# Contents

# Chapter 1

# Introduction

The central concepts in this Master thesis is spin orbit induced topological insulators[1], RKKY interaction and spin-orbit effects. Spin orbit induced topological insulators are a new class of materials that recently has been theoretically predicted and produced in laboratory. An overview of topological insulators is given in chapter 2 and a simple tight binding model is used in chapter 3 to derive the bulk band structure of the two dimensional spin orbit induced topological insulator.

This is followed by a chapter in which it is shown how the spin-orbit interaction, or Thomas term, arises in the non-relativistic limit of the Dirac equation. One reason that the spin orbit interaction is derived here is that it is this term that is responsible for the band structure in the spin orbit induced topological insulators. Secondly, another interaction called the Rashba interaction also is a kind of spin orbit interaction that follows from this derivation, and this interaction is similar in form to an effect that occurs on the surface of the three dimensional topological insulator.

In chapter 5 an interaction called the RKKY interaction, which is a special type of interaction between two localized spins that is mediated by a surrounding "electron sea" is derived. This is followed by a final chapter where a general method for solving such problems when the "electron sea" has a linear spectrum. The motivation for these two last chapters are that the electrons on the surface of a three dimensional topological insulator satisfies a linear spectrum, and thus is a special case of such a system.

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[1]I choose here to use the term spin orbit induced topological insulators instead of topological insulators because this makes it possible to differentiate between these and the quantum Hall systems that also will be briefly described later.

# Chapter 2

# Topological insulators - Overview

## 2.1 Introduction

In recent years a new type of material, spin-orbit induced topological insulators, has attracted a large interest in the community of condensed matter physicists. This class of materials has the special property that they are insulators in the bulk, but allows conducting states to exist on the boundary. This is interesting for several reasons, among them that this could allow for "electrical manipulation of spins and spin currents with little or no dissipation"[8].

Both two and three dimensional versions of these materials have been theoretically predicted[2] and subsequently produced in laboratories[9, 15], and the two dimensional versions has close analogies with the quantum Hall effect[8]. In this chapter an overview of some of the essential properties of these new types of materials as well as related properties of quantum Hall insulators is given. This chapter does in no way try to give a complete description of the topological insulators, neither is it intended to give detailed theoretical descriptions of why the phenomenas occur. The purpose of this chapter is instead to give an introduction to some of the most important properties, and to give a hint on the analogies and difference between the different systems.

## 2.2 The quantum Hall insulator

An early example of a class of topological insulators is provided by the quantum Hall insulators[8, 5]. In these systems a strong magnetic field gives rise to Landau quantization, where each electron falls into one of several degenerate and widely separated energy levels. See figure 2.1. As long as none of these energy levels coincides with the Fermi energy, the bulk of the material is in an insulating state in which all Landau levels below the Fermi surface are fully occupied and those above are empty.

In contrast, there exist conducting states at the edges of a quantum Hall insula-
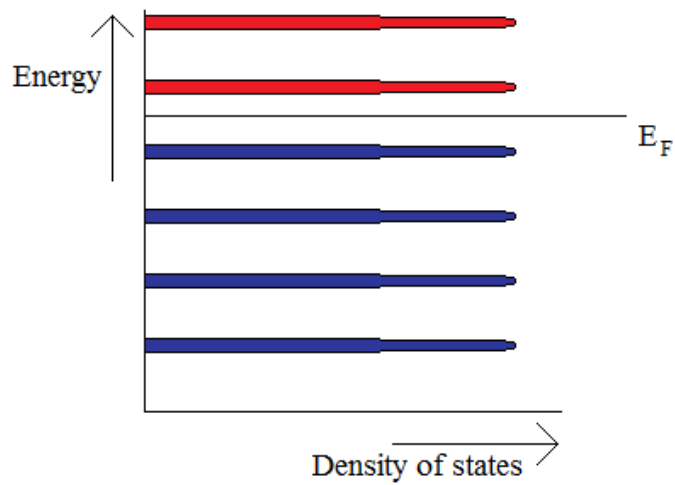
Figure 2.1: For strong magnetic fields, the energy spectrum in the bulk of a quantum Hall insulator consists of Landau levels with large amounts of electrons in each level. As the magnetic field is further increased the Landau levels are pushed upward, and each time a Landau level is pushed above the Fermi energy it gets emptied of electrons. Those levels that lies below the Fermi energy is therefore fully occupied (blue), while those above are empty (red). In this way there is an energy gap between the highest occupied and lowest unoccupied Landau level, as long as the Fermi energy not happens to fall within one of the Landau levels. The later happens at those critical values of the magnetic field strength at which the levels are emptied.
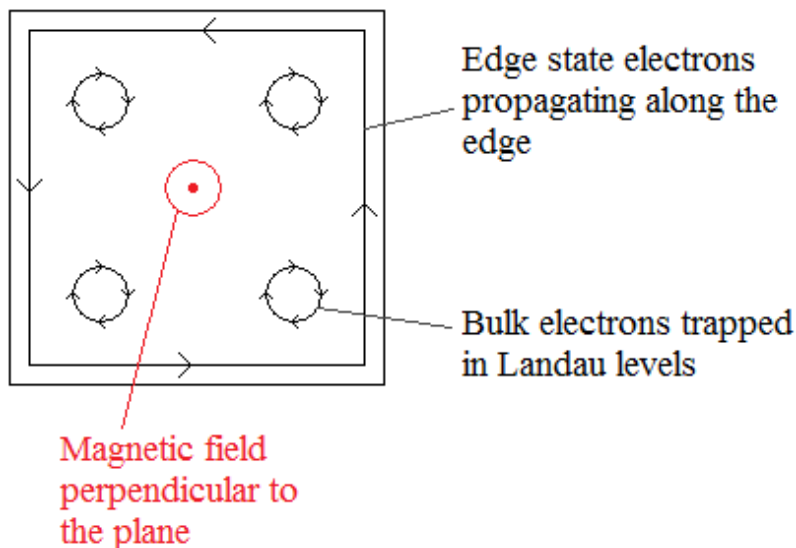
Figure 2.2: In the Quantum Hall effect the bulk electrons are trapped in filled Landau levels. There is however edge states in which electrons can propagate in one direction. Because the states only can propagate in one direction, they are insensitive to scattering from impurities. This results in very precise quantization of the resistance for the system.

tor. These states do however only allow for conduction in one direction and forbids backscattering. This in turn leads to a very precise quantization of the resistance for the system, so precise that it allows for an international standard of resistance to be based on it[1]. See figure 2.2.

## 2.3  Two dimensional quantum spin Hall insulator

The two dimensional quantum spin Hall insulator has many similarities with the quantum Hall insulator. Just as the quantum Hall insulator, the two dimensional quantum spin Hall insulator has an insulating bulk and conducting edge states. But in contrast to the quantum Hall insulator, it has two sets of edge states that propagates in opposite directions. See figure 2.3. Further these sets of edge states has a definite spin direction, each opposite to the other. In this way there is two conduction channels at the edge of a two dimensional quantum spin Hall insulator, where in one channel spin up electrons are conducted in one direction, while in the other channel spin down electrons are conducted in the opposite direction.

Similar to the edge states on a quantum Hall insulator, the edge states on the quantum spin Hall insulator are protected against scattering. At least this is true as long as there not is any magnetic scatterers along the edge. In this case there do exist conduction channels in both direction, but for an electron to be scattered into the opposite
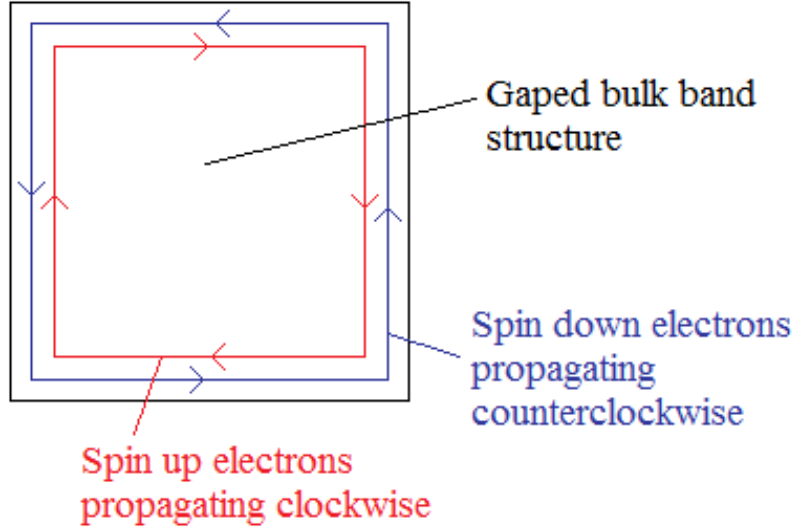
Figure 2.3: Similarly to the quantum Hall insulator, the two dimensional quantum spin Hall insulator is gaped in the bulk. However, in contrast to the quantum Hall insulator there exists two sets of edge states. One for each spin direction, and these propagates in opposite directions.

direction it has to reverse it's spin, which would require scattering against magnetic impurities.

The band structure that supports the quantum spin Hall insulator state is however quite different from that of the quantum Hall insulator. While the later band structure consists of Landau levels induced by an external magnetic field, the important part of the former one can be described by two bands that are intrinsic to the material itself. To understand the important parts of these, imagine two parabolic bands that bends away from each other, one with even and one with odd parity. Further imagine that they overlap each other so that they cross at some two points in $k$-space. At these points the two pure parity bands combine to form gaps, and the result is two bands like those depicted in figure 2.4. This kind of band structure is called an inverted band structure with a negative mass gap, and an important parameter related to this is labeled $\frac{M}{B}$. In terms of the description given here, this parameter describing the amount of overlap of the odd and even parity states. As $\frac{M}{B}$ makes a transition from $\frac{M}{B} < 0$ to $\frac{M}{B} > 0$ the even and odd states begins to overlap and the inverted band structure that supports the edge states appear. It is however also important that the band gap not is to large, so there is an upper limit $\frac{M}{B} < 4$ that also has to be satisfied in order to get the quantum spin Hall state[2].

The effect that creates this kind of band structure in the quantum spin Hall insulators is a strong spin-orbit interaction[9, 10, 2, 12], an interaction that is derived in chapter 4. In these materials two bands constructed from p-like and s-like orbitals, with odd and even parity respectively, corresponds to the odd and even bands described
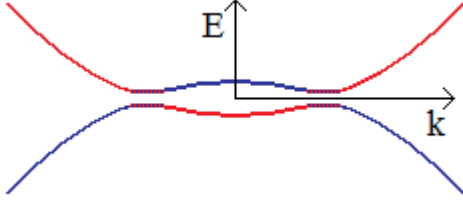
Figure 2.4: The bulk band structure in a spin Hall insulator can be thought of as consisting of two bands, one with even and one with odd parity, that overlaps each other. But where the two bands intersect, they combine to form a gap at the intersection of the pure parity bands. Each color refers to a definite parity.

above. Normally the bands do not overlap, as in the case of the material CdTe. But for some special types of materials, for example HgTe, the spin-orbit interaction is so strong that the $p$-like band is shifted so much in energy that the two bands overlap and creates the situation in figure 2.4.

One of the advantages of the quantum spin Hall insulator over the quantum Hall insulator is that the property is intrinsic to the material. While the quantum Hall effect requires a strong external magnetic field to be applied perpendicular to the material, the quantum spin Hall effect is achieved simply by the right choice of material.

## 2.4 Three dimensional topological insulator

The three dimensional quantum spin Hall insulator[15, 4, 6, 16, 12, 7] is very similar to the two dimensional version. The main difference from the description there is obviously that it is three dimensional, and that it therefore has a two dimensional surface on which the surface states propagates. This means that the notion of two spin channels with opposite spin and propagation directions not makes sense here. Two spins with opposite direction does however propagate in opposite directions on these surfaces too. The relation between the spin and propagation direction is such that the spin direction lies in the surface direction but is perpendicular to the propagation direction[15, 4, 16, 7], as displayed in 2.5. Moreover, as also depicted in the same figure, the surface states has a cone like energy spectrum. Altogether the spectrum on the surface of a topological insulator can be written as

$$H = \hbar v_F (k_x \sigma_y - k_y \sigma_x). \tag{2.1}$$

It is this property of the three dimensional topological insulator that serves as motivation for the derivation of the RKKY interaction between two localized spin in a two dimensional system with linear spectrum in chapter 6.

Side view                              Top view
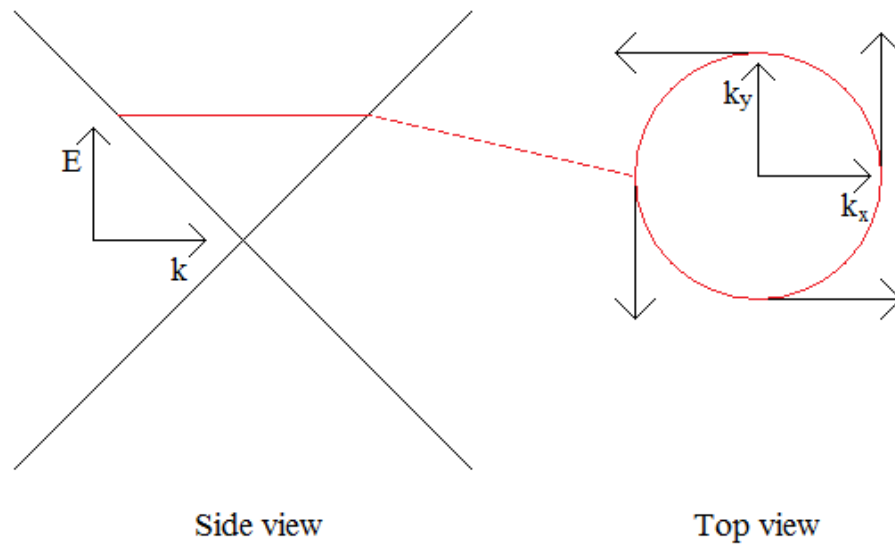
Figure 2.5: The energy spectrum on the surface of a three dimensional topological insulator, as seen in the "side" and "top" view. The energy spectrum is a cone, and for each $\mathbf{k}$ the spin is perpendicular to the $k$-vector as shown in the top view. From the top view it is clear that counter propagating spins is pointing in opposite direction.

# Chapter 3

# Bulk band structure in a 2D spin orbit induced topological insulator

## 3.1 Introduction

In this chapter a simple model for the bulk band structure in the two dimensional spin orbit induced topological insulator is derived to display the main building blocks that are involved in this construction. The model starts from a tight binding model on a square lattice with two orbitals per lattice site, where one of the orbitals has odd parity and the other has even parity. The one with odd parity has higher energy than the one with even parity. This system is a simplification of for example HgTe-CdTe quantum wells which essentially has a band structure constructed from two orbitals per lattice site, one with even and one with odd parity[2].

## 3.2 Orbitals and parity

Before the tight binding model can be constructed there is a few things that has to be settled. The atoms which the lattice is constructed from are supposed to bind to each other through sharing s- and p-orbitals. The electrons are therefore supposed to be able to occupy the s- and p-orbitals on each lattice site. However, because the system is two-dimensional, the p orbital with m=0 (as measured with an axis perpendicular to the plane) will have its orbital "pointing" out of the plane. This orbital is therefore not assumed to contribute to the binding as it would give a minimal overlap with orbitals on neighboring lattice sites. The electrons are therefore assumed to occupy only the s-orbitals and p-orbitals with $m = \pm 1$. Moreover the strong spin-orbit interaction will split the $m = \pm 1$ orbitals into two different energy levels, one with the spin of the electron parallel with the angular momentum, and one anti-parallel. Of these two possibilities, only the parallel is assumed to be involved in the binding. This gives a

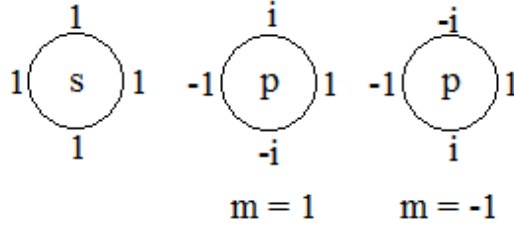Figure 3.1: The s- and p-orbitals have different parity. The s-orbital is spherically symmetric, while the p-orbital has an angular dependence that goes as $e^{im\phi}$. Viewed from $+z$.

total of two s-orbitals and two p-orbitals contributing to the binding, namely the two spin up and down configurations of the s-orbital, the spin up $m = 1$ p-orbital and the spin down $m = -1$ p-orbital.

