RASHBA SPIN-ORBIT INTERACTION IN TWO-DIMENSION ELECTRON GAS

By

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The undersigned hereby certify that they have read and recommend to the Faculty of Graduate Studies for acceptance a thesis entitled "**Rashba Spin-Orbit Interaction in Two-Dimension Electron Gas**" by **Belay Gemechu** in partial fulfillment of the requirements for the degree of **Master of Science**.

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Abstract

We have studied the spin orbit-coupling from the Dirac equation, Understanding the properties of electronic states in quantum wires is a central issue in nanoscience. In the ballistic region, with low electronic densities, electron-electron interactions are not very important, and wire conductance is determined by the transmission of electrons as independent particles and the effects of spin-orbit interaction (SOI) on the energy bands,a system of two dimensional equations with respect to the spinor components $\Psi_{\uparrow\downarrow}(t)$, in the case of $\alpha = 0$, $\alpha \neq 0$ and ballistic conductance.

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Chapter 1

Introduction

As its name already implies, spin-orbit interaction (SOI) gives rise to a coupling between the spin dynamics of an electron and its (orbital) motion in space. If an electron is travelling through an electric field, it "sees" in its rest frame a moving electric field, i.e., moving charges,the moving charges give rise to an internal magnetic field in the rest frame of the electron[1]. This internal magnetic field couples, in return, to the spin of the electron[2]. The magnitude and the direction of this internal magnetic field depend on the velocity and travel the direction of the electron in a material, i.e., SOI gives rise to a wave vector dependent internal magnetic field. When electrons are confined to a thin layer two dimension electron gas (2DEG) by an asymmetric confinement potential, their spin- and orbital degrees of freedom are coupled. This effect is known as Rashba SOI. The spin-orbit interaction has a relativistic origin [3]. In the presence of an external electric field, the relativistic correction introduces a coupling of the electron spin with its own momentum. In the absence of a magnetic field, the spin degeneracy of the two dimensional electron gas energy bands at $k \neq 0$ is lifted by the coupling of the electron spin with its orbital motion. This coupling arises because of the inversion asymmetry of the potential that confines the two dimensional electron gas system. This is described by Hamiltonian which is given [4] by:

$$H_{so} = \frac{\alpha}{\hbar}(\overrightarrow{\sigma} \times \overrightarrow{p})_z = i\alpha(\sigma_y \frac{\partial}{\partial_x} - \sigma_x \frac{\partial}{\partial_y}). \tag{1.0.1}$$

Here the z axis is chosen perpendicular to the two dimension electron gas system lying in the x-y plane α is the spin-orbit coupling constant, which is sample dependent and is proportional to the interface electric field and $\hat{p}$ is the momentum operator. The value of α determines the contribution of the Rashba spin -orbit coupling to the total electron Hamiltonian .This constant may have values from (1-10) meV/ nm. The electronic transport and photonic properties of a two-dimensional electron gas (2DEG) such as that found at a semiconductor heterojunction of GaAs/AlGaAs have been the subject of interest and discussion for many years now [4]. Related physical properties of narrow quantum wires of 2DEG have also been the subject of experimental and theoretical investigations because of their potential for device applications in the field of nanotechnology [5,6]. It is thus necessary to specify the model for the edge of a narrow quantum wire [7-9]. Here, we analyze the role played by the boundaries on the ballistic electron transport in a nanowire of 2DEG where the Rashba spin-orbit interaction (SOI) is included. The role of SOI on collective properties of the 2DEG has been investigated [10-12]. It is well established that the spin-orbit coupling is an essentially relativistic effect: an electron moving in an external electric field sees a magnetic field in its rest frame. In a semiconductor, the interaction causes an electron's spin to precess as it moves through the material, which is the basis of various proposed ”spintronic” devices. In nanostructures, quantum confinement can change the symmetry of the spin-orbit interaction. The relativistic motion of an electron is described by a Dirac equation. These effects combine to form both an electric dipole moment and the Thomas precession which is due to the rotational kinetic energy in the electric field [13-15]. The two mechanisms accidentally have very close mathematical form and consequently combine in a very elegant way. The SOI Hamiltonian can be obtained from the Dirac equation by taking the non-relativistic limit up to terms quadratic in v/c. This limit can be achieved either by expanding the Dirac equation in powers of v/c or by making use of the asymptotically exact Foldy-Wouthousen transformation [16]. We include the effects due to edges through sharp and high potentials at the boundaries. So, to solve the Rashba SOI model Hamiltonian to obtain analytic solutions is not mandator. Because the solution manifestly contains quantum interference effects from multiple scattering off the edges. we discuss a system of two dimensional equations with respect to the spinor components $\Psi_{\uparrow\downarrow}(t)$,in the case of $\alpha = 0$,$\alpha \neq 0$ and ballistic conductance.

1.1 Organization of the thesis.

The thesis is organized in the following manner. In Chapter two we discuss the spin-orbit coupling ,inversion symmetry and time reversal symmetry, Rashba effect in two dimension electron gas, properties of the Rashba Hamiltonian, while spin orbit coupling in the Dirac equation are discussed in Chapter three. Chapter four presents Rashba spin orbit coupling for a quantum wire, energy band structure for quantum wire,square quantum well and in this section, we discuss a system of two dimensional equations with respect to the spinor components $\Psi_{\uparrow\downarrow}(t)$ for both $\alpha = 0$ and $\alpha \neq 0$ and we discuss the SOI in the dependence of the ballistic conductance of a quasi-one dimensional electron system on the Fermi energy. Finally, in Chapter five we conclude the results.

Chapter 2

Spin orbit coupling.

2.1 Origin of spin orbit coupling

The spin-orbit coupling is a well-known phenomenon that manifests itself in lifting the degeneracy of one-electron energy levels in atoms, molecules, and solids. In solid-state physics, the non relativistic Schrodinger equation is frequently used as a first approximation, e.g. in electron band-structure calculations[1]. Without relativistic corrections, it leads to doubly-degenerated bands, spin-up and spin-down, which can be split by a spin-dependent term in the Hamiltonian. In this approach, spin-orbit interaction can be included as a relativistic correction to the Schrodinger equation. For this purpose we use the Dirac equation, which is the basic equation for electronic systems, including the electron spin and its relativistic behavior. We can obtain the Dirac equation by linearizing the relativistic generalization of the Schrodinger equation. It is Lorentz-invariant and describes the electron spin and spin-orbit coupling from first principles[17]. One naturally arrives at the Dirac equation when starting from the relativistic expression for the kinetic energy

$$E^2 = c^2p^2 + m^2c^4. \tag{2.1.1}$$

Inclusion of the electric potential, *phi* and magnetic potentials, A, by substituting P-$(\frac{e}{c})A$ for P (P is the canonical momentum) and $E - e\phi$ for electric potential, electron charge $(-e)$ in equation,(2.1.1) leads to:

$$(E - e\phi)^2 = (cP - eA)^2 + m^2c^4. \tag{2.1.2}$$

By interpreting P and E as operators

$$P = -i\hbar\overrightarrow{\nabla} and E = i\hbar\frac{\partial}{\partial t}. \qquad (2.1.3)$$

one can write the force-free form of the wave equation as

$$(E^2 - c^4\sum_{\mu} P_{\mu}^2 - m^2c^4)\psi = 0. \qquad (2.1.4)$$

$p_{\mu} = p_x, p_y$ and p_z are components of the momentum operator. From equation,(2.1.2)and Equation,(2.1.4) can be expressed as

$$(E - C\sum_{\mu}\alpha_{\mu}P_{\mu} - \beta mc^2)\psi(E + c\sum_{\mu}\alpha_{\mu}p_{\mu} - \beta mc^2)\psi = 0 \qquad (2.1.5)$$

with the conditions,

$$\alpha_{\mu}\alpha_{\mu} + \alpha_{\mu}\alpha_{\mu} = 2\delta\mu\mu, \alpha_{\mu}\beta + \beta\alpha_{\mu} = 0, \beta^2 = 1. \qquad (2.1.6)$$

