian of a quantum dot in the plane of a 2DEG of asymmetric distortion potential in presence of external magnetic field. For this case, the Hamiltonian can be written as

$$H_0 = \frac{\Omega_1}{2m^*\omega_0} [\hat{h}] - G + \frac{1}{2}g_0\mu_B\sigma_z B$$ (5.56)

Here, $g_0$ is the Bulk $g$-factor, $\mu_B$ is the Bohr magneton and $\sigma_z$ is the pauli matrix
along z-direction. With the help of creation and annihilation operators given in Eq 5.42, the Berry Phase of Eq. (5.55) is given by

$$\gamma_n(C) = \int_{\alpha} \int_{\beta} d\varrho_x d\varrho_y \frac{1}{\frac{1}{2}h\Omega \alpha [b + 1 - d] + g_0 \mu_B B}$$

(5.57)

Here $\Omega = \sqrt{\omega_0^2 + \omega_c^2}/4$ and $\omega_c = eB/m^*$ is the cyclotron frequency. The energy spectrum present in the denominator of the Berry Phase has been calculated numerically and is shown in the figure 5.1. From the figure, we clearly see the level crossing of spin up and spin down in the energy spectrum. This approach is only valid for the non-degenerate case.

5.7 Extension of Berry Phase for Degenerate Case

For the system of interest here (a single spin in a 2D electrostatically defined quantum dot) degeneracies exist for various parameter values [161, 172] and one must properly consider the generalization that was developed by Wilczek and others to handle the situation with degenerate states. [177, 178, 180–182] Then the geometric phase is replaced by a non-Abelian unitary transformation $U_{ad}$ of the initial state within the degenerate subspace.
The wave function now takes the form:

\[ |\Psi_\alpha(T)\rangle = \exp\left\{ -\frac{i}{\hbar} \int^T_0 E(t) dt \right\} U_{ad} |\Psi_\beta(0)\rangle. \]  

(5.58)

In the present work, we study the propagator on the right hand side of Eq. 5.58 using the Feynman disentangling technique and give analytical and numerical results. We now turn to a discussion of the Feynman disentangling technique and its application to the present problem. [164, 169–171]

5.8 The Spin Transition Probability via the Feynman Didentangling Method

To discuss a geometric-phase-induced spin rotation, we consider a GaAs quantum dot formed in the plane of a two-dimensional electron gas (2DEG), the center of mass of which, moves adiabatically along a closed path due to the application of appropriate potentials. An electron in the 2DEG plane experiences an effective local magnetic field as it moves due to spin-orbit coupling. The Hamiltonian for the spin-orbit coupling is of the form:

\[ H_{SO} = 2\alpha(P_y S_x - P_x S_y) - 2\beta(P_x S_x - P_y S_y), \]  

(5.59)

where \(P\) is the momentum of the electron in the \(xy\) plane in which the electron is confined, and \(S\) is the \(SU(2)\) spin operator whose components obey the \(SU(2)\) algebra:

\[ [S_+, S_-] = 2S_0, \quad [S_0, S_\pm] = \pm S_\pm, \]  

(5.60)

where \(S_\pm = S_x \pm iS_y\) and \(S_0 = S_z\). The Hamiltonian (5.59) consists of the Rashba coupling \((\alpha)\) and the Dresselhaus coupling \((\beta)\) whose coupling parameters are dependent on the electric field \(E\) of the quantum well confining potential (i.e. \(E = -\partial V/\partial z\)) as:

\[ \alpha = \frac{\alpha_R e}{\hbar} E, \quad \beta = \frac{0.7794 \gamma_c}{\hbar} \left( \frac{2m^* e}{\hbar^2} \right)^{2/3} E^{2/3} \]  

(5.61)

where \(\alpha_R = 4.4^2\) and \(\gamma_c = 26eV^3\) for the GaAs quantum dot [161]. \(H_{SO}\) may also be expressed as:

\[ H_{SO} = H_+(t)S_+ + H_-(t)S_-, \]  

(5.62)

with

\[ H_\pm = \{(\alpha P_y - \beta P_x) \mp i(\beta P_y - \alpha P_x)\}. \]  

(5.63)

Suppose the quantum dot orbits around a closed circular path of radius \(R_0\), \(r(t) = R_0(\cos \omega t, \sin \omega t, 0)\), in the \(xy\) plane under the influence of gate potentials, then the
semi-classical momentum $\mathbf{P} = m^* \dot{\mathbf{r}}(t)$ has components [173]

$$
P_x = -R_0 m^* \omega \sin \omega t, \quad P_y = R_0 m^* \omega \cos \omega t, \quad P_z = 0, \quad (5.64)
$$

where $m^*$ is the effective mass of the electron in the plane of 2DEG gas. Substitution of
(5.64) into (5.63) yields

$$
H_\pm = R_0 m^* \omega \left( \alpha e^{\mp i \omega t} \mp i \beta e^{\pm i \omega t} \right). \quad (5.65)
$$

The evolution operator (propagator) for this spin-orbit system is:

$$
U(t) = T \exp \left\{ -\frac{i}{\hbar} \int_0^t H_{SO}(t') dt' \right\}, \quad (5.66)
$$

where $T$ denotes the time-ordered product. Note, that both the geometric and dynamical
phases are contained in this expression, unlike the situation in Eq. 5.58 where the dynamical
phase has been factored out. Since $S_+$ and $S_-$ do not commute, the evaluation of the
time-ordered exponential for the evolution operator (5.66) is cumbersome.

For the case where the Hamiltonian is given by

$$
\dot{H} = \alpha(t) A + \beta(t) B + \gamma(t) C + \cdots, \quad (5.67)
$$

where $A, B, C, \ldots$ are non-commuting operators, and $\alpha, \beta, \gamma, \ldots$ are time-dependent
parameters, Feynman [164] devised an operator calculus by which the time-ordered exponen-
tial can be disentangled into the form

$$
U(t) = e^{a(t) A} e^{b(t) B} e^{c(t) C} \cdots \quad (5.68)
$$

where $a(t), b(t), c(t), \cdots$ are time-dependent scalar coefficients which can be determined
by solving relevant differential equations. This procedure is called the Feynman disentan-
gling method[164, 169–171].