The s-orbital is spherically symmetric, and has therefore even parity. But the p-orbitals are proportional to a factor $e^{im\phi}$ where $\phi$ is the polar coordinate in the $x, y$-plane. This means that the parity of the $p$-orbital is odd. For our purposes the values of $e^{im\phi}$ at the angels $0, \frac{\pi}{2}, \pi$ and $\frac{3\pi}{2}$ will be of interest because these are the angels at which the overlap integrals between the neighboring orbitals has to be evaluated. Theses properties are depicted in figure 3.1

## 3.3   Overlap integrals

To get the hopping amplitudes for the tight binding model, the overlap integrals between neighboring orbitals has to be evaluated. These will not be evaluated here, but will be left as arbitrary parameters. It is however assumed that the overlap between orbitals with opposite spins are zero[1]. The relation between many of the remaining parameters can be found from symmetry arguments. The main characteristics of the overlap integrals are depicted in figure 3.2. Apart from the information given in that picture, the only remaining relations needed to write down all the overlap integrals are the value of the overlap integrals $\langle s_{((x,y)}|H|s_{(x+a,y)}\rangle$, $\langle p_{((x,y)}|H|p_{(x+a,y)}\rangle$, $\langle s_{((x,y)}|H|p_{(x+a,y)}\rangle$ and $\langle p_{(x,y)}|H|s_{(x+a,y)}\rangle$, as the rest of the information can be deduced from the symmetry relations depicted in the figure. But note that the relation $\langle s_{(x,y)}|H|p_{(x+a)}\rangle^* = \langle p_{(x+a,y)}|H|s_{(x,y)}\rangle = \langle p_{(x,y)}|H|s_{(x-a,y)}\rangle$ has to be satisfied which reduces the four independent parameters to three independent parameters. As already stated, these overlap integrals will not be evaluated, but given as arbitrary parameters. Lets call these

$$\begin{aligned} S &= \langle s_{(x,y)}|H|s_{(x+a,y)}\rangle, \\ P &= \langle p_{(x,y)}|H|p_{(x+a,y)}\rangle, \\ A &= \langle s_{(x,y)}|H|p_{(x,y)}\rangle. \end{aligned} \tag{3.1}$$

---

[1]This might be an exact result, but I don't know how to show this.

From these parameters, together with the symmetry arguments the following overlap integrals follows

**Spin up and m = 1:**

$$
\begin{aligned}
\langle s_{(x,y)}|H|s_{(x+a,y)}\rangle = \langle s_{(x,y)}|H|s_{(x,y+a)}\rangle = \langle s_{(x,y)}|H|s_{(x-a,y)}\rangle = \\
= \langle s_{(x,y)}|H|s_{(x,y-a)}\rangle = S, \\
\langle p_{(x,y)}|H|p_{(x+a,y)}\rangle = \langle p_{(x,y)}|H|p_{(x,y+a)}\rangle = \langle p_{(x,y)}|H|p_{(x-a,y)}\rangle = \\
= \langle p_{(x,y)}|H|p_{(x,y-a)}\rangle = P, \\
\langle s_{(x,y)}|H|p_{(x+a,y)}\rangle = -i\langle s_{(x,y)}|H|p_{(x,y+a)}\rangle = -\langle s_{(x,y)}|H|p_{(x-a,y)}\rangle = \\
= i\langle s_{(x,y)}|H|p_{(x,y-a)}\rangle = A, \\
\langle p_{(x,y)}|H|s_{(x+a,y)}\rangle = i\langle p_{(x,y)}|H|s_{(x,y+a)}\rangle = -\langle p_{(x,y)}|H|s_{(x-a,y)}\rangle = \\
= -i\langle p_{(x,y)}|H|s_{(x,y-a)}\rangle = -A^*.
\end{aligned}
\tag{3.2}
$$

**Spin down and m = -1:**

$$
\begin{aligned}
\langle s_{(x,y)}|H|s_{(x+a,y)}\rangle = \langle s_{(x,y)}|H|s_{(x,y+a)}\rangle = \langle s_{(x,y)}|H|s_{(x-a,y)}\rangle = \\
= \langle s_{(x,y)}|H|s_{(x,y-a)}\rangle = S, \\
\langle p_{(x,y)}|H|p_{(x+a,y)}\rangle = \langle p_{(x,y)}|H|p_{(x,y+a)}\rangle = \langle p_{(x,y)}|H|p_{(x-a,y)}\rangle = \\
= \langle p_{(x,y)}|H|p_{(x,y-a)}\rangle = P, \\
\langle s_{(x,y)}|H|p_{(x+a,y)}\rangle = i\langle s_{(x,y)}|H|p_{(x,y+a)}\rangle = -\langle s_{(x,y)}|H|p_{(x-a,y)}\rangle = \\
= -i\langle s_{(x,y)}|H|p_{(x,y-a)}\rangle = A^*, \\
\langle p_{(x,y)}|H|s_{(x+a,y)}\rangle = -i\langle p_{(x,y)}|H|s_{(x,y+a)}\rangle = -\langle p_{(x,y)}|H|s_{(x-a,y)}\rangle = \\
= i\langle p_{(x,y)}|H|s_{(x,y-a)}\rangle = -A.
\end{aligned}
\tag{3.3}
$$

These overlap integrals, or hopping amplitudes, are depicted and more easily seen in figure 3.3. In addition to the overlap integrals considered above, the matrix elements

$$
\begin{aligned}
\tilde{S} = \langle s_{(x,y)}|H|s_{(x,y)}\rangle, \\
\tilde{P} = \langle p_{(x,y)}|H|p_{(x,y)}\rangle,
\end{aligned}
\tag{3.4}
$$

are needed for the complete model. These are the on site energy contributions associated with placing an electron in the corresponding orbitals.

## 3.4 Tight binding on a square lattice

With all the relations arrived at in the previous section the tight binding Hamiltonian can be written down. Because the up and down spin orbitals not couple to each others the Hamiltonian can be split into two parts, $H_\uparrow$ and $H_\downarrow$. From the two matrix elements

$\langle s_{(x,y)}|H|s_{(x+a,y)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|s_{(x,y+a)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|s_{(x-a,y)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|s_{(x,y-a)}\rangle$

s (x,y)  s
1x1=1

1x1=1
s
s (x,y)

s  s (x,y)
1x1=1

1x1=1
s (x,y)
s

$\langle p_{(x,y)}|H|p_{(x+a,y)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|p_{(x,y+a)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|p_{(x-a,y)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|p_{(x,y-a)}\rangle$

p (x,y)  p
1x-1=-1

±i*x∓i=-1
p
p (x,y)

p  p (x,y)
∓i*x±i=-1

-1x1=-1
p (x,y)
p

$\langle s_{(x,y)}|H|p_{(x+a,y)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|p_{(x,y+a)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|p_{(x-a,y)}\rangle$ $\qquad$ $\langle s_{(x,y)}|H|p_{(x,y-a)}\rangle$

s (x,y)  p
1x-1=-1

1x∓i=∓i
p
s (x,y)

p  s (x,y)
1x1=1

1x±i=±i
s (x,y)
p

$\langle p_{(x,y)}|H|s_{(x+a,y)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|s_{(x,y+a)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|s_{(x-a,y)}\rangle$ $\qquad$ $\langle p_{(x,y)}|H|s_{(x,y-a)}\rangle$

p (x,y)  s
1x1=1

±i*x1=∓i
s
p (x,y)

s  p (x,y)
∓i*x1=±i

-1x1=-1
p (x,y)
s
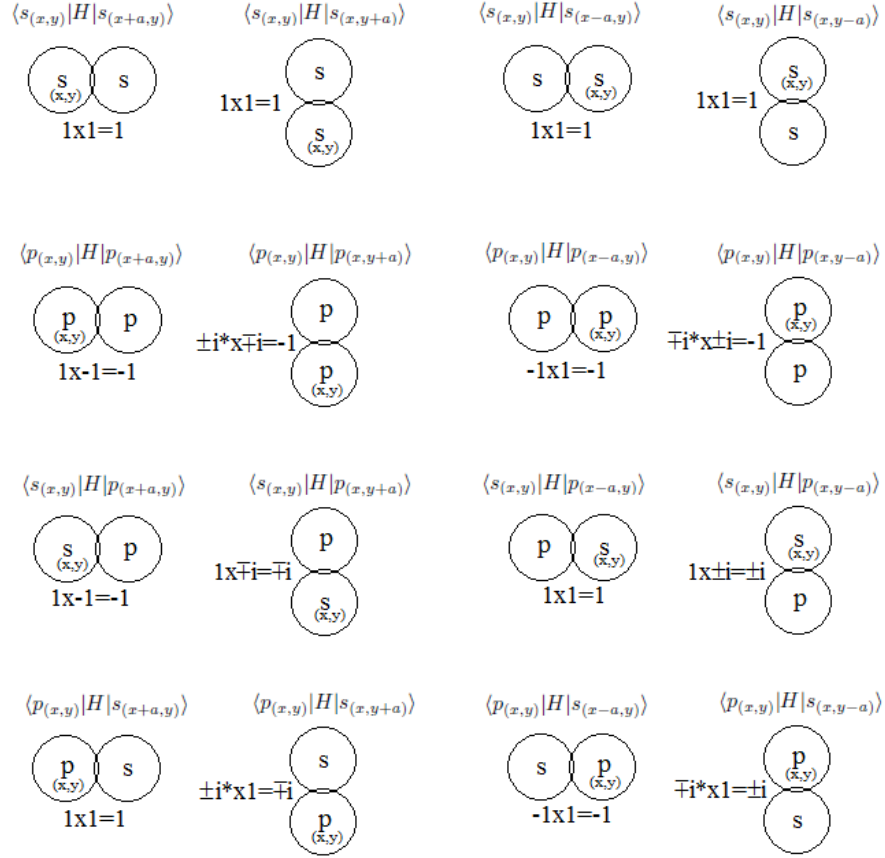
Figure 3.2: In this figure the nearest neighbor overlaps are depicted. The matrix element and a schematic view of the overlap is given, together with an equation for the relative phase between the orbitals in the overlap regions. The phase dependence is that depicted in figure 3.1, and the complex conjugation comes from the bra-expressions. The phase dependence on $\phi$ gives relative signs between some of the hopping amplitudes. As depicted in the picture, the s-s and p-p overlaps has the same phase in all directions. But the s-p and p-s hoppings acquires a phase $e^{\pm i\phi}$ as the hopping in different directions are considered.

Figure 3.3: Hopping amplitudes between neighboring lattice sites. The complex conjugation of the whole expression depends on whether spin up or spin down orbitals are considered.

above and figure 3.3, the tight binding Hamiltonian is seen to be

$$
H_\uparrow = \sum_i \left( \tilde{S} c^\dagger_{i,s} c_{i,s} + \sum_{j \in J} \left( S c^\dagger_{i,s} c_{i+j,s} + \frac{A}{a}(j_x + ij_y) c^\dagger_{i,s} c_{i+j,p} \right) + \right.
$$

$$
\left. + \tilde{P} c^\dagger_{i,p} c_{i,p} + \sum_{j \in J} \left( P c^\dagger_{i,p} c_{i+j,p} + \frac{A^*}{a}(-j_x + ij_y) c^\dagger_{i,p} c_{i+j,s} \right) \right),
$$

$$
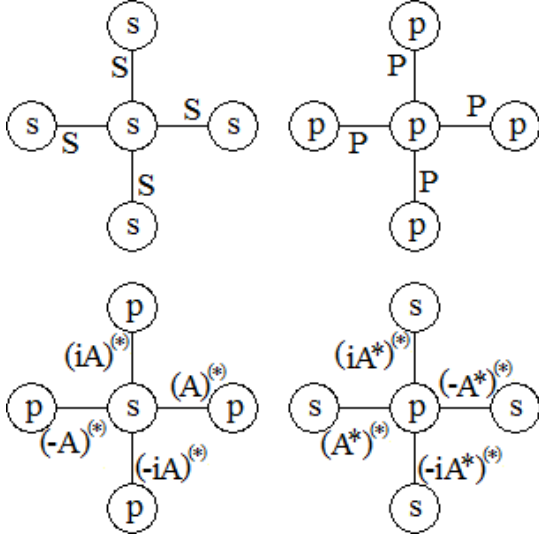H_\downarrow = \sum_i \left( \tilde{S} c^\dagger_{i,s} c_{i,s} + \sum_{j \in J} \left( S c^\dagger_{i,s} c_{i+j,s} + \frac{A^*}{a}(j_x - ij_y) c^\dagger_{i,s} c_{i+j,p} \right) + \right.
$$

$$
\left. + \tilde{P} c^\dagger_{i,p} c_{i,p} + \sum_{j \in J} \left( P c^\dagger_{i,p} c_{i+j,p} + \frac{A}{a}(-j_x - ij_y) c^\dagger_{i,p} c_{i+j,s} \right) \right),
$$

(3.5)

where $i = (x, y)$ is the lattice index and $J = \{(a, 0), (-a, 0), (0, a), (0, -a)\}$.

Now denote the probability amplitude that an electron is in the $s$-orbital on site $(x, y)$ with $\phi_s(x, y)$ and in the $p$-orbital on site $(x, y)$ with $\phi_p(x, y)$. In the limit $A = 0$ the tight binding Hamiltonian above would have been solved by plane wave solutions on the form $\phi_{ks}(x, y) \propto e^{i(k_x x + k_y y)}$ and $\phi_{kp}(x, y) \propto e^{i(k_x x + k_y y)}$. The solutions would in other words be solutions of the $s$- and $p$-bands. When $A$ is non zero the $s$- and $p$-bands does however mix. To see this mixing explicitly, the Hamiltonian can be

rewritten in the "plane wave-pure orbital"-basis. The result is[2]

$$
\begin{aligned}
H_\uparrow = \sum_k \Big( & \tilde{S} c_{ks}^\dagger c_{ks} + S \left( e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right) c_{ks}^\dagger c_{ks} + \\
& + A \left( e^{ik_x a} - e^{-ik_x a} + i e^{ik_y a} - i e^{-ik_y a} \right) c_{ks}^\dagger c_{kp} + \\
& + \tilde{P} c_{kp}^\dagger c_{kp} + P \left( e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right) c_{kp}^\dagger c_{kp} + \\
& + A^* \left( -e^{ik_x a} + e^{-ik_x a} + i e^{ik_y a} - i e^{-ik_y a} \right) c_{kp}^\dagger c_{ks} \Big), \\
H_\downarrow = \sum_k \Big( & \tilde{S} c_{ks}^\dagger c_{ks} + S \left( e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right) c_{ks}^\dagger c_{ks} + \\
& + A^* \left( e^{ik_x a} - e^{-ik_x a} - i e^{ik_y a} + i e^{-ik_y a} \right) c_{ks}^\dagger c_{kp} + \\
& + \tilde{P} c_{kp}^\dagger c_{kp} + P \left( e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right) c_{kp}^\dagger c_{kp} + \\
& - A \left( e^{ik_x a} - e^{-ik_x a} + i e^{ik_y a} - i e^{-ik_y a} \right) c_{kp}^\dagger c_{ks} \Big).
\end{aligned}
\tag{3.6}
$$

This is more compactly written as

$$
\begin{aligned}
H_\uparrow = \sum_k \Big( & \left( \tilde{S} + 2S \left( \cos(k_x a) + \cos(k_y a) \right) \right) c_{ks}^\dagger c_{ks} + \\
& + 2iA \left( \sin(k_x a) + i \sin(k_y a) \right) c_{ks}^\dagger c_{kp} + \\
& + \left( \tilde{P} + 2P \left( \cos(k_x a) + \cos(k_y a) \right) \right) c_{kp}^\dagger c_{kp} + \\
& + 2iA^* \left( -\sin(k_x a) + i \sin(k_y a) \right) c_{kp}^\dagger c_{ks} \Big), \\
H_\downarrow = \sum_k \Big( & \left( \tilde{S} + 2S \left( \cos(k_x a) + \cos(k_y a) \right) \right) c_{ks}^\dagger c_{ks} + \\
& + 2iA^* \left( \sin(k_z a) - i \sin(k_y a) \right) c_{ks}^\dagger c_{kp} + \\
& + \left( \tilde{P} + 2P \left( \cos(k_x a) + \cos(k_y a) \right) \right) c_{kp}^\dagger c_{kp} + \\
& - 2iA \left( \sin(k_x a) + i \sin(k_y a) \right) c_{kp}^\dagger c_{ks} \Big).
\end{aligned}
\tag{3.7}
$$

To further rewrite this expression, define

$$
\begin{aligned}
S - P &= 2B, \\
\tilde{S} - \tilde{P} + 4S - 4P &= 2M, \\
A(k) &= 2iA \left( \sin(k_x a) + i \sin(k_y a) \right), \\
\epsilon(k) &= \frac{\tilde{S} + \tilde{P}}{2} + (S + P) \left( \cos(k_x a) + \cos(k_y a) \right)
\end{aligned}
\tag{3.8}
$$

---

[2]Evaluate the matrix elements $\langle \phi_{k's} | H | \phi_{ks} \rangle$, $\langle \phi_{k'p} | H | \phi_{kp} \rangle$, $\langle \phi_{k's} | H | \phi_{kp} \rangle$, $\langle \phi_{k'p} | H | \phi_{ks} \rangle$ with the Hamiltonian in the lattice site basis to arrive at this expression. The of diagonal elements are zero because of the sum over $i$, and the sum over $k$ and $k'$ in the momentum-basis therefore reduces to a sum over $k$. The momentum-basis states has to be assumed to be normalized so that $\sum_i \langle \phi_{k's} | \phi_{ks} \rangle = \sum_i \langle \phi_{k'p} | \phi_{kp} \rangle = 1$.