We can linearize it by taking only the first part of equation ,(2.1.5). Solution of the first part will give the solution of whole equation. The linearized equation has the advantage that is of first order in $\frac{\partial}{\partial t}$, similar to the Schrodinger equation; it is referred to as Dirac equation:

$$(E - c\sum_{\mu}\alpha_{\mu}P_{\mu} - \beta mc^2)\psi = 0. \qquad (2.1.7)$$

Let us now compare the Dirac equation with the Schrodinger equation. For this we use the non-linear zed form

$$(E - e\phi - c\alpha\cdot(P - \frac{e}{c}A) - \beta mc^2)[E - e\phi + c\alpha\cdot(P - \frac{e}{c}A) + \beta mc^2]\psi = 0. \quad (2.1.8)$$

Using the approximation that the kinetic and potential energies are small compared to mc^2,two components of the spin function can be neglected, and equation ,(2.1.8) takes the form

$$(\frac{1}{2m})(P - \frac{e}{c}A)^2 + e\phi - \frac{eh}{2mc}\sigma\cdot B + i\frac{eh}{4m^2c^2}E\cdot P - \frac{eh}{4m^2c^2}\sigma\cdot(E\cdot P)\psi = E\psi. \quad (2.1.9)$$

The first two terms in the parentheses are equivalent to those in the Schrodinger equation for external fields. The third term corresponds to the interaction energy $-\overrightarrow{\mu}.\overrightarrow{B}$

of the magnetic dipole, whose moment is presented by operator $\overrightarrow{\mu}=\frac{eh}{2mc\overrightarrow{\sigma}}=\frac{e}{mc\overrightarrow{s}}$. The fourth term is a relativistic correction to the energy and does not have a classical analogy. The fifth term describes the spin-orbit coupling. It can be illustrated in framework of the classical electrodynamics, where the vectors of the electromagnetic field depend on the reference system. In a reference system that moves with velocity $\overrightarrow{V}$ relative to an electric field $\overrightarrow{E}$, the magnetic field is

$$\overrightarrow{B}=\frac{1}{c}\overrightarrow{V}\times\overrightarrow{E}=\frac{1}{mc}(\overrightarrow{E}\times\overrightarrow{P}) \tag{2.1.10}$$

Where terms of order $(v/c)^2$ and higher order terms are neglected. In other words, the moving electron experiences a magnetic field in its rest frame that arises from the Lorentz transformation of the static (external) electric field; this field will affect the electron spin. The energy of the electron in this field, due to its magnetic moment , is

$$-\overrightarrow{\mu}\cdot\overrightarrow{B}=\frac{e}{mc}\overrightarrow{S}\cdot\overrightarrow{B}=-\frac{e}{m^2c^2}\overrightarrow{S}\cdot(\overrightarrow{E}\times\overrightarrow{P}) \tag{2.1.11}$$

This additional energy term in the Hamiltonian is essentially the spin-orbit term in equation,(2.1.9), except for a factor of 2. This factor (Thomas factor) is missing because we have not taken into account that changing the frame of reference also leads to a time transformation and, consequently, the precession frequency of the electron spin in the magnetic field changes. For example the orbital motion of an electron in the electric field of an atomic nucleus has

$$E=-\frac{1}{e}\frac{1}{r}\frac{dV}{dr} \tag{2.1.12}$$

and the term can be written in the form

$$(S=\frac{h}{2}\sigma),-\frac{eh}{4m^2}\sigma\cdot(\overrightarrow{E}\times\overrightarrow{P})=\frac{e}{2m^2c^2}S\cdot(-\frac{1}{e}\frac{\mathbf{r}}{r}\frac{d\mathbf{v}}{dr}\times P)=\frac{1}{2m^2c^2}\frac{1}{r}\frac{dv}{dr}(S\cdot L). \tag{2.1.13}$$

This is called spin-orbit energy, as it results from an interaction of the spin with the magnetic field that is experienced by the moving electron.

2.2 Inversion symmetry and time reversal symmetry

In the absence of a magnetic field, the spin degeneracy of the two dimension electron gas energy bands at $k\neq 0$ is lifted by the coupling of the electron spin with its orbital motion. This coupling arises because of the inversion asymmetry of the potential that confines the two dimension electron gas system. In a free atom, spin-orbit interaction can lift the degeneracy of states with the same orbital wave function but with opposite spins. In solids, however, such a splitting can be forbidden due to crystal symmetry. At any point of the Brillouin zone, energy becomes

$$E(k,\uparrow) = E(-k,\downarrow). \tag{2.2.1}$$

The Kramer's degeneracy remains unaffected when including the spin-orbit interaction term in the Hamiltonian. If the crystal lattice has inversion symmetry (i.e. if the operation $\overrightarrow{r} \rightarrow -\overrightarrow{r}$ does not change the crystal lattice), we will obtain

$$E(k,\uparrow) = E(-k,\uparrow) and E(k,\downarrow) = E(-k,\downarrow). \tag{2.2.2}$$

From combination of the equations [2.2.1] and [2.2.2] it becomes clear that if both time reversal symmetry and inversion symmetry are present, the band structure should satisfy to the condition

$$E(k,\uparrow) = E(k,\downarrow). \tag{2.2.3}$$

In other words, the energy cannot depend on the electron spin. Consequently, for crystals which have inversion symmetry, spin splitting is not allowed in the bulk, and these solids keep their spin degeneracy.

2.3 Rashba effect in two dimension electron gas

The spin splitting in the two dimension electron gas presents two distinct contributions. One contribution is due to the inversion asymmetry of the zinc-blende crystal structure of the bulk host material. In the lowest order in the momentum k, this splitting is described in the bulk by a term of the form [18,19].

$$H_k^3 = \frac{\gamma}{\hbar}[\sigma_x P_x(k_y^2 - k_z^2)] + [\sigma_y P_y(k_z^2 - k_x^2) + \sigma_z P_z(k_x^2 - k_y^2) \tag{2.3.1}$$

Where σi stands for the Pauli matrices,γ is a material constant, and the coordinated axis are now assumed parallel to the crystallographic cubic axis. In a sufficiently narrow quantum well grown along the [001] direction, it is possible to approximate the operator p_z and p_z^2 by their expectation values $< P_z >, < p_z^2 >$. This leads to the following two contributions to SO coupling resulting from the bulk inversion asymmetry: the Dresselhaus term

$$H_D = \frac{\beta}{\hbar}(\sigma_x P_x - \sigma_y P_y) \tag{2.3.2}$$

linear in the moment with $\beta = \gamma < p_z^2 >$ and the trilinear term

$$H_D^{(3)} = \frac{\gamma}{\hbar}(\sigma_x P_x P_y^2 - \sigma_y P_y P_x^2) \tag{2.3.3}$$

Clearly the typical magnitude of $H_D^{(3)}$ compared to the linear term H_D is given by the ratio of the Fermi energy ε_F of the in plane motion to the kinetic energy of the quantized degree of freedom in the growth direction. For typical values of ε_F of about 10 meV and not too broad quantum wells this ratio is small, therefore is the Dresselhaus trilinear term is usually neglected. The other kind of spin orbit coupling present in two dimension electron gas is due to the Rashba effect. Contrary to the Dresselhaus effect, the Rashba spin orbit interaction is not due to bulk properties. In fact it has been demonstrated by de Andrada e Silva et al. [21] that it is present only in semiconductor hereto structures where there is a lack of inversion symmetry in the growth direction. So far those two models of spin orbit interaction in semiconductor heterostructures have been introduced; in the following their essential difference is underlined. The Dresselhaus term is due to bulk properties of the semiconductors so that its coupling constant β is fixed and cannot be tuned. Instead the Rashba term depends of the shape of the confining potential and the coupling constant α can be tuned by means metallic gate since the confining potential can be modified using electric field (see Fig.2.1).