Here we apply Feynman’s method for disentangling the time-ordered exponential in
(5.66) with the Hamiltonian (5.62). First we rewrite the Hamiltonian (5.62) as

$$
H_{SO} = \xi S_+ + (H_+ - \xi) S_+ + H_- S_- \quad (5.69)
$$

where $\xi$ is a time-dependent function to be determined appropriately. According to Feyn-
man’s procedure, the evolution operator may be put into the form,

$$
U(t) = e^{a(t) S_+} \exp \left\{ \frac{1}{i \hbar} \int_0^t dt' \left[ (H_+ - \xi) S'_+ + H_- S'_- \right] \right\} \quad (5.70)
$$
where
\[ a(t) = \frac{1}{i\hbar} \int_0^t \xi(t') dt', \quad (5.71) \]
\[ S_+ = e^{-aS_+}S_+e^{aS_+} = S_+ \quad (5.72) \]
and
\[ S_- = e^{-aS_-}S_-e^{aS_-} = S_- - 2aS_0 - a^2 S_+. \quad (5.73) \]
Substituting (5.72) and (5.73) into (5.70) and choosing \( \xi(t) \) such that the coefficient of \( S_+ \) in the integrand vanishes, we get
\[ U(t) = e^{a(t)S_+} T \exp \left\{ \frac{1}{i\hbar} \int_0^t dt' \left[ -2aH_-S_0 + H_-S_- \right] \right\}, \quad (5.74) \]
in which the term containing \( S_+ \) is disentangled. In a similar fashion, we disentangle the time-ordered exponential involving the mutually non-commuting operators \( S_0 \) and \( S_- \) by letting
\[
U(t) = e^{a(t)S_+} e^{b(t)S_0} T 
\exp \left\{ \frac{1}{i\hbar} \int_0^t dt' \left[ -2aH_- - \eta \right] S''_0 + H_-S''_- \right\} \quad (5.75)
\]
where
\[ b(t) = \frac{1}{i\hbar} \int_0^t \eta(t') dt' \quad (5.76) \]
\[ S''_0 = e^{-bS_0}S_0e^{bS_0} = S_0 \quad (5.77) \]
and
\[ S''_- = e^{-bS_0}S_-e^{bS_0} = S_-e^b. \quad (5.78) \]
Again choosing \( \eta(t) = -2aH_- \), we reduce the evolution operator (5.70) into the completely disentangled form,
\[ U(t) = e^{a(t)S_+} e^{b(t)S_0} e^{c(t)S_-} \quad (5.79) \]
where
\[ a(t) = \frac{1}{i\hbar} \int_0^t \left[ H_+(t') - a^2(t')H_-(t') \right] dt' \quad (5.80) \]
\[ b(t) = -\frac{2}{i\hbar} \int_0^t a(t')H_-(t') dt' \quad (5.81) \]
and
\[ c(t) = \frac{1}{i\hbar} \int_0^t H_-(t')e^{b(t')} dt'. \quad (5.82) \]
Although the time-ordered exponential is disentangled, the evaluation of the evolution operator remains incomplete until the coefficients \( a(t) \), \( b(t) \) and \( c(t) \) are determined.
Following Popov[171], we show that the spin flip probability can be expressed in the form of Eq. (5.96).

Since the time-evolution of the spin state can be achieved by a time-dependent rotation. The transition amplitude for spin \( \sigma \) to \( \sigma' \) is given by

\[
\langle \sigma | U(t) | \sigma' \rangle = D_{\sigma \sigma'}^{s}(\varphi, \vartheta, \psi) = \exp[-i(\sigma \varphi + \sigma' \psi)]d_{\sigma \sigma'}(\vartheta) \tag{5.83}
\]

where \( \varphi, \vartheta, \psi \) are the time-dependent Eulerian angles, and \( D_{\sigma \sigma'}^{(s)} \) are the elements of the Wigner D- matrix being the irreducible unitary representations of the SU(2) group, and \( d_{\sigma \sigma'}^{s} \) are Wigner’s d-function.

The corresponding transition probability along the z-axis is

\[
w_{\sigma \sigma'} = |d_{\sigma \sigma'}^{s}(\vartheta)(t)|^2. \tag{5.84}
\]

In particular, the transition probability from spin \( 1/2 \) to \( \pm 1/2 \) is

\[
w_{1/2,1/2} = \cos^2 \left( \frac{\vartheta(t)}{2} \right), \tag{5.85}
\]

and

\[
w_{1/2,-1/2} = \sin^2 \left( \frac{\vartheta(t)}{2} \right), \tag{5.86}
\]

because

\[
d_{1/2,1/2}^{1/2}(\vartheta) = \cos \frac{\vartheta}{2}, \quad d_{1/2,-1/2}^{1/2}(\vartheta) = i \sin \frac{\vartheta}{2}. \tag{5.87}
\]

For spin \( s = 1/2 \), the rotation matrix is given in the standard form [171],

\[
D(\varphi, \vartheta, \psi) = \begin{pmatrix}
\hat{\alpha} & -\hat{\beta}^* \\
\hat{\beta} & \hat{\alpha}^*
\end{pmatrix}
\tag{5.88}
\]

where

\[
\hat{\alpha} = \cos \frac{\vartheta}{2} \exp \left[i \frac{\psi + \varphi}{2} \right], \quad \hat{\beta} = i \sin \frac{\vartheta}{2} \exp \left[i \frac{\psi - \varphi}{2} \right]. \tag{5.89}
\]

Comparison of the evolution operator for the spin \( 1/2 \) transition expressed in the matrix form,

\[
U = \begin{pmatrix}
e^{\varphi/2} + a e^{i \varphi} & a e^{i \varphi} \\
e^{i \varphi} & e^{-\varphi/2}
\end{pmatrix}, \tag{5.90}
\]

and the rotation matrix yields

\[
|a|^2 = \tan^2 \frac{\vartheta}{2}. \tag{5.91}
\]

Again comparing this result with (5.99) and (5.100), we arrive at

\[
w_{1/2,1/2} = \frac{1}{1 + |a|^2}, \quad w_{1/2,-1/2} = \frac{|a|^2}{1 + |a|^2}. \tag{5.92}
\]
Note that $w_{1/2,1/2} + w_{1/2,-1/2} = 1$.