The expression then becomes

$$H_\uparrow = \sum_k \left( (\epsilon(k) + M - 2B(2 - \cos(k_x a) - \cos(k_y a))) c_{ks}^\dagger c_{ks} + A(k) c_{ks}^\dagger c_{kp} + \right.$$

$$+ (\epsilon(k) - M + 2B (2 - \cos(k_x a) - \cos(k_y a))) c_{kp}^\dagger c_{kp} + A^*(k) c_{kp}^\dagger c_{ks} \right),$$

$$H_\downarrow = \sum_k \left( (\epsilon(k) + M - 2B (2 - \cos(k_x a) - \cos(k_y a))) c_{ks}^\dagger c_{ks} - A^*(k) c_{ks}^\dagger c_{kp} + \right.$$

$$+ (\epsilon(k) - M + 2B (2 - \cos(k_x a) - \cos(k_y a))) c_{kp}^\dagger c_{kp} - A(k) c_{kp}^\dagger c_{ks} \right). \tag{3.9}$$

One further definition

$$M(k) = M - 2B(2 - \cos(k_x a) - \cos(k_y a)), \tag{3.10}$$

gives the expression

$$H_\uparrow = \sum_k \left( (\epsilon(k) + M(k)) c_{ks}^\dagger c_{ks} + A(k) c_{ks}^\dagger c_{kp} + \right.$$

$$+ (\epsilon(k) - M(k)) c_{kp}^\dagger c_{kp} + A^*(k) c_{kp}^\dagger c_{ks} \right),$$

$$H_\downarrow = \sum_k \left( (\epsilon(k) + M(k)) c_{ks}^\dagger c_{ks} - A^*(k) c_{ks}^\dagger c_{kp} + \right.$$

$$+ (\epsilon(k) - M(k)) c_{kp}^\dagger c_{kp} - A(k) c_{kp}^\dagger c_{ks} \right). \tag{3.11}$$

In matrix notation this is

$$H = \epsilon(k)I + \begin{bmatrix} M(k) & A(k) & 0 & 0 \\ A^*(k) & -M(k) & 0 & 0 \\ 0 & 0 & M(k) & -A^*(k) \\ 0 & 0 & -A(k) & -M(k) \end{bmatrix}. \tag{3.12}$$

Now looking back at the definitions it is easy to see that $M(k) = M(-k)$ and $A(k) = -A(-k)$. This means that the Hamiltonian as well can be written as

$$H = \epsilon(k)I + \begin{bmatrix} M(k) & A(k) & 0 & 0 \\ A^*(k) & -M(k) & 0 & 0 \\ 0 & 0 & M(-k) & A^*(-k) \\ 0 & 0 & A(-k) & -M(-k) \end{bmatrix}. \tag{3.13}$$

## 3.5   Summary

The tight binding model considered gives the following Hamiltonian

$$H = \epsilon(k)I + \begin{bmatrix} M(k) & A(k) & 0 & 0 \\ A^*(k) & -M(k) & 0 & 0 \\ 0 & 0 & M(-k) & A^*(-k) \\ 0 & 0 & A(-k) & -M(-k) \end{bmatrix}, \tag{3.14}$$

where[3]

$$M(k) = M - 2B\left(2 - \cos(k_x a) - \cos(k_y a)\right),$$
$$A(k) = 2iA\left(\sin(k_x a) + i\sin(k_y a)\right),$$
$$\epsilon(k) = \frac{\tilde{S} + \tilde{P}}{2} + (S + P)\left(\cos(k_x a) + \cos(k_y a)\right),$$
$$M = \frac{\tilde{S} - \tilde{P}}{2} + 2S - 2P,$$
$$B = \frac{S - P}{2}, \tag{3.15}$$
$$S = \langle s_{(x,y)}|H|s_{(x+a,y)}\rangle,$$
$$P = \langle p_{(x,y)}|H|p_{(x+a,y)}\rangle,$$
$$A = \langle s_{(x,y)}|H|p_{(x,y)}\rangle,$$
$$\tilde{S} = \langle s_{(x,y)}|H|s_{(x,y)}\rangle,$$
$$\tilde{P} = \langle p_{(x,y)}|H|p_{(x,y)}\rangle.$$

---

[3]Note that this result appears to differ slightly from given in for example [10] in that there we have $M(k) = M - 2Ba$

# Chapter 4

# Spin-orbit interaction

## 4.1 Introduction

When a charged particle moves in an electric field, the charge interacts with the electric field in a momentum dependent way. In the non-relativistic limit this interaction is described by a Hamiltonian called the Thomas term, or the spin-orbit interaction. Here this Thomas term will be derived, closely following the derivation given in section 3.3 in J.J. Sakurai's "Advanced quantum physics"[13].

Starting from the relativistic Dirac equation and pulling out the first corrections in the non-relativistic limit one arrives at the non-relativistic Schrödinger equation with some terms added. Among these extra terms there will be one term that reads

$$H_{Thomas} = -\frac{e\hbar\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p})}{4m^2c^2}.$$
(4.1)

This is the Spin-orbit interaction. The reason that it is called the Spin-orbit interaction is that in the case of an electron orbiting an atom with a spherically symmetric potential, the equation can also be written

$$H_{Thomas} = H_{SO} = -\frac{1}{2m^2c^2r}\frac{dV}{dr}\mathbf{S} \cdot \mathbf{L}.$$
(4.2)

This has exactly the same form as the spin-orbit interaction that otherwise is added ad-hoc to the non-relativistic equation. Strictly speaking the spin-orbit interaction is a special case of the Thomas-term. However, in condensed matter physics all kinds of Thomas terms are generally called spin-orbit interaction.

As one special case of the Thomas term, the Rashba interaction is also derived in this chapter. This interaction is one example of an interaction that is referred to as a spin-orbit interaction in condensed matter physics, but which more appropriately would be called a Thomas term. The Rashba interaction describes the interaction between a moving charge in a uniform electric field, and in the case this field is oriented along the $z$-direction, the interaction can be written as

$$H_{Rashba} = \frac{e\hbar^2 E}{4m^2c^2}(\sigma_x k_y - \sigma_y k_x).$$
(4.3)

### 4.1.1   Outline of the derivation

Writing down the Dirac equation in matrix notation the structure of the Dirac equation as two two-component spinors that interacts with each other through a first order differential equation will appear. This much resembles the way the electric and magnetic fields interact with each other through first order differential equations in Maxwell's theory. The two-component spinors will be called $\Psi_A$ and $\Psi_B$ and will together make up the four-component spinor $\Psi = (\Psi_A, \Psi_B)$ of the Dirac equation. Just like for the electric and magnetic fields in Maxwell's theory the two two-compont spinors can then be substituted into each others differential equation in order to obtain two uncoupled second order equations. The two fields therefore ends up being coupled only through possible boundary condition. The $\Psi_B$ field will further show to go to zero in the non-relativistic limit, leaving $\Psi_A$ as the non-relativistic solution. Consulting the normalization condition for $\Psi$, the first order correction to $\Psi_A$ from the non-zero value of $\Psi_B$ will then be found. Finally, after inserting the first order corrected $\Psi_A$ into it's second order equation the non-relativistic Shrödinger equation with some correction terms is arrived at. Among the correction terms is the Thomas term, which also is called the spin-orbit interaction.

## 4.2   Derivation of the spin-orbit interaction

### 4.2.1   Dirac equation

As discussed in the outline of the derivation, the Dirac equation can be written in the form of two coupled first order differential equations. To see how this comes about, the Dirac equation will here be written down, transfered into matrix notation, and finally the two coupled equations explicitly extracted.

To begin with the Dirac equation can be written as[1]

$$i\hbar\gamma^\mu\frac{\partial}{\partial x^\mu}\Psi = mc\Psi, \tag{4.4}$$

where $\Psi$ is a four component spinor and $\gamma^\mu$ can be represented by the matrices

$$\gamma^0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \gamma^i = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}. \tag{4.5}$$

Notice that each entry in the matrix is a two-by-two matrix, the 1's are unit matrices. Making the substitution $\frac{\partial}{\partial x^\mu} \rightarrow \frac{\partial}{\partial x^\mu} + \frac{ie}{\hbar c}A_\mu$ in order to account for interactions with the electromagnetic field this expression becomes

$$\gamma^\mu\left(i\hbar\frac{\partial}{\partial x^\mu} - \frac{e}{c}A_\mu\right)\Psi = mc\Psi. \tag{4.6}$$

In the matrix representation this is

$$\begin{bmatrix} i\frac{\hbar}{c}\frac{\partial}{\partial t} - \frac{e}{c}A_0 & -i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A} \\ i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A} & -i\frac{\hbar}{c}\frac{\partial}{\partial t} + \frac{e}{c}A_0 \end{bmatrix}\begin{bmatrix} \Psi_A \\ \Psi_B \end{bmatrix} = mc\begin{bmatrix} \Psi_A \\ \Psi_B \end{bmatrix}, \tag{4.7}$$

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[1]3.31 in Advanced Quantum Mechanics by J.J. Sakurai

where the first and last two components of $\Psi$ has been grouped together into two-component spinors labeled $\Psi_A$ and $\Psi_B$.

From this equation it is seen that the Dirac equation can be written as two coupled first order equations that reads[2]

$$\frac{1}{c}\left(mc^2 - i\hbar\frac{\partial}{\partial t} + eA_0\right)\Psi_A = \left(-i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_B,$$
$$\frac{1}{c}\left(mc^2 + i\hbar\frac{\partial}{\partial t} - eA_0\right)\Psi_B = \left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A.$$
(4.8)

The first step of writing the Dirac equation as a set of two coupled first order differential equations is thereby done.

## 4.2.2 Eigenmode analysis and the vanishing of $\Psi_B$ for small energies

Now that the two coupled equations are arrived at, the next step is to simplify the expression a bit in the following way. Because

$$\Psi = \Psi(x)e^{-iEt/\hbar}$$
(4.9)

is an eigenfunction to the time derivative, the Dirac equation (4.4) can actually be analyzed for a single $E$ and then solved generally by superposition of such solutions. The explicit expression of the factor $e^{-iEt/\hbar}$ carries over to the $\Psi_A$ and $\Psi_B$ expressions. This results in a problem where the time derivatives are replaced by $-i\frac{E}{\hbar}$, and only the space coordinates of the sought for solutions $\Psi_A$ and $\Psi_B$ are of importance:

$$\frac{1}{c}\left(mc^2 - E + eA_0\right)\Psi_A = \left(-i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_B,$$
$$\frac{1}{c}\left(mc^2 + E - eA_0\right)\Psi_B = \left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A.$$
(4.10)

The $E$ that is introduced here is of course the energy of the corresponding mode and the equations arrived at are the equations for the position space eigenfunctions.

Now note that as $E - eA_0 \to mc^2$ the equation becomes

$$0 = \left(-i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_B,$$
$$2mc\Psi_B = \left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\mathbf{A}\right)\Psi_A.$$
(4.11)

For this to hold $\Psi_B$ must approach zero in the same limit, for the right hand side of the second equation goes to zero as $v \to 0$. As long as $\Psi_B$ is very small, which it will be close to this limit, it does not affect the full differential equation for $\Psi_A$ in (4.11) very much. The $\Psi_A$ expression can therefore be said to contain all relevant information

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[2]I find it quite amusing to see that the time derivative of $\Psi_A$ depends on the space derivatives of $\Psi_B$ and vice versa, just as for $\mathbf{E}$ and $\mathbf{B}$ in Maxwell's equations. Corresponding to the source term in Maxwell's equation does however the field itself do here, and there is a "source" term for both $\Psi_A$ and $\Psi_B$.

and the interaction with the $\Psi_B$ part can be seen as a perturbation. However, before treating it as a perturbation there remains one step, to decouple the equations. Because even though $\Psi_B$ is very small in the second equation, it is multiplied by $2mc$ and might through the first equation carry over a significant influence of $\Psi_A$ upon itself.

Before proceeding to the decoupling it is time to comment on how the limit $E - eA_0 \to mc^2$ relates to the non-relativistic physics. One could imagine that $E$ is far away from $mc^2$ but that $eA_0$ is just so large as to cancel this contribution. However, the case that will be interesting here is when $A_0$ is small and $E$ is close to $mc^2$. This is exactly the limit that we expect in non-relativistic physics, where the total energy consists mainly of the mass term and the electric fields are weak.[3]

### 4.2.3   Decoupling the equations

Having performed the simplification above, it is now time to decouple the equations by substituting one of the expressions into the other. Doing this for both the expressions gives

$$
\left( -i\hbar\boldsymbol{\sigma} \cdot \nabla + \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \frac{c^2}{mc^2 + E - eA_0} \left( i\hbar\boldsymbol{\sigma} \cdot \nabla - \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \Psi_A =
$$
$$
= \left( mc^2 - E + eA_0 \right) \Psi_A,
$$
$$
\left( i\hbar\boldsymbol{\sigma} \cdot \nabla - \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \frac{c^2}{mc^2 - E + eA_0} \left( -i\hbar\boldsymbol{\sigma} \cdot \nabla + \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \Psi_B =
$$
$$
= \left( mc^2 + E - eA_0 \right) \Psi_B.
$$
$$(4.12)$$

Both these equations are exact, but as $\Psi_A$ contains all the interesting information in the non-relativistic limit the second equation can be dropped from now on. The $\Psi_B$ function will however, as said, be incorporated as a first order perturbation. To do this the second of the two coupled relations will be used to express $\Psi_B$ in terms of $\Psi_A$. The equations used to describe the evolution of the system will therefore be the first of the equations above and the second of the coupled equations, giving the set

$$
\left( -i\hbar\boldsymbol{\sigma} \cdot \nabla + \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \frac{c^2}{mc^2 + E - eA_0} \left( i\hbar\boldsymbol{\sigma} \cdot \nabla - \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \Psi_A =
$$
$$
= \left( mc^2 - E + eA_0 \right) \Psi_A, \qquad (4.13)
$$
$$
\Psi_B = \frac{c}{mc^2 + E - eA_0} \left( i\hbar\boldsymbol{\sigma} \cdot \nabla - \frac{e}{c}\boldsymbol{\sigma} \cdot \mathbf{A} \right) \Psi_A
$$

### 4.2.4   Expanding in the non-relativistic limit and restricting to the case $\mathbf{A} = 0$

Even though the differential equations now have been decoupled and the equation governing the evolution of $\Psi_B$ has been dropped, the remaining equation (4.13) is still

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[3]I have not checked this, but I guess that the gauge term in the exponential will put a strict requirement on $E$ to be close to $mc^2$ for this approximation to hold. But if this is not so, then the derivation actually is a bit more general than here. Allowing for the option of fine tuning the electromagnetic potential so that the same approximation is valid even at higher energies.

exact. It is now time to expand this equation around $E - eA_0 = mc^2$. In the first equation terms to first order will be kept. In the second equation $\Psi_B$ is however assumed to be small already at zeroth order because $\Psi_B$ is close to zero, so that expression is only expanded to zeroth order. After expansion the expression becomes

$$\left(-i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\frac{1}{2m}\left(1 - \frac{E - eA_0 - mc^2}{2mc^2}\right) \times$$
$$\times \left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A = \left(mc^2 - E + eA_0\right)\Psi_A, \tag{4.14}$$
$$\Psi_B = \frac{1}{2mc}\left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A.$$

Switching to non-relativistic energy $E^{(NR)} = E - mc^2$ the expression becomes

$$\left(-i\hbar\boldsymbol{\sigma}\cdot\nabla + \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\frac{1}{2m}\left(1 - \frac{E^{(NR)} - eA_0}{2mc^2}\right) \times$$
$$\times \left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A = -\left(E^{(NR)} - eA_0\right)\Psi_A, \tag{4.15}$$
$$\Psi_B = \frac{1}{2mc}\left(i\hbar\boldsymbol{\sigma}\cdot\nabla - \frac{e}{c}\boldsymbol{\sigma}\cdot\mathbf{A}\right)\Psi_A.$$

The expression is becoming increasingly complex. Moreover the effects that are of interest here will be how an electric field influences an electron, not the magnetic field. Therefore the derivation will from this point on be restricted to the case $\mathbf{A} = 0$. To further clean up the expressions $-i\hbar\nabla$ will from now on be denoted $\mathbf{p}$. The equations then are

$$\left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m}\left(1 - \frac{E^{(NR)} - eA_0}{2mc^2}\right)\boldsymbol{\sigma}\cdot\mathbf{p} + eA_0\right)\Psi_A = E^{(NR)}\Psi_A, \tag{4.16}$$
$$\Psi_B = -\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc}\Psi_A.$$

### 4.2.5 Including $\Psi_B$ as a perturbation

At $E - eA_0 = mc^2$ physics has been seen to be described by $\Psi_A$. As this limit is left, $\Psi_B$ is however expected to play an increasing role. It is now time to see how this is incorporated into the equations.

