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Coulomb Interaction Effects in Semiconductor Heterostructures with Spin-Orbit Interaction

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Coulomb Interaction Effects In Semiconductor Heterostructures With Spin-Orbit Interaction

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Physics

by
Jeremy Patrick Capps
May 2015

Accepted by:
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Abstract

In this thesis we analyze two different situations where the interplay between the spin-orbit coupling (SOI) of the Rashba and Dresselhaus type, linear in the electron momentum, and the Coulomb interaction generates a specific macroscopic phenomenology that can be experimentally observed. In the first problem, we investigate the Friedel oscillations that can be sustained in the presence of the Coulomb repulsion in a two-dimensional lateral superlattice with SOI and analyze the dependence on several system parameters. Then, we are concerned with the properties of a single quantum well in the special regime where the coupling strengths of the Rashba and Dresselhaus interactions are equal. Starting from general total-energy considerations, we demonstrate that the SU(2) spin-rotation symmetry and the resulting persistent helical state (PHS) predicted to occur are not in fact realized; the actual spin order being that of an itinerant antiferromagnet (IAF). We obtain numerical results that describe the temperature evolution of the order parameter in the IAF state and determine the critical temperature of the transition to the paramagnetic order. Transport in this state is modeled by using the solutions of a Boltzmann equation obtained within the relaxation time approximation. Numerical estimates performed for realistic GaAs and InAs samples indicate that at low temperatures, the amplitude of the spin-Seebeck coefficient can be increased by scattering on magnetic impurities.
Dedication

I dedicate this thesis to my parents, Jerry and Patricia Capps, for their continuous support throughout my graduate career. I also dedicate this thesis to my friends for their willingness to have ideas constantly bounced off of them and the occasional sparks of inspiration that came to life through these conversations.
Acknowledgments

I would like to thank my advisor Dr. Catalina Marinescu for all of the insights, guidance, and inspiration she has provided me while working together. Her unwavering dedication to our group and research is second to none, and I am honored to have worked alongside her.
# Table of Contents

Title Page ................................................................. i  
Abstract ................................................................. ii  
Dedication ................................................................. iii  
Acknowledgments ....................................................... iv  
List of Figures .......................................................... vi  

1 Introduction ........................................................... 1  

2 Friedel Oscillations in Lateral Superlattices with Spin-Orbit Interaction .................................................. 7  
2.1 Semiconductor Superlattices ....................................... 7  
2.2 Friedel Oscillations .................................................. 9  
2.3 System Description .................................................. 12  
2.4 The Density Response Function .................................... 18  
2.5 Real-Space Density Fluctuations ................................... 24  

3 Spin Instabilities in Interacting Electron Systems ................. 34  

4 Spin Instabilities and Spin-Orbit Interactions ..................... 42  
4.1 The Single-Particle Spectrum .................................... 47  
4.2 The Many-Body Interaction ....................................... 49  

5 Thermoelectric Transport at Equal Rashba and Dresselhaus Coupling Strengths ........................................... 62  
5.1 Thermoelectric Effects ........................................... 62  
5.2 Boltzmann Transport Equation .................................... 63  
5.3 Thermoelectric Transport in the $\alpha = \beta$ Regime .................... 67  

6 Conclusions and Discussion ............................................ 84  

Bibliography .............................................................. 86
List of Figures

1.1 Band structure and band splitting due to spin-orbit coupling in GaAs close to the fundamental gap. [From [5]] 3

1.2 Chiral behavior of the spin in the presence of the spin-orbit interaction. [From [9]] 4

2.1 Type I SL in GaAs. [From [23]] 8

2.2 The lateral superlattice is a 2D reduction of the general 3D superlattice that retains a periodic potential along the lateral superlattice axis. [From [25]] 9

2.3 Screening in an interacting electron system. [From [39]] 11

2.4 Analytic results for the single-particle state in a 2D lateral superlattice with SOI in arbitrary units. 16

2.5 Band structure calculated numerically for a 2D superlattice system with no SOI (left), and SOI (right). Energy is of the order meV. [From [48]] 16

2.6 The variation of the Fermi energy in a lateral superlattice with $\Delta = 20$ meV as a function of the spin-orbit coupling $\alpha = 5$ for $a = 30$nm, $a = 40$nm and $a = 50$nm. 18

2.7 The static polarization function in a SL with $\Delta = 20.0$ meV and $\alpha = 5$ for $a = 30$nm in (a), $a = 40$ nm in (b) and $a = 50$nm in (c). 28

2.8 The static density response function in a SL with $\Delta = 20.0$ meV for $\alpha = 5.0$ for $a = 30$nm in (a), $a = 40$ nm in (b) and $a = 50$nm in (c). 29

2.9 Friedel oscillations induced along the axis of a lateral SL by an impurity located at $x = 0$. The system parameters are $\Delta = 20$ meV, $a = 30$ nm and $\alpha = 5$. 30

2.10 Friedel oscillations induced in a lateral superlattice by an impurity located at $x = 0$ for different SOI coupling values $\alpha$. The SL parameters are $\Delta = 20$ meV and $a = 30$nm. 30

2.11 Friedel oscillations induced in a lateral superlattice by an impurity located at $x = 0$ for different SL constants for the same value of the spin-orbit interaction constant, $\alpha = 5$ and $\Delta = 20$ meV. 31

2.12 Friedel oscillations induced along the SL axis as a function of the miniband width for $a = 30$ nm and $\alpha = 0, 10$. 31
2.13 Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of the spin-orbit coupling, for $\Delta = 20$ meV and $a = 30 \text{nm}$. 32

2.14 Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of the lattice constant, for $\Delta = 20$ meV and $\alpha = 5$. 32

2.15 Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of different SL constants and bandwidths. 33

3.1 An Electron Gas With Giant Spiral Spin-Density Wave. 41

3.2 Single-particle Energy spectrum In a Spiral Spin-Density Wave. 41

4.1 The single-particle spectrum of a 2D electron system with equal Rashba-Dresselhaus linear couplings. The opposite-spin energies $\varepsilon_\uparrow$ and $\varepsilon_\downarrow$ are degenerate at $k = 0$, the source of a spin instability that leads to the formation of two new quasiparticles of energies $E_-$ and $E_+$. The states that overlap at $k = 0$ are plane waves of the same momentum. 43

4.2 The variation of the gap in GaAs at the center of the Fermi surface, $g(0,0)$, as a function of temperature for two different screening constants. 57

4.3 (color online) The variation of the gap function vs temperature for two different screening constants. For $\mu_1 = 10^{-3}$ (left panel) the temperatures are $T = 0$, $T_{\text{max}} = 13.4 \text{K}$, and $T_c = 90 \text{K}$, while for $\mu_2 = 10^{-2}$ (right panel) the temperatures are $T = 0$, $T_{\text{max}} = 5.97 \text{K}$, and $T_c = 29 \text{K}$, respectively. 59

4.4 (color online) The variation of the coupling angle vs temperature for two different screening constants. For $\mu_1 = 10^{-3}$ (left panel) the temperatures are $T = 0$, $T_{\text{max}} = 13.4 \text{K}$, and $T_c = 90 \text{K}$, while for $\mu_2 = 10^{-2}$ (right panel) the temperatures are $T = 0$, $T_{\text{max}} = 5.97 \text{K}$, and $T_c = 29 \text{K}$, respectively. 60

4.5 The fractional spin polarization along the $\hat{x}$ direction as a function of temperature for two different screening constants. 61

5.1 The variation of the inclination angle $\theta$ along $k_x$ for two different screening constants $\mu$ in an InAs quantum well with $n = 2.5 \times 10^{14} \text{m}^{-2}$. The momentum unit is $k_F = Q = \sqrt{2\pi n} = 2 \times 10^7 \text{m}^{-1}$. 74

5.2 The variation of the gap function along $k_x$ for two different screening constants $\mu$ in an InAs quantum well with $n = 2.5 \times 10^{14} \text{m}^{-2}$. The energy unit is $E_F = \hbar^2 k_F^2 / 2m^* = 0.6 \text{meV}$. 75

5.3 The variation of the relative Seebeck coefficient for the normal and parallel charge and spin modes with temperature for different values of the ratio $J/V_0$. $S_0$ is the value of the Seebeck coefficient in an isotropic system with the same particle density. 77
5.4 The variation of the relative Seebeck coefficient for the normal (a) and parallel (b) charge and normal (c) and parallel (d) spin modes with temperature for different values of the ratio $J/V_0$. $S_0$ is the value of the Seebeck coefficient in the isotropic system.

5.5 The variation of the gap function at the center of the Fermi surface and of the fractional spin polarization for a screening constants $\mu_1 = 10^{-3}$ in a InAs quantum well with $n = 4 \times 10^{15} \text{m}^{-2}$. $Q = 7.2\times 10^{-3} k_F$ as a function of temperature.

5.6 The variation of the gap in GaAs at the center of the Fermi surface, $g(0,0)$, as a function of temperature for two different screening constants.

5.7 The variation of the spin Seebeck coefficient for the normal in (a) and parallel in (b) mode with temperature for different values of the ratio $J/V$. The gap value is $0.2E_F$, while the polarization is 10%. The temperature unit is set by the spin-flip energy and corresponds to 35K.
Chapter 1

Introduction

Finding ways of exploiting the electronic spin degree of freedom in solid state structures has been one of the major thrust areas in condensed matter research in the last ten years. The fundamental issues of this effort were centered on the creation and control of spin-separated electron populations by external electromagnetic fields in systems that ideally could be easily integrated in the present semiconductor-based technology. Although encouraging results were obtained within various configurations, definitive conclusions have yet to be drawn.

One of the most important developments has been without a doubt the “rediscovery” of the spin-orbit interaction (SOI). Known to exist in solids for a long time, SOI was put forward in the context of spintronic applications by its anticipated role in spin control [1], in such devices as the spin field transistor. The origin of this coupling is the inversion asymmetry that occurs in certain crystals or artificially grown structures such as quantum wells. Since it acts as an effective magnetic field whose strength is proportional to the momentum of the electron, SOI is responsible for a series of interesting effects that involve the spin manipulation by electric fields, and more recently, by temperature gradients.
Several newer remarkable discoveries, starting with the existence of a persistent spin current in the spin-Hall effect [2] or the thermal generation of spin currents through the spin Seebeck effect [3, 4] have showcased novel ways in which physics was enhanced.

The basic phenomenology of the spin-orbit coupling in solids originates in the non-relativistic approximation of the Dirac equation which leads to the Pauli formula [5],

$$H_{SO} = -\frac{\hbar}{4m_0^2c^2} \vec{\sigma} \cdot \vec{p} \times (\nabla V_0),$$

where $\hbar$ is Planck’s reduced constant, $m_0$ is the free electron mass, $c$ is the speed of light, $\vec{p}$ is the electron momentum, $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$, and $V_0$ is the Coulomb potential from the core.

Extending similar considerations to the electron motion in solids had to take into account the structure of single-particle energies, $E_n(k)$, characterized by a band index $n$ and wave vector $k$. In semiconductor systems such as GaAs, the coupling of the orbital motion with the spin generates the splitting of the topmost valance band, as shown in Fig. (1.1), where the two mini-bands correspond to total $j = 3/2$ and $j = 1/2$.

In zinc-blende structures that lack inversion symmetry, the spin-splitting of the electron and hole states can occur at finite wave-vectors even in the absence of a magnetic field, a result first discussed by Dresselhaus [6]. Similarly, in two dimensional quantum wells without inversion symmetry, a spin-orbit coupling was discovered by Rashba [7].

Here we study effects that originate in the interplay between the Rashba (R) and Dresselhaus (D) SOI linear in the electron momentum, which in terms of the Pauli spin operators $\{\sigma_x, \sigma_y, \sigma_z\}$, are written for an electron of momentum $\vec{p} = \{p_x, p_y, p_z\}$.
Figure 1.1: Band structure and band splitting due to spin-orbit coupling in GaAs close to the fundamental gap. [From [5]]

as

\[ H_{\text{SOR}} = \alpha (\sigma_x p_y - \sigma_y p_x), \]  

(1.2)

and

\[ H_{\text{SOD}} = \beta (\sigma_x p_x - \sigma_y p_y), \]  

(1.3)

respectively. The coupling constant \( \alpha \) is determined by the quantum well parameters, and was shown to be quite sensitive to an applied electric field [8] whereas \( \beta \) is determined by the properties of the crystal lattice.

In the presence of the spin-orbit coupling the single-particle Hamiltonian of an electron of effective mass \( m^* \) is written as

\[ H_0 = \frac{p^2}{2m^*} + \alpha (\sigma_x p_y - \sigma_y p_x) + \beta (\sigma_x p_x - \sigma_y p_y). \]  

(1.4)

Its eigenstates are plane waves multiplied by linear combinations of up and down
spins indexed by the chiral number $\mu = \pm 1$, and written as

$$\psi_{p,\mu} = \frac{1}{\sqrt{V}} e^{ip \cdot r / \hbar} \left( |\uparrow\rangle + \mu e^{i\varphi_p} |\downarrow\rangle \right),$$

(1.5)

where the dephasing angle $\varphi_p$ is given by

$$\tan \varphi_p = \frac{\beta_p y - \alpha_p x}{\beta_p x + \alpha_p y},$$

(1.6)

The energy eigenvalues are given by

$$\epsilon_p = \frac{p^2}{2m^*} + \mu \sqrt{(\beta_p x + \alpha_p y)^2 + (\beta_p y - \alpha_p x)^2}.$$  

(1.7)

As shown in Fig. (1.2), along with the split in the single-particle energies, the spin-orbit coupling induces the chiral motion of the spin.

In real electron systems the simple single-particle picture outlined above needs to be completed by considering the Coulomb interaction. Although spin independent
in real-space, the Fourier transform of the interaction will be, however, modified by
the spin structure of the eigenstates in Eq. (1.7). Consequently, the effects of the
Coulomb repulsion on the physical properties of the homogeneous electron systems
with SOI have been explored in great detail both in terms of single-particle properties
[10] or as collective phenomenology [11, 12, 13, 14, 15] in complementary numerical
and analytical approaches [16, 17].

In this thesis, we analyze two different instances in which a distinct phe-
nomenology is observed that originates in the confluence of spin-orbit interaction and
the Coulomb repulsion. Firstly, we offer an analysis of the effect of the spin-orbit
in screening in lateral superlattices as reflected in the Friedel oscillations. We inves-
tigate the Friedel oscillations that can be sustained in the presence of the Coulomb
interaction in a two-dimensional lateral superlattice (SL) with Rashba spin-orbit in-
teraction. The superlattice is modeled as a periodic array of infinitely attractive
quantum wells whose periodicity determines the apparition of energy minibands in
the single-particle spectrum that are further spin-split by SOI. The Friedel oscillations
are obtained from the static real-space density response function \( \Delta \nu(r) \) to an external
perturbation, evaluated self-consistently within the random-phase approximation of
the Coulomb interaction. The interplay in the momentum-space between the spin-
orbit coupling and periodicity determines the overall characteristics of the density
fluctuations. Previously, the superposition of SOI and spatial confinement has been
shown to produce specific phenomena that are absent in homogeneous systems such
as the induced spin accumulation in the presence of an electric field [18, 19, 20] and
the enhancement of the excitation frequency of the collective plasma modes [21]. In
a singly occupied, chiral-split miniband approximation, the amplitude and phase of
the oscillations are studied numerically as functions of several significant parameters
of the system such as the miniband width, the strength of the spin-orbit coupling and
In a second problem, we investigate the properties of the many-body electron system in the presence of the Coulomb interaction in the special case when the Rashba and Dresselhaus interactions are equal. Starting from general total-energy considerations, we demonstrate that the SU(2) spin-rotation symmetry and the resulting persistent helical state (PHS) predicted to occur in an electron system with equal Rashba-Dresselhaus coupling constants are not in fact realized. On account of the accidental degeneracy that appears in the single-particle spectrum, the Coulomb interaction favors the apparition of an itinerant antiferromagnetic (IAF) order characterized by a fractional polarization of fixed spatial orientation. Within the Hartree-Fock approximation, we obtain numerical results that describe the temperature evolution of the order parameter in the IAF state and determine the critical temperature of the transition to the paramagnetic state.