As is seen in above, the spin transition probability depends only on $a(t)$. Therefore the full form of the evolution operator is not needed. To determine $a(t)$, we convert the integral equation (5.80) together with (5.65) into a Riccati equation of the form,

$$\frac{da}{dt} = -R\omega [f(t) + f^*(t) \alpha^2(t)]$$

(5.93)

where $R = m^* R_0 / \hbar$,

$$f(t) = \beta \alpha e^{-i\omega t},$$

(5.94)

and

$$f^*(t) = \beta^{-i\omega t} - i\alpha e^i\omega t,$$

(5.95)

Solving (5.93) for $a(t)$, we can get to the spin transition probabilities, $w_{s,s'}$. In particular, the transition probabilities from spin 1/2 to $\pm 1/2$ are calculated by

$$w_{1/2,1/2} = \frac{1}{1 + |a|^2}, \quad w_{1/2,-1/2} = \frac{|a|^2}{1 + |a|^2}.$$  

(5.96)

### 5.9 Computational Method for Matrix Berry Phase

In general the Riccati equation (5.93) is not exactly solvable. Therefore numerical analysis is needed. As is shown in Appendix B, however, exact solutions are obtained for special cases, which include those for the Rashba limit ($\beta = 0$), the Dresselhaus limit ($\alpha = 0$) and the symmetric case ($\alpha = \beta$).

In what follows, as an illustration, we present calculations of the spin flip probability (5.96) from $s = 1/2$ to $s' = -1/2$ for the exact cases and numerical results directly obtained from (5.93).

Following Popov [171], we show that the spin flip probability can be expressed in the form of Eq. (5.96).

Since the time-evolution of the spin state can be achieved by a time-dependent rotation. The transition amplitude for spin $\sigma$ to $\sigma'$ is given by

$$\langle \sigma | U(t) | \sigma' \rangle = D_{\sigma\sigma'}^s(\varphi, \vartheta, \psi) = \exp[-i(\sigma \varphi + \sigma' \psi)]d_{\sigma\sigma'}(\vartheta)$$

(5.97)

where $\varphi, \vartheta, \psi$ are the time-dependent Eulerian angles, and $D_{\sigma\sigma'}^s$ are the elements of the Wigner D-matrix being the irreducible unitary representations of the SU(2) group, and $d_{\sigma\sigma'}$ are Wigner’s d-function.

The corresponding transition probability along the z-axis is

$$w_{\sigma\sigma'} = |d_{\sigma\sigma'}(\vartheta)(t)|^2.$$  

(5.98)

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In particular, the transition probability from spin \(1/2\) to \(\pm 1/2\) is

\[ w_{1/2,1/2} = \cos^2 \left( \frac{\vartheta(t)}{2} \right), \quad (5.99) \]

and

\[ w_{1/2,-1/2} = \sin^2 \left( \frac{\vartheta(t)}{2} \right), \quad (5.100) \]

because

\[ d_{1/2,1/2}^{1/2}(\vartheta) = \cos \frac{\vartheta}{2}, \quad d_{1/2,-1/2}^{1/2}(\vartheta) = i \sin \frac{\vartheta}{2}. \quad (5.101) \]

For spin \(s = 1/2\), the rotation matrix is given in the standard form

\[ D(\varphi, \vartheta, \psi) = \begin{pmatrix} \hat{\alpha} & -\hat{\beta} \hat{\star} \\ \hat{\beta} & \hat{\alpha} \hat{\star} \end{pmatrix} \quad (5.102) \]

where

\[ \hat{\alpha} = \cos \frac{\vartheta}{2} \exp \left[ i \frac{\psi + \varphi}{2} \right], \quad \hat{\beta} = i \sin \frac{\vartheta}{2} \exp \left[ i \frac{\psi - \varphi}{2} \right]. \quad (5.103) \]

Comparison of the evolution operator for the spin \(1/2\) transition expressed in the matrix form,

\[ U = \begin{pmatrix} e^{b/2} + ace^{-b/2} & ae^{-b/2} \\ ce^{-b/2} & e^{-b/2} \end{pmatrix}, \quad (5.104) \]

and the rotation matrix yields

\[ |a|^2 = \tan^2 \frac{\vartheta}{2}. \quad (5.105) \]

Again comparing this result with (5.99) and (5.100), we arrive at

\[ w_{1/2,1/2} = \frac{1}{1 + |a|^2}, \quad w_{1/2,-1/2} = \frac{|a|^2}{1 + |a|^2}. \quad (5.106) \]

Note that \(w_{1/2,1/2} + w_{1/2,-1/2} = 1\).

### 5.10 Special Solutions of the \(\alpha - \beta\) Riccati Equation

Here we wish to solve under a special condition the Riccati equation (5.93)

\[ \frac{da(t)}{dt} = -R\omega \{ f(t) + f^*(t) a^2(t) \} \quad (5.107) \]

where

\[ f(t) = \beta e^{i \omega t} + i \alpha e^{-i \omega t}, \quad f^*(t) = \beta e^{-i \omega t} - i \alpha e^{i \omega t}. \quad (5.108) \]

This equation contains the Rashba limit \((\alpha \neq 0, \beta = 0)\), and the Dresselhaus limit \((\alpha = 0, \beta \neq 0)\), both of which have exact solutions.