First note that the normalization condition for $\Psi$ is

$$1 = \int \Psi^\dagger\Psi d^3x = \int \left(\Psi_A^\dagger\Psi_A + \Psi_B^\dagger\Psi_B\right)d^3x, \tag{4.17}$$

and that by using the first and zeroth order expansions of $\Psi_A$ and $\Psi_B$ (4.16), this expression becomes

$$1 = \int \Psi_A\left(1 + \frac{\mathbf{p}^2}{4m^2c^2}\right)\Psi_A d^3x. \tag{4.18}$$

The wave function that to second order in $\mathbf{p}$ satisfies this normalization condition is

$$\Psi = \left(1 + \frac{\mathbf{p}^2}{8m^2c^2}\right)\Psi_A, \tag{4.19}$$

which strongly indicates that this might be the wave function that to this order describes the system. To the same order this expression can also be written

$$\Psi_A = \left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)\Psi. \tag{4.20}$$

Using this together with the first equation in (4.16) and multiplying the whole result by $\left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)$, the expression becomes

$$\left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)\left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m}\left(1 - \frac{E^{(NR)} - eA_0}{2mc^2}\right)\boldsymbol{\sigma}\cdot\mathbf{p} + eA_0\right)\times$$
$$\times\left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)\Psi = \left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)E^{(NR)}\left(1 - \frac{\mathbf{p}^2}{8m^2c^2}\right)\Psi. \tag{4.21}$$

Multiplying this out and ignoring most terms with higher order than $\frac{\mathbf{p}^2}{c^2}$ this is[4]

$$\left(\frac{\mathbf{p}^2}{2m} - \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2m}\frac{E^{(NR)} - eA_0}{2mc^2}\boldsymbol{\sigma}\cdot\mathbf{p} + eA_0 - \frac{\mathbf{p}^4}{8m^3c^2} - \frac{\mathbf{p}^2 eA_0}{8m^2c^2} - \frac{eA_0\mathbf{p}^2}{8m^2c^2}\right)\Psi =$$
$$= E^{(NR)}\left(1 - \frac{\mathbf{p}^2}{4m^2c^2}\right)\Psi. \tag{4.22}$$

The non-relativistic Schrödinger equation begins to be visible. At least the $\frac{\mathbf{p}^2}{2m}$ and $eA_0$ terms that are expected are there, and further the $\frac{\mathbf{p}^4}{8m^3c^2}$ term can be recognized as the first relativistic correction to the kinetic energy. After some manipulations in the next section the other terms will show up to give two other relativistic corrections, one of them the Thomas term.

### 4.2.6   Manipulating the expression and extracting the Thomas term

In the last section an expression that at least plausibly was the non-relativistic limit of the Dirac equation was derived. After some manipulations in this section the plausibility will be further strengthened. Because among the terms not realized as obvious non-relativistic terms, one term called the Thomas term will appear which in the case of an electron in a spherically symmetric potential will turn out to be the spin-orbit interaction, a term that has to be added ad-hoc in non-relativistic quantum physics.

But before starting the manipulation, a few things has to be settled. First of all $eA_0$ is nothing other than the the electric potential $V(x)$. Secondly the relations

$$[\boldsymbol{\sigma}\cdot\mathbf{p}, eA_0] = [\boldsymbol{\sigma}\cdot\mathbf{p}, V(x)] = i\hbar\boldsymbol{\sigma}\cdot\nabla V(x) = i\hbar\boldsymbol{\sigma}\cdot\mathbf{E} \tag{4.23}$$

and[5]

$$[\boldsymbol{\sigma}\cdot\mathbf{p}, \boldsymbol{\sigma}\cdot\mathbf{E}] = -i\hbar\nabla\cdot\mathbf{E} - 2i\boldsymbol{\sigma}\cdot(\mathbf{E}\times\mathbf{p}) \tag{4.24}$$

---

[4]Notice that the $\mathbf{p}^4$ term that is kept really not should be dropped because it only is divided by $c^2$.

[5]Consult the appendix to see how to arrive at this expression

will be used.

Having arrived at these commutation relations, it is now time to manipulate (4.22). First of all the second term becomes

$$\frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{2m} \frac{E^{(NR)} - eA_0}{2mc^2} \boldsymbol{\sigma} \cdot \mathbf{p} = E^{(NR)} \frac{\mathbf{p}^2}{4m^2c^2} - \frac{eA_0\mathbf{p}^2}{4m^2c^2} - \frac{ie\hbar\boldsymbol{\sigma} \cdot \mathbf{E}}{4m^2c^2} \boldsymbol{\sigma} \cdot \mathbf{p}. \quad (4.25)$$

Now, to be able to use the commutation relations above to manipulate the fifth term, write $\mathbf{p}^2$ as $(\boldsymbol{\sigma} \cdot \mathbf{p})^2$ and perform the commutation in two steps:

$$\mathbf{p}^2 eA_0 = \boldsymbol{\sigma} \cdot \mathbf{p} eA_0 \boldsymbol{\sigma} \cdot \mathbf{p} + ie\hbar\boldsymbol{\sigma} \cdot \mathbf{p} \boldsymbol{\sigma} \cdot \mathbf{E} =$$
$$= eA_0 \mathbf{p}^2 + ie\hbar\boldsymbol{\sigma} \cdot \mathbf{E} \boldsymbol{\sigma} \cdot \boldsymbol{p} + ie\hbar\boldsymbol{\sigma} \cdot \mathbf{p} \boldsymbol{\sigma} \cdot \mathbf{E} = \quad (4.26)$$
$$= eA_0 \mathbf{p}^2 + 2ie\hbar\boldsymbol{\sigma} \cdot \mathbf{E} \boldsymbol{\sigma} \cdot \mathbf{p} + e\hbar^2 \nabla \cdot \mathbf{E} + 2e\hbar\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p}).$$

Replacing the non commuted terms in (4.22) with these the expression becomes

$$\left( \frac{\mathbf{p}^2}{2m} + eA_0 - \frac{\mathbf{p}^4}{8m^3c^2} - \frac{e\hbar^2 \nabla \cdot \mathbf{E}}{8m^2c^2} - \frac{e\hbar\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p})}{4m^2c^2} \right) \Psi =$$
$$= E^{(NR)}\Psi. \quad (4.27)$$

The fifth term here is the Thomas term. To see that this really gives the spin-orbit interaction for an electron in a spherically symmetric potential write

$$\mathbf{E} = -\frac{dV(r)}{dr} \frac{\mathbf{r}}{r}, \quad (4.28)$$
$$\mathbf{r} \times \mathbf{p} = \mathbf{L},$$

which is valid in such a situation. The Thomas term can then be written

$$H_{Thomas} = -\frac{e\hbar\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p})}{4m^2c^2} = \frac{e\hbar}{4m^2c^2r} \frac{dV(r)}{dr} \mathbf{r} \times \mathbf{p} = \frac{e\hbar}{4m^2c^2r} \frac{dV(r)}{dr} \mathbf{L}, \quad (4.29)$$

which is exactly the spin-orbit interaction that otherwise is added ad-hoc to the non-relativistic equation.

## 4.3 Rashba interaction

The Thomas term is the general expression that can be used to calculate how the motion of a charged particle couples to an electric field in the non-relativistic limit. When making calculations it might however turn out to be a good idea to have expressions that are special cases of this expression. The spin-orbit interaction derived above is one such expression that is valid for charged particles in spherically symmetric potentials. Here another special case that later will be used is derived, the Rashba interaction.

The Rashba interaction describes how a charged particle interacts with an electric field of constant strength and direction. To derive the expression one simply has to assume that the electric field of strength $E$ is oriented in the $\hat{\mathbf{z}}$ direction:

$$\mathbf{E} = E\hat{\mathbf{z}}. \quad (4.30)$$

Now insert this electric field into the expression for the Thomas term to obtain

$$H_{Rashba} = -\frac{e\hbar E\boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \mathbf{p})}{4m^2c^2} = i\frac{e\hbar^2 E}{4m^2c^2}\left(\sigma_y\frac{\partial}{\partial x} - \sigma_x\frac{\partial}{\partial y}\right). \qquad (4.31)$$

Denoting $k_i = -i\frac{\partial}{\partial i}$ this can be written

$$H_{Rashba} = \frac{e\hbar^2 E}{4m^2c^2}\left(\sigma_x k_y - \sigma_y k_x\right). \qquad (4.32)$$

# Chapter 5

# The RKKY interaction

## 5.1 Introduction

In this chapter field theoretical methods will be used to derive the RKKY interaction, an indirect interaction between two localized spins that is mediated by conduction electrons. It relies heavily on the presentation of quantum field theory given by Michael Peskin and Daniel Shroeder in "An Introduction to Quantum Field Theory"[11]. Their presentation is however relativistic while this calculation is non-relativistic. Among the difference from their calculations will be that the Hamiltonian here is non-relativistic, spinors has two instead of four components and the expansion of the position space creation and annihilation operators are expanded in eigenfunctions of the non-relativistic Hamiltonian. Another book that has been very useful is Gerald Mahan's book "Many-Particle Physics"[3], which was a good reference when trying to translate the language in condensed matter physics articles into the language used in "An Introduction to Quantum Field Theory". Further it was Mahan's book that inspired me to try to calculate the energy by the method used here.

### 5.1.1 Description of the interaction

The RKKY interaction between two spins can be understood in the following way. Start with a conducting material in its ground state and add a localized spin to it. The localized spin could for example be an impurity atom with a bound but unpaired electron. Before the spin is added the ground state is a solution to some Hamiltonian $H_0$ of the system, but after adding the spin the ground state will be the solution to a new Hamiltonian that includes the effect of the interaction between the localized spin and the conduction electrons. In the Kondo model such an interaction is accounted for by adding

$$H_{Kondo} = \psi^\dagger(\mathbf{r})(JS) \cdot \boldsymbol{\sigma}\psi(\mathbf{r}), \tag{5.1}$$

to the ordinary Hamiltonian. Here $\mathbf{r}$ is the position of the localized spin and

$$JS = (J_x S_x, J_y S_y, J_z S_z) \tag{5.2}$$

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is a vector where $S_\alpha$ are the expectation value of the spin components of the local-
ized spin, and the $J$ terms has been included to account for the possibility of different
coupling strength in different directions.

The form of this Hamiltonian can be understood if we imagine that the operators
where classical fields and write

$$\int_{S^2} d^2 s |\psi_s(\mathbf{r})|^2 s \cdot (JS),\tag{5.3}$$

where $s$ is a classical spin[1] of the conduction field. In this expression it is seen how
$|\psi(r)|^2$ denotes the particle density of electrons with spin $s$ at $r$, and how it gives
an energy term that is proportional to that density and the scalar product between the
classical spins. There is two differences between these two expressions. The first is
that the former consists of quantum operators, while the other is that the spin degrees of
freedom has been absorbed into the creation and annihilation operators of the quantum
expression.

Now add a second spin to the system, but do not immediately bother about how the
second spin disturbs the ground state. Instead concentrate on another effect, how the
correction of the ground state due to the first spin alters the energy needed to place the
second spin where it is placed. If the first spin had not been present the ground state
would have been different and thus the energy associated with adding the "second"
spin at some site would have been different from the case when the first spin disturbs
the ground state. This energy will also depend on the direction of the two spins and in
this way the two electrons indirectly interacts with each other through the conduction
electrons. The same argument with the notion of first and second spin interchanged
will also give a similar contribution of the energy from adding the first spin.

The RKKY interaction derived here is the main energy contribution to the system
from this kind of interaction. It will be the term arising from calculating the energy
change of the two spins that is due to the first order correction of the ground state from
the other spin. One could imagine a more general expression for the RKKY interaction
where also higher order interactions between the two localized spins are included, these
higher order terms are however not considered here.

### 5.1.2  The idea behind the derivation

The idea behind the derivation that follows will be to start with the ground state of the
Hamiltonian that not includes the localized spins and evolve this state from $-\infty \to 0$
with the full Hamiltonian, treating the Kondo term as a perturbation. Then multiply the
ground state by the Hamiltonian corresponding to the energy that is wanted to calculate,
and finally multiply by the Hermitian conjugate of the evolved ground state. That is, if
the unperturbed ground state is denoted by $|G\rangle$ and the perturbed ground state by $|I\rangle$
we will evolve $|G\rangle \to |I\rangle$, then sandwich the Hamiltonian $H$ that corresponds to the
energy we want to calculate between the evolved states to get

$$E = \langle I|H|I\rangle.\tag{5.4}$$

---

[1]Here I mean for example a magnetic dipole of fixed strength arising from a small current carrying loop,
which is representable by a three dimensional vector with its tip on the unit sphere.
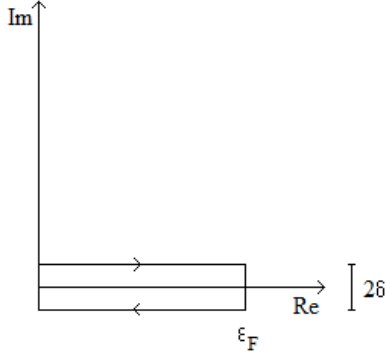
Figure 5.1: Integration contour for the energy integral in the calculation of $H_{RKKY}$.

The energy calculated in this way would be the total energy of the system, and because the RKKY interaction is just one part[2] of this energy, the full energy expression will be written down and then the RKKY terms will be extracted.

After the expression for the RKKY interaction has been extracted the expression is rewritten in terms of Green's functions and the final expression becomes

$$H_{RKKY} =$$

$$= \frac{i}{\pi} \int_\Gamma dE \sum_{i \neq j} Tr[(JS_i) \cdot \boldsymbol{\sigma} G(\mathbf{R}_{ij})(JS_j) \cdot \boldsymbol{\sigma} G(-\mathbf{R}_{ij})], \tag{5.5}$$

where $\Gamma$ is the contour in figure (5.1.2), $\mathbf{R}_{ij}$ is the vector between the two localized spins, and

$$G(\mathbf{R}_{ij}) = \int \frac{d^2 k}{(2\pi)^2} \frac{1}{E - H_0} e^{-i\mathbf{k}\cdot\mathbf{R}_{ij}}. \tag{5.6}$$

### 5.1.3 The particle picture

The calculations that follows will be in a wave picture of quantum physics. Creation and annihilation operators can with the wave picture in mind be seen as correcting the Fourier coefficients in the mathematical description of the system, rather than really creating and annihilating particles. A correction that has to be done because we start with a false ground state. It is however very interesting to see what an analysis of the same derivation with the particle picture in mind[3] has to say. In this framework one can interpret the interaction as arising from creation of electron-hole pairs at one of the localized spins, which then propagates to the other localized spin where they recombine.

---

[2]First order correction to the energy needed to place the localized spins at their sites, arising from the perturbation of the ground state by the other spin.

[3]It is up to the reader to read the derivation that follows with a particle picture in mind.