Next, in the same system, we discuss the possible existence of an anomalously high low-temperature charge and spin thermopower. The transport in this state is modeled by using the solutions of a Boltzmann equation obtained within the relaxation time approximation. We show that when scattering on magnetic impurities is introduced, the energy dependence of the relaxation time enhances the value of the thermoelectric coefficient for both charge and spin currents. An estimate of the effect is provided for two different quantum wells, GaAs and InAs, with different characteristics. In each case, the variation of the effect with the strength of the magnetic scattering is studied.
Chapter 2

Friedel Oscillations in Lateral Superlattices with Spin-Orbit Interaction

2.1 Semiconductor Superlattices

First introduced in the experimental physics world in the early 70’s by Esaki and Tsu [22], superlattices (SL) are composed of alternating layers of two (or more) different constituents having different energy-band parameters, with a periodicity much greater than the fundamental lattice constants. The coupling between successive quantum wells aligned along one spatial direction by molecular beam epitaxy (MBE) alters the electronic properties and band structures of the individual components leading to essentially new materials, with properties that are intermediate between those of the constituents.

Early on, two types of superlattices were created and studied, known as type I and II. Type-I superlattices are exemplified by a GaAs/Al$_x$Ga$_{1-x}$As system as
Figure 2.1: Type I SL in GaAs. [From [23]]

in Fig. (2.1), in which the band gap of GaAs is smaller than, and contained within, that of Al$_x$Ga$_{1-x}$As giving rise to band-gap discontinuities in both the valence and conduction bands of the resultant superlattice. In type-II superlattices, as exemplified by the InAs/GaSb system the band match-up is such that the conduction band minimum of InAs is below the valence band maximum of GaSb. In this case there is a transfer of electrons from one layer (GaSb) to another (InAs), resulting in a spatial separation of electrons and holes in adjacent potential wells, with the formation of electron and hole minibands.

In 1989 K. von Klitzing [24] realized the first lateral superlattice by patterning the surface of a 2D electron system by a periodic potential, as shown in Fig. (2.2). The gates induce a 1D periodic potential that confines the electrons along quasi 1D wires. When conditions allow tunneling between the wires, minibands emerge similar to those at the interfaces in the 3D superlattice. The new physics explored in the lateral superlattice is a consequence of introducing additional geometric constraints to the 2D electrons in the real and momentum spaces.
2.2 Friedel Oscillations

As a real-space manifestation of the many-body Coulomb interaction, Friedel oscillations originate in the electron density fluctuations induced by external potentials. They were observed in many STM measurements at surfaces, where steps, impurities, surface dislocations, and point defects can give rise to its characteristic Fermi wavelength-dependent oscillatory signature in tunneling spectroscopy scans [26, 27, 28, 29, 30, 31, 32, 33]. On their account, modulation effects have been registered on other phenomena, such as quantum confinement and charge spilling, which appear in the so-called “electronic growth” model for thin metallic films on semiconductors. This model has been used to understand the critical thicknesses observed in the growth modes of Ag and Pb films [34, 35]. More recently, it has been proposed that the Friedel oscillation may similarly modulate the growth modes for graphene films on vicinal surfaces [36].

In the presence of a charged impurity at the origin of a 2D electron system, electrons experience simultaneously the potential of the impurity as well as the repulsion of the other electrons. This effective potential determines a specific behavior
of the density fluctuation induced in the electron system as seen in Fig. (2.3), a phenomenon known as Friedel oscillations. The effective potential in general will be less than the bare $1/r$ dependence for electrons far from the impurity. It can be shown mathematically to have the following form:

$$\delta \phi(r) = \frac{qe^{-k_{TF}r}}{r}, \quad (2.1)$$

where we have introduced the Thomas-Fermi screening length parameter $k_{TF}^{-1}$, defined by $k_{TF}^2 = \frac{2e^2m^*/\hbar^2}{2}$ in $2D$.

A favorable consequence of accounting for screening is that it effectively removes the divergence of the bare long-range Coulomb interaction, such that when a potential $\phi^{\text{ext}}(q) = 4\pi e/q^2$ is introduced the effective potential experienced by an electron is

$$\phi(q) = \phi^{\text{ext}}(q)/\varepsilon(q) = \frac{4\pi e/q^2}{1 + k_{TF}^2/q^2} = \frac{4\pi e}{k_{TF}^2 + q^2}, \quad (2.2)$$

which is well defined for all values of $q$. This is very useful for numerical integration routines used to study the properties of the system.

The behavior of Friedel oscillations in $2D$ homogeneous systems is well understood as a consequence of the non-analyticity of the static polarization function $\Pi(\mathbf{q},0)$, whose first order derivative is discontinuous at a wavevector $\mathbf{q}$ equal to the diameter of the Fermi surface [37]. This characteristic is responsible for the $r^{-d}$ decay of the oscillations at large distances in a $d$-dimensional space.

Here we are inspired by recent experimental investigations of the vicinal stepped Au (111) [38] surface that probed the physics of a periodic quasi-two dimensional system endowed with spin-orbit interaction to study the Friedel oscillations that can be supported in this context. To extend the applicability limit of our results, the theory
is formulated for a standard template of a periodic system, a semiconductor lateral
superlattice with SOI, essentially a 2D electron layer patterned by a periodic array of
electrostatic gates [24] that is simultaneously characterized by the redistribution in
\(\mathbf{k}\)-space of the single-particle state energies on account of the spin-orbit interaction,
and by a geometric real-space periodic confinement that introduces a mini-band en-
ergy structure. Because the characteristic parameters of this system, such as particle
density, miniband width, and periodicity, can be externally controlled, it presents
a good test case for theoretical predictions and experimental observation. Results
derived in this framework can serve then as guidance for similar problems in metallic
surfaces where the particle concentration is fixed.

In systems with SOI, several particular features of the electrostatic screening
and of the Friedel oscillations have been identified as a consequence of the modified
single-particle spectrum. Significant examples are the small-q high-temperature osc-
cillations [40] and the beatings of the Friedel oscillations predicted to appear, under
certain circumstances, in the simultaneous presence of the Rashba and Dresselhaus
interactions [41].
In this work, we analyze the principal characteristics of the Friedel oscillations in a lateral superlattice with spin-orbit interaction, a system that allows a momentum-space interplay between the mini-band distortion introduced by the spin-orbit coupling and the SL periodicity. Following the traditional approach, we evaluate the the static polarization function of the system within the random-phase-approximation (RPA) of the many-body Coulomb interaction and calculate the real-space density fluctuations as the Fourier transform of the response function. In a singly occupied, spin-split miniband approximation, the density oscillations are studied numerically as a function of several system parameters, such as the strength of the interaction, the miniband width and the lattice periodicity.

2.3 System Description

The system under consideration is obtained by subjecting a 2D electron layer to an additional attractive potential that is periodic along the \( \hat{x} \) direction. The confining potential acts on a finite region of width \( b \) and has periodicity \( a \). We will assume that \( b \ll a \), but remains finite, such that the Coulomb interaction is that of a 2D system. A suitable choice of potential and \( b \) can be made, assuring that the energy difference between the ground state level in the well and the next excited state is much larger than any of the broadening effects induced by tunneling and spin-orbit effects. In this case, we can write

\[
V(x) = -\lambda \sum_l \delta(x - la),
\]

where \( \lambda \) is a parameter describing the well. Moreover, this approximation allows one to consider that in the presence of an electric potential, density excitations that occur
within the lowest miniband are decoupled from other possible excitations and they constitute our present interest [42, 43, 44]. Tunneling occurs between the quasi-one-dimensional wires thus constructed and, as a result, the single-particle states inside the wells broaden into minibands that are spin-split by the spin-orbit interaction.

In the absence of SOI, the eigenstate of an electron of momentum \( \mathbf{k} = \{k_x, k_y\} \), spin \( \sigma \) and effective mass \( m^* \) in the lateral superlattice is built as a Bloch function from the single-particle state inside the wire \( \nu(x) \), multiplying an up or down spin state \( \chi_\sigma = \{|\uparrow\rangle, |\downarrow\rangle\} \),

\[
\psi_{k_x,k_y,\sigma} = \frac{1}{\sqrt{L_y}} e^{ik_y y} \xi_{k_x}(x) \chi_\sigma ,
\]

with

\[
\xi_{k_x}(x) = \frac{R_{k_x}}{\sqrt{N}} \sum_l e^{ik_x la} \nu(x-la) .
\]

\( k_x \) is subject to periodic boundary conditions, and is given by \( k_x = \frac{2\pi}{Na} j \), where \( j \in [-N/2, N/2] \). The normalization factor \( R_{k_x} \) differs from 1 by the overlap between states in two adjacent wells, \( \gamma = \int_{-\infty}^{\infty} dx \nu(x) \nu(x-a) \),

\[
R_{k_x} = [1 + 2\gamma \cos k_x a]^{-1/2} .
\]

With \( \Delta = 4 \int_{-b/2}^{b/2} dx \nu(x)V(x)\nu(x-a) \), the single-particle energy is written, in respect with the minimum of the band, as

\[
\epsilon_{k\sigma} = \frac{\hbar^2 k_y^2}{2m} + \frac{\Delta}{2} (1 - \cos k_x a) .
\]

When a Rasba-type interaction of coupling constant \( \alpha \) is present, \( H_R = \alpha (\sigma \times \mathbf{p}) \hat{z} \), the the spin-degenerate miniband splits. In a perturbative approach [18, 45], the
energy spectrum is determined within the tight-binding approximation by performing a diagonalization of the Rashba-interaction within the Hilbert space of the single-particle states, Eq. (2.4). The electron momenta that participate in the spin-orbit coupling are

\[
\begin{align*}
p_y &= \hbar k_y, \\
p_x &= m^* \frac{\partial \epsilon_{k_x,k_y,\sigma}}{\partial k_x} = \left( \frac{m^* a \Delta}{2\hbar} \right) \sin k_x a. \tag{2.8}
\end{align*}
\]

Two new chiral minibands corresponding to chiral quantum number \( \mu = \pm 1 \) emerge, their associated single-particle energy being

\[
E_{k,\mu} = \epsilon_k + \alpha \mu \sqrt{(\hbar k_y)^2 + \left( \frac{m^* a \Delta}{2\hbar} \right)^2 \sin^2 k_x a}. \tag{2.9}
\]

In Fig. 2.4 we display the spectrum of the single-particle chiral states in an amplified representation. The corresponding eigenstate is given by

\[
\psi_{k,\mu}(x,y) = e^{ik_y y} \xi_{k_x}(x)|\mu>_k,
\]

where the spinor \(|\mu>_k\) represents a linear combination of up and down spin states whose coefficients are momentum dependent,

\[
|\mu>_k = \frac{1}{\sqrt{2}} \left[ |\uparrow>_k + \mu e^{i\varphi_k} |\downarrow>_k \right]. \tag{2.10}
\]

The chiral angle \( \varphi_k \) is specified through its trigonometric functions,

\[
\begin{align*}
\sin \varphi_k &= \frac{p_y}{p} = \frac{\hbar k_y}{\sqrt{(\hbar k_y)^2 + \left( \frac{m^* a \Delta}{2\hbar} \right)^2 \sin^2 k_x a}}, \\
\cos \varphi_k &= \frac{p_x}{p} = \frac{m^* a \Delta}{\hbar} \frac{\sin k_x a}{\sqrt{(\hbar k_y)^2 + \left( \frac{m^* a \Delta}{2\hbar} \right)^2 \sin^2 k_x a}}, \tag{2.11}
\end{align*}
\]

where \( p = \sqrt{p_x^2 + p_y^2} \) is the magnitude of the electron momentum.
The limits of this approximation were tested in Ref. [20]. There the electron Bloch functions in the superlattice were constructed from the single-particle eigenstates of the Rashba Hamiltonian in each wire, the spin coefficients and the single-particle energies being calculated in the tight-binding approximation. The dispersion relations for the lowest-two chiral mini-bands found in this way are similar to those expressed in Eq. (2.9). Moreover, the points of chiral-spin degeneracy, at $k_x = 0, \pm \pi/a$, are preserved. Since the physical properties discussed in this chapter are obtained through an algorithm that integrates over all the energy states within the two lowest-lying mini-bands, the analytic model presented above is expected to provide an adequate qualitative and quantitative description of the problem for a large range of values of $\Delta$ and $\alpha$.

The broadening of the single energy eigenstate into a miniband on account of tunneling in the simultaneous presence of the periodic potential in Eq. (2.3) and SOI in Eq. (1.2) has been obtained by both numerical [46] and analytical methods [45, 47]. Conceptually, the difference in the two approaches is established by the balance between the magnitude of the two competing effects that determine the exact shape of the spectrum, namely the strength of the tunneling which affects the widening of the single-particle levels embodied by the miniband width $\Delta$ and the strength of SOI which couples the electron momentum to its spin. In both instances, however, the salient characteristics of the spectrum, i.e. degeneracy at $k_x = 0$ and $k_x = \pm \pi/a$, as well as the overall shape of the dispersion curves are similar as shown in Fig. 2.4 and Fig. 2.5. Based on these findings, we anticipate that the validity of our results, derived analytically within the approximation of the dominance of the band effects on the spin-orbit coupling will maintain even in strongly SOI-coupled systems when the situation can be reversed.

In the following considerations, we will assume that the two minibands of
Figure 2.4: Analytic results for the single-particle state in a 2D lateral superlattice with SOI in arbitrary units.

Figure 2.5: Band structure calculated numerically for a 2D superlattice system with no SOI (left), and SOI (right). Energy is of the order meV. [From [48]]
opposite chirality are fully occupied. This condition determines the maximum value of the \( x \)-axis momentum, \( k_{x\mu}^{\text{max}} = \pi/a \) at the edge of the Brillouin zone, the same for both chiralities. For a given total particle density \( n_0 \), and implicitly a set Fermi energy \( E_F \), the maximum value of the \( y \)-axis wavevector is determined by solutions of the equation \( E_F = E_{k_x,k_{y\mu}^{\text{max}}} \) for each value of \( k_x \). The maximum momentum along the \( y \)-axis, as function of \( k_x \), is calculated to be

\[
\hbar k_{y\mu}^{\text{max}}(k_x a) = \left\{ 2m^* \left( E_F - \Delta \sin^2 \frac{k_x a}{2} + m^* \alpha^2 \right) - \alpha \mu \left[ 2m^* \left( E_F - \Delta \sin^2 \frac{k_x a}{2} \right) + \left( \frac{m^* a \Delta}{2\hbar} \right)^2 \sin^2 k_x a a + m^* \alpha^2 \right]^{1/2} \right\}^{1/2}.
\]

(2.12)

The existence of solutions for both values of \( \mu \) when \( k_x \in [-\pi/a, \pi/a] \) requires that the Fermi energy satisfies \( E_F > \Delta [1 + \arctan(\alpha m^* a/\hbar)] \), a condition that constrains the relationship between the equilibrium particle density, \( \nu \), and the structure parameters of the superlattice, \( \Delta, a \) and \( \alpha \). At \( T = 0K \), when the particle occupation number is represented by the product of two independent Heaviside functions, \( n_{k,\mu}^0 = \theta(\pi/a - |k_x|) \theta(k_{y\mu}^{\text{max}} - |k_y|) \), the particle density is given by

\[
\nu = \sum_{k,\mu} n_{k,\mu}^0 = \frac{1}{2\pi^2} \int_0^{\pi/a} dk_x \left[ k_{y+}^{\text{max}}(k_x a) + k_{y-}^{\text{max}}(k_x a) \right],
\]

(2.13)

where the second equality is obtained by transforming the sum into an integral over the momentum-state in the usual fashion.