First we let \(a(t) = g(t) X(t)\) in (5.107). If we further let \(g(t) = -i f / |f|\), then we see
that \( X(t) \) obeys
\[
\frac{dX}{dt} = iR\omega |f(t)| \left\{ X^2 - 2h(t)X - 1 \right\}, \tag{5.109}
\]
where
\[
|f(t)| = \left[ \alpha^2 + \beta^2 + 2\alpha\beta \sin(2\omega t) \right]^{1/2} \tag{5.110}
\]
and
\[
h(t) = \frac{\beta^2 - \alpha^2}{2R\omega(\alpha^2 + \beta^2)^{3/2}} \left[ 1 + \frac{2\alpha\beta}{\alpha^2 + \beta^2} \sin(2\omega t) \right]^{-3/2}. \tag{5.111}
\]

Now we consider a special case where \( h(t) \) is a constant, say, \( h_0 \). In this case, (5.109) can be expressed as
\[
\frac{dX}{(X - n_1)(X - n_2)} = iR\omega |f(t)| dt \tag{5.112}
\]
where \( n_1 \) and \( n_2 \) are roots of
\[
X^2 - 2h_0X - 1 = 0, \tag{5.113}
\]
that is,
\[
n_1, n_2 = h_0 \pm \sqrt{h_0^2 + 1}. \tag{5.114}
\]
Note that
\[
n_1n_2 = -1, \quad n_1 + n_2 = 2h_0, \quad n_1 - n_2 = 2\sqrt{h_0^2 + 1}. \tag{5.115}
\]
Upon integration, we obtain with the condition \( X(0) = 0 \),
\[
X(t) = -\frac{1 - e^{i\phi(t)}}{n_2 - n_1 e^{i\phi(t)}}. \tag{5.116}
\]
The phase function \( \phi(t) \) is
\[
\phi(t) = R\omega(n_1 - n_2) \int_0^t |f(\tau)| d\tau \tag{5.117}
\]
which can be expressed in closed form,
\[
\phi(t) = 2R\omega \sqrt{h_0^2 + 1} \left( \alpha + \beta \right)
\left\{ E \left( \omega t - \frac{\pi}{4}, \frac{2\sqrt{\alpha\beta}}{\alpha + \beta} \right) - E \left( -\frac{\pi}{4}, \frac{2\sqrt{\alpha\beta}}{\alpha + \beta} \right) \right\} \tag{5.118}
\]
where \( E(\varphi, k) \) is the elliptic function of the second kind defined by
\[
E(\varphi, k) = \int_0^\varphi \sqrt{1 - k^2 \sin^2 \theta} d\theta.
\]

Consequently, for the case where \( h(t) = h_0 \), the starting Riccati equation (5.107) is
exactly solved, the result being of the form,

\[ a(t) = \frac{e^{i\phi/2} - e^{-i\phi/2}}{|f|} \left( n_1 e^{i\phi/2} - n_2 e^{-i\phi/2} \right) = \frac{ih_0 + i\sqrt{h_0^2 + 1} \cot(\phi/2)}{|f|} \left( h_0^2 + (h_0^2 + 1) \cot(\phi/2) \right). \]  

(5.119)

Since \( \phi(0) = 0 \), it is evident that \( a(0) = 0 \). The transition probabilities from spin 1/2 to ±1/2 are given by

\[ w_{1/2,1/2} = 1 - \frac{1}{h_0^2 + 1} \sin^2 \left( \frac{1}{2} \phi(t) \right) \]  

(5.120)

and

\[ w_{1/2,-1/2} = \frac{1}{h_0^2 + 1} \sin^2 \left( \frac{1}{2} \phi(t) \right), \]  

(5.121)

which are characterized only by the constant \( h_0 \) and the phase function \( \phi(t) \).

Although the above results are exact under the assumption that \( h(t) = h_0 \) is a constant, it may be taken as approximate results when \( h(t) \approx h_0 \).

Finally, specifying the values of \( h_0 \) and \( \phi(t) \), we shall obtain the exact results for the Rashba, the Dresselhaus and the symmetric cases.

**The Rashba limit** \( (\alpha \neq 0, \beta = 0) \): In this case, from (5.111) follows

\[ h_0 = -\frac{1}{2\alpha R}. \]  

(5.122)

Furthermore the right-hand side of (5.117) easily integrates, so that

\[ \phi(t) = \sqrt{1 + 4R^2\alpha^2} \omega t. \]  

(5.123)

Thus the spin flip probability is obtained in the form,

\[ w_{1/2,-1/2}^R = \frac{4R^2\alpha^2}{1 + 4R^2\alpha^2} \sin^2 \left( \frac{1}{2} \sqrt{1 + 4R^2\alpha^2} \theta \right), \]  

(5.124)

**The Dresselhaus limit** \( (\alpha = 0, \beta \neq 0) \): In this case, (5.111) leads to

\[ h_0 = \frac{1}{2\beta R}. \]  

(5.125)

The integral of (5.117) yields

\[ \phi(t) = \sqrt{1 + 4R^2\beta^2} \omega t. \]  

(5.126)

Hence the spin flip probability is

\[ w_{1/2,-1/2}^D = \frac{4R^2\beta^2}{1 + 4R^2\beta^2} \sin^2 \left( \frac{1}{2} \sqrt{1 + 4R^2\beta^2} \theta \right), \]  

(5.127)
The symmetric case \((\alpha = \beta \neq 0)\): In this particular case,

\[ h_0 = 0. \]  

(5.128)

The phase factor becomes

\[ \phi(t) = 2\sqrt{2} \alpha R \left[ \sin(\omega t) - \cos(\omega t) + 1 \right]. \]  

(5.129)

The corresponding spin flip probability is

\[ w_{1/2,-1/2}^{sym} = \sin^2 \left\{ \sqrt{2} \alpha R \left( \sin \theta - \cos \theta + 1 \right) \right\}. \]  