## 5.2   Derivation of the RKKY interaction

Now that the preliminaries are settled the total Hamiltonian of the system can be written down. If $H_0$ is the Hamiltonian for the conduction electrons and $H_{Kondo}$ is the Kondo Hamiltonian (5.1), then the total Hamiltonian can be written as

$$H = H_0 + \sum_i H_{Kondo}(\mathbf{r}_i), \tag{5.7}$$

where $i$ runs over the indices of the two localized spins. Writing out the Kondo term this is

$$H = H_0 + \sum_i \psi^\dagger(\mathbf{r}_i)(JS_i) \cdot \sigma \psi(\mathbf{r}_i). \tag{5.8}$$

To not be forced to explicitly write out the summation sign through the derivation that follows we now define

$$H_{2Kondo} = \sum_i \psi^\dagger(\mathbf{r}_i)(JS_i) \cdot \sigma \psi(\mathbf{r}_i), \tag{5.9}$$

so that the Hamiltonian can be written as

$$H = H_0 + H_{2Kondo}. \tag{5.10}$$

### 5.2.1   Interaction picture

Now the problem is to be formulated in the interaction picture. To do this we begin with the Shrödinger equation in the Schrödinger representation,

$$\frac{\partial \psi(t)}{\partial t} = H\psi(t). \tag{5.11}$$

Knowing the initial condition at some time $t = t_0$, the solution to the Shrödinger equation above can be written as

$$\psi(t) = e^{-iH(t-t_0)}\psi(t_0). \tag{5.12}$$

Further, the following calculation[4]

$$\frac{\partial}{\partial t} e^{iH_0(t-t_0)} e^{-iH(t-t_0)} \psi(t_0) = e^{iH_0(t-t_0)} \left(iH_0 - iH\right) e^{-iH(t-t_0)} \psi(t_0) =$$
$$= -i e^{iH_0(t-t_0)} H_{2Kondo} e^{-iH_0(t-t_0)} e^{iH_0(t-t_0)} e^{-iH(t-t_0)} \psi(t_0), \tag{5.13}$$

---

[4]There is a slight asymmetry in the derivation performed here. It is important to realize that $e^{iH_0(t-t_0)}$ is the inverse of $e^{-iH_0(t-t_0)}$ and that the derivation therefore places $iH_0$ on the right hand side of the exponential. For the same reason $iH$ is placed to the left of $e^{-iH(t-t_0)}$. The asymmetry is however not present if the Hamiltonian is time invariant, as the Hamiltonian then commutes with the exponential. The asymmetry is most easily understood if the exponential is written down as $e^{-iH(t-t_0)} = (1 - iH(t - dt)dt)...(1 - iH(t_0 + dt)dt)(1 - iH(t_0)dt)$. Some more information about the exponentiation of Hamiltonians is provided in the section on Dyson expansion that follows.

shows that we can write

$$\frac{\partial \hat{\psi}(t)}{\partial t} = -i\hat{H}_{2Kondo}(t)\hat{\psi}(t), \tag{5.14}$$

where

$$\hat{\psi}(t) = e^{iH_0(t-t_0)}e^{-iH(t-t_0)}\psi(t_0),$$
$$\hat{H}_{2Kondo}(t) = e^{iH_0(t-t_0)}H_{2Kondo}e^{-iH_0(t-t_0)}. \tag{5.15}$$

Going over to bracket notation, these equation are written as

$$\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = -i\hat{H}_{2Kondo}(t)U(t,t_0)|\psi(t_0)\rangle, \tag{5.16}$$

where

$$U(t,t_0) = e^{iH_0(t-t_0)}e^{-iH(t-t_0)}. \tag{5.17}$$

Especially we will be interested in the equation

$$\frac{\partial}{\partial t}U(t,t_0)|G\rangle = -i\hat{H}_{2Kondo}(t)U(t,t_0)|G\rangle, \tag{5.18}$$

where $|G\rangle$ is the ground state of $H_0$. This gives us the equation

$$\frac{\partial U(t,t_0)}{\partial t} = -i\hat{H}_{2Kondo}(t)U(t,t_0), \tag{5.19}$$

which completes our reformulation of the problem in the interaction picture.


## 5.2.2 Dyson expansion

The expression above is a compact formulation of the problem. An exact solution to it would be an exact solution to the whole system of conduction and localized electrons. To solve this is however not so easy, neither is it what we are trying to do. We are not interested in the solution to the whole system, rather in a specific part of the energy that arises from this solution. In the introduction I said that we were interested in the first order correction of the wave function from one electron and how it affects the energy associated with the other, and vice versa. But what do we mean by first order correction to the wave function? That is what will be explained in this section. The first order correction refers to the first order term in the Dyson expansion of the problem, and we will see here what that means.

In a system where the Hamiltonians varies with time, the exponential expressions involving the Hamiltonian above does not make much sense if we don't know what they really mean. A much more elusive way of writing down the solution, which also is required to really understand what the exponentials means in case of time dependent Hamiltonians, is to write the solution of (5.19) as

$$U(t,t_0) = U(t_0,t_0) - i\int_{t_0}^{t} d\tau \hat{H}_{2Kondo}(\tau)U(\tau,t_0) = 1 - i\int_{t_0}^{t} d\tau \hat{H}_{2Kondo}(\tau)U(\tau,t_0), \tag{5.20}$$

which after iterative insertion of $U(\tau, t_0)$ becomes

$$U(t, t_0) = \sum_{n=0}^{\infty} (-i)^n \int_{t_0}^{t} dt_1 ... \int_{t_0}^{t_{n-1}} dt_n \hat{H}_{2Kondo}(t_1)...\hat{H}_{2Kondo}(t_n). \qquad (5.21)$$

This is the Dyson expansion of the solution, and the first order correction is the term with $n = 1$. Now we have seen what the first order correction is and have come one step closer to the calculation we are about to do. But first it would be nice to see how the exponential form fits together with this. Therefore we use the notion of a time ordering operator which puts the operators in time order (latest time to the left) and writes the above equation as

$$U(t, t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 ... \int_{t_0}^{t} T \left[ \hat{H}_{2Kondo}(t_1)...\hat{H}_{2Kondo}(t_n) \right]. \qquad (5.22)$$

What we have done is to extend all integral limits to $t$ now that we don't have to worry about the time order explicitly, at the same time we have introduced a factor of $\frac{1}{n!}$ and these two modifications cancels each other. Looking at this last expression it is very similar in form to the expansion of an exponential. Therefore we define

$$e^{-i \int_{t_0}^{t} \hat{H}_{2Kondo} dt} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 ... \int_{t_0}^{t} dt_n T \left[ \hat{H}_{2Kondo}(t_1)...\hat{H}_{2Kondo}(t_n) \right],$$
$$(5.23)$$

and keeps in mind that the left hand side is an abbreviation of the right hand expression. Further we note that as long as the Hamiltonians are time invariant the time ordering operator is unimportant. The integrations can then easily be performed and we arrive at the expression

$$U(t, t_0) = e^{-i\hat{H}_{2Kondo}(t-t_0)} = \sum_{n} \frac{(-i)^n}{n!} \hat{H}_{2Kondo}(t - t_0)^n. \qquad (5.24)$$

Now we have seen how the solution of the Schrödinger equation in the interaction picture can be expanded into Dyson series where corrections of different order can be calculated. We have also connected this solution method with the method of multiplying the ground state with an exponential of a Hamiltonian and given much more sense to such expressions. Giving the method validity also for time dependent Hamiltonian as long as it is seen as an abbreviation of the Dyson series expansion.

### 5.2.3 Constructing the ground state

Assume that the the ground state $|G\rangle$ of $H_0$ is known. Is there then a way in which the ground state $|I\rangle$ of $H$ can be determined? The idea of the following construction will be to start with the ground state at some time $t' < 0$, introduce the perturbation $H_{2Kondo}$ into the system and evolve it until $t = 0$. Assuming that the overlap between $|I\rangle$ and $|G\rangle$ is nonzero and introducing a term that causes all energy states that are

higher than the new ground state to decay, this procedure allows us to calculate $|I\rangle$. The derivation will be done in the Heisenberg picture but the result can then be translated to the interaction picture as soon as it is done.

To see how this is done, expand the ground state of $H_0$ in eigenstates $|J\rangle$ of $H$ and evolve it from $t' \to 0$,

$$e^{iHt'}|G\rangle = e^{iE_I t'}\langle I|G\rangle|I\rangle + \sum_{J\neq I} e^{iE_J t'}\langle J|G\rangle|J\rangle. \tag{5.25}$$

However, making a slight redefinition of $t'$ so that the $t'$ above lies along the line $1 + i\epsilon$ in the complex plane, the expression becomes

$$e^{iH(1+i\epsilon)t'}|G\rangle = e^{iE_I(1+i\epsilon)t'}\langle G|I\rangle|I\rangle + \sum_{J\neq I} e^{iE_J(1+i\epsilon)t'}\langle J|G\rangle|J\rangle. \tag{5.26}$$

The effect of this is to make the egeinstates decay with the rate $e^{-E_J \epsilon}$ from $t = t'$ to $t = 0$. The state that will decay slowest is $|I\rangle$ and by a renormalization of the evolved state, that will be done in a moment, we can remove the decay of $|I\rangle$ completely. Leaving the rest of the states decaying slightly slower, but still decaying. For $t' \to -\infty$ (i.e. giving the system a long time to settle down to adopt to the new Hamiltonian) the expression can therefore be written as

$$e^{iH(1+i\epsilon)t'}|G\rangle = e^{iE_I(1+i\epsilon)t'}\langle G|I\rangle|I\rangle. \tag{5.27}$$

After a rearrangement this reads[5]

$$|I\rangle = (e^{iE_I(1+i\epsilon)t'}\langle G|I\rangle)^{-1}e^{iH(1+i\epsilon)t'}|G\rangle, \tag{5.28}$$

and the corresponding bra expression reads

$$\langle I| = (e^{iE_I(1-i\epsilon)t'}\langle G|I\rangle)^{-1}\langle G|e^{-iH(1+i\epsilon)t'}. \tag{5.29}$$

The perturbed ground state is now expressed in terms of the unperturbed one and it is seen how the new ground state is arrived at through evolving the unperturbed ground state for a long time with the perturbed Hamiltonian and letting the states decay proportionally to their energy.

### 5.2.4 Calculating expectation values

Now, to calculate any expectation value of an operator at $t = 0$, simply sandwich it between the brackets in the ordinary way, which gives

$$<\hat{O}> = \langle I|\hat{O}|I\rangle = (e^{-iE_I(1-i\epsilon)t'}\langle G|I\rangle)^{-2}\langle G|U(t',0)\hat{O}U(0,t')|G\rangle. \tag{5.30}$$

The effect of the normalization factor in front of the expression will be to cancel terms in the rest of the expression that arises from terms corresponding to disconnected Feynman diagrams.[6] Therefore, as long as it is kept in mind that only terms corresponding

---

[5]This is the renormalization mentioned above

[6]For a more thorough description of how this comes about, consult section 4.2 and 4.4 in "An Introduction to Quantum Field Theory"[11]

to fully connected Feynman diagrams should be calculated, the expression can with a slight abuse of notation be written as

$$< \hat{O} >= \langle I|\hat{O}|I\rangle = \langle G|U(t',0)\hat{O}U(0,t')|G\rangle. \tag{5.31}$$

### 5.2.5   Expanding the ground state to first order

The expressions above are exact. Now it is time to begin to approximate and find the terms that we are interested in calculating. Therefore begin by expressing the correction of the ground state up to first order[7]

$$|I\rangle = (1 - i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(t_1))|G\rangle. \tag{5.32}$$

The corresponding bra expression is

$$\langle I| = \langle G|(1 + i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(t_1)), \tag{5.33}$$

### 5.2.6   Finding the RKKY interaction

The energy we are interested in calculating resides inside $H_{2Kondo}$ and we therefore begin by writing down the full expression for this energy and filters in a moment out the part that is the RKKY term. The expectation value for the $H_{2Kondo}$ Hamiltonian is

$$< \hat{H}_{2Kondo}(0) >= \langle I|\hat{H}_{2Kondo}(0)|I\rangle. \tag{5.34}$$

To first order correction in the ground state this is

$$
\begin{aligned}
< \hat{H}_{2Kondo}(0) >= \langle G| \left(1 + i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(t_1)\right) \hat{H}_{2Kondo}(0) \times \\
\times \left(1 - i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(t_1)\right)|G\rangle = \\
= \langle G| \left(\hat{H}_{2Kondo}(0) + i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(t_1)\hat{H}_{2Kondo}(0) - \right. \\
\left. -i \int_{-\infty}^{0} dt_1 \hat{H}_{2Kondo}(0)\hat{H}_{2Kondo}(t_1) + ...\right)|G\rangle,
\end{aligned}
\tag{5.35}
$$

where ... denotes terms with higher order than 2 in $\hat{H}_{2Kondo}$. By introducing the loop ordering operator $T_l$, that orders the operators so that those with largest integration

---

[7]From now on $t'$ is sent to $-(1 + i\epsilon)\infty$ and all calculations are performed along the line $(1 + i\epsilon)t$, but the prefactor is not explicitly written out. $-\infty$ therefore actually means $-(1 + i\epsilon)\infty$.

parameter stands to the left, we can rewrite this expression as

$$< \hat{H}_{2Kondo}(0) >= \langle G| \left( \hat{H}_{2Kondo}(0) - i \int_0^{-\infty} dt_1 \hat{H}_{2Kondo}(t_1) \hat{H}_{2Kondo}(0) - \right.$$
$$\left. -i \int_{-\infty}^0 \hat{H}_{2Kondo}(0) \hat{H}_{2Kondo}(t_1) \right) |G\rangle =$$
$$= \langle G| \left( \hat{H}_{2Kondo}(0) - i \int_{-\infty \to 0 \to -\infty} dt_1 T_l \left[ \hat{H}_{2Kondo}(t_1) \hat{H}_{2Kondo}(0) \right] \right) |G\rangle. \tag{5.36}$$

The first term is just the energy contribution that arises from putting two spins into the unperturbed ground state without taking into consideration the modification of the ground state. We are interested in the part of the energy shift that arises from the first order correction of the wave function and that is given by the second term. So lets call that term $\hat{H}_{2Kondo,FOC}(0)$[8]

$$< \hat{H}_{2Kondo,FOC}(0) >= -i\langle G| \int_{loop} dt_1 T_l \left[ \hat{H}_{2Kondo}(t_1) \hat{H}_{2Kondo}(0) \right] |G\rangle, \tag{5.37}$$

where loop means integration over $-\infty \to 0 \to -\infty$. Explicitly writing out the $\hat{H}_{2Kondo}$ expressions we have

$$< \hat{H}_{2Kondo,FOC}(0) >=$$
$$= -i\langle G| \int_{loop} dt_1 T_l \left[ \sum_{i,j} \hat{\psi}^\dagger(\boldsymbol{r}_i, t_1) \left( J\hat{S}_i \right) \cdot \hat{\boldsymbol{\sigma}} \hat{\psi}(\boldsymbol{r}_i, t_1) \hat{\psi}^\dagger(\boldsymbol{r}_j, 0) \left( J\hat{S}_j \right) \cdot \hat{\boldsymbol{\sigma}} \hat{\psi}(\boldsymbol{r}_j, 0) \right] |G\rangle. \tag{5.38}$$

Finally we are ready to make the final reduction of this expression to obtain the RKKY interaction. We do not bother about how the energy of inserting a spin is influenced by the first order correction of the ground state due to itself, but only how that energy is affected by the first order correction arising from the other spin. Therefore we restricting the summation to $i \neq j$ and call this term $H_{RKKY}(0)$. The RKKY interaction energy is therefore given by

$$< \hat{H}_{RKKY}(0) >=$$
$$= -i\langle G| \int_{loop} dt_1 T_l \left[ \sum_{i \neq j} \hat{\psi}^\dagger(\boldsymbol{r}_i, t_1) \left( J\hat{S}_i \right) \cdot \hat{\boldsymbol{\sigma}} \hat{\psi}(\boldsymbol{r}_i, t_1) \hat{\psi}^\dagger(\boldsymbol{r}_j, 0) \left( J\hat{S}_j \right) \cdot \hat{\boldsymbol{\sigma}} \hat{\psi}(\boldsymbol{r}_j, 0) \right] |G\rangle. \tag{5.39}$$

## 5.3 Manipulating the expression

Having arrived at the RKKY interaction it is time to turn it into an expression that can be calculated. However, before we can do this we have to go through some notation

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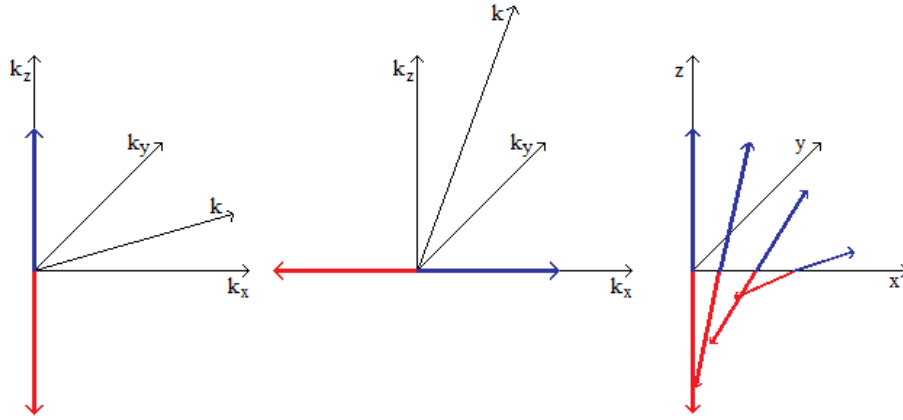
[8]FOC for First Order Correction.