To illustrate the results of Eq. (2.13) we introduce the standard system for our simulations: a 2D InAs lateral superlattice (effective mass \( m^* = 0.023m_e \), with \( m_e \) the electron mass) with particle density \( \nu = 2.5 \times 10^{11}\text{cm}^{-2} \). While the particle
density remains constant, the rest of the SL characteristics, i.e. miniband width $\Delta$ and the SL constant $a$ are considered the variable parameters of the problem along with the spin-orbit coupling $\alpha$. The latter is measured in units of $10^{-11}\text{eVm}/\hbar$ that will not be declared henceforth.

In Fig. 2.6 we show the variation of the Fermi energy $E_F$ with the strength of the spin-orbit coupling $\alpha$ for a SL with miniband width $\Delta = 20\text{ meV}$ and three SL constants, $a = 30\text{ nm}$, $40\text{ nm}$ and $50\text{ nm}$. Within the limits of the analytical model used to determine the single-particle states, for a given particle density we register a weak evolution of the Fermi energy with $\alpha$, an outcome consistent with the assumption that the the spin-orbit coupling effect is secondary to the miniband formation in the system. In the following considerations, this SL description will be the template used in all our numerical simulations.

![Figure 2.6: The variation of the Fermi energy in a lateral superlattice with $\Delta = 20\text{ meV}$ as a function of the spin-orbit coupling $\alpha = 5$ for $a = 30\text{nm}$, $a = 40\text{nm}$ and $a = 50\text{nm}$.](image)

### 2.4 The Density Response Function

The linear response of the electron system to a perturbation is described in the Fourier transform space, by a simple proportionality relation that connects the
induced density fluctuations self-consistently with the effective potential experienced by the electrons. In the random-phase approximation (RPA) of the Coulomb interaction, the effective potential is the superposition between the external potential and the potential associated with the charge fluctuations themselves, leading to the well-known self-consistent equation,

\[
\Delta \nu(q, \omega) = \Pi(q, \omega) [V_{ex}(q, \omega) + \Delta \nu(q, \omega)\tilde{v}(q)] ,
\]

(2.14)

where \( \tilde{v}(q) = \frac{1}{N} \sum_l 2\pi e^2/\sqrt{(q_x + 2\pi l/a)^2 + q_y^2} \) is the Fourier transform of the Coulomb interaction in 2D that explicitly incorporates the fact that along the superlattice axis the conservation of the electron momenta in the electrostatic scattering is realized only up to an integer multiple of the reciprocal lattice vector, \( 2\pi/a \) [21].

The self-consistent density response function to an electric field within the RPA can be evaluated by following the equation-of-motion method [49, 50, 51]. In the case of a lateral superlattice, this algorithm was explicitly explained in Ref. [21], so here we will outline only the salient parts of the derivation.

The particle density fluctuations induced by a perturbation are expressed as the difference between the average of the density operator on the unperturbed ground state, denoted by \( \langle \cdots \rangle_0 \), and the equilibrium density,

\[
n(r, t) = \langle H(r, t) \rangle_0 - n^0 .
\]

(2.15)

The field operator \( \Psi(r, t) \) is a linear combination of single-particle states \( \psi_k(x, y) \) multiplying destruction (creation) operators \( c_{k, \mu}^{\dagger}(t) \),

\[
\Psi(r, t) = \sum_{k, \mu} \psi_k(x, y)c_{k, \mu}(t) .
\]

(2.16)
\[ n(q, t) = \sum_{k\mu, k'\nu} \langle k\mu | e^{-i q \cdot r} | k'\nu \rangle \langle \hat{c}_{k\mu}(t) \hat{c}_{k'\nu}(t) \rangle_0 - n^0_{q, 0} \]  

(2.17)

An electric potential \(-e\nu(r)\) generates the interaction Hamiltonian

\[ H_{int} = -e \int dr \nu(r) n(r, t) = \sum_{k\mu, k'\nu} \langle k\mu | \nu(r) | k'\nu \rangle \langle \hat{c}_{k\mu}(t) \hat{c}_{k'\nu}(t) \rangle \]  

(2.18)

which determines the time evolution of the density fluctuations through the equation of motion,

\[ i\hbar \langle \frac{\partial n}{\partial t} \rangle_0 = \langle [H, n(t)] \rangle_0 \]  

(2.19)

The result of this algorithm is expressed in terms of the frequency- and wavevector-dependent density fluctuation \(n(q, \omega)\),

\[ n(q, \omega) = \sum_{k\mu, k'\nu} \frac{n^0_{k\mu} - n^0_{k'\nu}}{E_{k\mu} - E_{k'\nu} + \hbar \omega} \langle k\mu | e^{-i q \cdot r} | k'\nu \rangle \langle \hat{c}_{k\mu}(t) \hat{c}_{k'\nu}(t) \rangle \]  

(2.20)

\(n^0_{k\mu} = \langle c_{k\mu}^\dagger c_{k\mu} \rangle_0\) represents the equilibrium occupation number for a given single-particle state \(|k, \mu\rangle\) of energy \(E_{k\mu}\). Within the RPA, the electric potential \(-e\nu(r)\) is self-consistently induced by the fluctuations:

\[ -e\nu(r) = \int dr' \frac{e^2}{|r - r'|} n(r', t) = \sum_{q_0} v(q_0) e^{i q_0 \cdot r} n(q_0, t) \]  

(2.21)

where \(v(q_0) = 2\pi e^2/\epsilon q_0\) is the Fourier transform of the Coulomb interaction in a 2D system of dielectric constant \(\epsilon\). The matrix element of the self-consistent potential

\[ < ... >_0 \] denotes the average on the unperturbed ground state. The Fourier transform of the time-dependent density fluctuation is given by

\[ n(q, t) = \sum_{k\mu, k'\nu} \langle k\mu | e^{-i q \cdot r} | k'\nu \rangle \langle \hat{c}_{k\mu}(t) \hat{c}_{k'\nu}(t) \rangle_0 - n^0_{q, 0} \]  

(2.17)
between the states labeled by \{k_\mu\} and \{k'_\nu\} is

\[
<k'_\nu| - e v(r)|k_\mu> = - \sum_{q_0} v(q_0) <k'_\nu| e^{i q_0 \cdot r} |k_\mu > > n(q_0, \omega). \tag{2.22}
\]

Eqs. (2.20), (2.21), and (2.22), provide the self-consistent equation satisfied by the particle fluctuations in the RPA,

\[
n(q, \omega) = \sum_{k_\mu; k'_\nu} \frac{n_{k_\mu}^0 - n_{k'_\nu}^0}{E_{k_\mu} - E_{k'_\nu} + \hbar \omega} < k_\mu |e^{-i q_0 \cdot r} |k'_\nu > \times \sum_{q_0} v(q_0) <k'_\nu| e^{i q_0 \cdot r} |k_\mu > > n(q_0, \omega). \tag{2.23}
\]

For a given pair of states \{k_\mu\}, \{k'_\nu\}, the simultaneous existence of the two matrix elements, \(< k_\mu |e^{-i q_0 \cdot r} |k'_\nu > > and \(< k'_\nu| e^{i q_0 \cdot r} |k_\mu > >, implies, \(q = q_0 \) \cite{51}. Hence,

\[
n(q, \omega) = \sum_{k_\mu; k'_\nu} \frac{n_{k_\mu}^0 - n_{k'_\nu}^0}{E_{k_\mu} - E_{k'_\nu} + \hbar \omega} < k_\mu |e^{-i q_0 \cdot r} |k'_\nu > >^2 v(q)n(q, \omega). \tag{2.24}
\]

The matrix element that appears in the above expression is calculated explicitly when the components of \(k = \{k_x, k_y\}\) are introduced. We obtain

\[
<k_x, k_y, \mu | e^{-i q_0 \cdot r} |k'_x, k'_y, \nu > = < k'_x | e^{-i q_0 \cdot x} |k_x > < k'_y | e^{-i q_0 \cdot y} |k_y > F_{\mu \nu}(k_x, k_y, k'_x, k'_y). \tag{2.25}
\]

The chiral form factor \(F_{\mu \nu}(k_x, k_y, k'_x, k'_y)\) is produced by the overlap of the two spinors \(|\mu >_k\) and \(|\nu >_{k'}\) in the spin space, Eq. (2.10),

\[
F_{\mu \nu}(k_x, k_y, k'_x, k'_y) = \sum_{k} < \mu | e^{ - i \phi_k + i \phi_{k'}} > = \frac{1}{2} \left[ 1 + \mu e^{-i \phi_k + i \phi_{k'}} \right]. \tag{2.26}
\]

The orthogonality of the single-particle states imposes the conservation of the mo-
mentum $k' = k + q$, which implies, $< k_y | e^{-iq_y} | k'_y > = \delta_{k'_y,k_y+q_y}$ and $< k_x | e^{-iq_x} | k'_x > = \delta_{k'_x,k_x+q_x} A(k_x,k_x+q_x)$, where $A(k_x,q_x)$ results from the overlap of the single-electron states, Eq. (2.5), along the $\hat{x}$ direction,

$$A(k_x,q_x+k_x) = R_{k_x}R_{k_x+q_x}\sum_l e^{-ik_x l a}\int_{-\infty}^{\infty} dx \nu(x) e^{-iq_x x}(x - la).$$

(2.27)

In the tight-binding approximation, $A(k_x,q_x+k_x)$ can be calculated to be

$$A(k_x,q_x) = R_{k_x}R_{k_x+q_x} \left[ \int_{-\infty}^{\infty} dx \nu(x)^2 e^{iq_x x} + 2Re \left( e^{ik_x a} \int_{-\infty}^{\infty} dx \nu(x)e^{iq_x x}\nu(x-a) \right) \right].$$

(2.28)

($Re$ denotes the real part of a complex number.)

Because of the superlattice periodicity along the $\hat{x}$ direction, the momentum transfer $q_x$ can be defined only up to a reciprocal lattice vector $2\pi s/a$ when umklapp processes are included. Therefore, if $q$ is restricted to reside in the first Brillouin zone, the self-consistent equation satisfied by the intra-band density fluctuations is obtained, with input from Eqs. (2.24), (2.25), (2.26) and (2.27) written for $q_x \rightarrow q_x + 2\pi s/a$, to be

$$n(q,\omega) \left[ 1 - \sum_{\mu\nu} \sum_{k_x,k_y} \frac{n^0_{k-q/2,\mu} - n^0_{k+q/2,\nu}}{E_{k-q/2,\mu} - E_{k+q/2,\nu} + \hbar\omega} \times |F_{\mu\nu}(k_x,k_y,q_x,q_y)|^2 \sum_s \frac{2\pi e^2 |A(k_x,q_x+2\pi s/a)|^2}{\sqrt{(q_x+2\pi s/a)^2 + q_y^2}} \right] = 0.$$  

(2.29)

This final form takes advantage of the fact that with the exception of the longitudinal
form factor $A$ and the Coulomb interaction Fourier transform, $v(q)$, all the functions are periodic in the reciprocal space and are left invariant by umklapp scattering.

The result of Eq. (2.29) is characteristic for single-miniband superlattices previously discussed in Refs. [50, 42, 43, 44]. An important simplification occurs in the weak tunneling regime, where only nearest-neighbor tunneling is considered. Then, in first order in the tunneling probability, the form factor $A(k_x, q_x)$ in Eq. (2.27) is independent of $k_x$, regardless of the exact analytic form of the single well function $\nu(x)$ [42, 43, 44]. This approximation allows the factorization of the double sum in Eq. (2.29) and enable the direct definition of the total polarization of the 2D lateral superlattice,

$$P(q_x, q_y, \omega) = \sum_{k_x \mu, k_y \nu} \frac{n_{k+q/2, \mu}^0 - n_{k+q/2, \nu}^0}{E_{k+q/2, \mu} - E_{k+q/2, \nu} + \hbar \omega} |F_{\mu \nu}(k_x, k_y, q_x, q_y)|^2,$$  

(2.30)

where, from Eq. (2.26),

$$|F_{\mu \nu}(k, q)|^2 = \frac{1}{2} \left[ 1 + \mu \nu \cos(\varphi_{k-q/2} - \varphi_{k+q/2}) \right].$$  

(2.31)

The structure of Eq. (2.30) is that of the usual real-part of the polarization function of a 2D free electron system with SOI [52], except for the different dispersion of the single-particle energies.

Numerical estimates of the static polarization function presented below are obtained for the InAs SL described above. For a given strength of the SOI coupling and for a given SL periodicity, Eq. 2.13 was used to obtain the Fermi energy and the values of the maximum $k_y$ momenta in Eq. (2.12). Moreover, we denote by $k_{Fy}$ the absolute maximum value of the electron momentum along the $y$-axis, $k_{y, \text{max}}$ and use it as a scale reference for $q_y$. In Fig. 2.7 the polarization surfaces are shown for three
different values of the SL constant \(a\) for the same value of the SOI constant \(\alpha = 5\). The polarization values are expressed in terms of the density of states at the Fermi surface, \(n_0\) calculated in the absence of SOI coupling. In general, \(n_0\) is given by

\[
n_0(\alpha) = \frac{1}{(2\pi)^2} \sum_{k,\mu} \delta(\epsilon_F - E_{k,\mu}) = \frac{1}{2\pi^2} \sum_{\mu} \int_{0}^{\pi/a} dk_x \frac{1}{|\nabla_{k_y}\mu - k_{y\mu}|}.
\]

These pictures reproduce the characteristic behavior of 2D systems with SOI, in which the polarization shows an increase in respect to the value at \(\alpha = 0\), on account of the possible transitions between states of opposite chirality. This contribution is magnified by the increase in the SL constant \(a\) which enhances the spin-orbit coupling through its effect on the \(x\)-axis momentum \(p_x\), Eq. (2.8). The static density response function is then evaluated from Eq. (2.14) as

\[
\chi(q,\omega) = \frac{\Pi(q,\omega)}{1 - \tilde{v}(q)\Pi(q,\omega)}.
\]

Using the polarization values obtained before in Fig. 2.7, the density response function is plotted in Fig. 2.8.

### 2.5 Real-Space Density Fluctuations

In the linear regime approximation, the Friedel oscillations result from the density fluctuations registered in response to a perturbing potential \(V_{ex}\). They are given by

\[
\Delta \nu(\vec{R}) = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}} \chi(\vec{q}) V_{ex}(\vec{q}) .
\]

As before, in the periodic system, the sum over \(q\) has to take into account the fact that the wave vector \(q_x\) is defined only up to a multiple of the reciprocal lattice vector,
$2\pi l/a$, where $l$ is an integer. In the following considerations we take the perturbing potential to be that of an impurity localized at the origin at the system, $V_{\text{ex}} = C\delta(r)$, whose Fourier transform is a constant $C$. With this choice the quantities involved in Eq. (2.34) are periodic with $2\pi/a$ and consequently the sum over $q_x$ can be separated into an integral over the first Brillouin zone and a sum over all its periodic iterations. With this, Eq. (2.34) becomes

$$
\Delta \nu(\mathbf{R}) = C \sum_{q_x,q_y} \chi(q_x,q_y) e^{i(q_x R_x + q_y R_y)} \left( \frac{1}{N} \sum_l e^{i2\pi l a R_x} \right). \quad (2.35)
$$

The latter sum can be evaluated exactly for a $N$-well SL,

$$
I(R_x) = \frac{1}{N} \sum_l e^{i2\pi l a R_x} = \frac{\sin \left( \frac{(N+1)\pi R_x}{a} \right)}{N \sin \frac{\pi R_x}{a}}. \quad (2.36)
$$

The function $I(R_x)$ describes an interference term of the single-particle states in the SL and reaches a maximum for integer values of the SL constant, $R_x = la$, at the location of the gates. With this, we finally write,

$$
\Delta \nu(\mathbf{R}) = \frac{C I(R_x)}{4\pi^2} \int_{-\infty}^{\infty} dq_x \int_{-\infty}^{\infty} dq_y \chi(q_x,q_y) e^{i(q_x R_x + q_y R_y)}, \quad (2.37)
$$

which is the basic equation that describes the Friedel oscillations in the SL. It is easy to see in this configuration that the overall behavior of the density fluctuations is the result of two distinct factors, the interference effects that occur on the account of the geometric periodicity and the real-space variation produced by the non-analytical points of the polarization function within the first Brillouin zone.