(5.130)

Figures 5.3(a) and (b) present the results for the spin flip transition probability vs. the angle of rotation, for pure Rashba and for pure Dresselhaus cases, for one complete revolution of the quantum dot center of mass in the plane of the 2DEG. These results were obtained from Eqs. 5.124 and 5.127. Since the Riccati equation for non-zero \(\alpha\) and \(\beta\) is non-trivial, we carry out numerical simulations of ‘a’ from Eq. 5.93. The results for the transition probability vs. the angle of rotation for non-zero \(\alpha\) and \(\beta\) are plotted from Eq. 5.96 and are shown in Fig. 5.3(c). In these figures, we keep the orbit radius fixed at 60 nm and vary the electric field. For the three curves, the electric field takes on the values: \(1 \times 10^3\), \(5 \times 10^5\) and \(10^6\) V/cm. From Figs. 5.3(a), (b) and (c), one sees that the transition probability increases with electric field as expected.

Results from Fig. 5.3(c) show that the spin transition probability for the non-zero \(\alpha\) and \(\beta\) is larger than for the case of pure Rashba (Fig. 5.3(a)) or pure Dresselhaus(Fig. 5.3(b)) cases considered separately. Similar plots for different orbit radii are shown in Figs. 5.4 and Fig. 5.5. In these cases, we keep the electric field the same as in Fig. 5.3 and vary the orbit radius as: 125 nm in Fig. 5.4, and 250 nm in Fig. 5.5.

Another important observation from these plots regards the period of spin flipping vs. angle in the plane. We note that the periods for the pure Rashba and for pure Dresselhaus cases are different. One sees from Fig. 5.4(c) and Fig. 5.5(c) that the result for non-zero \(\alpha\) and \(\beta\) appears to be a superposition of the two cases considered separately.

The strength of the Rashba and Dresselhaus spin orbit coupling can be calculated from Eq. 5.61 and becomes equal at \(E = 3.02 \times 10^6\) V/cm . For the situation in which the two mechanisms have equal strength (i.e. \(\alpha = \beta\)), the Riccati Eq. 5.93 becomes exactly solvable and the transition probability is given by equation Eq. 5.130. The transition probability vs. angle of rotation is obtained from equation Eq. 5.130 and is plotted in Fig. 5.6. Simulation results shows that one can enhance the transition probability by increasing the orbit radius. This makes intuitive sense because, for a given angular velocity, a larger orbit radius implies a larger momentum and, in turn, a larger spin-orbit interaction.

One again sees from Fig. 5.6 what appears to be a superposition effect resulting from
the presence of both interactions that separately have different periods. By superposition, we are referring to the fact that the amplitude varies with angle in a more complicated way than it does for the two interactions considered separately.

Fig. 5.7 is a further comparison study of the transition probability for pure Rashba, pure Dresselhaus, and non-zero $\alpha$ and $\beta$. For this case, the values of $\alpha$ and $\beta$ are determined by the strength of the electric field. Here we choose to fix the orbit radius at 125 nm and we consider two different electric field strengths: $1 \times 10^5$ V/cm in Fig. 5.7(a) and $5 \times 10^5$ V/cm in Fig. 5.7(b). Again, we note that the transition probability is greater when both mechanisms are acting and the amplitude variation suggests a superposition effect.

5.11 Analytical Expressions for the Electron Propagator via Feynman Disentangling Method

After getting the analytical expressions of the three different Riccati equations (5.80), (5.81), (5.82) in several cases, we are now ready to give the analytical expressions for the evolution operator $U_{ad}(t)$, sometimes refer to as matrix Berry Phase as appear in equation (5.58). One can find the disentangled operators $S_+$, $S_0$ and $S_-$ in the SU(2) matrix form by choosing $\hat{S}_x = \frac{1}{2}(\sigma_x \pm i\sigma_y)$, $\hat{S}_0 = \frac{1}{2}\sigma_z$ where $\sigma_i$ are pauli matrices as,

\begin{equation}
S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S_0 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},
\end{equation}

Substituting Eq. (5.131) into Eq. (5.79), we get the evolution operator in more compact form as

\begin{equation}
\hat{U}_{ad}(t, 0) = \begin{pmatrix} e^{b/2} + a e^{-b/2} & a e^{-b/2} \\ c e^{-b/2} & e^{-b/2} \end{pmatrix} = F(\theta)I + G(\theta)\sigma_x + J(\theta)\sigma_y + L(\theta)\sigma_z
\end{equation}

Here F,G,J and L are the coefficients of constant term, $\sigma_x, \sigma_y, \sigma_z$ in the series expansion of the evolution operator.

For pure Rashba case ($\beta = 0$), the unitary transformation for any angle of rotation can be found from equation (5.66) and can be written as

\begin{equation}
U^R_{ad}(t_0) = exp \left[ -iR\alpha \int_{\phi=0}^{\theta} d\phi (\sigma_x \cos \phi + \sigma_y \sin \phi) \right]
\end{equation}
In this case, the coefficients \(a(t), b(t)\) and \(c(t)\) in Eq. (5.132) are given by

\[
a(\tau) = \frac{e^{-i\omega \tau} - e^{-i\mu t}}{n_1 e^{i(\omega - \mu)t} - n_2}
\]
\[\text{(5.134)}\]
\[
e^b(\tau) = \frac{(n_1 - n_2)^2 e^{-i\mu t}}{(n_2 - n_1 e^{i(\omega - \mu)t})^2}
\]
\[\text{(5.135)}\]
\[
c = \frac{1 - e^{i(\omega - \mu)t}}{n_1 e^{i(\omega - \mu)t} - n_2}
\]
\[\text{(5.136)}\]

where \(\mu = \omega \left(1 - 2R\alpha \sqrt{h_0^2 + 1}\right)\) and \(h_0 = -\frac{1}{2R\alpha}\) for pure Rashba case.