Figure 5.2: Blue and red arrows, representing high and low energy configuration of the spin for a conduction electron. The first two figures shows how the direction for the high and low levels can depend on the **k**-vector associated with the electron. The third figure shows how the high and low energy configuration of the spin can vary with position. The direction could also depend on both **k** and the position at the same time.

that will enable us to make the manipulations that then follows. Therefore begin by denoting the eigenstates of the unperturbed Hamiltonian with $u(s)\psi_n^s$, where n is an index that runs over the momentum-position degrees of freedom, s is a spin index and u(s) is a two component spinor. In the case that is going to be treated later the energy is dependent on the spin direction, moreover the quantization axis that separates the two spin states into lower and higher energy states will depend on the $n$ index. The state referred to as $s =\uparrow$ should throughout this derivation therefore be understood to have a spin up in a direction that is dependent on $n$. To be completely general the quantization direction could also depend on the position, and as long as this is kept in mind the derivation is valid for such cases too (see figure (5.3)). One only has to be careful to not take any intermediate step in the derivation, fix quantization axis and expect to be able to use the expression to calculate the RKKY interaction energy. Any intermediate state is however obviously valid to use for evaluating the RKKY interaction if the variable spin quantization axis is taken into account. The final expression derived will be expressed in such a way that the quantization axis can be chosen in a single and arbitrary direction and makes it the most suitable for actual calculations.

### 5.3.1 Expansion of operators

Now that the notion of the eigenstates are clear, the operators we are about to use can be expanded in this basis. For the creation and annihilation operators we have

$$
\psi(x_i) = \sum_{n,s} a_n^s u(s) \psi_n^s(\mathbf{r}_i),
$$
$$
\psi^\dagger(\mathbf{r}_i) = \sum_{n,s} a_n^{s\dagger} u^\dagger(s) \psi_n^s(\mathbf{r}_i),
$$

(5.40)

where $a_n^{s\dagger}$ and $a_n^s$ are the creation and annihilation operators of the corresponding eigenstates, and they satisfies the anti-commutation relations

$$
\{a_m^{s\dagger}, a_n^{t\dagger}\} = \{a_m^s, a_n^t\} = 0,
$$
$$
\{a_m^{s\dagger}, a_n^t\} = \delta^{nm}\delta^{st}.
$$

(5.41)

The reason for including the summation over the spins inside the definition of $\psi(x_i)$ and $\psi^\dagger(x_i)$ used in (5.1) was that the spin direction could be dependent on $n$. However, now that we have this in mind we write out the summation explicitly. In this basis the Hamiltonian also becomes

$$
H_0 = \sum_{n,s} E_n^s a_n^{s\dagger} a_n^s.
$$

(5.42)

Further the ground state $|G\rangle$ of the unperturbed Hamiltonian is written as

$$
|G\rangle = \prod_{E_n < \epsilon_F, s} a_n^{s\dagger} |0\rangle.
$$

(5.43)

These are general expansions for the expansion in the eigenbasis of the unperturbed Hamiltonian. The expansions of the creation and annihilation operators in the free electron basis is also interesting. Comparing it with the expression above is also useful for understanding the notation because we switch between summation and integration notation. Summation in the first for the general nature of the $n$ index which is hard to account for in an integral notation, and integration in the one that follows because it is a notion that will be used for the actual calculations later. With free electrons as basis the expansion can be written

$$
\psi(\mathbf{r}_i) = \int \frac{d^2k}{(2\pi)^2} \sum_s a_k^s u(s) e^{i\mathbf{k}\cdot\mathbf{r}_i},
$$
$$
\psi^\dagger(\mathbf{r}_i) = \int \frac{d^2k}{(2\pi)^2} \sum_s a_k^{s\dagger} u^\dagger(s) e^{-i\mathbf{k}\cdot\mathbf{r}_i}.
$$

(5.44)

The summation is replaced by an integral, but the anti-commutation relations must also be redefined to agree with the normalization of the integrals. The new anti-commutation relations are

$$
\{a_m^{k\dagger}, a_l^{t\dagger}\} = \{a_k^s, a_l^t\} = 0,
$$
$$
\{a_k^{s\dagger}, a_l^t\} = (2\pi)^2 \delta(k-l)\delta^{st}.
$$

(5.45)

## 5.3.2   The explicit expression

At last it is time to manipulate the expression into a form suitable for performing calculations. This will be done in four steps. First (5.39) will be expressed explicitly in the expansion of its operators and ground state, then the integral will be divided into two parts just as before the loop order operator was introduced and each integral calculated alone. Finally the two results will be combined into the complete solution.

So lets begin with writing out the terms involved explicitly

$$
< \hat{H}_{RKKY}(0) > = -i\langle 0| \prod_{E_k<\epsilon_F,r} a_k^r \int_{loop} dt_1 T_l \left[ \sum_{i\neq j} e^{iH_0 t_1} \times \right.
$$
$$
\times \sum_{p,t} a_p^{t\dagger} u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)(JS_i)\cdot\boldsymbol{\sigma} \sum_{q,u} a_q^u u(u)\psi_q^u(\mathbf{r}_i)e^{-iH_0 t_1} \times
$$
$$
\left. \times \sum_{P,v} a_P^{v\dagger} u^\dagger(v)\psi_P^{v\dagger}(\mathbf{r}_j)\left(JS_j\right)\cdot\boldsymbol{\sigma} \sum_{Q,w} a_Q^w u(w)\psi_Q^w(\mathbf{r}_j) \right] \prod_{E_l<k_F,s} a_l^{s\dagger}|0\rangle
$$

(5.46)

Now it is time to divide the calculation into two parts, what follows is the calculation for the case $t_1 \in [0, -\infty]$ followed by the case $t_1 \in [-\infty, 0]$. That is the late and early part of the time loop respectively. These two parts will be denoted $< \hat{H}_{RKKY}(0) >_{[0,-\infty]}$ and $< \hat{H}_{RKKY}(0) >_{[-\infty,0]}$ to distinguish them from $< \hat{H}_{RKKY}(0) >$.

## 5.3.3   The late expression, $[0, -\infty]$

When $t_1 \in [0, -\infty]$ the operator ordering is the same as inside the loop ordering expression above, because $t = t_1$ then is "after" $t = 0$. Simply removing the loop ordering operator from the expression we have

$$
< \hat{H}_{RKKY}(0) >_{[0,-\infty]} =
$$
$$
= -i\langle 0| \prod_{E_k<\epsilon_F,r} a_k^r \int_0^{-\infty} dt_1 \sum_{i\neq j} e^{iH_0 t_1} \times
$$
$$
\times \sum_{p,t} a_p^{t\dagger} u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)(JS_i)\cdot\boldsymbol{\sigma} \sum_{q,u} a_q^u u(u)\psi_q^u(\mathbf{r}_i)e^{-iH_0 t_1} \times
$$

(5.47)

$$
\times \sum_{P,v} a_P^{v\dagger} u^\dagger(v)\psi_P^{v\dagger}(\mathbf{r}_j)\left(JS_j\right)\cdot\boldsymbol{\sigma} \sum_{Q,w} a_Q^w u(w)\psi_Q^w(\mathbf{r}_j) \prod_{E_l<k_F,s} a_l^{s\dagger}|0\rangle =
$$

Now insert the identity $e^{-iH_0 t_1} e^{iH_0 t_1}$ between $a_p^{t\dagger}$ and $a_q^u$ and move the exponentials next to these operators

$$
= -i\langle 0| \prod_{E_k < \epsilon_F, r} a_k^r \int_0^{-\infty} dt_1 \sum_{i \neq j} \times
$$

$$
\times \sum_{p,t} e^{iH_0 t_1} a_p^{t\dagger} e^{-iH_0 t_1} u^\dagger(t) \psi_p^{t\dagger}(\mathbf{r}_i)(JS_i) \cdot \boldsymbol{\sigma} \times
$$

$$
\times \sum_{q,u} e^{iH_0 t_1} a_q^u e^{-iH_0 t_1} u(u) \psi_q^u(\mathbf{r}_i) \times
$$

$$
\times \sum_{P,v} a_P^{v\dagger} u^\dagger(v) \psi_P^{v\dagger}(\mathbf{r}_j) (JS_j) \cdot \boldsymbol{\sigma} \sum_{Q,w} a_Q^w u(w) \psi_Q^w(\mathbf{r}_j) \prod_{E_l < k_F, s} a_l^{s\dagger} |0\rangle = \quad (5.48)
$$

$$
= -i\langle 0| \prod_{E_k < \epsilon_F, r} a_k^r \int_0^{-\infty} dt_1 \sum_{i \neq j} \times
$$

$$
\times \sum_{p,t} a_p^{t\dagger} e^{iE_p^t t_1} u^\dagger(t) \psi_p^{t\dagger}(\mathbf{r}_i)(JS_i) \cdot \boldsymbol{\sigma} \sum_{q,u} a_q^u e^{-iE_q^u t_1} u(u) \psi_q^u(\mathbf{r}_i) \times
$$

$$
\times \sum_{P,v} a_P^{v\dagger} u^\dagger(v) \psi_P^{v\dagger}(\mathbf{r}_j) (JS_j) \cdot \boldsymbol{\sigma} \sum_{Q,w} a_Q^w u(w) \psi_Q^w(\mathbf{r}_j) \prod_{E_l < k_F, s} a_l^{s\dagger} |0\rangle.
$$

For this to be non zero we see that $a_Q^w$ has to annihilate a state below the Fermi level so that $E_Q \leq \epsilon_F$. Further $a_P^{v\dagger}$ can recreate the same state, but that corresponds to a disconnected Feynman diagram which we ignore[9], so the only other possibility is that it creates a state above the Fermi level so that $E_P > \epsilon_F$. $a_q^u$ then has to destroy the state created by $a_P^{v\dagger}$. This means that we have to have $q = P$ and $t = w$. Finally a similar argument gives us that $p = Q$ and $u = v$. The arguments given are the same as removing the ground states and operators from the expression and inserting $\delta^{pQ} \delta^{tw}$

---

[9]Reread the section "Calculating expectation values" and consult the note given there if this is unclear.

and $\delta^{qP}\delta^{uv}$ into the $P$ and $Q$ sums. Which after summation gives us[10]

$$< \hat{H}_{RKKY}(0) >_{[0,-\infty]}=$$

$$-i\int_0^{-\infty} dt_1 \sum_{i\neq j} \sum_{E_p^t<\epsilon_F,t} e^{iE_p^t t_1} u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)(JS_i)\cdot\boldsymbol{\sigma}\times$$

$$\times \sum_{E_q^u>\epsilon_F,u} e^{-iE_q^u t_1} u(u)\psi_q^u(\mathbf{r}_i)u^\dagger(u)\psi_q^{u\dagger}(\mathbf{r}_j)\,(JS_j)\cdot\boldsymbol{\sigma}u(t)\psi_p^t(\mathbf{r}_j)=$$

$$=-i\int_0^{-\infty} dt_1 \sum_{i\neq j}\sum_{E_p^t<\epsilon_F,t}\sum_{E_q^u>\epsilon_F,u} e^{i(E_p^t-E_q^u)t_1} u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)\times$$

$$\times(JS_i)\cdot\boldsymbol{\sigma}u(u)\psi_q^u(\mathbf{r}_i)u^\dagger(u)\psi_q^{u\dagger}(\mathbf{r}_j)\,(JS_j)\cdot\boldsymbol{\sigma}u(t)\psi_p^t(\mathbf{r}_j)=$$

$$=\sum_{i\neq j}\sum_{E_p^t<\epsilon_F,t}\sum_{E_q^u>\epsilon_F,u}\frac{1}{E_p^t-E_q^u}u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)(JS_i)\cdot\boldsymbol{\sigma}u(u)\psi_q^u(\mathbf{r}_i)\times \qquad (5.49)$$

$$\times u^\dagger(u)\psi_q^{u\dagger}(\mathbf{r}_j)\,(JS_j)\cdot\boldsymbol{\sigma}u(t)\psi_p^t(\mathbf{r}_j)=$$

$$=-\frac{1}{4\pi i}\int_\Gamma dE\sum_{i\neq j}\sum_{p,t}\sum_{q,u}\frac{1}{E-E_p^t}u^\dagger(t)\psi_p^{t\dagger}(\mathbf{r}_i)(JS_i)\cdot\boldsymbol{\sigma}u(u)\times$$

$$\times\psi_q^u(\mathbf{r}_i)\frac{1}{E-E_q^u}u^\dagger(u)\psi_q^{u\dagger}(\mathbf{r}_j)\,(JS_j)\cdot\boldsymbol{\sigma}u(t)\psi_p^t(\mathbf{r}_j)=$$

$$=-\frac{1}{4\pi i}\int_\Gamma dE\sum_{i\neq j}\sum_{p,t}\sum_{q,u}u^\dagger(t)(JS_i)\cdot\boldsymbol{\sigma}\frac{1}{E-E_q^u}\psi_q^{u\dagger}(\mathbf{r}_j)\psi_q^u(\mathbf{r}_i)\times$$

$$\times u(u)u^\dagger(u)\,(JS_j)\cdot\boldsymbol{\sigma}\frac{1}{E-E_p^t}\psi_p^{t\dagger}(\mathbf{r}_i)\psi_p^t(\mathbf{r}_j)u(t)=$$

The $\Gamma$-contour integrated along here is that shown in figure (5.1.2).

Denoting the unperturbed Hamiltonian expressed in momentum-position-spin space coordinates (i.e. with derivatives, position coordinates and spin matrices) with $\tilde{H}_0$ this can be written

$$=-\frac{1}{4\pi i}\int_\Gamma dE\sum_{i\neq j}\sum_{p,t}\sum_{q,u}u^\dagger(t)(JS_i)\cdot\boldsymbol{\sigma}\frac{1}{E-\tilde{H}_0}\psi_q^{u\dagger}(\mathbf{r}_j)\psi_q^u(\mathbf{r}_i)\times$$

$$\times u(u)u^\dagger(u)\,(JS_j)\cdot\boldsymbol{\sigma}\frac{1}{E-\tilde{H}_0}\psi_p^{t\dagger}(\mathbf{r}_i)\psi_p^t(\mathbf{r}_j)u(t)= \qquad (5.50)$$

---

[10]In the second step a convergence factor $e^{\epsilon t_1}$ has to be added to the integral to assure that the integral converges and not oscillates in the integration limit $-\infty$. This is to get rid of oscillating terms similar to those that are ignored in the calculation of $\delta(x)=\frac{1}{2\pi}\int_{-\infty}^\infty e^{ikx}dk$ and is similar to require that the wave function we actually are considering is $L^2$ convergent. Also, the third step actually is a bit more involved than it at first sight might appear. To arrive at the fourth expression an integration along the $\Gamma$-contour is performed. The antisymmetric relations $E_p^t<\epsilon_F$, $E_q^u>\epsilon_F$ and term $\frac{1}{E_p-E_q}$ are replaced by the symmetric term $\frac{1}{E-E_p^t}\frac{1}{E-E_q^u}$. To to do this the relations $\int_\Gamma dE\frac{1}{E-E_p^t}\frac{1}{E-E_q^u}=0$ for $E_p^t,E_q^u<\epsilon_F$ and $E_p^t,E_q^u>\epsilon_F$, $\int_\Gamma dE\frac{1}{E-E_p^t}\frac{1}{E-E_q^u}=\frac{1}{E_p^t-E_q^u}$ for $E_p^t<\epsilon_F$ and $E_q^u>\epsilon_F$, $\int_\Gamma dE\frac{1}{E-E_p^t}\frac{1}{E-E_q^u}=\frac{1}{E_q^u-E_p^t}$ for $E_p^t>\epsilon_F$ and $E_q^u<\epsilon_F$, and $\frac{1}{E_q^u-E_p^t}\leftrightarrow\frac{1}{E_p^u-E_q^t}$ under interchange of $E_p^t-E_q^u$.