The basic idea is that the magneto conductance of a two dimension electron gas at T = 0 is given by

$$\sigma_{xx} \propto \sum_{n\pm}(n + \frac{1}{2})exp\frac{-(E_F - E_{n\pm})^2}{\Gamma^2}. \tag{2.3.4}$$

where E_F is the Fermi energy,$E_n\pm$ is the energy of the nth Landau level with spin up (+) and spin down (-) and Γ is the Landau level broadening that is assumed constant. In a magnetic field B, the energy spectrum for the nth Landau level is described by

$$E_0 = \frac{1}{2}\hbar\omega_c, \tag{2.3.5}$$

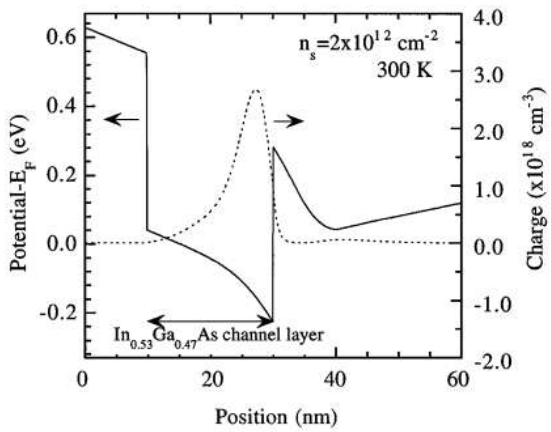

Figure 2.1: Calculated conduction band diagram and electron distribution [20].

where n=0

$$E_n^{\pm} = \hbar(n + \frac{1}{2}\sqrt{(1 - \frac{gm*}{2})^2} + n\frac{\Delta_R^2}{E_F \hbar\omega_c}) \quad (2.3.6)$$

Where ω_c is the cyclotron frequency which is given by $\omega_c = eB/m*$, and g is the effective g factor. In the last equation the information relative to the spin-splitting is taken in account through the factor $\delta_R = 2k_F\alpha$ with α Rashba spin orbit coupling constant.

The way to measure the tunability of the Rashba spin orbit interaction takes in account that the conductivity of low-dimensional system shows significant of quantum interference that depend on magnetic field and spin orbit coupling [24]. In particular, constructive backscattering associated with pairs of time-reversed closed-loop electron trajectories in the absence of significant spin orbit interaction leads to negative magneto resistance measurement known as weak localization.

On the contrary, when it is present a significant spin orbit interaction the backscattering becomes destructive and the positive magneto resistance change is known as anti-weak localization. It has been demonstrated by Miller et al. [25] that controlling the spin orbit coupling in a moderately high-mobility GaAs/AlGaAs two dimension electron gas through the applications of top-gate voltage it is possible to induce a crossover from weak localization to anti-localization (see Fig. 2.3).

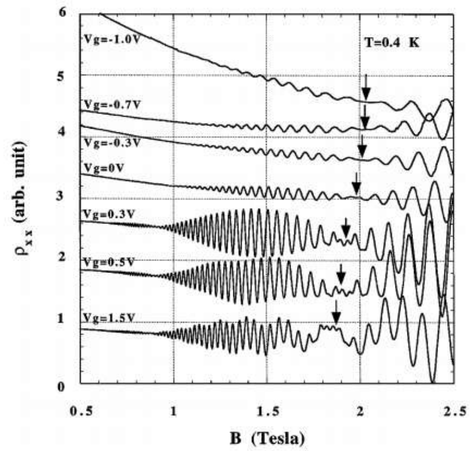

Figure 2.2: Schubnikov-de Haas oscillations as function of the gate voltages. [20].

2.4 Properties of the Rashba Hamiltonian

The Hamiltonian of the systems of two dimension electron gas in the plane (x,y) in the presence of the Rashba spin orbit term ($H = \frac{\alpha}{\hbar}(\overrightarrow{\sigma_x} \times \overrightarrow{p}).\hat{z}$),

$$H = \frac{\overrightarrow{p}^2}{2m} + \frac{\alpha}{\hbar}(\overrightarrow{\sigma} \times p).\hat{z}. \tag{2.4.1}$$

The eigenvalues of this Hamiltonian is

$$E \pm (\overrightarrow{k}) = \frac{\hbar^2 k^2}{2m} \pm \sigma k = \frac{\hbar^2}{2m}(k_x \pm k_{so})^2 - \delta_s o. \tag{2.4.2}$$

Where k $= \sqrt{k_x^2 + k_y^2}$ is the modulus of the electron momentum, $k_{so} = \frac{\alpha m}{\hbar^2}$ is a recast form of the spin orbit coupling constant and $\delta_s o = (\frac{\alpha m}{\hbar})^2$ which is neglected because of spin orbit coupling α is small. The eigenvectors of the Hamiltonian (2.4.1) relative to the spectrum (2.4.2) are plane wave's function of the momentum $\overrightarrow{k}$.

$$\psi_+(x,y) = e^{i(k_x+k_y)}\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} ie^- i\theta \tag{2.4.3}$$

$$\psi_-(x,y) = e^{i(k_x+k_y)}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} e^- i\theta \tag{2.4.4}$$

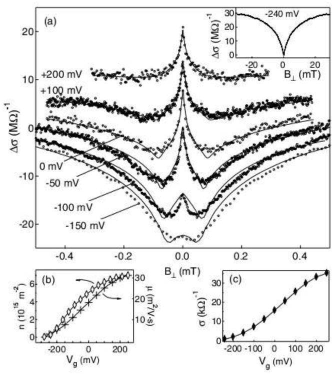

Figure 2.3: (a) Experimental magneto conductance, $\Delta\sigma = \sigma(B) - \sigma(0)$ (circles), offset for clarity, along with three-parameter fits (solid line) for several gate voltages. Inset: Experimental magneto conductance data for the most negative gate voltage, showing pure weak localization. (b) Density and mobility as function of Vg, extracted from longitudinal and Hall volt-age measurements. (c) Experimental conductivity, showing strong dependence on Vg [25].

where $\theta = \arctan(\frac{k_x}{k_y})$ is the angle between the momentum vector and the k_x direction. When the electron moves along x direction the spinor part of the eigenvectors become $\begin{pmatrix} 1 \\ i \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -i \end{pmatrix}$ that is the spin up and spin down in the y direction, on the contrary when the electron moves along the y direction the eigenvectors become $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ that is the spin up and spin down state in the x direction.

Chapter 3

SPIN-ORBIT COUPLING IN THE DIRAC EQUATION

3.1 Introduction

In this chapter we will study the Dirac equation which describes spin-1/2 particles such as quarks and leptons. We will refer to the particle represented by the Dirac equation as an 'electron', but the discussions apply to any point-like spin-1/2 particle which is not antiparticle of itself. It is now well established that spin-orbit coupling is an essentially relativistic effect. The relativistic motion of an electron is described by the Dirac equation that contains both effects (electric dipole and Thomas precession) in the spin-orbit interaction and does so in a very elegant way [27, 28].

3.2 Spin-orbit coupling in the Dirac equation

The spin orbit interaction Hamiltonian can be obtained from the Dirac equation by taking the non-relativistic limit of the Dirac equation up to terms quadratic in v/c inclusive. This limit can be attained in two different ways: either by direct expansion of the Dirac equation in powers of v/c or by the asymptotically exact Foldy-Wouthuysen transformation [26].