Similarly, for pure Dresselhaus case (\(\alpha = 0\)), the unitary transformation for any angle of rotation can be found from equation (5.66) and can be written as

\[
U_{ad}^D(t_0) = \exp \left[ -iR\beta \int_{\phi=0}^{\theta} d\phi \left( \sigma_x \sin \phi + \sigma_y \cos \phi \right) \right]
\]
\[\text{(5.137)}\]

In this case, the coefficients \(a(t), b(t)\) and \(c(t)\) in Eq. (5.132) are given by

\[
a(\tau) = i \left[ \frac{e^{i\omega \tau} - e^{i\mu t}}{n_2 - n_1 e^{i(\mu - \omega)t}} \right]
\]
\[\text{(5.138)}\]
\[
e^b(\tau) = \frac{(n_1 - n_2)^2 e^{i\mu t}}{(n_2 - n_1 e^{i(\mu - \omega)t})^2}
\]
\[\text{(5.139)}\]
\[
c = i \left[ \frac{1 - e^{-i(\mu - \omega)t}}{n_1 e^{-i(\omega - \mu)t} - n_2} \right]
\]
\[\text{(5.140)}\]

where \(\mu = \omega \left(1 + 2R\beta \sqrt{h_0^2 + 1}\right)\) and \(h_0 = \frac{1}{2R\beta}\) for pure Dresselhaus case.

Based on Feynman [163, 164] path integral, non-abelian unitary transformations expressed in Eq. (5.133) and Eq. (5.137) for pure Rashba and for pure Dresselhaus cases are expanded in several orders of \(R\). Finally the coefficients of \(\sigma_x, \sigma_y, \sigma_z\) and constant terms appear in Eq. (5.133) and Eq. (5.137) are compared to that appear in Eq. (5.132) for pure Dresselhaus and Pure Rashba cases separately and found the same result from both approaches. This type of comparison studies have been carried out to support the extra evidence of correctness of our calculations of the propagator based on Feynman disentangling technique.

The coefficients of constant term, \(\sigma_x\) and \(\sigma_y\) and \(\sigma_z\) for pure Dresselhaus case are represented by \(F^D, G^D, J^D\) and \(L^D\) and can be written as

The coefficients of constant term:

\[
F^D(\theta) = F_0^D(\theta) + F_2^D(\theta) - F_4^D(\theta) + F_6^D(\theta) - F_8^D(\theta) + F_{10}^D(\theta) + \cdots
\]
\[\text{(5.141)}\]

odd terms \(F_1^D, F_3^D, F_5^D\) ... are zero. Starting values: \(F_0^D = 1, F_2^D = -\frac{R^2\beta^2}{2}(1 - \cos \theta), \ldots \)
\[F^D_m(\theta) = \frac{iR\beta}{2}(-i)^m \int_{\phi=0}^{\theta} d\phi [\sin \phi G^D_{m-1}(\phi) + \cos \phi J^D_{m-1}(\phi)] \quad (5.142)\]

The coefficients of \(\sigma_z\):

\[G^D(\theta) = G^D_1(\theta) - G^D_3(\theta) + G^D_5(\theta) - G^D_7(\theta) + G^D_9(\theta) - G^D_{11}(\theta) + \cdots \quad (5.143)\]

even terms \(G^D_0, G^D_2, G^D_4, \ldots \) are zero. Starting values: \(G^D_1 = -iR\beta(1 - \cos \theta)\)

\[G^D_n(\theta) = R\beta(-i)^n \int_{\phi=0}^{\theta} d\phi \left[ \sin \phi F^D_{n-1}(\phi) + i \cos \phi L^D_{n-1}(\phi) \right] \quad (5.144)\]

The coefficients of \(\sigma_y\):

\[J^D(\theta) = J^D_1(\theta) - J^D_3(\theta) + J^D_5(\theta) - J^D_7(\theta) + J^D_9(\theta) - J^D_{11}(\theta) + \cdots \quad (5.145)\]

even terms \(J^D_0, J^D_2, J^D_4, \ldots \) are zero. Starting values: \(J^D_1 = -iR\beta \sin \theta\)

\[J^D_n(\theta) = R(-i)^n \int_{\phi=0}^{\theta} d\phi [\cos \phi F^D_{n-1}(\phi) - i \sin \phi L^D_{n-1}(\phi)] \quad (5.146)\]

The coefficients of \(\sigma_z\):

\[L^D(\theta) = L^D_2(\theta) + L^D_4(\theta) - L^D_6(\theta) + L^D_8(\theta) - L^D_{10}(\theta) + L^D_{12}(\theta) + \cdots \quad (5.147)\]

even terms \(L^D_1, L^D_3, L^D_5, \ldots \) are zero. Starting values: \(L^D_2 = -\frac{iR^2\beta^2}{2^2}(\theta - \sin \theta)\)

\[L^D_m(\theta) = \frac{R}{2}(-i)^m \int_{\phi=0}^{\theta} d\phi [\sin \phi J^D_{m-1}(\phi) - \cos \phi G^D_{m-1}(\phi)] \quad (5.148)\]

where superscript ‘D’ represents for Dresselhaus case.