Now that the Hamiltonian acts on the states instead of having the energy explicitly written out it is no longer important to expand the solution in an eigenbasis. Therefore the spin quantization axis from now on can be chosen to point in a single arbitrary direction and the waves can be expanded in the free electron basis which is much easier to use for calculation. Going over to free electron expansion the expression becomes

$$
= -\frac{1}{4\pi i} \int_\Gamma \sum_{i\neq j} \sum_{t,u} u^\dagger(t)(JS_i) \cdot \boldsymbol{\sigma} \int \frac{d^2q}{(2\pi)^2} \frac{1}{E - \tilde{H}_0} e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \times
$$

$$
\times u(u)u^\dagger(u)\,(JS_j) \cdot \boldsymbol{\sigma} \int \frac{d^2p}{(2\pi)^2} \frac{1}{E - \tilde{H}_0} e^{-i\mathbf{p}\cdot(\mathbf{r}_i-\mathbf{r}_j)} u(t) =
$$

$$
= -\frac{1}{4\pi i} \int_\Gamma \sum_{i\neq j} \sum_{t} u^\dagger(t)(JS_i) \cdot \boldsymbol{\sigma} \int \frac{d^2q}{(2\pi)^2} \frac{1}{E - \tilde{H}_0} e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \times \tag{5.51}
$$

$$
\times (JS_j) \cdot \boldsymbol{\sigma} \int \frac{d^2p}{(2\pi)^2} \frac{1}{E - \tilde{H}_0} e^{-i\mathbf{p}\cdot(\mathbf{r}_i-\mathbf{r}_j)} u(t) =
$$

$$
= -\frac{1}{4\pi i} \int_\Gamma \sum_{i\neq j} Tr[(JS_i) \cdot \boldsymbol{\sigma} G(-\mathbf{R}_{ij})\,(JS_j) \cdot \boldsymbol{\sigma} G(\mathbf{R}_{ij})],
$$

where $\mathbf{R}_{ij} = \mathbf{r}_i - \mathbf{r_j}$, and

$$
G(\mathbf{R}_{ij}) = \int \frac{d^2k}{(2\pi)^2} \frac{1}{E - H_0} e^{-i\mathbf{k}\cdot\mathbf{R}_{ij}}. \tag{5.52}
$$

### 5.3.4 The early expression, $[-\infty, 0]$

When $t' \in [-\infty, 0]$ the operators at $t_1$ should stand to the right of the operators at $t = 0$. In this case the expression becomes

$$
< \hat{H}_{RKKY}(0) >_{[-\infty,0]} = -i\langle 0| \prod_{E_k < \epsilon_F, r} a_k^r \int_{-\infty}^0 dt_1 \sum_{i\neq j} \times
$$

$$
\times \sum_{P,v} a_P^{v\dagger} u^\dagger(v) \psi_P^{v\dagger}(\mathbf{r}_j)\,(JS_j) \cdot \boldsymbol{\sigma} \sum_{Q,w} a_Q^w u(w) \psi_Q^w(\mathbf{r}_j) e^{iH_0 t_1} \times \tag{5.53}
$$

$$
\times \sum_{p,t} a_p^{t\dagger} u^\dagger(t) \psi_p^{t\dagger}(\mathbf{r}_i)(JS_i) \cdot \boldsymbol{\sigma} \sum_{q,u} a_q^u u(u) \psi_q^u(\mathbf{r}_i) e^{-iH_0 t_1} \prod_{E_l < k_F, s} a_l^{s\dagger} |0\rangle =
$$

Mimicking the calculation above this becomes

$$
= -\frac{1}{4\pi i} \int_\Gamma \sum_{i\neq j} Tr[(JS_i) \cdot \boldsymbol{\sigma} G(-\mathbf{R}_{ij})\,(JS_j) \cdot \boldsymbol{\sigma} G(\mathbf{R}_{ij})]. \tag{5.54}
$$

### 5.3.5 The final answer

Now that both contributions are calculated, all that remains is to add these together. The result is

$$
< \hat{H}_{RKKY}(0) > = \frac{i}{2\pi} \int_\Gamma \sum_{i\neq j} Tr[(JS_i) \cdot \boldsymbol{\sigma} G(-\mathbf{R}_{ij})\,(JS_j) \cdot \boldsymbol{\sigma} G(\mathbf{R}_{ij})], \tag{5.55}
$$

where $\mathbf{R}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and

$$G(\mathbf{R}_{ij}) = \int \frac{d^2k}{(2\pi)^2} \frac{1}{E - H_0} e^{-i\mathbf{k}\cdot\mathbf{R}_{ij}}. \tag{5.56}$$

This is the final expression for the RKKY interaction energy, applicable to any Hamiltonian $H_0$. Something that ain't obvious from this expression but can be seen in (5.49) is that the states far from the Fermi surface are suppressed ($E_p^t$ is bellow the Fermi energy and $E_q^u$ above, therefore the term $E_p^t - E_q^u$ that divides the third expression becomes large if any of them ain't close to that energy). In calculations the Hamiltonian $H_0$ can therefore be approximated by the Hamiltonian around the Fermi energy. An exception occurs however if the density of states increases as fast or faster than the energy difference from the Fermi energy.

# Chapter 6

# General method for reducing RKKY-interaction problems

## 6.1 Introduction

The Hamiltonian derived in chapter 5 describes the effective spin interaction between two localized spins on a two dimensional surface, where the interaction is mediated by the conduction electrons that surrounds both the spins. The set of equations that was derived there was

$$H_{RKKY} = \frac{i}{2\pi} \int_{\Gamma} dE \sum_{i \neq j} Tr \left[ (JS_i) \cdot \boldsymbol{\sigma} G(-\boldsymbol{R}_{ij})(JS_j) \cdot \boldsymbol{\sigma} G(\boldsymbol{R}_{ij}) \right],$$

$$G(\mathbf{R}) = \int \frac{d^2 k}{(2\pi)^2} G(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}}, \qquad (6.1)$$

$$G(\mathbf{k}) = \frac{1}{E - H},$$

where $H$ is the Hamiltonian that describes the motion of the surrounding conduction electrons.

In this chapter a general method for reducing this set of equations, for a large class of Hamiltonians, to a new set of equations on the form

$$H_{RKKY} = S_1 \Phi S_2, \qquad (6.2)$$

is given. Here $\Phi$ is a three by three matrix with entries consisting of terms with at most one-dimensional integrals. Which should be compared with the five dimensional integral in the original Hamiltonian[1]. In some cases the entries can be further analytically integrated to give analytically obtained values. In the other cases the entries are on a simple enough form to allow straight forward and quick numerical integration. The

---

[1] One energy integral, and two momentum integrals for each Green's function

requirement on $H$ is that it is on the form

$$H = C + \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K}, \qquad (6.3)$$

where $\mathbf{A}$ is a constant $3x3$-matrix with linearly independent second and third column, and $\mathbf{K}^T = (1, \mathbf{k})$. This kind of Hamiltonian is able to describe a large set of conduction electron settings. For example a linear spectrum, spin-orbit interactions, interactions between a magnetic field and a spin, and many more types of interactions gives linear terms, as well as superpositions of such interactions, which makes the method quite general.[2] This derivation builds upon that given in [14].

## 6.2   Step 1: Rewriting the Green's function

From 6.1 the momentum space Green's function with 6.3 inserted is seen to be

$$G(\mathbf{k}) = \frac{1}{E - C - \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K}}. \qquad (6.4)$$

The first step in the reduction process is to rewrite this so that the sigma matrices appears above the division sign instead of below. This is done by multiplying the expression from above and below by $E - C + \mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma}$, which gives[3]

$$G(\mathbf{k}) = (E - C + \mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma}) \times$$
$$\times \frac{1}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma} \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K} + (E - C)(\mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma} - \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K})}. \qquad (6.5)$$

First it is easy to see that

$$E(\mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma} - \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K}) = 0. \qquad (6.6)$$

Further $\boldsymbol{\sigma}^T \boldsymbol{\sigma}$ is an anti-symmetric matrix of matrices, with identity matrices on the diagonal. For some anti-symmetric matrix $\mathbf{a}$ without diagonal entries, the middle expression below the division sign can therefore be written as

$$\mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma} \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K} = \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K} + \mathbf{K}^T \mathbf{A}^T \mathbf{a} \mathbf{A} \mathbf{K}. \qquad (6.7)$$

But because of the structure of $\mathbf{a}$, the second term is zero. The momentum space Green's function can therefore be written

$$G(\mathbf{k}) = \frac{E - C + \mathbf{K}^T \mathbf{A}^T \boldsymbol{\sigma}}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}}, \qquad (6.8)$$

where the identity matrix that multiplies each expression below the division sign has been factored out and inverted to allow the two expressions to be written on top of each other.

---

[2]Even though I haven't examined this case, I find it quite likely that the method also can be extended to parabolic spectrum. Giving the method almost universal applicability in two-dimensional systems.

[3]Note that these are matrix equations, this is the reason that the first term on the right hand side not is on top of the division expression, but to the left of it.

Now that the momentum Green's function has been brought to a form where all sigma matrices are above the division sign it is possible to write the momentum space function as

$$G(\mathbf{k}) = G_I(\mathbf{k}) + G_x(\mathbf{k})\sigma_x + G_y(\mathbf{y})\sigma_y + G_z(\mathbf{z})\sigma_z, \qquad (6.9)$$

where

$$
\begin{aligned}
G_I(\mathbf{k}) &= \frac{E - C}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}}, \\
G_x(\mathbf{k}) &= \frac{(\mathbf{A}\mathbf{K})_x}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}}, \\
G_y(\mathbf{k}) &= \frac{(\mathbf{A}\mathbf{K})_y}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}}, \\
G_z(\mathbf{k}) &= \frac{(\mathbf{A}\mathbf{K})_z}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}}.
\end{aligned}
\qquad (6.10)
$$

Because the position space Green's functions are the Fourier transforms of the momentum space Green's functions, this division of the Green's function is carried over into position space. The position space Green's functions can therefore be written as

$$G(\mathbf{R}) = G_I(\mathbf{R}) + G_x(\mathbf{R})\sigma_x + G_y(\mathbf{R})\sigma_y + G_z(\mathbf{R})\sigma_z, \qquad (6.11)$$

where

$$
\begin{aligned}
G_I(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} G_I(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_x(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} G_x(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_y(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} G_y(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_z(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} G_z(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{R}}.
\end{aligned}
\qquad (6.12)
$$

## 6.3 Step 2: Factoring out the numerator outside of the integral

The four components of the position space Green's function obtained above, becomes with the expressions for the momentum space Green's functions inserted

$$
\begin{aligned}
G_I(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} \frac{E - C}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}} e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_x(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} \frac{(\mathbf{A}\mathbf{K})_x}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}} e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_y(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} \frac{(\mathbf{A}\mathbf{K})_y}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}} e^{-i\mathbf{k}\cdot\mathbf{R}}, \\
G_z(\mathbf{R}) &= \int \frac{d^2 k}{(2\pi)^2} \frac{(\mathbf{A}\mathbf{K})_z}{(E - C)^2 - \mathbf{K}^T \mathbf{A}^T \mathbf{A} \mathbf{K}} e^{-i\mathbf{k}\cdot\mathbf{R}}.
\end{aligned}
\qquad (6.13)
$$

The first step in evaluating these is to factor out the numerator out of the integral. But for the $x-, y-$ and $z$-component the numerator depends on $\mathbf{AK}$, which in turn depends on $\mathbf{k}$, and this forbids the term to be factored out of the integral. But noting that replacing the $\mathbf{AK}$ term in the numerator by

$$\mathbf{AK} \to \mathbf{A}\mathbb{K} = \mathbf{A}(1, i\frac{\partial}{\partial x}, i\frac{\partial}{\partial y}),$$ (6.14)

makes the differentiation act on the exponential and brings down the same factor in front of it. The only difference is that this differential operator can be brought out of the integral so that the expression can be written as

$$\begin{aligned}
G_I(\mathbf{R}) &= (E - C)I_0, \\
G_x(\mathbf{R}) &= (\mathbf{A}\mathbb{K})_x I_0, \\
G_y(\mathbf{R}) &= (\mathbf{A}\mathbb{K})_y I_0, \\
G_z(\mathbf{R}) &= (\mathbf{A}\mathbb{K})_z I_0,
\end{aligned}$$ (6.15)

where

$$I_0 = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-i\mathbf{k}\cdot\mathbf{R}}}{(E - C)^2 - \mathbf{K}^T\mathbf{A}^T\mathbf{AK}}.$$ (6.16)

## 6.4   Step 3: Transforming K

The next step in the evaluation of the momentum integrals is to change integration variable. To do this, define

$$\tilde{\mathbf{K}} = \mathbf{TAK},$$ (6.17)

where $\mathbf{T}$ is a rotation matrix that makes $\mathbf{TA}$ lower triangular.[4] Further label the entries in $\tilde{K}$ by

$$\tilde{K}^T = (\tilde{k}_0, \tilde{\mathbf{k}}).$$ (6.18)

Because $\mathbf{T}$ is a rotation Matrix it satisfies $\mathbf{T}^T\mathbf{T} = \mathbf{I}$. Using this together with $\tilde{\mathbf{K}}^2 = \tilde{k}_0^2 + \tilde{\mathbf{k}}^2$, the integral $I$ can be written as

$$I_0 = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-i\mathbf{k}\cdot\mathbf{R}}}{(E - C)^2 - \tilde{k}_0^2 - \tilde{\mathbf{k}}^2}.$$ (6.19)

Because the second and third column of $\mathbf{A}$ are linearly independent and $\mathbf{T}$ is a rotation matrix, the second and third column of $\mathbf{TA}$ are linearly independent as well. This property makes it possible to find a matrix $\mathbf{M}$ and a constant vector $\mathbf{n}$ such that

$$\mathbf{k} = \mathbf{M}\tilde{\mathbf{k}} + \mathbf{n}.$$ (6.20)

---

[4]This is always possible, think of the three columns as three vectors. I is always possible to find a rotation that rotates the third vector into the $z$-direction and the second vector into the $y, z$-plane.

Using this expression, $I$ can be rewritten as

$$I_0 = \det(\mathbf{M}) e^{-i\mathbf{R}\cdot\mathbf{n}} \int \frac{d^2\tilde{k}}{(2\pi)^2} \frac{e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{R}}}}{(E-C)^2 - \tilde{k}_0^2 - \tilde{k}^2}, \tag{6.21}$$

where

$$\tilde{\mathbf{R}}^T = \mathbf{R}^T \mathbf{M}. \tag{6.22}$$

## 6.5   Step 4: Integrating over the momentum

It is now time to perform the momentum integral. Switching to polar coordinates, noting that the denominator in the integral is constant for constant $\tilde{k}$, and using the relation[5]

$$J_0(\tilde{k}\tilde{R}) = \int_\pi^\pi \frac{d\theta}{2\pi} e^{-i\tilde{k}\tilde{R}\sin(\theta)}, \tag{6.23}$$

the angular coordinate can be integrated out to give

$$I_0 = \det(\mathbf{M}) e^{-i\mathbf{n}\cdot\mathbf{R}} \int_0^\infty \frac{d\tilde{k}}{2\pi} \frac{\tilde{k} J_0(\tilde{k}\tilde{R})}{(E-C)^2 - \tilde{k}_0^2 - \tilde{k}^2}. \tag{6.24}$$

The $J_0(\tilde{k}\tilde{R})$ in these equations are the zeroth order Bessel function of first kind, and in what follows the first order Bessel function of first kind, $J_1(\tilde{k}\tilde{R})$, the Bessel function of first and second order of the second kind, $Y_0(\tilde{k}\tilde{R})$ and $Y_1(\tilde{k}\tilde{R})$, as well as a set of related Hankel functions will be used. Before preceding with the calculation a few properties of these functions will therefore be presented.