Using the same InAs SL template as before, Eq. (2.37) is computed numerically to illustrate the behavior of the oscillations induced by an impurity of potential $C =$
1meV/m² located at the $N = 0$ gate, considered the origin of the system.

In Fig. 2.9 we show a representative picture of the interference effect between the oscillatory pattern imposed by the SL periodicity and the density variation determined by the Fourier transform of the density response function within the first Brillouin zone. The interference effect described by Eq. (2.36) generates the fast variation of the oscillations with a period proportional to $2a/(N + 1)$. They reach significant amplitudes near the position of the gates where the interference factor approaches $(N + 1)/N$. $I(R_x)$ modulates the density oscillations that result from the Fourier transform in the first Brillouin zone amplifying the opposite-sign density oscillations that occur in the vicinity of $R_x = la$ points. Since this pattern results from the periodicity of the SL, it is reproduced identically in the presence of the spin-orbit interaction of any strength. As we show below, the spin-orbit interaction changes only the relative amplitude of the oscillations, and for this reason, in the following pictures we present only the oscillations that result from the integration of the polarization function over the momentum $q$ restricted to the first Brillouin zone.

The relative variation of the density oscillations in respect to the equilibrium values is plotted for different values of the SOI coupling strength for the same SL parameters, $\Delta = 20$ meV and $a = 30$ nm in Fig. 2.10. The amplitude of the oscillations decreases compared with the case of $\alpha = 0$, a result of the stronger coupling between the single-particle electron states mediated by the spin-orbit interaction. This outcome reproduces the behavior of a 2D homogeneous system, where the amplitude of the Friedel oscillations is known to decrease with $\alpha$ [12]. The density fluctuations are commensurate with the SL period, the zeroes in $\Delta \nu$ being realized at integer and half integer lattice constants. This is a consequence of the periodicity of the polarization function in the momentum-space with $\pi/a$. The difference in the amplitudes as a function of $\alpha$ decreases with the distance from the impurity.
In Fig. 2.11 we present the variation of the Friedel oscillations with the SL constant $a$ for the same value of the SOI coupling strength $\alpha = 5$ and miniband width $\Delta = 20$ meV. As the SL constant increases, the amplitude of the oscillations decreases indicating a stronger screening. This feature is a consequence of the $\Delta$ dependence of the $x$-axis momentum involved in the SOI coupling. As before, the periodicity of the polarization in the momentum-space localizes the nodes in the density fluctuations at integer and half-integer lattice constants uniformly.

Further, we plot the oscillations induced along the $x$-axis as a function of the SL miniband width, by comparison with the variation induced by SOI, in Fig. 2.12 for the same values of the SL constant. These results indicate a stronger effect of the spin-orbit coupling in enhancing the screening than the miniband width variation.

These general characteristics also describe the density fluctuations registered along the central $y$-axis. That spectrum, however, carries the imprint of $y$ maximum momentum being a function of $k_x$ leading to an established pattern of oscillations further from the potential. The variation $\Delta \nu$ is presented in Fig. 2.13 as a function of SOI for a same SL with $\Delta = 20$ nm and $a = 30$nm and for different SL constants at the same value of the SOI coupling, $\alpha = 5$, and $\Delta = 20$ meV in Fig. 2.14. In Fig. 2.15 we present by comparison the change in the amplitude of the oscillations for two miniband widths at two SOI coupling values.
Figure 2.7: The static polarization function in a SL with $\Delta = 20.0$ meV and $\alpha = 5$ for $a = 30$nm in (a), $a = 40$ nm in (b) and $a = 50$nm in (c).
Figure 2.8: The static density response function in a SL with $\Delta = 20.0$ meV for $\alpha = 5.0$ for $a = 30$ nm in (a), $a = 40$ nm in (b) and $a = 50$ nm in (c).
Figure 2.9: Friedel oscillations induced along the axis of a lateral SL by an impurity located at $x = 0$. The system parameters are $\Delta = 20$ meV, $a = 30$ nm and $\alpha = 5$.

Figure 2.10: Friedel oscillations induced in a lateral superlattice by an impurity located at $x = 0$ for different SOI coupling values $\alpha$. The SL parameters are $\Delta = 20$ meV and $a = 30$ nm.
Figure 2.11: Friedel oscillations induced in a lateral superlattice by an impurity located at $x = 0$ for different SL constants for the same value of the spin-orbit interaction constant, $\alpha = 5$ and $\Delta = 20$ meV.

Figure 2.12: Friedel oscillations induced along the SL axis as a function of the mini-band width for $a = 30$ nm and $\alpha = 0, 10$. 
Figure 2.13: Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of the spin-orbit coupling, for $\Delta = 20$ meV and $a = 30$ nm.

Figure 2.14: Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of the lattice constant, for $\Delta = 20$ meV and $\alpha = 5$. 

32
Figure 2.15: Friedel oscillations induced perpendicular on the SL axis at $x = 0$ as a function of different SL constants and bandwidths.
Chapter 3

Spin Instabilities in Interacting Electron Systems

A predictor of spin instabilities in an interacting electron system is the single-point accidental degeneracy realized in the single-particle energy spectra corresponding to opposite spins. Thus it is possible to lower the total energy of the system in the presence of the Coulomb interaction, by maximizing the negative exchange energy which occurs between parallel spins. Consequently, by flipping spin at the point of degeneracy, with no cost in the kinetic energy, an electron establishes exchange interactions in each region of the momentum-space with the corresponding parallel spin population. The phenomenology outlined here is the basis of the spin-density wave theory (SDW) first elaborated by Overhauser [53, 54]. Its details are presented below.

The ground state of an interacting electron system is essentially determined by its density, since the fundamental many-body interaction, the Coulomb repulsion, is dependent on the number of particles that participate. In the standard representation of the jellium model, the electron system is described by a collection of $N$ particles
inside a volume $V$ superimposed on a positive background. The electronic wave functions are normalized spinors of wave-vector $\vec{k}$ and spin function $\chi_\sigma$, where the latter is either one of the eigenstates of the $\hat{z}$ component of the spin operator $|\uparrow\rangle$ and $|\downarrow\rangle$ associated with eigenvalues $\sigma = +1$ and $\sigma = -1$ respectively, written as

$$\varphi_{\vec{k},\sigma}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \chi_\sigma.$$  \hfill (3.1)

The single non-interacting electron energy is $\epsilon_{\vec{k},\sigma} = \frac{\hbar^2 \vec{k}^2}{2m}$.

The many-body Hamiltonian of the system, is written, in the second quantization language that introduces the creation and destruction operators for the electron states, $c_{\vec{k}}^\dagger$ and $c_{\vec{k}}$, respectively, as

$$H = \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}} - \frac{1}{2} \sum_{\vec{q},\vec{k},\sigma,\vec{k}',\sigma'} v(\vec{q}) c_{-\frac{\vec{q}}{2},\sigma}^\dagger c_{\frac{\vec{q}}{2}+\frac{\vec{k}'}{2},\sigma'}^\dagger c_{\frac{\vec{k}'}{2}-\frac{\vec{q}}{2},\sigma'} c_{\vec{k}'+\vec{q},\sigma} c_{\vec{k}+\vec{q},\sigma}, \hfill (3.2)$$

where the first term is the kinetic energy of the electrons, while the second term describes the Coulomb interaction between two electrons that exchange a momentum $\vec{q}$. $v(\vec{q}) = 4\pi e^2/q^2$ is the matrix element of the Coulomb interaction between states given by Eq. (3.1).

The challenge involved in solving the quantum mechanical problem anchored by the above Hamiltonian is finding an exact solution for the interaction part. Therefore, over the past sixty years various methods of approximation have been developed, which we briefly review below.

In the simplest picture, an electron experiences just an averaged field created by all the other electrons. This statement defines the mean-field approximation or the random phase approximation (RPA), in which the full interaction potential is
replaced by a sum of single-particle terms,

\[ V_{\vec{k},\sigma} = \sum_{\vec{k},\vec{q}} v(q)c_{\vec{k} - \frac{\vec{q}}{2},\sigma}^\dagger c_{\vec{k} + \frac{\vec{q}}{2},\sigma} \sum_{\vec{k}',\sigma} <c_{\vec{k}' - \frac{\vec{q}}{2},\sigma'}^\dagger c_{\vec{k}' + \frac{\vec{q}}{2},\sigma'}^\dagger >_0 \; , \]  

(3.3)

where \(< \ldots >_0\) represents the average on the ground state of the system. The latter is itself dependent on the solution obtained for the electron motion, leading to a self-consistent set of equations. Eq. (3.3) represents the interaction between an electron and an average density of other electrons in the system defined by

\[ \Delta n(\vec{q}) = \sum_{\vec{k}} <c_{\vec{k} - \frac{\vec{q}}{2},\sigma}^\dagger c_{\vec{k} + \frac{\vec{q}}{2},\sigma}^\dagger >_0 \]  

(3.4)

The next level of approximation of the many-body interaction is to consider the Pauli exclusion principle which prohibits two electrons with the same quantum numbers, here the wave-vector \(\vec{k}\) and spin \(\sigma\), from occupying the same spatial coordinates. In this approximation, the ground state average of the four-operator product involved in the interaction part of Eq. (3.2) is replaced by a product of two averages of two operators estimated on the same ground state. Thus, by applying Wick’s theorem,

\[ <c_{\vec{k} - \frac{\vec{q}}{2},\sigma}^\dagger c_{\vec{k}' - \frac{\vec{q}}{2},\sigma'}^\dagger c_{\vec{k}' - \frac{\vec{q}}{2},\sigma'} c_{\vec{k}' + \frac{\vec{q}}{2},\sigma}^\dagger >_0 \approx <c_{\vec{k}' - \frac{\vec{q}}{2},\sigma}^\dagger c_{\vec{k}' + \frac{\vec{q}}{2},\sigma}^\dagger >_0 <c_{\vec{k}' + \frac{\vec{q}}{2},\sigma'} c_{\vec{k}' - \frac{\vec{q}}{2},\sigma'}^\dagger >_0 \]  

(3.5)

The first term on the right-hand-side of Eq. (3.5) is non-zero only for \(\vec{q} = 0\). It represents the divergent direct interaction which is fully compensated by the interaction with the positive background. The value of the second term is entirely dependent on the nature of the ground state, as yet unknown. So at this point, an \textit{apriori}
assumption is needed to be made about the ground state of the system.

In the simplest picture, two opposite-spin electrons share the same state described by the same wave-vector \( \vec{k} \). Thus, in the paramagnetic state electrons occupy states of progressively increasing energy in the 3D momentum-space, up to the maximum wave-vector \( k_F \), related to the electron density by

\[
 n = \frac{k_F^3}{3\pi^2}.
\]  

(3.6)

This is the familiar Fermi sphere description of the Fermi liquid in the 3D momentum-space. Consequently, when this happens, the only non-zero value for the average of two operators in Eq. (3.5) occurs when the two electrons have parallel spins,

\[
< c_{\vec{k}+\frac{q_2}{2},\sigma}^\dagger c_{\vec{k}+\frac{q_2}{2},\sigma'} > = < c_{\vec{k}'+\frac{q_2}{2},\sigma'}^\dagger c_{\vec{k}+\frac{q_2}{2},\sigma} > \delta_{\vec{kk}'} \delta_{\sigma\sigma'} = n_{\vec{k}+\frac{q_2}{2},\sigma}^0 \delta_{\sigma\sigma'},
\]  

(3.7)

where \( n_{\vec{k}}^0 \) is the occupation number of the state indexed by \( \vec{k} \). At low temperatures, the distribution function is a step function, \( n_{\vec{k}}^0 = \theta(k_F - k) \). Thus, the Hartree-Fock exchange potential is

\[
V_{\vec{k},\sigma} = -\sum_{\vec{q}} v(\vec{q}) n_{\vec{k}+\vec{q},\sigma}^0.
\]  

(3.8)

Eq. (3.8) allows the separation of the original Hamiltonian of the problem, Eq. (3.2) into a sum of single-particle energies given by,

\[
\tilde{\epsilon}_{\vec{k},\sigma} = \epsilon_{\vec{k},\sigma} - V_{\vec{k},\sigma}.
\]  

(3.9)

The Hartree-Fock energy per electron in the paramagnetic state is obtained by sum-
ming all the energies Eq. (3.9) in the momentum space, leading to

\[
\frac{W}{N_p} = \frac{3\hbar^2k_F^2}{10m} - \frac{3e^2k_F}{4\pi} .
\] (3.10)

From Eq. (3.9) it is also clear that, within the Hartree-Fock approximation, minimizing the total energy of the system is a competition between the kinetic energy term and the exchange potential \(V_{k\sigma}\).

An alternative configuration in the momentum-space, for the same density \(N\), is obtained by allowing only one electron in each state described by momentum \(\vec{k}\). In the ferromagnetic state, electrons occupy single-spin states inside a sphere within a radius of \(2^{1/3}k_F\). The HF energy per electron of the ferromagnetic state is

\[
\frac{W}{N_f} = \frac{2^{1/3}3\hbar^2k_F^2}{10m} - \frac{2^{1/3}3e^2k_F}{4\pi} .
\] (3.11)

Eqs. (3.10) and (3.11) indicate that the ferromagnetic state has lower energy than the paramagnetic state when

\[
k_F < \frac{5me^2}{(2^{1/3} + 1)2\pi\hbar^2} .
\] (3.12)

Consequently, a high density electron gas would be paramagnetic and a low density one would be ferromagnetic. This criterion was first derived by Bloch [55].

If in Eq. (3.5), however, one imagines that there exists such a ground state for which

\[
< c_{\vec{k}'+\vec{q},\sigma}^\dagger c_{\vec{k}+\vec{q},\sigma} > \neq 0 ,
\] (3.13)

when \(\sigma \neq \sigma'\), the outcome of the HF approximation is entirely different.

This concept was first introduced by Overhauser [53, 54], who showed that
the Hartree-Fock ground state of a Fermi gas with Coulomb interactions is not the familiar sphere of occupied momentum states, but rather a state in which there are large static spin-density waves and in which large energy gaps exist in the single-particle excitation spectrum.

The fundamental intuition behind this proof is that a degeneracy that occurs between energy levels occupied by opposite-spin electrons favors a pairing between states $|\vec{k}, \uparrow\rangle$ and $|\vec{k} + \vec{Q}, \downarrow\rangle$ that minimizes the total energy by increasing the negative exchange energy with a relatively low increase in the kinetic energy. In a SDW state the electron gas has a finite fractional polarization at each point $\vec{P}(\vec{r})$ whose direction varies continuously with the position,

$$\vec{P} = P(\hat{x} \cos Qz + \hat{y} \sin Qz).$$  \hspace{1cm} (3.14)

Here the axis of the SDW is taken to be $\hat{z}$.