The coefficients of constant term, \(\sigma_x\) and \(\sigma_y\) for pure Rashba case are represented by \(F^R, G^R, J^R\) and \(L^R\) and can be written as

The coefficients of constant term:

\[F^R(\theta) = F^R_0(\theta) + F^R_2(\theta) - F^R_4(\theta) + F^R_6(\theta) - F^R_8(\theta) + F^R_{10}(\theta) + \cdots \quad (5.149)\]

odd terms \(F^R_1, F^R_3, F^R_5, \ldots\) are zero. Starting values: \(F^R_0 = 1, \ F^R_2 = -\frac{R^2\alpha^2}{2^2} (1 - \cos \theta)\)

\[F^R_m(\theta) = \frac{iR\alpha}{2}(-i)^m \int_{\phi=0}^{\theta} d\phi \left[ \cos \phi G^R_{m-1}(\phi) + \sin \phi J^R_{m-1}(\phi) \right] \quad (5.150)\]

The coefficients of \(\sigma_z\):

\[G^R(\theta) = G^R_1(\theta) - G^R_3(\theta) + G^R_5(\theta) - G^R_7(\theta) + G^R_9(\theta) - G^R_{11}(\theta) + \cdots \quad (5.151)\]
even terms $G_0^R, G_2^R, G_4^R \ldots$ are zero. Starting values: $G_1^R = -\frac{i\alpha}{2} \sin \theta$

$$G_n^R(\theta) = \frac{R\alpha}{2} (-i)^n \int_{\phi=0}^{\theta} d\phi \left[ \cos \phi F_{n-1}^R(\phi) + i \sin \phi L_{n-1}^R(\phi) \right]$$  \hspace{1cm} (5.152)

The coefficients of $\sigma_y^i$:

$$J_n^R(\theta) = J_1^R(\theta) - J_2^R(\theta) + J_3^R(\theta) - J_4^R(\theta) + J_5^R(\theta) - J_6^R(\theta) + \cdots$$  \hspace{1cm} (5.153)

even terms $J_0^R, J_2^R, J_4^R \ldots$ are zero. Starting values: $J_1^R = -\frac{i\alpha}{2} (1 - \cos \theta)$

$$J_n^R(\theta) = \frac{R\alpha}{2} (-i)^n \int_{\phi=0}^{\theta} d\phi \left[ \sin \phi F_{n-1}^R(\phi) - i \cos \phi L_{n-1}^R(\phi) \right]$$ \hspace{1cm} (5.154)

The coefficients of $\sigma_z^i$:

$$L_n^R(\theta) = L_2^R(\theta) + L_3^R(\theta) - L_5^R(\theta) + L_6^R(\theta) - L_8^R(\theta) + L_9^R(\theta) + \cdots$$ \hspace{1cm} (5.155)

even terms $L_1^R, L_3^R, L_5^R \ldots$ are zero. Starting values: $L_2^R = -\frac{R^2\alpha^2}{2} (\sin \theta \theta)$

$$L_n^R(\theta) = \frac{R\alpha}{2} (-i)^n \int_{\phi=0}^{\theta} d\phi \left[ \cos \phi J_{m-1}^R(\phi) - \sin \phi G_{m-1}^R(\phi) \right]$$ \hspace{1cm} (5.156)

where superscript ‘$R$’ represents for Rashba case.

### 5.12 Summary and Conclusion

In summary, we first exactly diagonalized the Hamiltonian of a quantum dot confined in an asymmetric distortion potential and presented analytical expression for the Berry Phase. For degenerate case, we considered spin manipulation via non-abelian matrix Berry phases induced by adiabatic transport of a single spin in the 2D plane in the presence of the Rashba and Dresselhaus spin-orbit coupling. We solved the problem exactly by using the Feynman disentangling technique in three cases: (a) pure Rashba coupling, (b) pure Dresselhaus coupling, and (c) equal strength of Rashba and Dresselhaus coupling. For the most general case, when the solution becomes non-trivial, we carried out numerical simulations of the transition probabilities vs. the various parameters such as electric field strength and the radius of the circular loop in the 2D plane.
Figure 5.2: The geometric spin precession due to spin orbit interaction for an electron in a quantum dot moving adiabatically in the plane of 2DEG is equivalent to the changing orientation of a sphere rolling on a plane [171].

Figure 5.3: Transition probability of $w_{1/2,-1/2}$ vs $\theta$ for three cases: (a) pure Rashba ($\beta = 0$), (b) pure Dresselhaus ($\alpha = 0$) and (c) mixed (non zero $\alpha$ and $\beta$) spin orbit interactions. The Orbital radius is 60 nm. The three curves represent the following electric field strengths: $1 \times 10^5$ V/cm (solid black line), $5 \times 10^5$ V/cm (dashed red line), and $1 \times 10^6$ V/cm (dot-dashed blue line) respectively.
Figure 5.4: Transition probability $w_{-1/2,1/2}$ vs. theta for the following cases: (a) pure Rashba ($\beta = 0$), (b) pure Dresselhaus ($\alpha = 0$), and (c) mixed (non-zero $\alpha$ and $\beta$). The orbit radius is chosen to be 125 nm and the following values of the electric field are considered: $1 \times 10^5$ V/cm (solid black line), $5 \times 10^5$ V/cm (dashed red line), and $1 \times 10^6$ V/cm (dash-dot blue line).

Figure 5.5: Transition probability $w_{-1/2,1/2}$ vs. theta for the following cases: (a) pure Rashba ($\beta = 0$), (b) pure Dresselhaus ($\alpha = 0$), and (c) mixed (non-zero $\alpha$ and $\beta$). The orbit radius was chosen to be 250 nm and the following values of the electric field were chosen: $1 \times 10^5$ V/cm (solid black line), $5 \times 10^5$ V/cm (dashed red line), and $1 \times 10^6$ V/cm (dash-dot blue line).
Figure 5.6: Transition probability $w_{-1/2,1/2}$ vs. theta for $\alpha = \beta$. Physically, this situation occurs for electric field strength given by $E = 3.02 \times 10^6$ V/cm. The following orbit radii were chosen: 60 nm (solid black line), 175 nm (dashed red line), and, 250 nm (dash-dot blue line).