Here,we will only present the method using the Dirac equation. Since the Dirac equation is useful for describing electrons, let us insert the potential for the electron in the hydrogen atom,$\hat{V} = \frac{(-e^2)}{r}$. (Note that we are still approximating the proton as infinitely massive.) The Dirac equation is then

$$(c\hat{\alpha}.\hat{p} + \hat{\beta}mc^2 + \hat{V})|\psi\rangle = E|\psi\rangle. \tag{3.2.1}$$

Where α and β represent four- by-four matrices and $\psi(r)$ is a four component Dirac eigenfunction. The momentum operator is defined as $p = i\hbar\overrightarrow{\nabla}$. The Dirac alpha matrix is a vector defined to be $\alpha_x\hat{i} + \alpha_y\hat{j} + \alpha_z\hat{k}$. where the α matrices are defined to be

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}, \alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}, \alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \tag{3.2.2}$$

The two components Pauli matrices are defined to be

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.2.3}$$

We will need some properties of Pauli matrices

$$\sigma = \sigma_x\hat{i} + \sigma_y\hat{j} + \sigma_z\hat{k} = \begin{pmatrix} \hat{k} & \hat{i} - i\hat{j} \\ \hat{i} + i\hat{j} & -\hat{k} \end{pmatrix}. \tag{3.2.4}$$

$$\begin{aligned}(\sigma.p)^2 &= (-i\hbar)^2 \begin{pmatrix} \partial_z & \partial_x - i\partial_y \\ \partial_x + i\partial_y & -\partial_z \end{pmatrix} \begin{pmatrix} \partial_z & \partial_x - i\partial_y \\ \partial_x + i\partial_y & -\partial_z \end{pmatrix} \\ &= -\hbar^2 \begin{pmatrix} \partial_x^2 + \partial_y^2 + \partial_z^2 & 0 \\ 0 & \partial_x^2 + \partial_y^2 + \partial_z^2 \end{pmatrix} \\ &= -\hbar^2\nabla^2 \end{aligned} \tag{3.2.5}$$

The α matrix may also be written in the alternate from

$$\alpha = -\gamma^5\sigma,$$

where

$$\gamma = \begin{pmatrix} 0 & -I_2 \\ I_2 & 0 \end{pmatrix} \tag{3.2.6}$$

and the Dirac β matrix is a scalar defined to be

$$\beta = \begin{pmatrix} 0 & -I_2 \\ I_2 & 0 \end{pmatrix},$$

where

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.2.7}$$

If we again write $|\psi\rangle$ as

$$|\psi\rangle = \begin{pmatrix} \chi \\ \phi \end{pmatrix}. \tag{3.2.8}$$

By combining equation, (3.2.1), (3.2.2),(3.2.3),and equation (3.2.4), (the Dirac equation can be written in a matrix form) the Dirac equation becomes

$$\begin{pmatrix} E - \hat{V} - mc^2 & c\hat{\sigma}.\hat{p} \\ -c\hat{\sigma}.\hat{p} & E - \hat{V} + mc^2 \end{pmatrix} \begin{pmatrix} \chi \\ \phi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.2.9}$$

which leads to two coupled deferential equations:

$$(E - \hat{V} - mc^2)\chi + c\hat{\sigma}.\hat{p}\phi = 0 \tag{3.2.10}$$

$$(E - \hat{V} + mc^2)\phi - c\hat{\sigma}.\hat{p}\chi = 0 \tag{3.2.11}$$

Combining these equations by eliminating phi , we get

$$(E - \hat{V} - mc^2)\chi = c\hat{\sigma}.\hat{p}[\frac{1}{(E - \hat{V} + mc^2)}]c\hat{\sigma}.\hat{p}\chi \tag{3.2.12}$$

On the left hand side,we make the substitution $E_s = E - mc^2$, where E_s is the energy from Schrodinger's equation, and on the right hand side we approximate

$$\begin{aligned} \frac{1}{(E - \hat{V} + mc^2)} &= \frac{1}{2mc^2 + E_s - \hat{V}} \\ &= \frac{1}{2mc^2(1\frac{+E_s - \hat{V}}{2mc^2})^{-1}} \approx \frac{1}{2mc^2}(1 + \frac{E_s - \hat{V}}{2mc^2}) \\ &= \frac{1}{2mc^2} + \frac{E_s - \hat{V}}{4m^2c^4} \end{aligned} \tag{3.2.13}$$

If we only kept the lowest term in this expansion, $\frac{1}{2}mc^2$, we would get the familiar non relativistic Schrodinger equation. Keeping the higher order term allows us to see the fine structure. Now we make our substitutions into Equation, (3.2.12) to get

$$E_s\chi = (\frac{\hat{p}^2}{2m} + V - \frac{\hat{\sigma}.\hat{p}(E_s - \hat{V})\hat{\sigma}.\hat{p}}{4m^2c^4})\chi \tag{3.2.14}$$

In order to get rid of the E_S on the right hand side, we use the fact that $\hat{V}$ and $\hat{\sigma}$ commute and that we only need $E_s - V$ to lower $(v/c)^2$ order to write

$$(E_s - \hat{V})\hat{\sigma}.\hat{p}\chi = \hat{\sigma}.\hat{p}(E_s - \hat{V})\chi + \hat{\sigma}.(E_s - \hat{V}, \hat{p})\chi = (\hat{\sigma}.\hat{p})\frac{\hat{p}^2}{2m}\chi + \hat{\sigma}.[\hat{p}, \hat{V}]\chi. \tag{3.2.15}$$

Now,equation (3.2.14) becomes

$$E_s = [\frac{\hat{p}^2}{2m} + \hat{V} - \frac{\hat{p}^4}{8m^3c^2} - i\frac{\hat{\sigma}.\hat{p}\chi[\hat{p}, \hat{V}]}{4m^2c^2} - \frac{\hat{p}.[\hat{p}, \hat{V}]}{4m^2c^2}]\chi \tag{3.2.16}$$

The first two terms are just the Hamiltonian for the non relativistic Schrodinger equation. The third term is the relativistic correction to the kinetic energy. We are concerned with the fourth term, the spin- orbit interaction H_{so}. To analyze this term, we note first that

$$\begin{aligned} [\hat{p}, \hat{V}]|\psi\rangle &= (\hat{p}\hat{V}, \hat{V}\hat{p})|\psi\rangle \\ &= (i\hbar\nabla\frac{e^2}{r} - \frac{e^2}{r}i\hbar\nabla)|\psi\rangle \\ &= i\hbar e^2((\nabla\frac{1}{r})|\psi\rangle + (\frac{1}{r}\nabla)|\psi\rangle - (\frac{1}{r}\nabla)|\psi\rangle \\ &= -i\hbar e^2\frac{\hat{r}}{r^3}|\psi\rangle. \end{aligned} \tag{3.2.17}$$

This gives

$$\begin{aligned} H_{so} &= -i\hat{\sigma}.\hat{p}\chi\frac{[\hat{p}, \hat{V}]}{4m^2c^2} \\ &= -\frac{i\hat{\sigma}.\hat{p}\chi(-i\hbar e^2\frac{\hat{r}}{r^3})}{4m^2c^2} \\ &= -\frac{\hbar e^2\hat{\sigma}.\hat{p}\times\hat{r}}{4m^2c^2r^3} \\ &= \frac{e^2}{2m^2c^2r^3}(\frac{\hbar}{2}\hat{\sigma}).(\hat{r}\times\hat{p}) \\ &= \frac{e^2}{2m^2c^2r^3}\hat{S}.\hat{L}. \end{aligned} \tag{3.2.18}$$

The Dirac equation allows us drop the Thomas factor. The last equation we obtained describes the spin orbit interaction within the material and includes both contributions to the spin orbit coupling from the electric dipole and the Thomas precession (caused by the electric field) mechanisms and it is a relativistic equation for the electron. For electron gas confined in some plane, say x-y plane, the electrostatic potential is uniform along the heterostructure interface and varies only along the z-axis. Hence, the obtained Hamiltonian in (3.2.12) contains just the contribution arising from its confinement along the z-direction.

Chapter 4

RASHBA SPIN-ORBIT COUPLING FOR A QUANTUM Wire and Square quantum Well

When the two-dimensional (2D) electron gas lying at the interface of a semiconductor hetero structure is further confined along one of the two directions, a quantum wire is formed. To-day's nanolithographic techniques can manufacture quantum wires that have a high structural perfection and are largely free from impurities. These nanostructures are therefore close to ideal electron waveguides where propagation is allowed in one direction (along the wire) while, in the other directions, confinement induces the quantization of the energy states. The transverse quantization manifests itself in the formation of energy sub bands occupied by electrons up to a maximum energy for a given wire density [28, 29].