In the Overhauser theory, the spin polarization of the above form leads to an off-diagonal contribution to the single-electron exchange potential, Eq. (3.13) that can be written as

$$V' = -g \begin{pmatrix} 0 & e^{-iQz} \\ e^{iQz} & 0 \end{pmatrix}.$$  \hspace{1cm} (3.15)

For this potential, the single-particle Schrödinger equation is written as

$$\left[ \frac{\vec{P}^2}{2m} + V' \right] \psi_k = E_k \psi_k.$$  \hspace{1cm} (3.16)
The energy eigenvalues are

\[ E^+_k = \frac{1}{2}(\epsilon_k + \epsilon_{k+Q}) \pm \left[ \frac{1}{4}(\epsilon_k - \epsilon_{k+Q})^2 + g^2 \right]^{1/2}, \quad (3.17) \]

where \( \epsilon_k \) is the energy of an electron of momentum \( k \) written within the Hartree-Fock approximation. The associated wave functions for the lower branch is

\[ \varphi_k = \frac{1}{\sqrt{V}} [ | \uparrow > \cos \theta e^{ik \cdot r} + | \downarrow > \sin \theta e^{i(k+Q) \cdot r} ] , \quad (3.18) \]

where

\[ \cos \theta(k) \equiv \frac{g}{\left[ g^2 + (\epsilon_k - E_k)^2 \right]^{1/2}} . \quad (3.19) \]

The wave function of the upper branch is

\[ \varphi_k = \frac{1}{\sqrt{V}} [ | \uparrow > \cos \left( \theta + \frac{\pi}{2} \right) e^{i\tilde{k} \cdot \tilde{r}} + | \downarrow > \sin \left( \theta + \frac{\pi}{2} \right) e^{i(\tilde{k}+\tilde{Q}) \cdot \tilde{r}} ] . \quad (3.20) \]

The single-particle energy spectrum is shown in the Fig. 3.1.

A more clear demonstration for the spin-density wave formation is shown in Fig. 3.2 The spin-down have been displaced by \( Q \) to the left of the spin-up branch. Only the lower branch states are occupied in a SDW ground states.
Figure 3.1: An Electron Gas With Giant Spiral Spin-Density Wave

Figure 3.2: Single-particle Energy Level Spectrum In a Spiral Spin-Density Wave.
Chapter 4

Spin Instabilities and Spin-Orbit Interactions

Since the Rashba and Dresselhaus spin-orbit interactions rotate the electron spin in a two-dimensional plane in opposite directions, early on, the state with equal (R)-(D) coupling amplitudes was flagged as having special properties such as the absence of the antilocalization term in the corrections to the conductivity [56, 57, 58, 59] or the long spin relaxation time [60].

A more recent effort resuscitated the interest in understanding the physics of this particular situation, when it reported that the SU(2) spin-rotational symmetry is recovered along with the creation of a permanent spin-helix (PSH) in real-space [61]. This phenomenology was deemed possible through the existence of a uniform displacement in the momentum-space of the opposite-spin single-particle energies, indexed by momentum $\hbar k$, by a constant wave vector $2Q = 4m^*\alpha/\hbar\hat{x}$ proportional to the common SOI coupling constant $\alpha$ ($m^*$ is the electron mass). As shown in
Figure 4.1: The single-particle spectrum of a 2D electron system with equal Rashba-Dresselhaus linear couplings. The opposite-spin energies $\varepsilon_{\uparrow}$ and $\varepsilon_{\downarrow}$ are degenerate at $k = 0$, the source of a spin instability that leads to the formation of two new quasiparticles of energies $E_-$ and $E_+$. The states that overlap at $k = 0$ are plane waves of the same momentum.

Fig. 4.1, for all momenta $k$, they satisfy

$$\varepsilon_{\uparrow}(k + 2Q) = \varepsilon_{\downarrow}(k). \quad (4.1)$$

Thus, the argument proceeds in Ref. [61], if a uniform translation of $2Q$ is applied in the momentum-space, the whole spin-up Fermi disk will be perfectly superimposed over the whole spin-down Fermi disk. This configuration, that corresponds to each state $k$ being occupied simultaneously by two electrons of opposite spin, guarantees the SU(2) spin-rotation symmetry, whereby all total-spin components $S_z = \sum_k c_{k\uparrow}^\dagger c_{k\downarrow} - c_{k+2Q\uparrow}^\dagger c_{k+2Q\downarrow}$, $S_Q^\dagger = \sum_k c_{k+2Q\uparrow}^\dagger c_{k\downarrow}$ and $S_Q = \sum_k c_{k\uparrow}^\dagger c_{k+2Q\downarrow}$ (expressed in terms of the creation and destruction operators for the electron states
involved) commute with the single-particle Hamiltonian

\[ H_0 = \sum_k \left[ \epsilon_{k,\downarrow} c_{k,\downarrow}^\dagger c_{k,\downarrow} + \epsilon_{k+2Q,\uparrow} c_{k+2Q,\uparrow}^\dagger c_{k+2Q,\uparrow} \right] . \]  

(4.2)

Based on the commutation of the spin operators with the particle density \( \rho_q = \sum_{k,\sigma} c_{k+q,\sigma}^\dagger c_{k,\sigma} \), they also commute with the single-particle potential scattering terms such as \( \sum_q V_q \rho_q \), as well as many-body interaction terms such as \( \sum_q V_q \rho_q^\dagger \rho_{-q} \), implying that the SU(2) symmetry is robust against these perturbations.

Simultaneously, as a consequence of the translation in the momentum-space, the spin-up eigenstates acquire an additional phase \( e^{2iQ \cdot r} \), which, when carried over in the matrix elements of \( S_Q, S_Q^\dagger, S_z \) generates a spin polarization whose components are proportional to \( \sin 2Q \cdot r \) and \( \cos 2Q \cdot r \) leading to the creation of a spin-helix in real-space.

Ulterior experimental evidence seemed to support this conclusion by testing several characteristic features of this state, such as the existence of very long spin relaxation rates [62, 63].

The beautiful math aside, one has to wonder about the physical reason that would make, in reality, all the electrons in the spin-up Fermi disk decide to transform their wave functions simultaneously, such as to accommodate our imagined translation. Historical precedent developed for the first time in the spin density wave (SDW) theory [53, 54] demonstrates that such collective behavior will be justified only if a lower total energy of the system is obtained in the new configuration, whereas in this problem the energy remains constant, including potential interactions that are left invariant by the momentum translation.

Further, as a totally degenerate Fermi liquid is created through the superposition of the two Fermi disks, the existence of non-zero matrix elements of \( S_Q^\dagger \) and \( S_Q \)
in this paramagnetic state, required to generate the spin-helix, imply that spin-flips occur at the same location in the momentum-space. This incurs a great cost in kinetic energy, since on account of the Pauli principle two same-spin particles cannot occupy the same momentum state and consequently the whole Fermi surface has to expand. Only in the presence of the Coulomb interaction, that mediates the negative exchange energy also enhanced by the parallel spin alignment, the conditions underlying a possible paramagnetic to ferromagnetic transition can be determined. Even in the ferromagnetic case, the system would not support a helical spin distribution periodic in real-space, as the matrix elements of the off-diagonal spin operators $S_Q^\dagger$ and $S_Q$ are zero. Since the ferromagnetic alignment has usually a higher energy, a normal Fermi liquid system, like the one analyzed here, has a paramagnetic ground state, a conclusion supported by the fact that the $2Q$ translation leaves the Hamiltonian invariant. We also note that in the limit $Q = 0$ which describes the usual paramagnetic Fermi liquid, the same arguments as those in Ref. [61] hold, leading to the un-physical result of a non-zero off-diagonal spin polarization.

Based on these general considerations, one has to conclude therefore that neither the SU(2) spin-symmetry nor the associated helical spin state are realized by translating the up-spin disk in the momentum-space (or for that matter, by any translation that overlaps the two disks), on account of producing a higher total-energy state than that of the initial paramagnetic configuration.

Here we propose a different analysis of the problem that considers the degeneracy of the opposite-spin single-particle states at $k = 0$, $\varepsilon_\uparrow(0) = \varepsilon_\downarrow(0)$, as seen in Fig. 4.1. Extensive theoretical and experimental literature developed within the context of interacting Fermi liquids discussed many instances in which, in the presence of the Coulomb interaction, opposite-spin degeneracies in the single-particle spectrum signaled a magnetic phase transition from the usual paramagnetic many-body state to
a lower total energy configuration characterized by a particular spin arrangement [64]. This phenomenology can be simply understood by recognizing that the no-kinetic energy spin-flip enabled by the degeneracy decreases the total exchange energy as it allows a given spin electron to interact with both spin-segregated populations in the corresponding regions of the momentum-space. In the many-body system, the process is optimized by allowing for the continuous rotation of the electron spin in the momentum-space, the original idea behind the spin-density wave formation first proposed by Overhauser in Refs. [53, 54] as an even lower total energy alternative to the paramagnetic alignment.

Later, spin instabilities were extensively investigated, in both theoretical and experimental works, in two-dimensional semiconductor heterostructures subjected to a tilted magnetic field in the quantum Hall regime. Such driven magnetic phases were studied both theoretically and observed experimentally in single quantum wells [65, 66], double layers [67, 68, 69], and in multilayers [70, 71, 72]. Depending on the nature of the single-particle states involved in the creation of the spin-degeneracy, the resulting magnetic phases were found to be either spiral spin density waves (SDW) [71, 72] or canted antiferromagnetic [67, 68].

In the present case the opposite-spin single-particle spectra are naturally separated in the momentum-space by $2Q$, proportional to the strength of the spin-orbit coupling. Therefore, we follow the traditional approach described in the spin-instability literature [64] to explore the existence of a low-temperature magnetic long-range order induced by the degeneracy in the single-particle states shown in Fig. 4.1. To this end we use the Hartree-Fock approximation of the Coulomb interaction, an adequate standard in the spin-instability theory [64, 53, 54, 65, 67, 68, 70, 71, 72] as well as in determining the ground state properties of electron systems with Rashba interaction [73], to calculate the modified single-particle states and derive the self-
consistent condition that describes the long range magnetic order, embodied by a non-zero gap function.

Our analysis is completed by numerical results performed for realistic samples currently used in experiments that probe the equal Rashba-Dresselhaus coupling regime. They show that at low temperatures the ground state of the system is described by an itinerant antiferromagnetic (IAF) order that is replaced by the usual paramagnetic configuration above a critical temperature. Moreover, in the IAF state, the spin-polarization is found to be aligned along the direction of the displacement vector $Q$.

4.1 The Single-Particle Spectrum

The basic physical system for our calculation is a $2D$ electron system in a semiconductor quantum well with Rashba-Dresselhaus spin-orbit of strengths $\alpha$ and $\beta$, respectively, placed in the $\hat{x} - \hat{z}$ plane. Throughout this calculation we neglect the cubic Dresselhaus term, known to produce only a small perturbation to the $\alpha = \beta$ phenomenology \cite{59, 74}. A positive background is understood to assure charge neutrality. The single-particle Hamiltonian of an electron of wave-vector $k = \{k_x, k_z\}$ and spin $\sigma = \{\sigma_x, \sigma_y, \sigma_z\}$ is given by

$$H_1 = \frac{\hbar^2 k^2}{2m^*} + \hbar \alpha (\sigma_z k_x - \sigma_x k_z) + \hbar \beta (\sigma_z k_z - \sigma_x k_x).$$ \hspace{1cm} (4.3)

A real-space rotation (clock-wise about $\hat{y}$) in the $x - z$ plane is used to introduce the new momentum coordinates $k'_x = (k_x + k_z)/\sqrt{2}$ and $k'_z = (k_z - k_x)/\sqrt{2}$ and the new spin projections, $\sigma'_x = (\sigma_x + \sigma_z)/\sqrt{2}$ and $\sigma'_z = (\sigma_z - \sigma_x)/\sqrt{2}$. In this frame, the
expression of the Hamiltonian becomes

\[ H_1 = \frac{\hbar^2 (k'_x)^2}{2m^*} + \frac{\hbar^2 (k'_z)^2}{2m^*} + (\alpha + \beta)\sigma'_z p'_x - (\alpha - \beta)\sigma'_x p'_z. \] (4.4)

When \( \alpha = \pm \beta \), one of the two spin-orbit terms cancels and the Hamiltonian commutes with the remaining component of the spin operator. For simplicity, we select \( \alpha = \beta \), drop the prime indices, and rewrite the Hamiltonian in a simplified form,

\[ H_1 = \frac{\hbar^2}{2m^*} (k_x - Q_x \sigma_z)^2 + \frac{\hbar^2 k_z^2}{2m^*} - \frac{\hbar^2 Q_x^2}{2m^*}, \] (4.5)

where \( Q = (2m^* \alpha/\hbar, 0) \) is a displacement vector in the momentum-space parallel to the \( \hat{x} \)-axis. Henceforth we will refer to Eq. (4.5) as the fundamental single-particle Hamiltonian of the problem.

For a sample of unit area, the spin-dependent eigenstates of Eq. (4.5) are plane waves,

\[ \psi_{k,\sigma}(r) = e^{i k \cdot r} |\sigma\rangle, \] (4.6)

of energy eigenvalues, written in respect with the constant \( -\hbar^2 Q^2/2m^* \), as

\[ \varepsilon_{k,\sigma} = \frac{\hbar^2 (k_x - \sigma Q)^2}{2m^*} + \frac{\hbar^2 k_z^2}{2m^*}, \] (4.7)

where \( \sigma \) is 1 for \( |\uparrow\rangle \) and \(-1\) for \( |\downarrow\rangle \).

The energies shown above in Eq. (4.7) satisfy two important relations. First, a translation by \( 2Q \) in the momentum-space leads to \( \varepsilon_{\uparrow}(k + 2Q) = \varepsilon_{\downarrow}(k) \), a situation that replicates the totally spin-degenerate spectrum of a normal Fermi liquid. As detailed in the introduction, this equation underlies the theory presented in Ref. [61].

In this chapter we focus on the second important property of the single-particle
energies, Eq. (4.7), the degeneracy that occurs only at \( k = 0 \), where the kinetic energies of two opposite-spin states become equal. This situation is completely similar with the underlying physics of the spin density wave theory (SDW) where a single point degeneracy of the particle spectrum was found to lead, in the presence of the Coulomb interaction, to a long range magnetic order with a lower energy than that of the paramagnetic state. Since in the SDW calculation, the single-particle degeneracy is created by artificially displacing the opposite-spin electron spectra by \( 2k_F \) in the momentum-space, the result was a periodically modulated magnetization in real-space. In this instance, however, the plane waves that are involved in the degeneracy are both of momentum \( k \), so no real-space dependence should result. We also remark that here the spin-orbit interaction, intrinsic to the system, plays the role of the external magnetic field in the study of spin instabilities in quantum Hall heterostructures [65].

It is important to note that the existence of a spin degeneracy in the single-particle kinetic energy spectrum is not by itself sufficient to predict the formation of a long-range many-body coherent state, but rather only an indicator that such a state might exist. A many-body calculation that includes the Coulomb interaction is necessary.