Figure 5.7: Transition probability $w_{-1/2,1/2}$ vs. theta for the following cases: pure Rashba ($\beta = 0$: dot-dashed blue line), pure Dresselhaus ($\alpha = 0$: red dashed line) and mixed (non-zero $\alpha$ and $\beta$: solid black line). The orbit radius was chosen to be 125 nm and the following values of the electric field were chosen: (a) $E = 1 \times 10^5$ V/cm and, (b) $E = 5 \times 10^5$ V/cm.
Chapter 6

Results and Conclusions

In Chapter 3, we reported the numerical calculation of the conduction band diagram of an AlGaAs/GaAs heterojunction based on the Finite Element simulation method. We found the asymmetric triangular quantum well and reported some of the numerical values of the ground and first excited states of electron eigenvalues and its wave functions [189]. There we used the numerical values of AlGaAs/GaAs heterojunction for the realistic design of the device such as $5 \times 10^{11}$ electrons per square centimeter for channel electrons and 0.3 ev for a band offset between the AlGaAs/GaAs heterojunction. Our numerical simulations agree with the results published by Stern and Das Sarma [190].

Also, we solved the Schrodinger-Poisson equation self-consistently on the basis of effective mass and local density functional approximations where the potentials of electron-electron interactions were included in order to take account of exchange-correlation effects.

We considered the three dimensional geometry of a realistic device consisting of a single electron transistor, which is also under investigation by experimentalists at the College of Nanoscale Science and Engineering at Albany [189].

In Chapter 4, we solved the Schrodinger equation coupled with the Maxwell-Poisson electrostatic equation self-consistently in three dimensional geometry. In order to obtain the electrostatic solution for the confining potential, we approximate the 2DEG as a classical perfect conductor and give it a finite width. The width ($\approx 0.05\mu m$) is unrealistically large from a quantum perspective but is assumed to give a reasonable description of the spatial variation of the potential a 2DEG. In a subsequent step we treat the 2DEG from a realistic quantum mechanical point of view [190]. The main conclusion of this study is that the electrostatic potential for a realistic device is asymmetric both along and perpendicular to the growth direction.

Finally, the electrostatic potentials found in this device were fitted to a polynomial form and compared to the harmonic oscillator quadratic potential. We found the analytical value of the coefficient of degree of anisotropy, which is $\alpha = 1$ and $\beta^2 = 2.8$. We chose this value as the benchmark to find the numerical simulation of our g-value calculation.

Also, in Chapter 4, we carried out numerical simulations of the energy spectrum with
respect to variation of the magnetic field applied to a single electron confined in a GaAs quantum dot in the absence of spin-orbit interactions. Our numerical simulation of the Fock-Darwin energy spectrum has been carried out for two different potentials: (a) the circular quadratic potential, and (b) the realistic potential. We found that the realistic potential removes the degeneracy in the Fock-Darwin energy spectrum at zero magnetic field [185, 187].

We have studied the influence of spin orbit interaction terms in the Hamiltonian of the Fock-Darwin energy spectrum—namely the Bychkov-Rashba [184] and the linear and cubic Dresselhaus terms [186]—on the g-value calculation for the several parameters such as electric fields, magnetic fields and degree of anisotropy [189]. We have elaborated three principal effects involved in electron g-value calculations in a symmetric confining potential for a single electron present in a GaAs and InAs quantum dots. First, Dresselhaus spin-orbit coupling is a dominating parameter for the negative g-value. Second, Rashba spin orbit coupling is a dominating parameter for the positive g-value. Third, we can demonstrated level crossings in the g-value calculation for larger radii of the quantum dot.

We extended the above g-value analysis for realistic potentials for realistic device with high degrees of anisotropy. We found that anisotropic effects extend the tunability of this electron g-value, which breaks down in-plane symmetry in both GaAs and InAs quantum dots. A decrease in the energy gap between the ground and first excited states in the energy eigenvalues for realistic confining potentials shows that this spin-orbit coupling dominates in the manipulation of electron spin in the gate control logic devices.

The most important result we found in this Chapter is to remove the degeneracy for spin up and spin down states for the GaAs quantum dot via the variation of several parameters such as magnetic fields, electric fields, and gate potentials. Note that the gate potential helps in designing logic devices based on single electron transistors.

Another means of manipulating the electron spin in a GaAs quantum dot is through geometric phases. Here, we explored the manipulation of electron spin through geometric phases by rotating the quantum dot center of mass adiabatically in a closed loop via several variable parameters such as quantum dot radius and electric fields. We presented numerical simulations and analytical expressions of the Berry phase with respect to the quantum dot radius of the orbit in the plane, to electric fields and to the degree of anisotropy for the non-degenerate Hamiltonian. We consider a very strong confining potential along the z- direction in a quantum dot. Accordingly only ground and first excited states of electron spins are considered for the numerical simulation of the Berry phase [188].

In Chapter 5, We calculated the matrix Berry phase for degenerate states of GaAs quantum dot in the presence of spin-orbit interaction. We presented the exact analytical expressions for the matrix Berry phase and the transition probability of electron spin in three different cases: (a) pure Rashba coupling; (b) pure Dresselhaus coupling; and
(c) a combination of equally strong Rashba and Dresselhaus couplings. These analytical expressions are obtained by using the Feynman disentangling technique. For general cases, when the states becomes degenerate, we carry out numerical simulations of such matrix Berry phase and of such spin transition probabilities.

From numerical simulations, we see that one can enhance the transition probability of electron spin in the presence of spin-orbit interaction over the pure Rashba and pure Dresselhaus cases. We also quantify numerically that even though, the Rashba spin orbit coupling is smaller in magnitude than the Dresselhaus spin orbit coupling, its period during the revolution of a quantum dot is different, which gives the superposition effect [188].

So far we have considered the Hamiltonian of a quantum dot which is isolated from the environment. We showed some numerical simulations and analytical expressions of the control of electron spin via two different approaches such as the g-value and geometric phase calculations with the help of gate potentials. In a realistic design of the device, these quantum dots are coupled to the environment. Hence one needs to include the Hamiltonian of the environment as a heat reservoir, and needs to see the quantum dissipation effect to the isolated Hamiltonian. This effect will reduce the performance of the device. To quantify the effects of the environment, we wish to continue this project.
Bibliography


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