4.1 Rashba spin orbit coupling for a quantum wire

Understanding the properties of electronic states in quantum wires is a central issue in nanoscience. In the ballistic region, with low electronic densities, electron-electron interactions are not very important, and wire conductance is determined by the transmission of electrons as independent particles. This leads to the celebrated conductance quantization in multiples of the conductance quantum $\frac{e^2}{h}$, as predicted by Landauer [30] and measured in the narrow channels formed by quantum point contacts [31, 32]. Deviations from a perfect staircase quantization of the conductance can be due to various causes, such as impurities, localized states and spin-orbit interactions. The analysis of these deviations has been drawing much interest in nanoscience for many years [33-35] and we try to address the this deviation from this curve due to spin-orbit interaction.

4.2 Energy band structure for quantum wire

The relativistic motion of an electron is described by the Dirac equation that contains both effects (electric dipole and Thomas precession) in the spin-orbit interaction and does so in a very elegant way [27,28]. The Hamiltonian for an electron in the quadratic $[O(v^2/c^2)]$ approximation is the sum [26]

$$\hat{H} = \hat{H}_{so} + \Delta\hat{H}, \tag{4.2.1}$$

where $\Delta\hat{H}$ is the free-particle Hamiltonian and

$$\hat{H}_{so} = \frac{\hbar}{4m^2c^2}[\vec{\nabla}\hat{V}(r) \times \hat{p}].\hat{\sigma} \tag{4.2.2}$$

describes the SOI within the material and includes both contributions to the spin-orbit coupling from the electric dipole and the Thomas precession. For a quasi-one-dimensional model, we have to account for the extra local confinement produced by both the electric field within the x y-plane. When we take into account that the quantum well electric field is perpendicular to the heterojunction interface, the spin-orbit Hamiltonian has a contribution which can be written for the Rashba coupling as

$$\hat{H}^{\alpha}_{so} = \alpha R/\hbar(\hat{\sigma} \times \hat{p})_z. \tag{4.2.3}$$

The value of α determines the contribution of the Rashba spin-orbit coupling to the total electron Hamiltonian. This constant may have values running from $(1 - 10) \times 10^{-10}\ eV \times cm$. Within the single-band effective mass approximation [36, 37], the total Hamiltonian of a quasi-one-dimensional electron system (Q1DES) can be written as

$$\hat{H} = \frac{\hat{p}^2}{2m*} + \hat{V}_c(r) + \hat{H}_{so}, \tag{4.2.4}$$

where the electron effective mass ($m*$) incorporates both the crystal lattice and interaction effects. Moroz and Barnes [37] chose the lateral confining potential $\hat{V}_c(r) = (M\omega^2 x^2)/2$, a parabolic potential which would be appropriate for very narrow wires since the electrons would be concentrated at the bottom of the potential. But, here we consider the in-plane electric field $\vec{E}_c(r)$ associated with $\hat{V}_c(r)$ that is given by $E_c(r) = -\vec{\nabla}\hat{V}_c(r)$. We assume that the SOI Hamiltonian in Equation, (4.2.4) is formed by two contributions:$\hat{H}_{so} = \hat{H}^{\alpha}_{so} + \hat{H}^{\beta}_{so}$. $\hat{H}^{\alpha}_{so}$ arises from the asymmetry of the quantum well, i.e., from the Rashba mechanism [36] for the spin-orbit coupling. For strong lateral confinement, narrow and deep potentials or sharp and high potentials at the edges, the electric field associated with it may not be negligible compared with the interface-induced (Rashba) field. We use [41]

$$\hat{V}_c(x) = V_0\{erfc(\frac{x}{l_0\sqrt{2}}) + erfc(\frac{W-x}{l_0\sqrt{2}})\} \tag{4.2.5}$$

for a conducting channel of width W with well depth V_0. Here, $erfc(x)$ is the complimentary error function. For this potential, the Hamiltonian (4.2.2) gives a term

$$\frac{\partial}{\partial_x}[erfc(\frac{x}{l_0\sqrt{2}}) + erfc(\frac{W-x}{l_0\sqrt{2}})] = \left\{ \exp\left(- \frac{(W-x)^2}{2l_0} \right) - \exp\left(- \frac{x^2}{2l_0^2} \right) \right\} \frac{\sqrt{2}}{\sqrt{\pi}}$$

$$\begin{aligned} \hat{H}^{\beta}_{so} &= \frac{-i\hbar^2 V_0 \sqrt{2}}{4m^{*2}c^2 l_0 \sqrt{\pi}}[\exp\left(- \frac{(W-x)^2}{2l_0^2} \right) - \exp\left(\frac{-x^2}{2l_0^2} \right)] \frac{\partial}{\partial_y}(\hat{i} \times \hat{j}) \cdot \hat{\sigma} \\ &= \frac{-i\hbar^2 V_0 \sqrt{2}}{4m^{*2}c^2 W}(\frac{W}{l_0})\sigma_z \left[\exp\left(- \frac{(W-x)^2}{2l_0^2} \right) - \exp\left(\frac{-x^2}{2l_0^2} \right) \right] \frac{\partial}{\partial_y}. \end{aligned}$$

$$\hat{H}^{\beta}_{so} \equiv i\beta(\frac{W}{l_0}) f(x) \sigma_z \frac{\partial}{\partial_y}, \tag{4.2.6}$$

where $\beta = \frac{\hbar^2 V_0}{4m*^2 c^2 W} \frac{\sqrt{2}}{\sqrt{\Pi}}$.

From this figure we deduced that,when the width of the wire conductor decreases as,the length of the wire conductor increases, then the potential becomes narrow and deep. In Equation, (4.2.6), $f(x)$ is related to the electric field due to lateral confinement in the x direction. The ratio $l_0 << W$ characterizes the steepness of the potentials at the two edge and we are free to use a range of values of the ratio of these two lengths, keeping in mind that the in-plane confinement must be appreciable if the β -term is to play a role. Therefore, we use only one small value of l_o/W to

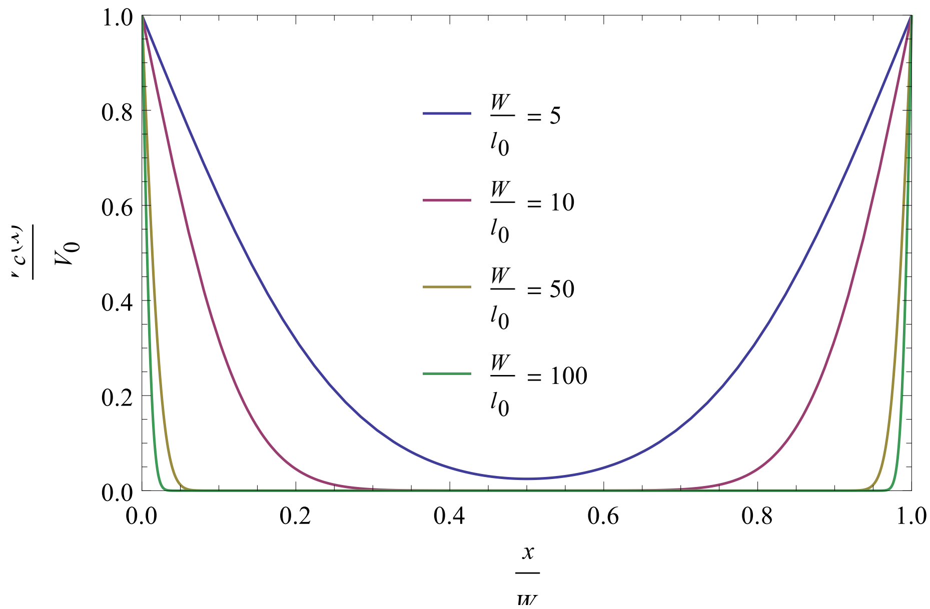

Figure 4.1: (Color online)Plots of $V_c(x)/V_0$, defined in Equation,(4.2.5), as a function of x/W for $W/l_0 = 5$ (blue curve), $W/l_0 = 10$ (violet curve), $W/l_0 = 50$ (brown curve), and $W/l_0 = 100$ (green curve)

illustrate the effects arising from our model on the conductance and thermoelectric power. The β is another Rashba parameter due to the electric confinement along the x direction. Comparison of typical electric fields originating from the quantum well and lateral confining potentials allows one to conclude that a reasonable estimate [38] for β should be roughly 10% of α. The β_{SOI} term in equation, (4.2.6) is asymmetric about the mid-plane $x = \frac{W}{2}$ and varies quadratically with the displacement from either edge (see Fig. 4.1). In this quasi-square well potential, the electron wave functions slightly penetrate into the barrier regions. However, we only need energy levels for the calculations of ballistic transport electrons, not the wave functions, if we assume electronic system is a spatially-uniform quasi-one-dimensional one.