4.2 The Many-Body Interaction

We consider therefore the many-body Hamiltonian of the system written in terms of the single-particle eigenstates identified in Eq. (4.6) represented by the creation and destruction operators \( c_{k,\sigma}^\dagger, c_{k,\sigma} \). The equilibrium many-body Hamiltonian
is composed of a kinetic energy part and the usual Coulomb repulsion, written as

\[ H = \sum_{k,\sigma} \varepsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{1}{2} \sum_{\substack{k,q,k',\sigma,\sigma'}} v(q) c_{k+q,\sigma}^\dagger c_{k',\sigma'}^\dagger c_{k',\sigma+q,\sigma'} c_{k,\sigma} , \]  

(4.8)

where \( v(q) = \frac{2\pi e^2}{\kappa q} \) is the Coulomb interaction matrix element in two dimensions for an environment of static dielectric constant \( \kappa \). The ground state energy of the system is obtained by averaging the total Hamiltonian on the ground state wave function, a process that involves certain approximations of the interaction terms. In Hartree-Fock, the ground-state average of the product of four operators is factorized into a product of two two-particle operators [64]. For now, no assumption is made on the nature of the ground state. Thus, with \( < \ldots, \ldots > \) representing the ground state average, the interaction becomes

\[ \langle H_{\text{int}} \rangle = \frac{1}{2} \sum_{k,q,\sigma,\sigma'} v(q) \left[ \langle c_{k+q,\sigma}^\dagger c_{k,\sigma} \rangle \langle c_{k',\sigma'}^\dagger c_{k'+q,\sigma'} \rangle - \langle c_{k+q,\sigma}^\dagger c_{k,\sigma} \rangle \langle c_{k',\sigma'}^\dagger c_{k,\sigma} \rangle \right] . \] 

(4.9)

In the first term of Eq. (4.9) one recognizes the direct interaction,

\[ \langle c_{k+q,\sigma}^\dagger c_{k,\sigma} \rangle \langle c_{k',\sigma'}^\dagger c_{k'+q,\sigma'} \rangle = n_{k,\sigma}^0 n_{k+q,\sigma'}^0 \delta_{q,0} , \] which is canceled out by the positive background \( (n_{k,\sigma}^0 \) is the ground state occupation number of the single-particle state). The second term represents the exchange interaction. Since in this formalism, the ground state averages are evaluated on a state that in itself is not known, a priori assumptions on the magnetic ordering of the ground state need to be made. A ground state that assumes only a parallel spin alignment, be it paramagnetic or ferromagnetic, will generate non-zero averages in \( \langle c_{k',\sigma'}^\dagger c_{k,\sigma} \rangle \) only for \( \sigma = \sigma' \), at \( k = k' \), which is the usual exchange in Fermi systems with paramagnetic or ferromagnetic configurations. If it is hypothesized, however, that the ground state is based on a non-parallel spin
alignment, then by default, one needs to assume that \( \langle c_{k,\sigma}^\dagger c_{k',\sigma'} \rangle \neq 0 \) even for \( \sigma \neq \sigma' \) at \( k' = k \). This is the fundamental paradigm of the SDW formation in simple metals [53], an assumption also pursued here, such that we write

\[
\langle H_{int} \rangle = -\frac{1}{2} \sum_{k,q,\sigma} v(q) \langle c_{k+q,\sigma}^\dagger c_{k,\sigma} \rangle \langle c_{k,\sigma}^\dagger c_{k,\sigma} \rangle - \frac{1}{2} \sum_{k,q} v(q) \langle c_{k+q,\sigma}^\dagger c_{k+q,\bar{\sigma}} \rangle \langle c_{k,\bar{\sigma}}^\dagger c_{k,\sigma} \rangle ,
\]

(4.10)

where \( \bar{\sigma} \) is the opposite of \( \sigma \). As we show below, the second term in Eq. (4.10) is responsible for the antiferromagnetic coupling of the electron spins.

The total Hartree-Fock Hamiltonian of the system is then linearized by means of a canonical Bogoliubov-Valatin (BV) transformation [64]. This introduces two new fermionic operators \( u_k \) and \( v_k \),

\[
u_k = \cos \theta_k c_{k,\uparrow} + \sin \theta_k c_{k,\downarrow} ,
\]

\[v_k = -\sin \theta_k c_{k,\uparrow} + \cos \theta_k c_{k,\downarrow} , \quad (4.11)\]

which are continuous functions of the spin inclination angle \( \theta_k \), the variational parameter of the transformation. In this form, it is transparent that \( u_k \) and \( v_k \) describe electron states whose spin composition varies continuously throughout the momentum-space. The electron operators that enter these expressions, \( c_{k,\sigma} \) have to be those of the opposite-spin states that are involved in the accidental spin degeneracy, i.e., the spin rotation is allowed only if there is no kinetic energy cost. In real-space, the state functions associated with \( u_k \) and \( v_k \) are written as linear superpositions of the single-particle eigenstates at the point of degeneracy, Eq. (4.6),

\[
\Psi_{k-} = (\cos \theta_k | \uparrow \rangle + \sin \theta_k | \downarrow \rangle) e^{ikr} ,
\]

\[
\Psi_{k+} = (-\sin \theta_k | \uparrow \rangle + \cos \theta_k | \downarrow \rangle) e^{ikr} . \quad (4.12)
\]
The spin polarization associated with the single-particle states in Eq. (4.12) is given by

$$ p_{\pm} = \hat{x} \langle \Psi_{k,\pm}^{} | \sigma_x | \Psi_{k,\pm}^{} \rangle + \hat{z} \langle \Psi_{k,\pm}^{} | \sigma_z | \Psi_{k,\pm}^{} \rangle $$

$$ = \pm \hat{x} \sin 2 \theta_k^{} \pm \hat{z} \cos 2 \theta_k^{} , $$

(4.13)

an expression that does not have any real-space dependence.

The substitution of the electron operators by the Eqs. (4.11) leads to an expression for the ground state energy that depends on averages of the newly introduced operators, $u_k$ and $v_k$. There are four types of terms that appear. Two represent the same-particle averages, $\langle u_k^{\dagger} u_k \rangle$ and $\langle v_k^{\dagger} v_k \rangle$, and two mixed-ones, $\langle u_k^{\dagger} v_k \rangle$ and $\langle v_k^{\dagger} u_k \rangle$. The first category can be easily associated with the occupation numbers of two new quasiparticles, while the second describes the excitation processes of these quasiparticles, neglected in a ground state calculation. Thus, by the means of the BV transformation, the system of interacting electrons is transformed into a system of non-interacting quasiparticles.

As a function of the quasiparticle occupation numbers, $f_{k,-} = \langle u_k^{\dagger} u_k \rangle$ and $f_{k,+} = \langle v_k^{\dagger} v_k \rangle$, the ground state energy becomes

$$ \langle H \rangle_{HF} = \sum_k \tilde{\epsilon}_{k,\downarrow} (\cos^2 \theta_k^{} f_{k,+}^{} + \sin^2 \theta_k^{} f_{k,-}^{}) + \sum_k \tilde{\epsilon}_{k,\uparrow} (\sin^2 \theta_k^{} f_{k,+}^{} + \cos^2 \theta_k^{} f_{k,-}^{}) $$

$$ - \frac{1}{4} \sum_{k,k'} v(k' - k) \sin 2 \theta_k^{} \sin 2 \theta_{k'}^{} (f_{k,+}^{} - f_{k,-}^{})(f_{k',+}^{} - f_{k',-}^{}), $$

(4.14)

where we introduced $q = k' - k$ and the single-particle energies in the HF approxi-
mation,
\[ \tilde{\varepsilon}_{k,\downarrow} = \varepsilon_{k,\downarrow} - \sum_{k'} v(k' - k) \left( \cos^2 \theta_{k'} f_{k',+,} + \sin^2 \theta_{k'} f_{k',-,} \right), \tag{4.15} \]
and
\[ \tilde{\varepsilon}_{k,\uparrow} = \varepsilon_{k,\uparrow} - \sum_{k'} v(k' - k) \left( \sin^2 \theta_{k'} f_{k',+,} + \cos^2 \theta_{k'} f_{k',-,} \right). \tag{4.16} \]

We note that the canonical transformation, Eq. (4.11) preserves the total number of particles since
\[ N = \sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} = \sum_{k,i=\pm} f_{k,i}. \tag{4.17} \]

At finite temperature \( T \), a fermionic entropy term can be added to the ground state energy,
\[ S = -k_B \sum_{k,i=\pm} \left[ f_{k,i} \ln f_{k,i} + (1 - f_{k,i}) \ln(1 - f_{k,i}) \right]. \tag{4.18} \]

By minimizing the grand canonical thermodynamic function, written for a chemical potential \( \mu \),
\[ \Omega(T, V, \mu) = \langle H \rangle_{HF} - \varepsilon N - TS, \tag{4.19} \]
in respect with \( \theta_k \) and the two quasiparticle occupation numbers \( f_{k,+} \) and \( f_{k,-} \), a set of three coupled self-consistent equations are obtained. First, by minimizing in respect with \( \theta_k \) one obtains the gap equation,
\[ \tan (2\theta_k) = \frac{g_k}{\tilde{\varepsilon}_{k,\downarrow} - \tilde{\varepsilon}_{k,\uparrow}}, \tag{4.20} \]
where the antiferromagnetic gap is
\[ g_k = \sum_{k'} v(k' - k) \sin 2\theta_{k'} (f_{k',+} - f_{k',-}). \tag{4.21} \]
Eq. (4.20) is a non-local, self-consistent expression, since the solution is dependent on the values of the inclination angle throughout the Brillouin zone. By minimizing $\Omega(T, A, \mu)$ in respect with the two occupation numbers, the single quasiparticle energies are obtained as

$$E_{k \pm} = \frac{1}{2} \left[ \tilde{\varepsilon}_{k,\downarrow} + \tilde{\varepsilon}_{k,\uparrow} \pm \sqrt{ (\tilde{\varepsilon}_{k,\downarrow} - \tilde{\varepsilon}_{k,\uparrow})^2 + g_k^2 } \right], \quad (4.22)$$

while the occupation numbers are $f_{k, \pm} = \left[ e^{(E_{k \pm} - \xi)/k_B T} + 1 \right]^{-1}$. As depicted by dashed lines in Fig. 4.1, $E_+$ and $E_-$ are separated at $k_x = 0$ by $g_k$, the antiferromagnetic gap.

One can combine Eqs. (4.20) and (4.21) in a single expression, known as the “gap equation”,

$$g_k = \sum_{k'} g_{k'} \frac{v(k - k')(f_{k',-} - f_{k',+})}{\sqrt{(\tilde{\varepsilon}_{k',\downarrow} - \tilde{\varepsilon}_{k',\uparrow})^2 + g_{k'}^2}}, \quad (4.23)$$

whose trivial solution $g_k = 0$ is immediate. Equivalently, $\tan 2\theta_k = 0$, a situation that corresponds either to a paramagnetic order at $\theta_k = 0$ or ferromagnetic at $\theta_k = \pi/2$.

Iterative solutions to Eq. (4.23) are discussed below for realistic structures.

At $T = 0$K, when it can be assumed that only the lowest quasiparticle level is occupied, i.e. $f_{k,-} = 1$ and $f_{k,+} = 0$, the stability condition for the antiferromagnetic phase is $\partial^2 < H >_{HF} / \partial \theta_{k_x}^2 < 0$, which is always realized when a solution to the gap equation is found, since

$$\frac{\partial^2 < H >_{HF}}{\partial \theta_{k_x}^2} = -\sqrt{(\tilde{\varepsilon}_{k,\downarrow} - \tilde{\varepsilon}_{k,\uparrow})^2 + g_k^2}. \quad (4.24)$$

Under the same circumstances, an easy analytical solution of Eq. (4.23) is obtained if one assumes a constant Coulomb interaction $2\pi e^2/|k - k'| = \gamma$, such that the right-hand side does not depend on $k_x$ anymore and the gap is a constant.
Following Ref. [54], the integration domain can be chosen to be a rectangle in \( \mathbf{k} \) centered at 0, of lengths \( L_x \) and \( L_z \), that incorporate the states that are likely to be distorted by the gap formation in Fig. 4.1. Then, the gap equation can be integrated directly and the gap is obtained as

\[
g = \frac{L_x \hbar^2 Q}{m^* \sinh \left( \frac{4\hbar^2 Q^2 \pi^2}{m^* \gamma L_y} \right)},
\]

(4.25)
a result which indicates the a non-zero \( g \) is conditioned by the existence of a finite \( Q \), as well as the non-perturbative nature of this effect in terms of the inclusion of the Coulomb interaction, since \( g \sim e^{-C/\gamma} \).

Finally, the spin-polarization in the system is obtained to be, from Eqs. (4.12),

\[
P = \hat{x} \sum_k \sin 2\theta_k (f_{k-} - f_{k+}) + \hat{z} \sum_k \cos 2\theta_k (f_{k-} - f_{k+}),
\]

(4.26)
a result that shows that the polarization maintains a constant direction in space. Further, since from Eq. (4.20) we obtain

\[
\sin 2\theta_k = \frac{g_k}{\sqrt{(\varepsilon_{k\downarrow} - \varepsilon_{k\uparrow})^2 + g_k^2}},
\]

\[
\cos 2\theta_k = \frac{(\varepsilon_{k\downarrow} - \varepsilon_{k\uparrow})}{\sqrt{(\varepsilon_{k\downarrow} - \varepsilon_{k\uparrow})^2 + g_k^2}}.
\]

(4.27)
The \( \hat{z} \) component of polarization is zero, on account of the oddness in \( \mathbf{k} \)-space of \( \cos 2\theta_k \). Consequently the direction of the polarization is parallel to that of the displacement vector \( \mathbf{Q} \).

We present numerical results of the gap equation for a GaAs (effective mass \( m^* = 0.067 \), dielectric constant \( \kappa = 13 \)) quantum well of electron density \( n = 4 \times 10^{15} \text{m}^{-2} \). The \( \alpha = \beta \) state was identified from the antilocalization peak of the
quantum corrections to the conductivity in the weak scattering regime and found to correspond to a value $\alpha = 9 \times 10^2$ m/s $[75]$. For the given particle concentration, we define the Fermi momentum of the isotropic system (in the absence of SOI), $k_F = \sqrt{2\pi n} = 1.58 \times 10^8$ m$^{-1}$ which henceforth will be used as a unit in the momentum-space. Correspondingly, the energy scale of the problem is set by the single-particle Fermi energy, $E_F = \hbar^2 k_F^2 / 2m^* = 12.88$ meV. For these parameters, $Q = 2m^*\alpha / \hbar = 2\alpha / v_F = 7.2 \times 10^{-3} k_F$.

We plot the solutions obtained in an iterative calculation of the gap equation in the usual approximation that considers in the kernel of Eq. (4.23) the single-particle states in the absence of the Hartree-Fock corrections, i.e. $\tilde{\epsilon}_k = \epsilon_k$ $[64]$. To provide a qualitative description of the additional screening that can appear in the system on account of short range Coulomb interaction effects beyond the Hartree-Fock approximation, our computation is performed with a Yukawa potential Fourier of variable screening constant $\mu$ (expressed throughout in $k_F$ units), such that $v(q) = 2\pi e^2 / \kappa \sqrt{q^2 + \mu^2}$. At each temperature, Eq. (4.17) is used to determine the Fermi level $\mathcal{E}$.

Since the gap at the center of the Fermi surface corresponds to the energy difference between the two quasiparticles, $g(0,0)$ is a de facto order parameter of the itinerant antiferromagnetic state and its temperature dependence suffices to describe the phase transition. The variation of $g(0,0)$ with temperature, calculated from Eq. (4.23), is shown in Fig. 4.2 for two different values of the screening constants, $\mu_1 = 10^{-3}$ and $\mu_2 = 10^{-2}$, chosen to be of the same order of magnitude with the displacement $Q$ and ten times higher. The temperature scale is expressed in units of the Fermi energy. The illustration shows a typical variation of an order parameter that presents a finite value at very low temperature, essentially $T = 0$K, reaches a maximum, and eventually becomes zero at a critical, higher temperature. As it is
well known [64], screening plays an important role in suppressing itinerant magnetic effects, a fact confirmed here where the maximum value of the gap function, as well as the critical temperature of the transition to the paramagnetic phase are lower at stronger screening, $T_c(\mu_1) = 90$ K and $T_c(\mu_2) = 29$K. The maximum gap is reached at $T_{\text{max}}(\mu_1) = 13.4$ K and $T_{\text{max}}(\mu_2) = 5.97$K, respectively.

The complete evolution of the gap function is presented for three different temperatures in Fig. 4.2 for the two different screening constants. The side by side comparison is realized for $\mu_1 = 10^{-3}$ and $\mu_2 = 10^{-2}$. The temperatures at which the heat-maps are plotted correspond to the $T = 0$K, $T = T_{\text{max}}$ and $T = T_c$ as given by
the plot of $g(0,0)$ in Fig. 4.2. This illustration shows the existence of a gap at the origin in the momentum-space which extends toward the edges as a measure of the difference between the single-quasiparticle energies, $E_+ - E_-$. A similar behavior is registered by the angle $\theta(k_x, k_z)$ that describes the angle between the electron spins defining the variable spin-polarization of the quasiparticles. While below the critical temperature the coupling angle has a quasi-uniform distribution, at $T_c$ its value drops sharply indicating a paramagnetic $\theta_k \rightarrow 0$ arrangement of the spins.

Another measure of the magnetic order can be provided by the fractional polarization, calculated from Eq. (4.13) and (4.17) as $p = P_x/N$. Its temperature variation is presented in Fig. 4.5 for the same screening constants previously employed. Although $p$ represents a collective property of the system its temperature variation is similar to that of $g(0,0)$, a result of the self-consistency of the calculation. At maximum, the fractional polarization reaches 18% for $\mu_1 = 10^{-3}$ and 12% for $\mu_2 = 10^{-2}$. 

58
\[ \mu = 10^{-3} \quad \mu = 10^{-2} \]

Figure 4.3: (color online) The variation of the gap function vs temperature for two different screening constants. For \( \mu_1 = 10^{-3} \) (left panel) the temperatures are \( T = 0, \) \( T_{\text{max}} = 13.4 \text{K}, \) and \( T_c = 90 \text{K}, \) while for \( \mu_2 = 10^{-2} \) (right panel) the temperatures are \( T = 0, \) \( T_{\text{max}} = 5.97 \text{K}, \) and \( T_c = 29 \text{K}, \) respectively.
\[ \mu = 10^{-3} k_F \quad \text{and} \quad \mu = 10^{-2} k_F \]

Figure 4.4: (color online) The variation of the coupling angle vs temperature for two different screening constants. For \( \mu_1 = 10^{-3} \) (left panel) the temperatures are \( T = 0, \quad T_{\text{max}} = 13.4 \text{K}, \) and \( T_c = 90 \text{K}, \) while for \( \mu_2 = 10^{-2} \) (right panel) the temperatures are \( T = 0, \quad T_{\text{max}} = 5.97 \text{K}, \) and \( T_c = 29 \text{K}, \) respectively.
Figure 4.5: The fractional spin polarization along the $\hat{x}$ direction as a function of temperature for two different screening constants.
Chapter 5

Thermoelectric Transport at Equal Rashba and Dresselhaus Coupling Strengths

5.1 Thermoelectric Effects

In the presence of an electric field and a temperature gradient, solid structures generate response functions that reflect the mutual interdependence of these perturbations. The phenomenological description of these response functions was done as early as the end of the 19th century. The Seebeck effect describes the appearance of an electric field in a circuit made of two different metals (denoted by $a$ and $b$), whose junctions are kept at different temperatures. The proportionality constant between the electric field and the temperature gradient is called the Seebeck coefficient or thermopower,

$$\vec{E} = S_{ab} \nabla T.$$  (5.1)
In a phenomenological description, the linear response functions for the charge and heat currents can be written as

\[ \vec{j}_e = \hat{L}_{11} \vec{E} + \hat{L}_{12} \left( -\frac{\nabla T}{T} \right); \quad (5.2) \]

\[ \vec{j}_Q = \hat{L}_{21} \vec{E} + \hat{L}_{22} \left( -\frac{\nabla T}{T} \right), \quad (5.3) \]

where by applying the Onsager symmetry relations, \( L_{12} = L_{21} \). If in the first equation we set \( \nabla T = 0 \) (no thermal gradient applied), \( L_{11} \) becomes the electrical conductivity. When \( \vec{j}_e = 0 \), the first equation generates the relation between the temperature gradient and the induced electric field,

\[ \vec{E} = \frac{L_{12}}{L_{11}} \frac{\nabla T}{T}; \quad (5.4) \]

The Seebeck coefficient is defined therefore as

\[ S = \frac{L_{12}}{L_{11} T}. \quad (5.5) \]

The microscopic origin of the phenomenological coefficients \( L_{ij} \) is clarified by the Boltzmann transport theory.

5.2 Boltzmann Transport Equation

The simplest, but qualitatively and quantitatively accurate, picture of thermo-electric transport is obtained within the semi-classical framework of the Boltzmann transport equation applied to a system of free fermions. For a system of \( n \) electrons per unit volume, superimposed on a positive background to assure charge neutrality, the single-particle states, indexed by momentum \( \mathbf{k} \) and spin \( \sigma \), are described in
equilibrium at temperature $T$ by the Fermi distribution function

$$f_k^0 = \frac{1}{e^{\frac{\epsilon_k - \mu}{k_B T}} + 1}. \quad (5.6)$$

The Boltzmann transport equation results from a semi-classical approximation that allows the treatment of electrons as classical objects moving in phase-space under the action of classical perturbations, such as forces and temperature gradients, whose momentum and position are simultaneously determined. At the same time, however, the state and energy of the electrons are calculated quantum mechanically.

When a perturbation is applied, the distribution function becomes a function of position, momentum and time, $f = f(\vec{r}, \vec{k}, t)$. The Boltzmann transport equation represents the conservation of the number of particles in a volume of phase-space:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} \bigg|_{coll}, \quad (5.7)$$

by expressing the fact that the total change of the distribution function results only from scattering events that take the particles outside the considered volume.

The left-hand side of this equation is obtained by expanding the total derivative of $f$ with respect to time, generating the drift terms:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \frac{\partial f}{\partial t} + \dot{\vec{k}} \nabla_{\vec{k}} f + \dot{\vec{r}} \nabla_{\vec{r}} f. \quad (5.8)$$

We identify $\dot{\vec{r}} = \vec{v}_k$ as the electron velocity, while $\dot{\vec{k}} = \frac{\vec{F}}{\hbar}$ expresses the second law of dynamics, whereby the time variation of the momentum is equal to the applied force, $\vec{F}$. The explicit time dependence, $\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t}$, is equal to zero in the stationary case. For
weak perturbations, the linear approximation applies to the drift terms,

\[ \nabla_{\vec{r}} f(\vec{r}, \vec{k}, t) \approx \nabla_{\vec{r}} f^0 \approx \nabla_{\vec{r}} f^0(\vec{r}, \vec{k}, t) = \frac{\partial f^0}{\partial T} \nabla T + \frac{\partial f^0}{\partial \mu} \nabla \mu ; \quad (5.9) \]

rewritten as,

\[ \nabla_{\vec{r}} f(\vec{r}, \vec{k}, t) = \left( -\frac{df^0}{d\epsilon_k} \right) \left( \nabla \mu + \frac{\epsilon_k - \mu}{T} \nabla T \right) ; \quad (5.10) \]

and,

\[ \nabla_{\vec{k}} f(\vec{r}, \vec{k}, t) \approx \nabla_{\vec{k}} f_k^0 = \nabla_{\vec{k}} \epsilon_k \frac{df^0}{d\epsilon_k} = \hbar \vec{v}_k \frac{df^0}{d\epsilon_k} , \quad (5.11) \]

where we recognized that the drift velocity \( \vec{v}_k = \frac{1}{\hbar} \nabla_{\vec{k}} \epsilon_k \).

From Eqs. (5.10) and (5.11) we obtain:

\[ \frac{df}{dt} = \left( -\frac{df^0}{d\epsilon_k} \right) \left( e\tilde{E} + \nabla \mu + \frac{\epsilon_k - \mu}{T} \nabla T \right) . \quad (5.12) \]

In the time relaxation approximation, the right-hand side of Eq. (5.7), the collision term can be written as

\[ \left. \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} \right|_{coll.} = -\frac{f(\vec{r}, \vec{k}, t) - f^0_k}{\tau(\vec{k})} . \quad (5.13) \]

In general, for elastic collisions, \( \tau \) is considered to dependent on the momentum \( \vec{k} \) only through energy.

Eqs. (5.12) and (5.13) conduce to what is known as the solution of the Boltzmann equation in the relaxation time approximation,

\[ f(\vec{r}, \vec{k}, t) = f^0(\epsilon_k) + \tau \vec{v}_k \frac{df^0}{d\epsilon_k} \left( e\tilde{E} + \frac{\epsilon_k - \mu}{T} \nabla T \right) , \quad (5.14) \]

where \( \tilde{E} = \vec{E} + \frac{1}{e} \nabla \mu \) is the electrochemical potential.
5.2.1 Transport Coefficients

The solution of the Boltzmann transport equation is necessary to calculate the electric and energy currents that appear in an electron system in the presence of an electric field and a temperature gradient. The electric current is proportional with the sum over all occupied states of the particle velocities, while the energy current sums all available energies (expressed with respect to the Fermi level) multiplied by the particle velocity, weighted by the occupancy function of those states:

\[
\vec{j} = -2e \sum_k \frac{\hbar \vec{k}}{m} f(\vec{r}, \vec{k}, t), \quad (5.15)
\]

\[
\vec{j}_Q = 2 \sum_k (\epsilon_k - \mu) \frac{\hbar \vec{k}}{m} f(\vec{r}, \vec{k}, t), \quad (5.16)
\]

where a factor of 2 was introduced to account for the spin degeneracy. Upon the insertion of Eq. (5.14), Eqs. (5.15) and (5.16) become,

\[
\vec{j} = \hat{\sigma} \vec{E} - \hat{\beta} \nabla T T, \quad (5.17)
\]

\[
\vec{j}_Q = \hat{\beta} \vec{E} - \hat{\kappa} \nabla T T.
\]

The cartesian components of the rank-2 tensors \( \hat{\sigma}, \hat{\beta} \) and \( \hat{\kappa} \) specified in respect with spatial directions \( i, j \) are given by

\[
\sigma_{ij} = 2e^2 \sum_k \tau(\epsilon) v_i(\vec{k}) v_j(\vec{k}) \left( -\frac{\partial f}{\partial \epsilon} \right) ; \quad (5.18)
\]

\[
\beta_{ij} = -2e \sum_k \tau(\epsilon) v_i(\vec{k}) v_j(\vec{k}) (\epsilon - \epsilon_F) \left( -\frac{\partial f}{\partial \epsilon} \right) ; \quad (5.19)
\]

\[
\kappa_{ij} = \frac{2}{k_B T} \sum_k \int d\vec{k} \tau(\epsilon) v_i(\vec{k}) v_j(\vec{k}) (\epsilon - \epsilon_F)^2 \left( -\frac{\partial f}{\partial \epsilon} \right) . \quad (5.20)
\]
For simplicity, in the following consideration we will assume isotropic response and reduce these tensors to scalar behavior. The physical significance of these quantities is immediately apparent from Eqs. (5.15) and (5.16). In the absence of the temperature gradient, Eq. (5.15) reduces to

\[ \vec{j} = \sigma \vec{E}, \] (5.21)

indicating that \( \sigma = L_{11} \) is the electric conductivity. Similarly, in the absence of any electrochemical fields, \( L_{22} = k/T \).

The presence of a temperature gradient \( \nabla T \), in an open circuit, when \( \vec{j} = 0 \), induces an electric field such that

\[ \vec{E} = \frac{\beta \sigma T}{\sigma T} \nabla T. \] (5.22)

The proportionality coefficient in Eq. (5.22) is the thermopower, from Eq. (5.1),

\[ S = \frac{\beta}{\sigma T}. \] (5.23)

Moreover, the phenomenological parameter \( L_{12} \) is found to be \( \beta/T \).

5.3 Thermoelectric Transport in the \( \alpha = \beta \) Regime

Energy efficient spin and charge transport has long been a desiderate of theoretical and experimental condensed matter research. If traditional thermoelectrics has been concerned with optimizing charge transport, the field of spin caloritronics [76] is exploring the confluence between temperature gradients and magnetic, spin-dependent phenomenology in an effort to increase the efficiency of spin flow in solid structures. In the last several years, experiments have showcased different ways of
producing spin currents or macroscopic spin-dependent effects by relying on temperature gradients applied to systems with magnetic order [77, 4, 78, 79].

Defined as the proportionality coefficient between the electric field that appears in a closed circuit and the thermal gradient that induces it, the Seebeck coefficient or thermopower $S$ was early on recognized as a measure of the efficiency of transport. In the standard theory based on the semi-classical Boltzmann transport equation solved in the relaxation-time approximation $S$ is given by

$$S_c = -\frac{1}{eT} \sum_k (\epsilon_k - \epsilon_F) \tau(\epsilon_k) v_k \cdot v_k \left( -\frac{\partial f_0^k}{\partial \epsilon_k} \right), \quad (5.24)$$

where $v_k$ and $\epsilon_k$ are the velocity and energy, respectively, of a single-particle state of wave-vector $k$, $\epsilon_F$ is the Fermi energy and $\tau(\epsilon_k)$ is the particle relaxation time, considered a function of energy only. $f_0^k = (\exp(\epsilon_k - \epsilon_F) + 1)^{-1}$ is the equilibrium occupation function. Eq. (5.24) makes it easy to see that in normal (degenerate) metallic systems, the weak variation with energy of both the particle velocity and the relaxation time enables a significant cancelation among the terms of the sum for energies above and below the Fermi energy, leading to a small result proportional to $(k_B T/\epsilon_F)^2$ at finite temperature.

Disrupting the cancelation discussed above requires the presence of two factors, as it was recognized long ago in Ref. [80]. First, it is necessary that two distinct, unequal groups of electrons exist, such as one can obtain through spin-polarization. Second, a scattering mechanism that provides a unidirectional energy transfer between these groups needs to be introduced, for example one that involves spin-flips. While the latter factor can be controlled rather easily through doping with magnetic impurities, it is the first criterion that drastically limits the number of systems that can
be susceptible to this approach, as naturally created and sustained spin-polarization is rare.

Here we provide a qualitative proof that a semiconductor quantum well with spin-orbit interactions of the Rashba and Dresselhaus type, linear in the electron momentum, and doped with magnetic impurities satisfies these conditions and consequently should exhibit an enhanced Seebeck coefficient at low temperatures. This is predicted to occur in the special case when the strengths of the two spin-orbit couplings are equal, a situation in which the minimum total-energy of the many-body system in the presence of the Coulomb interaction evaluated within the Hartree-Fock approximation can lead to a weak itinerant antiferromagnetic order. Thus the two opposite-spin, unequal electron populations are created. Through inelastic scattering on magnetic impurities that occurs with the flip of the impurity spin, a one-way energy transfer is then assured leading to the amplification of the numerator in the expression of the Seebeck coefficient, Eq. (5.24).