4.3 Square Quantum well

In this section, we discuss a system of two dimensional equations with respect to the spinor components $\Psi_{\uparrow\downarrow}(t)$ for both $\alpha = 0$ and $\alpha \neq 0$. The ballistic conductance is also our interest of discussion. The potential in the Schrodinger equation (4.2.4) for the case of lateral confining potential is modified as $V_{LC}(r) = \frac{MW^2}{2}x^2$ and the corresponding wave equation is $\Psi_{\uparrow\downarrow}(\overrightarrow{r})$=$e^(ik_y y)\phi_{\uparrow\downarrow}(t)$, where $t = \frac{x}{w}$, $\phi_{\uparrow\downarrow}(t)$ is spinor, and k_y is the longitudinal wave number. Substitute this in the Schrodinger equation we obtain a system of two differential equations i.e

$$\hat{H}\psi_{\uparrow\downarrow}(\overrightarrow{r}) = E\psi_{\uparrow\downarrow}(\overrightarrow{r})$$

$\Rightarrow \frac{-\hbar^2}{2M}[\frac{d^2}{d_{x^2}} - k_y^2]\phi_{\uparrow\downarrow} + (\frac{MW^2}{2}x^2)\phi_{\uparrow\downarrow} + i\alpha[\sigma_y\frac{\partial}{\partial_x} - \sigma_x ik_y]\phi_{\uparrow\downarrow} - \beta\frac{x}{L_w}\sigma_z k_y\phi_{\uparrow\downarrow} = E\phi_{\uparrow\downarrow}$

$\Rightarrow \frac{-\hbar^2}{2M}[\frac{d^2}{d_{x^2}} - k_y^2]\phi_{\uparrow\downarrow} + i\alpha\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{\partial}{\partial_x}\begin{pmatrix} \phi_{\uparrow\downarrow} \\ \phi_{\uparrow\downarrow} \end{pmatrix} +$

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\alpha k_y+\begin{pmatrix} \phi_{\uparrow\downarrow} \\ \phi_{\uparrow\downarrow} \end{pmatrix}$ - $\beta\frac{x}{L_w}k_y\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}+\begin{pmatrix} \phi_{\uparrow\downarrow} \\ \phi_{\uparrow\downarrow} \end{pmatrix}$=$E\begin{pmatrix} \phi_{\uparrow\downarrow} \\ \phi_{\uparrow\downarrow} \end{pmatrix}$.

$\Rightarrow \frac{-\hbar^2}{2M}[\frac{d^2}{d_{x^2}} - k_y^2]\phi_\uparrow + (\frac{MW^2}{2}x^2)\phi_\uparrow + \alpha\frac{\partial}{\partial_x}\phi_\downarrow + \alpha k_y\phi_\downarrow - \beta\frac{x}{L_w}k_y\phi_\uparrow = E\phi_\uparrow$. From this equation we get

$\frac{d^2}{d_x^2}\phi_\uparrow + (\frac{2ME}{\hbar^2} - k_y^2)\phi_\uparrow + (\frac{x}{w}\beta\frac{2M}{\hbar^2}k_y L_w)\phi_\uparrow - (\frac{M^2W^2x^2}{\hbar^2})\phi_\uparrow = \alpha\frac{2M}{\hbar^2}(\frac{\partial}{\partial_x} + k_y)\phi_\downarrow$

$$\Phi_\uparrow'' + (\varepsilon_x - t^2 + t_\beta t)\phi_{\uparrow(t)} = (\frac{l_w}{l_\alpha})[(k_y l_w)\phi_\downarrow' + \phi_\downarrow]. \qquad (4.3.1)$$

Here

$l_w = \frac{\hbar}{MW}, \varepsilon_x = \frac{2ME}{\hbar^2} - k_y^2, t_\beta = \frac{l_w}{l_\beta}(k_y l_w)$ and the prime denotes the derivative with respect to t.

$\Rightarrow \frac{-\hbar^2}{2M}[\frac{d^2}{d_{x^2}} - k_y^2]\phi_\downarrow + (\frac{MW^2}{2}x^2)\phi_\downarrow + \alpha\frac{\partial}{\partial_x}\phi_\uparrow - \alpha k_y\phi_\uparrow + \beta\frac{x}{L_w}k_y\phi_\uparrow = E\phi_\downarrow$

Similarly,from this equation we get

$$\Phi_\downarrow'' + (\varepsilon_x - t^2 - t_\beta t)\phi_{\downarrow(t)} = (\frac{l_w}{l_\alpha})[(k_y l_w)\phi_\uparrow' - \phi_\uparrow]. \qquad (4.3.2)$$

The α terms enter only on the right hand side while all the β terms are contained on the left side. This suggests that the β -coupling is responsible for forming independent wave functions $\Phi_{\uparrow\downarrow}(t)$, while the α-coupling mixes them together to form the solution of the whole system equation (4.3.1) and (4.3.2).

4.4 In case of $\alpha = 0$

When the spin orbit coupling constant is equal to zero in equation (4.3.1) and (4.3.2) the interface induced electric field vanishe and they transform into two independent Hermite equation[43] whose solutions are

$$\phi^n_{\uparrow\downarrow}(t) \equiv \phi^n_{\uparrow\downarrow}(t)|\frac{l_w}{l_\alpha} \to 0 = \frac{e^{[-(t\mp\frac{t_\beta}{2})^2]}}{\sqrt{2^n n!`\pi^{1/2}}} H_n(t \mp t_\beta), \tag{4.4.1}$$

n=0,1,2,and $H_n(t)$ is the Hermite polynomial of n^{th} order.
The real wave functions $\phi^n_\uparrow(t)$ and $\phi^n_\downarrow(t)$ form complete sets with respect to the discrete quantum number n and normalized by the following conditions:

$$\langle\phi^m_{\uparrow\downarrow}|\phi^n_{\uparrow\downarrow}\rangle \equiv \int_{-\infty}^{\infty} dt \phi^m_{\uparrow\downarrow}(t)\phi^n_{\uparrow\downarrow}(t) = \delta_{mn}, \tag{4.4.2}$$

where both $\phi^m_{\uparrow\downarrow}$ and $\phi^n_{\uparrow\downarrow}$ are taken at the same value of k_y. From equation (4.4.1) one can see that the both up ($\phi^n_\uparrow$) and down ($\phi^n_\downarrow$) spinor components have exactly the same shape as a functions of t but are spatially displaced with respect to each other by amount of t_β. This displacement is direct consequence of the β-coupling because it does not vanish as long as β different from zero except $k_y l_w = 0$. At the finite values of t_β, the complete sets of functions $\phi^n_\uparrow(t)\phi^n_\downarrow(t)$ turn out not to be mutually orthogonal. Instead of this the scalar product $\langle\phi^m_{\uparrow\downarrow}|\phi^n_{\uparrow\downarrow}\rangle$ in the case of sufficiently weak β coupling is governed by the following asymptots:

$$\langle\phi^n_{\uparrow\downarrow}|\phi^n_{\uparrow\downarrow}\rangle = 1 - o(t^2_\beta) \tag{4.4.3}$$

$$\langle\phi^n_{\uparrow\downarrow}|\phi^{n+1}_{\uparrow\downarrow}\rangle \simeq \pm\sqrt{\frac{n+1}{2}}t_\beta = \pm\sqrt{\frac{n+1}{2}}\frac{l_w}{l_\beta}(k_y l_w) \tag{4.4.4}$$

$$\langle\phi^n_{\uparrow\downarrow}|\phi^{n-1}_{\uparrow\downarrow}\rangle \simeq \mp\sqrt{\frac{n}{2}}t_\beta = \mp\sqrt{\frac{n}{2}}\frac{l_w}{l_\beta}(k_y l_w) \tag{4.4.5}$$

$$\langle\phi^n_{\uparrow\downarrow}|\phi^{n\pm p}_{\uparrow\downarrow}\rangle = o(t^p_\beta), \tag{4.4.6}$$

for $p \geq 2$.
The displacement effect of the β-coupling on spinor wave functions is similar to the effect of perpendicular magnetic field on the quasi-one dimensional system. The β-coupling shifts the spinor components and is not lifting their energy degeneracy. The

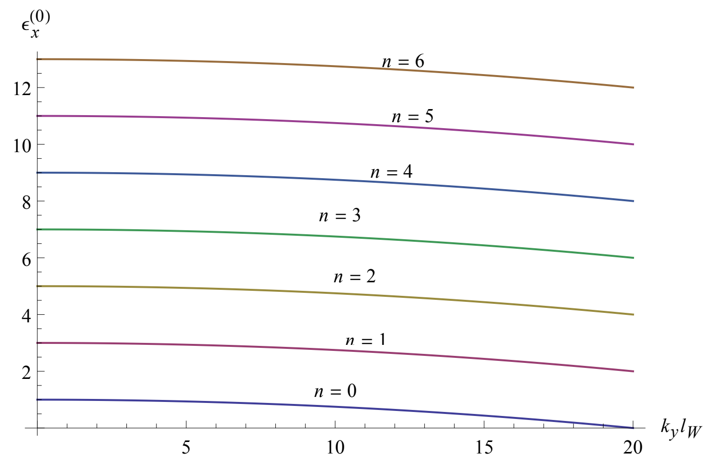

Figure 4.2: The transverse energy $\varepsilon_x^{(0)}$ vs. $k_y l_W$ for $l_W/l_\beta = 0.1$

dimensionless transverse energy $\varepsilon_x^{(o)}$ corresponding to both $\phi_{\uparrow\downarrow}^n(t)$ is given by (see Fig.4.2)

$$\varepsilon_x^{(o)} \equiv \varepsilon_x^{(o)}(n, k_y) = 2n + 1 - (\frac{t_\beta}{2})^2 = 2n + 1 - \frac{1}{4}(\frac{l_w}{l_\beta})^2(k_y l_w)^2 \tag{4.4.7}$$

The total electron energy E then forms parabolic sub-bands for each n^{th} transverse mode:

$$E \equiv E_n(k_y) = \frac{\hbar\omega}{2}\varepsilon_x^{(o)}(n, k_y) + \frac{\hbar^2 k_y^2}{2M}. \tag{4.4.8}$$

For $\beta = 0$, the equations (4.4.7) and (4.4.8) describe the well known electric sub-bands.

4.5 In case of $\alpha \neq 0$

We now discuss the situation where the interface-induced electric field is non-zero. This interface-induced field gives rise to a non zero α-coupling. To analyse the energy spectrum in the presence of α-coupling, we first expand the unknown functions $\Phi_{\uparrow\downarrow}(t)$ in terms the unperturbed solutions $\phi_{\uparrow\downarrow}(t)$ (4.4.1) of equations (4.3.1) and (4.3.2):

$$\Phi_{\uparrow\downarrow}(t) = \sum_{m=0}^{\infty} f_{\uparrow\downarrow}^m \phi_\uparrow^m(t) \tag{4.5.1}$$

$$\Phi_{\uparrow\downarrow}(t)=\sum_{m=0}^{\infty} g^{m}_{\uparrow\downarrow}\phi^{m}_{\downarrow}(t) \tag{4.5.2}$$

We substitute this expansions (4.5.1)and (4.5.2) into equations (4.3.1)and (4.3.2) respctively and use the property[43]

$$\frac{d}{d_t}\phi^{n}_{\uparrow\downarrow}(t)=\sqrt{\frac{n}{2}}\phi^{n-1}_{\uparrow\downarrow}(t)-\sqrt{\frac{n+1}{2}}\phi^{n+1}_{\uparrow\downarrow}(t) \tag{4.5.3}$$

to remove the derivative with respect to t in the equation (4.3.1) and (4.3.2). We next multiply the equations obtained by $\phi^{n}_{\uparrow}t$ and $\phi^{n}_{\downarrow}t$ respectively and integrate them over t from $-\infty$ to ∞. Owing to the orthogonality condition (4.4.2), the summation over m is removed by the delta function δ_{mn} and we find the simple vector relations:

$$f_{\uparrow}=\hat{U}_{\uparrow}f_{\downarrow} \tag{4.5.4}$$

$$g_{\downarrow}=\hat{U}_{\downarrow}g_{\uparrow} \tag{4.5.5}$$

where $f_{\uparrow\downarrow}\equiv({f_{\uparrow\downarrow}}^{0},{f_{\uparrow\downarrow}}^{1},{f_{\uparrow\downarrow}}^{2},....,{f_{\uparrow\downarrow}}^{n})$ and $g_{\uparrow\downarrow}\equiv({g_{\uparrow\downarrow}}^{0},{g_{\uparrow\downarrow}}^{1},{g_{\uparrow\downarrow}}^{2},....,{g_{\uparrow\downarrow}}^{n})$ are vectorised coefficients of the expansions (4.5.1)and(4.5.2) respectively,and $\hat{U}_{\uparrow\downarrow}$ are tridiagonal matrices defined by their elements:

$$\hat{U}^{nn}_{\uparrow\downarrow}=\frac{l_w}{l_\alpha}\frac{k_y l_w}{\varepsilon_x-\varepsilon^{(0)}_x(n)} \tag{4.5.6}$$

$$\hat{U}^{n,n+1}_{\uparrow\downarrow}=\pm\frac{l_w}{l_\alpha}(\frac{n+1}{2})^{1/2}\frac{1}{\varepsilon_x-\varepsilon^{(0)}_x(n)} \tag{4.5.7}$$

$$\hat{U}^{n+1,n}_{\uparrow\downarrow}=\mp\frac{l_w}{l_\alpha}(\frac{n+1}{2})^{1/2}\frac{1}{\varepsilon_x-\varepsilon^{(0)}_x(n)+1} \tag{4.5.8}$$

To find the relation ship between the vectors $f_{\uparrow\downarrow}$ and $g_{\uparrow\downarrow}$,we equate the right hand sides of equation (4.5.1) to that of equation (4.5.2) and take the scalar product of the resulting equation with $\phi^{n}_{\uparrow}(t)$. By using orthogonalisation condition,we find that

$$f_{\uparrow\downarrow}=\hat{W}_{\uparrow}g_{\uparrow\downarrow} \tag{4.5.9}$$

where the matrix $\hat{W}_{\uparrow}$ is defined by

$$W^{mn}_{\uparrow\downarrow}=\langle\phi^{m}_{\uparrow\downarrow}\mid\phi^{n}_{\uparrow\downarrow}\rangle. \tag{4.5.10}$$

Similarly, by taking a scalar product of the right hand side of equation(4.5.1) and equation (4.5.2) by $\phi_{\downarrow}^{n}(t)$, it can be shown that

$$g_{\uparrow\downarrow} = \hat{W}_{\uparrow} f_{\uparrow\downarrow}. \tag{4.5.11}$$

Finally,we combine relations (4.5.4),(4.5.5),(4.5.9) and (4.5.11) into a closed homogenous equation with respect to $f_{\uparrow}$: $f_{\uparrow} = \hat{U}_{\uparrow}\hat{W}_{\uparrow}\hat{U}_{\downarrow}\hat{W}_{\downarrow}f_{\uparrow}$. In order for this equation to have a non-trival solution,the Jacobian matrix must satisfy the following condition:

$$det(1 - \hat{U}_{\uparrow}\hat{W}_{\uparrow}\hat{U}_{\downarrow}\hat{W}_{\downarrow}) = 0 \tag{4.5.12}$$

The roots of this equation determine the dispersion law of electrons.