Since the single-particle states described by the canonical transformations Eq. (4.12) represent exact eigenstates of the non-interacting Hamiltonian, we define the spin and charge currents carried by these states as the averages of the generalized momentum \( p - \sigma_z \hbar \mathbf{Q} \) on these states. Consequently, the total charge and \( \hat{x} \)-polarized spin currents are given by,

\[ j = -e \sum_{k, \pm} \langle \psi^\pm | \frac{p - \sigma_z \hbar \mathbf{Q}}{m^*} | \psi^\pm \rangle \Delta f_{k\pm}, \tag{5.25} \]
\[ j_x = \frac{\hbar}{2} \sum_{k, \sigma, \pm} \frac{1}{2m^*} \langle \psi^\pm | (p - \sigma_z \hbar \mathbf{Q}) \sigma_x + \sigma_x (p - \sigma_z \hbar \mathbf{Q}) | \psi^\pm \rangle \Delta f_{k\pm}, \tag{5.26} \]

where \( \Delta f_{k\pm} \) is the deviation from equilibrium of the single-particle occupation number under the effect of the external perturbation. In equilibrium the occupation
number is the Fermi function written for energies $E_k^\pm$ in Eq. (4.22). In the following considerations, we will focus only on the deviation in the presence of an electric field, as the Seebeck coefficient is calculated by using the Mott formula which establishes the equivalence of Eq. (5.24) with the derivative of the logarithm of the electric conductivity,

$$S = \frac{\pi k_B}{3 e} \frac{k_B T}{E_F} \left( \frac{d \ln \sigma(E)}{dE} \right) \bigg|_{E=E_F} .$$

In the presence of an electric field $E$, the out-of-equilibrium part of the distribution function is written in the relaxation time approximation as

$$\Delta f_{k^\pm} = -e (E \cdot v_{k^\pm}) v_{k^\pm} \tau(E_{k^\pm}) \left( -\frac{d f_{k^\pm}^0}{dE_{k^\pm}} \right) ,$$

where the single-particle velocity is $v_{k^\pm} = \nabla_k E_{k^\pm}/\hbar$. Considering the temperature range of interest in this problem, henceforth we approximate $(-df_{k^\pm}/dE_{k^\pm}) = \delta(E_F - E_{k^\pm})$. Since the velocity is given by the same expression as the average of the canonical momentum on the eigenstate $|\psi_k^\pm\rangle$,

$$v_{k^\pm} = \frac{1}{\hbar} \nabla_k E_{k^\pm} = \frac{\hbar}{m^*} (k \pm Q \cos 2\theta_k) ,$$

there will be two different transport modes, normal and parallel, depending on the relative orientation of the electric field $E$ and the wave vector $Q$. While the normal mode velocity is simply $v_{k^\pm}^{(n)} = \hbar k/m^*$, the parallel mode velocity is

$$v_{k^\pm}^{(p)} = \frac{\hbar}{m^* Q} (k \cdot Q \pm Q^2 \cos 2\theta_k) = \frac{\hbar}{4m^* Q} (g \cot 2\theta_k \pm (2Q)^2 \cos 2\theta_k) .$$

We introduce the corresponding $n$ or $p$ conductivity expressions for the charge and
spin current, polarized along the \( \hat{x} \) direction,

\[
\sigma^{(n,p)}(E) = e^2 \sum_{k,\pm} v_{k,\pm}^{(n,p)} \tau^{(n,p)}(E_{k,\pm}) \delta(E - E_{k,\pm}),
\]

\[
\sigma_{x}^{(n,p)}(E) = -\frac{e \hbar}{2} \sum_{k,\pm} \operatorname{sgn}(\pm) \sin 2\theta_{k,\pm} v_{k,\pm}^{(n,p)} \tau^{(n,p)}(E_{k,\pm}) \delta(E - E_{k,\pm}),
\]

(5.31)

where \( \operatorname{sgn}(\pm) = \pm 1 \).

The weak variation of the electric conductivity, Eq. (5.31) as a function of energy generates the very small Seebeck coefficient in homogeneous systems. As argued in the introduction, maximizing the transport coefficients is realized by including scattering processes that preserve the population imbalance of up and down spin-states created through antiferromagnetic order. As shown in Ref. [80] this can be realized by considering a scattering potential that has a magnetic component, of the type

\[
\sum_{i} [V_0 \delta(r - R_i) + J \sigma \cdot S_i \delta(r - R_i)],
\]

(5.32)

where \( \sigma \) is the electron spin at the site of the magnetic scatterer of spin \( S \). \( V_0 \) is the isotropic scattering potential and \( J \) is the strength of the magnetic potential. For this choice of potential, a long but straightforward calculation based on applying the Fermi golden rule inside the collision integral of the Boltzmann transport equation.
provides values for the normal and parallel relaxation times \[80\]. Thus,

\[
\frac{1}{\tau^{(n)}(E_{k\pm})} = \frac{\pi N_i}{\hbar^2} \left\{ \left(V^2 + J^2 S_z^2\right) I_0(E_{k\pm}) + \sin 2\theta_k(V^2 - J^2 S_z^2) I_1(E_{k\pm}) \right. \\
+ \frac{(J S^-)^2}{2} \eta(E, \Delta E) \left[ I_0(E_{k\pm} - \Delta E) + \sin 2\theta_k I_1(E_{k\pm} - \Delta E) \right] \\
+ \frac{(J S^+)^2}{2} \eta(E_{k\pm}, -\Delta E) \left[ I_0(E_{k\pm} + \Delta E) + \sin 2\theta_k I_1(E_{k\pm} + \Delta E) \right] \right\} .
\]

(5.33)

This result assumes a concentration \(N_i\) of impurities with same spin \(S\) whose projection on the \(z\)-axis is \(S_z\), while its perpendicular components are \((S^\pm)^2 = S(S+1) - S_z^2\). In the numerical evaluations \(S_z\) is replaced by its thermal average. \(\Delta E\) is the Zeeman splitting in the presence of the magnetic impurity which parametrizes the function \(\eta(E_{k\pm}, \Delta E)\), a measure of the collision inelasticity given by

\[
\eta(E_{k\pm}, \Delta E) = \frac{e^{(E_{k\pm} - E_F)/k_B T} + 1}{e^{(E_{k\pm} - E_F)/k_B T} + e^{-\Delta E/k_B T}} .
\]

(5.34)

\(I_0(E_{k\pm})\) and \(I_1(E_{k\pm})\) represent the density of states and the fractional polarization at energy \(E_{k\pm}\),

\[
I_0(E_{k\pm}) = \sum_{k'} \delta(E_{k\pm} - E_{k'\pm}) , \\
I_1(E_{k\pm}) = \sum_{k'} \sin 2\theta_{k'} \delta(E_{k\pm} - E_{k'\pm}) .
\]

(5.35)

The parallel mode relaxation time is

\[
\tau^{(p)}(E_{k\pm}) = \frac{\tau^{(n)}(E_{k\pm})}{1 - \frac{\pi N_i}{\hbar} \left( V^2 - J^2 S_z^2 \right) \sum_{k'} \cos 2\theta_{k'} v_p(k') \tau^{(n)}(E_{k\pm}) \delta(E_{k\pm} - E_{k'\pm}) } \left( \int_{-\infty}^{\infty} \frac{\cos 2\theta_k v_p(k) \tau^{(n)}(E_{k\pm}) \delta(E_{k\pm} - E_{k'\pm})}{1 - \frac{\pi N_i}{\hbar} \left( V^2 - J^2 S_z^2 \right) \sum_{k'} \cos 2\theta_{k'} \tau^{(n)}(E_{k\pm}) \delta(E_{k\pm} - E_{k'\pm}) } \right) .
\]

(5.36)
5.3.1 The Case of InAs

We illustrate this approach in the case of an InAs quantum well (effective electron mass $m^* = 0.023 m_e$) with Rashba-Dresselhaus spin-orbit coupling constant $\alpha = 5 \times 10^4$ m/s, or equivalently, $Q = 2 \times 10^7$ m$^{-1}$, which are typical values for experiments that investigate the $\alpha = \beta$ state in SOI systems [62, 63]. The system is considered to be in a weak antiferromagnetic ground state whose gap function, for simplicity, is taken to be constant. In Fig. 5.5 we plot the self-consistent solution for the angle $\theta$ along $k_x$ for a system with $n = Q^2 / 2\pi = 2.5 \times 10^{14}$ m$^{-2}$ particles assuming that only the lowest energy level is occupied at $T = 0$K for two different values of the screening constant $\mu$, expressed in units of $k_F$. Here $k_F = Q = \sqrt{2\pi n}$ is the Fermi radius of a homogeneous electron system without spin-orbit coupling. The variation of the gap function along $k_x$ in the momentum-space is shown for the same values of the screening constants in Fig. 5.2. As expected, both $\theta_k$ and $g_k$ attain significant values in the vicinity of the degeneracy point, while decreasing to zero far from it. We note that $\theta = 0$ and $\theta = \pi/2$ are always solutions to the gap equation, as they correspond to the usual paramagnetic or ferromagnetic configurations of an electron system, depending on the particle density. Screening the Coulomb interaction reduces the amplitude of both $\theta_k$ and $g_k$.

The temperature variation of the gap is negligible over the temperature scale used in the problem, set by the Zeeman splitting induced by the scattering potential, $\Delta E/k_B$. We define as a momentum unit the Fermi wave-vector of a homogeneous electron system, $k_F = \sqrt{2\pi n} = 2.5 \times 10^8$ m$^{-1}$, and correspondingly the energy unit is $E_F = \hbar^2 k_F^2 / 2m^* = 93$meV. For the rather small ratio $Q/k_F = 0.08$ we calculate a gap constant equal to $0.013 E_F$ and a resulting spin-polarization of the system of the order of 1%. For these values, both single-particle energy levels $E^\pm$ are occupied and
Figure 5.1: The variation of the inclination angle $\theta$ along $k_x$ for two different screening constants $\mu$ in an InAs quantum well with $n = 2.5 \times 10^{14} \text{m}^{-2}$. The momentum unit is $k_F = Q = \sqrt{2\pi n} = 2 \times 10^7 \text{m}^{-1}$. 
Figure 5.2: The variation of the gap function along $k_x$ for two different screening constants $\mu$ in an InAs quantum well with $n = 2.5 \times 10^{14} \text{m}^{-2}$. The energy unit is $E_F = \hbar^2 k_F^2 / 2m^* = 0.6$ meV.
participate in transport. The parameter of the simulation is the ratio of the spin-dependent scattering potential $J$ to the isotropic potential $V_0$, $J/V_0$. The former is set $J = 0.03\text{eV}$, while $V_0$ is allowed to vary. The impurity spin is $S = 5/2$. The values of the Seebeck coefficient are given in respect with the value in the normal system $S_0$. The chosen values of $J$ and $p$ give the value of the Zeeman splitting $\Delta E = pJ$ and establish the temperature unit $\Delta E/k_B$. $T = 1$ corresponds to 4.5K.

In Fig. 5.3.1 we present the values of the Seebeck coefficient for different values of the ratio $J/V_0$. These results indicate a monotonous tracking of the amplitude of the Seebeck anomaly with the magnitude of the magnetic scattering $|J|$ for the same value of the isotropic scattering $V_0$. The amplitude is higher for $J < 0$ than for $J > 0$. The position of the peak varies very slowly, as it is essentially fixed by the ratio of the Zeeman splitting and the Fermi energy. The normal charge and spin Seebeck coefficients track an almost identical temperature dependence except for $J/V_0 = 2$ when their amplitudes are separated. The variation of each of the coefficients for a whole range of $J/V_0$ values is shown in Fig. 5.4.

### 5.3.2 The Case of GaAs

We also present numerical results of thermoelectric transport in a GaAs (effective mass $m^* = 0.067$, dielectric constant $\kappa = 13$) quantum well of electron density $n = 4 \times 10^{15}\text{m}^{-2}$. The $\alpha = \beta$ state was identified from the antilocalization peak of the quantum corrections to the conductivity in the weak scattering regime and found to correspond to a value $\alpha = 9 \times 10^2 \text{m/s}$ [75]. For the given particle concentration, we have $k_F = \sqrt{2\pi n} = 1.58 \times 10^8\text{m}^{-1}$. Correspondingly, the energy scale of the problem is set by the single-particle Fermi energy, $E_F = \hbar^2 k_F^2/2m^* = 12.88 \text{meV}$. For these parameters, $Q = 2m^*\alpha/\hbar = 2\alpha/v_F = 7.2 \times 10^{-3}k_F$, while the Fermi temperature
Figure 5.3: The variation of the relative Seebeck coefficient for the normal and parallel charge and spin modes with temperature for different values of the ratio $J/V_0$. $S_0$ is the value of the Seebeck coefficient in an isotropic system with the same particle density.
Figure 5.4: The variation of the relative Seebeck coefficient for the normal (a) and parallel (b) charge and normal (c) and parallel (d) spin modes with temperature for different values of the ratio $J/V_0$. $S_0$ is the value of the Seebeck coefficient in the isotropic system.
which sets the temperature scale is $T_F = 150K$.

An iterative calculation is first employed to obtain a solution of the gap equation plotted as a function of temperature in Fig. 5.6. To incorporate a qualitative description of the additional screening that can appear in the system on account of short range Coulomb interaction effects beyond the Hartree-Fock approximation, our computation is performed with a Yukawa potential of screening constant $\mu = 10^{-3}$ (expressed throughout in $k_F$ units), whose Fourier transform is $v(q) = 2\pi e^2/\kappa \sqrt{q^2 + \mu^2}$.

At each temperature, Eq. (4.17) is used to determine the Fermi level $E$. Here, we show the variation of the gap function at the center of the Fermi disk, a good indicator for the temperature range in which one expects to have an antiferromagnetic state. Our results indicate that the critical temperature of the system is about 90K. In the following evaluations the ratio of the spin-dependent scattering potential $J$ to the isotropic potential $V$, $J/V$, is used as a parameter. The former is set to $J = 0.03eV$, while $V$ is allowed to vary. The impurity spin is $S = 5/2$. The chosen values of $J$ and $p$ give the value of the Zeeman splitting $\Delta E = pJ$ and establish the temperature unit $\Delta E/k_B$. $T = 1$ corresponds to 35K. Here we present results obtained for negative values of the spin-dependent scattering coupling constant $J$, since for $J > 0$ there is hardly any effect on the current values. Moreover, for the numerical data available for this system, the effect on the charge current is small and we choose not to plot it here. Since the temperature unit imposed by the magnetic impurity scattering is much smaller than the critical temperature of the antiferromagnetic transition, we will assume that in the low temperature range we are interested in the gap variation with temperature is negligible and consequently the gap function is considered constant, equal to $0.2\epsilon_F$.

In Fig. 5.7 we present the values of the spin Seebeck coefficient for different values of the ratio $J/V$ for the normal and parallel spin currents. The current of
Figure 5.5: The variation of the gap function at the center of the Fermi surface and of the fractional spin polarization for a screening constants $\mu_1 = 10^{-3}$ in an InAs quantum well with $n = 4 \times 10^{15} \text{m}^{-2}$. $Q = 7.2 \times 10^{-3} k_F$ as a function of temperature.
Figure 5.6: The variation of the gap in GaAs at the center of the Fermi surface, $g(0, 0)$, as a function of temperature for two different screening constants.
course is spin polarized after \( \hat{x} \). The amplitude of the low-temperature peak in the Seebeck coefficient for each mode varies monotonically with the absolute value of \( J \). Higher values are obtained for negative \( J \). Such a result should not be surprising however since its existence is guaranteed by the general considerations presented in the introduction that involve fundamental principles of the energy transfer in the system are satisfied.
Figure 5.7: The variation of the spin Seebeck coefficient for the normal in (a) and parallel in (b) mode with temperature for different values of the ratio $J/V$. The gap value is $0.2E_F$, while the polarization is 10%. The temperature unit is set by the spin-flip energy and corresponds to 35K.
Chapter 6

Conclusions and Discussion

In this thesis we discuss two instances of macroscopic manifestations that involve the interplay between the spin-orbit interaction and the Coulomb interaction in semiconductor systems with zinc blende structure. In each case, the spin-orbit coupling was considered to be linear in the electron momentum, while the cubic Dresselhaus term was neglected. In the first problem we analyzed the influence of spin-orbit coupling on the real-space dependence of the particle density fluctuations in a lateral superlattice with spin-orbit interaction in the presence of the Coulomb interaction as a function of the miniband width, the SOI coupling and SL constant. We find the amplitude of the oscillations, as well as their phase, is affected by the presence of SOI which enhances the coupling between the single particle states indicating a stronger screening [81].

In a separate direction, we investigated the effect of the Coulomb interaction on the state where the Rashba-Dresselhaus interactions are of equal strengths. In that instance starting from general total-energy considerations, we demonstrate that the ground state of the electron system at low temperature is an itinerant antiferromagnet, with a fractional polarization oriented along the $\hat{x}$ axis, the direction in which the
single-electron spectrum is displaced. Above a critical temperature \( T_c \), the system transitions into a paramagnetic state [82, 83].

Using the solutions of a Boltzmann equation obtained within the relaxation time approximation, we evaluate the transport properties in this state. In realistic InAs and GaAs samples, we calculate the thermoelectric coefficients for spin and charge transport. Our results show that an unusual high value of the Seebeck coefficient is possible to exist at low temperature when the impurity scattering contains a magnetic component. This outcome originates in the confluence of the magnetic order imposed by the minimization of the total energy of the electron system in the presence of the Coulomb interaction and the unidirectional energy transfer in the spin-flip scattering. The overall amplitude of the effect is determined by the degree of polarization of the electron system and the strength of the magnetic scattering [84].
Bibliography


90