4.6 BALLISTIC CONDUCTANCE

Here we discuss the effect of the SOI on the ballistic conductance of along aquasi-one dimensional electron system at low temperatue,we must relate its conductance to its energy spectrum. So,to do this we use two landauer formula[43] that is

$$G \equiv G(\varepsilon_F) = \frac{e^2}{h} M(\varepsilon_F) \tag{4.6.1}$$

where G is the ballistic conductance, ε_F is the fermi energy,and $M(\varepsilon_F)$ is the number of occupied electron subbands which propagate in the same direction:

$$M(\varepsilon_F) = \sum_{n} \sum_{i} \sum_{s=\uparrow\downarrow} \theta[\varepsilon_F - \varepsilon_{min}^{s}(n, i)] \tag{4.6.2}$$

where $\varepsilon_{min}^{s}(n, i)$ is the energy of the $i^t h$ minimum in the $n^t h$ electron subband with the spin orientation S and $\theta(x)$ is the heaviside unit step function. Since $\varepsilon_{min}^{s}(n, i)$ can be found directly from the dispersion law of electrons the conductance G(4.6.1)turns out to be completely defined by the energy spectrum alone. The general scattering approach to quantum transport, is essentially based on the condition that the current must travel in any one dimension electron subband with out scattering into any other. To define the matrix elements of the current density $j_{mn}(r)$ for the case where the wave functions $\Psi_{mn}(r)$ are spinors,
$\Psi_{mn} = (\Psi_{\uparrow}^{mn}, \Psi_{\downarrow}^{mn})$:

$$j_{mn}(r) = \frac{1}{2M}(\Psi_{m}^{\dagger}\hat{\sigma}(\hat{\sigma}.\hat{p})\Psi_{n} + [(\hat{\sigma}.\hat{p})\Psi_{m}]^{\dagger}\hat{\sigma}\Psi_{n}). \tag{4.6.3}$$

Here the dagger denotes the hermitian conjugate and the divergence of the vector $j_{mn}(r)$ is given by

$$\nabla.j_{mn}(r) = \frac{i\hbar}{2M}((\nabla^2\Psi_m^\dagger)\Psi_n - \Psi_m^\dagger(\nabla^2\Psi_n)). \qquad (4.6.4)$$

By using the Hamiltonian equation, $\hat{H} = \frac{\hat{p}^2}{2M} + V_{lc} + \hat{H}_{so}$ and the schrodinger equation, $\hat{H}\Psi = E\Psi$, we express $\nabla^2\Psi_m^\dagger and \nabla^2\Psi_n$ interms of $\Psi_m^\dagger$and Ψ_n respectively and substitute the expression obtained into equation(4.6.4). As aresult, we have

$$\nabla.j_{mn}(r) = \frac{i}{\hbar}(E_m - E_n)\Psi_m^\dagger(r)\Psi_n(r) \qquad (4.6.5)$$

where E_m and E_n are energies corresponding to the states Ψ_m and Ψ_n respectively. In the absence of any inelastic collisions,any scattering occurs between states of the same energy. So, without loss of generality,we restrict ourselves to considering only equal energies $E_m = E_n$ in equation(4.6.5),in which case we find that

$$\nabla.j_{mn}(r) = 0 \qquad (4.6.6)$$

for $E_m = E_n$. The eigenstates of the Hamiltonian $\hat{H}$ are prefect current carrying states that are free from scattering even in the presence of arbitrary spin orbit coupling. This result implies that the spectrum of the Hamiltonian is directly relevant to and completely defines the ballistc conductance in the presence of the spin orbit coupling. So we can discuss the features of the ballistic conductance in a quasi one dimensional electron system subject to the spin orbit interaction and for illustrative purposes we use the case of zero spin orbit coupling. The corresponding subband energies $\varepsilon_n = 2n + 1 + (k_y l_w)^2$ are plotted in (Fig.4.3) as functions of $k_y l_w$. The dependence ballistic conductance can simple be deduced from this figure by moving a horizontal line ε=ε_F from zero upwards and counting the number of points at which this line crosses the spectral parabolas. Since all the subbands in an ideal system are two fold spin degenerate for any k_y this number coincides the number M of propagating modes in the quasi one dimensional electron system and we deduced that the β-coupling alone does not affect the ballistic conductance.

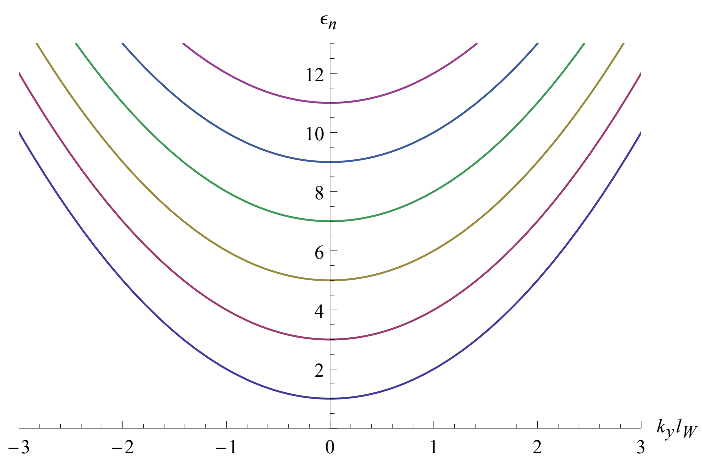

Figure 4.3: The subband energy ϵ in units of $\hbar\omega/2$ vs. $k_y l_W$ for $\alpha = 0$

Chapter 5

conclusion

We studied the spin orbit coupling, spin orbit coupling from the Dirac equation,and the spinor equation.Spin-orbit interaction gives rise to a coupling between the spin dynamics of an electron and its orbital motion in space. The moving charges gives rise to an internal magnetic in the rest frame of the electron. The magnitude and the direction of this internal magnetic field depends on the velocity and the direction of the electron in the material,i.e spin orbit interaction gives to a wave vector dependent internal magnetic field.

In the absence of a magnetic field,the spin degeneracy of the two dimension electron gas energy bands at $k \neq 0$ is lifted by the coupling of the electron spin with its orbital motion. This coupling arises because of the the inversion asymmetry of the potential that confines the two dimension electron gas system.In a free atom,spin orbit interaction can lift the degeneracy of states with the same orbital wave function but with opposite spins.

Their is a difference between Dresselhaus and Rashba term i.e the dresselhaus term is due to bulk properties of the semiconductors that its coupling constant β is fixed and can not be tuned.But the Rashba term depends on the shape of the confining potential and the coupling constant α can be tuned by means metallic gate since the confining potential can be modified using electric field.

We used a model in which edge effects for the nanowires are taken into account by solving numerically Dirac's equation in a quasi-square potential and we found that the energy bands are different. The influence of the spin orbit coupling on the spectrum and the ballistic conductance of the quasi one dimensional electron system formed by lateral electric confinement of a two dimensional electron gas.The electron eigenstates that were found as the solution to the spectral problem are perfect current -carrying states. A current can travel in any of these states without scattering into any other.This property allows the ballistic conductance to be calculated directly from the energy spectrum with the help of simple Landauer formula [43].

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