First of all the Bessel functions of first kind, $J_m$, can be analytically continued to the whole complex plane. When doing the same for the Bessel function of second kind, $Y_m$, a branch cut has to be introduced. In this case it is suitable to place this branch cut along the negative $x$-axis. Next the Hankel functions of first and second kind are defined as[6]

$$\begin{aligned} H_m^{(1)}(\tilde{k}\tilde{R}) &= J_m(\tilde{k}\tilde{R}) + iY_m(\tilde{k}\tilde{R}), \\ H_m^{(2)}(\tilde{k}\tilde{R}) &= J_m(\tilde{k}\tilde{R}) - iY_m(\tilde{k}\tilde{R}), \end{aligned} \tag{6.25}$$

and the branch cuts in $Y_m$ are carried over to these Hankel functions. From this expression it is clear that $J_0(\tilde{k}\tilde{R})$ can be written as

$$J_0(\tilde{k}\tilde{R}) = \frac{1}{2}\left( H_0^{(1)}(\tilde{k}\tilde{R}) + H_0^{(2)}(\tilde{k}\tilde{R}) \right). \tag{6.26}$$

Now keep in mind that the integral in $I$ is performed along the positive $x$-axis. This allows the branch cut in $H_0^{(2)}(\tilde{k}\tilde{R})$ to be turned around in the upper half plane until it coincides with the positive $x$-axis, as long as $H_0^{(2)}(\tilde{k}\tilde{R})$ is evaluated on the lower branch, see figure 6.1. After the branch cut has been turned in this way, the

---

[5]8.411.1 in Tables of integrals, series, and products by I.S. Gradshteyn and I.M. Ryzhik.
[6]8.405 in Tables of integrals, series, and products by I.S. Gradshteyn and I.M. Ryzhik.
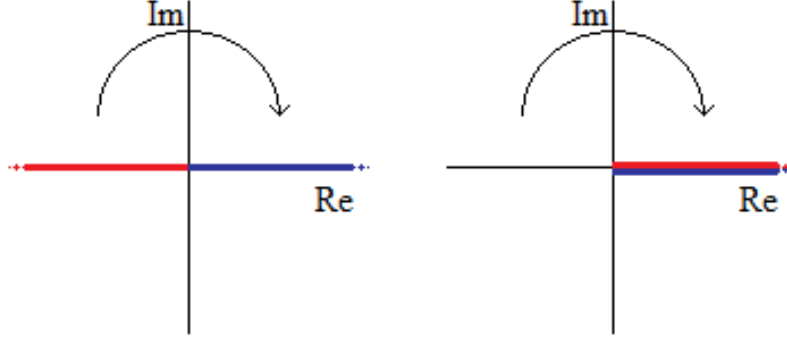
Figure 6.1: The red line shows the branch cut for the two Hankel functions, while the blue line shows the path that $J_0$, and therefore $H_0^{(1)}$ and $H_0^{(2)}$ will be integrated over. If the branch cut for $H_0^{(2)}$ is turned around in the upper half plane and the value of $H_0^{(2)}$ is evaluated on the lower branch there will be no difference in its value because the branch cut never sweeps over the path where $H_0^{(2)}$ is evaluated.

relation[7]

$$H_m^{(2)}(\tilde{k}\tilde{R}) = (-1)^{1+m} H_m^{(1)}(-\tilde{k}\tilde{R}) \tag{6.27}$$

can be used to give

$$J_0(\tilde{k}\tilde{R}) = \frac{1}{2} \left( H_0^{(1)}(\tilde{k}\tilde{R}) - H_0^{(1)}(-\tilde{k}\tilde{R}) \right). \tag{6.28}$$

Because $H_0^{(1)}(\tilde{k}\tilde{R})$ and $H_0^{(2)}(\tilde{k}\tilde{R})$ now has opposite branch cuts, $H_0^{(2)}(\tilde{k}\tilde{R})$ is evaluated on the lower branch cut, and $H_0^{(2)}(\tilde{k}\tilde{R}) = -H_0^{(1)}(-\tilde{k}\tilde{R})$ maps the lower branch of $H_0^{(2)}(\tilde{k}\tilde{R})$ onto the upper branch of $H_0^{(1)}(-\tilde{k}\tilde{R})$. This expression for $J_0(\tilde{k}\tilde{R})$ has to be thought of as being evaluated on the upper branch of $H_0^{(1)}(\tilde{k}\tilde{R})$ whenever there is a choice of branch. See figure 6.2.

With these considerations $I$ can be written

$$I_0 = \det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}} \int_0^\infty \frac{d\tilde{k}}{4\pi} \frac{\tilde{k}H_0^{(1)}(\tilde{k}\tilde{R})}{(E-C)^2 - \tilde{k}_0^2 - \tilde{k}^2} - \int_0^\infty \frac{d\tilde{k}}{4\pi} \frac{\tilde{k}H_0^{(1)}(-\tilde{k}\tilde{R})}{(E-C)^2 - \tilde{k}_0^2 - \tilde{k}^2}. \tag{6.29}$$

After a change of variables, $\tilde{k} \to -\tilde{k}$, in the second integral this becomes

$$I_0 = \det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}} \int_{-\infty}^\infty \frac{d\tilde{k}}{4\pi} \frac{\tilde{k}H_0^{(1)}(\tilde{k}\tilde{R})}{(E-C)^2 - \tilde{k}_0^2 - \tilde{k}^2}. \tag{6.30}$$

Now the integrand goes quickly enough to zero as $\tilde{k} \to \infty$ in the upper half plane to make a similar integral along the the path $\tilde{k}\tilde{R} \to \infty$ go to zero. This allows $I$ to be

---

[7]8.476.8 in Tables of integrals, series, and products by I.S. Gradshteyn and I.M. Ryzhik.
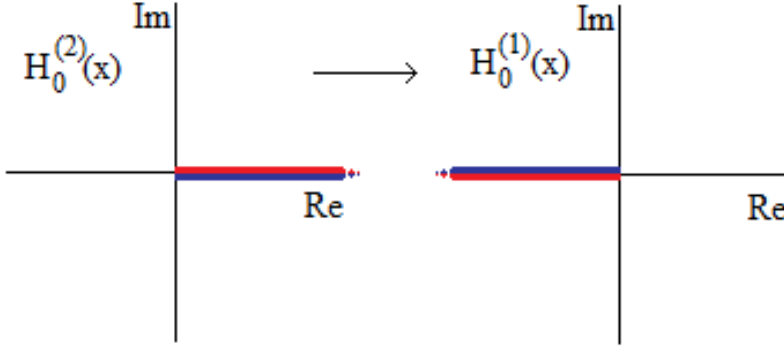
Figure 6.2: On the left hand side the integration path for $H_0^{(2)}$ is shown. When $H_0^{(2)}$ is replaced by $H_0^{(1)}$ by relation (6.27) the integration has to be performed along the path on the right hand side

evaluated with residue calculus, where the important poles are those in the upper half plane. Therefore the expression is rewritten as

$$I_0 = \det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}} \int_{-\infty}^{\infty} \frac{d\tilde{k}}{8\pi} \left( \frac{H_0^{(1)}(\tilde{k}\tilde{R})}{\sqrt{(E-C)^2 - \tilde{k}_0^2} - \tilde{k}} - \frac{H_0^{(1)}(\tilde{k}\tilde{R})}{\sqrt{(E-C)^2 - \tilde{k}_0^2} + \tilde{k}} \right),$$

(6.31)

which reveals the simple poles at $\tilde{k} = \pm\sqrt{(E-C)^2 - \tilde{k}_0^2}$. Residue calculus then gives[8]

$$I_0 = \begin{cases} \frac{i\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4} H_0^{(1)}(\sqrt[*]{(E-C)^2 - k_0^2}\,\tilde{R}) & \text{if } \text{Im}(E) > 0, \\ -\frac{i\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4} H_0^{(1)}(-\sqrt[*]{(E-C)^2 - k_0^2}\,\tilde{R}) & \text{if } \text{Im}(E) < 0. \end{cases}$$

(6.32)

## 6.6 Step 5: Taking the derivative of the momentum integral

Now that $I$ has been evaluated it is time to step back to equation 6.15 and evaluate the derivatives in these expressions. Using the relation[9]

$$\frac{dH_0^{(1)}(x)}{dx} = -H_1^{(1)}(x),$$

(6.33)

---

[8]In this step some care has to be taken about the imaginary part of $E$. The only entry inside the square root expression that is complex is $E$, which takes values in the first or fourth quadrant of the complex plane (see the definition of $\Gamma$). The square roots taken in these expression has to be considered to be defined so that it gives the same imaginary sign as $E$ has. The square root is therefore marked with an asterisk to remind that the square root has to be taken in this way.

[9]??? in Tables of integrals, series, and products by I.S. Gradshteyn and I.M. Ryzhik.

it is straight forward to check that 6.15 together with 6.32 can be written as

$$
\begin{aligned}
G_I(\mathbf{R}) &= (E - C)I_0, \\
G_x(\mathbf{R}) &= (\mathbf{A}\mathbb{G})_x, \\
G_y(\mathbf{R}) &= (\mathbf{A}\mathbb{G})_y, \\
G_z(\mathbf{R}) &= (\mathbf{A}\mathbb{G})_z,
\end{aligned}
\tag{6.34}
$$

where

$$
\mathbb{G}^T = (I_0,\, n_x I_0 + i\frac{\partial \tilde{R}}{\partial x}I_1,\, n_y I_0 + i\frac{\partial \tilde{R}}{\partial y}I_1),
\tag{6.35}
$$

and

$$
I_0 = \begin{cases}
\frac{i\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4}H_0^{(1)}(\sqrt[*]{(E-C)^2 - k_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) > 0, \\
-\frac{i\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4}H_0^{(1)}(-\sqrt{(E-C)^2 - k_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) < 0,
\end{cases}
$$

$$
I_1 = \begin{cases}
-\frac{i\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4}H_1^{(1)}(\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) > 0, \\
-\frac{i\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\det(\mathbf{M})e^{-i\mathbf{n}\cdot\mathbf{R}}}{4}H_1^{(1)}(-\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) < 0.
\end{cases}
\tag{6.36}
$$

It is also easy to see that inversion of $\mathbf{R}$ gives

$$
\begin{aligned}
G_I(-\mathbf{R}) &= (E - C)I_{0*}, \\
G_x(-\mathbf{R}) &= (\mathbf{A}\mathbb{G}_*)_x, \\
G_y(-\mathbf{R}) &= (\mathbf{A}\mathbb{G}_*)_y, \\
G_z(-\mathbf{R}) &= (\mathbf{A}\mathbb{G}_*)_z,
\end{aligned}
\tag{6.37}
$$

where[10]

$$
\mathbb{G}_* = (I_{0*},\, n_x I_{0*} - \frac{\partial \tilde{R}}{\partial x}I_{1*},\, n_y I_{0*} - \frac{\partial \tilde{R}}{\partial y}I_{1*}),
\tag{6.38}
$$

and

$$
I_{0*} = \begin{cases}
\frac{i\det(\mathbf{M})e^{i\mathbf{n}\cdot\mathbf{R}}}{4}H_0^{(1)}(\sqrt[*]{(E-C)^2 - k_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) > 0, \\
-\frac{i\det(\mathbf{M})e^{i\mathbf{n}\cdot\mathbf{R}}}{4}H_0^{(1)}(-\sqrt[*]{(E-C)^2 - k_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) < 0,
\end{cases}
$$

$$
I_{1*} = \begin{cases}
-\frac{i\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\det(\mathbf{M})e^{i\mathbf{n}\cdot\mathbf{R}}}{4}H_1^{(1)}(\sqrt{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) > 0, \\
-\frac{i\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\det(\mathbf{M})e^{i\mathbf{n}\cdot\mathbf{R}}}{4}H_1^{(1)}(\sqrt{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \mathrm{Im}(E) < 0.
\end{cases}
\tag{6.39}
$$

---

[10]The reason for the minus signs before the differentiations in this expressions stems from the introduction of $\mathbb{K}$ in 6.14. When $\mathbf{R}$ is inverted, the derivatives has to be multiplied by $-1$ for the substitution to be valid.

## 6.7 Step 6: Evaluating the trace and sum expression

Now that the components of the position space Green's functions has been evaluated, it is time to evaluate the trace and sum expression in 6.1. That is, the expression

$$TS = \sum_{i \neq j} Tr\left[(JS_i)\boldsymbol{\sigma}G(-\mathbf{R})(JS_j)\boldsymbol{\sigma}G(\mathbf{R})\right]. \tag{6.40}$$

A glance at the equations from step 5 together with 6.11, reveals that this also can be written as

$$TS = -\frac{\det^2(\mathbf{M})}{16} \sum_{i \neq j} Tr\left[(JS_i) \cdot \boldsymbol{\sigma}F_*(\mathbf{R})(JS_j) \cdot \boldsymbol{\sigma}F(\mathbf{R})\right], \tag{6.41}$$

where[11]

$$\begin{aligned} F(\mathbf{R}) &= (E - C)K_0 + (\mathbf{A}\mathbb{F}) \cdot \boldsymbol{\sigma}, \\ F_*(\mathbf{R}) &= (E - C)K_0 + (\mathbf{A}\mathbb{F}_*) \cdot \boldsymbol{\sigma}, \end{aligned} \tag{6.42}$$

and

$$\mathbb{F} = (K_0, n_x K_0 + i\frac{\partial \tilde{R}}{\partial x}K_1, n_y K_0 + i\frac{\partial \tilde{R}}{\partial y}K_1),$$

$$\mathbb{F}_* = (K_0, n_x K_0 - i\frac{\partial \tilde{R}}{\partial x}K_1, n_y K_0 - i\frac{\partial \tilde{R}}{\partial y}K_1),$$

$$K_0 = \begin{cases} H_0^{(1)}(\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \text{Im}(E) > 0, \quad (6.43) \\ -H_0^{(1)}(-\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \text{Im}(E) < 0, \end{cases}$$

$$K_1 = \begin{cases} -\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}H_1^{(1)}(\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \text{Im}(E) > 0, \\ -\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}H_1^{(1)}(-\sqrt[*]{(E-C)^2 - \tilde{k}_0^2}\tilde{R}) & \text{if } \text{Im}(E) < 0. \end{cases}$$

The evaluation of $TS$ now is a simple but tedious exercise in algebra, and the result is

$$TS = -\frac{\det^2(\mathbf{M})}{16}S_1\boldsymbol{\Phi}S_2, \tag{6.44}$$

where

$$\boldsymbol{\Phi} = \boldsymbol{\Phi}_{00}K_0^2 + \boldsymbol{\Phi}_{00}^{EC}(E-C)^2K_0^2 + \boldsymbol{\Phi}_{01}^{EC}(E-C)K_0K_1 + \boldsymbol{\Phi}_{11}K_1^2, \tag{6.45}$$

---

[11]It is implicitly assumed that $(E - C)K_0$ is multiplied by the unit matrix.

$$\Phi_{00} = 4 \begin{bmatrix} J_x^2(\phi_1^2 - \phi_S) & 2J_xJ_y\phi_1\phi_2 & 2J_xJ_z\phi_1\phi_3 \\ 2J_xJ_y\phi_1\phi_2 & J_y^2(\phi_2^2 - \phi_S) & 2J_yJ_z\phi_2\phi_3 \\ 2J_xJ_z\phi_1\phi_3 & 2J_yJ_z\phi_2\phi_3 & J_z^2(\phi_3^2 - \phi_S) \end{bmatrix},$$

$$\Phi_{00}^{EC} = 4 \begin{bmatrix} J_x^2 & 0 & 0 \\ 0 & J_y^2 & 0 \\ 0 & 0 & J_z^2 \end{bmatrix},$$

$$\Phi_{01}^{EC} = 8 \begin{bmatrix} 0 & -J_xJ_y\varphi_3 & J_xJ_z\varphi_2 \\ J_xJ_y\varphi_3 & 0 & -J_yJ_z\varphi_1 \\ -J_xJ_z\varphi_2 & J_yJ_z\varphi_1 & 0 \end{bmatrix},$$

$$\Phi_{11} = 4 \begin{bmatrix} J_x^2(2\varphi_1^2 - \varphi_S) & 2J_xJ_y\varphi_1\varphi_2 & 2J_xJ_z\varphi_1\varphi_3 \\ 2J_xJ_y\varphi_1\varphi_2 & J_y^2(2\varphi_2^2 - \varphi_S) & 2J_yJ_z\varphi_2\varphi_3 \\ 2J_xJ_z\varphi_1\varphi_3 & 2J_yJ_z\varphi_2\varphi_3 & J_z^2(2\varphi_3^2 - \varphi_S) \end{bmatrix},$$

(6.46)

and

$$\phi_i = a_{i1} + a_{i2}n_x + a_{i3}n_y,$$

$$\phi_S = \sum_{i=1}^{3} \phi_i^2,$$

$$\varphi_i = a_{i2}\frac{\partial \tilde{R}}{\partial x} + a_{i3}\frac{\partial \tilde{R}}{\partial y},$$

$$\varphi_S = \sum_{i=1}^{3} \varphi_i^2.$$

(6.47)

## 6.8 Step 7: Simplification of the energy integrals

The final step in this process is to integrate out the energy. Here the energy integral is simplified, but the actual integration is not carried out analytically for all cases. This is the only step where an analytical step in the evaluation of $H_{RKKY}$ not has been found for all cases. But in any way the integrals obtained here are on a simple enough form to allow for straight forward numerical integration.

From 6.1 and the equations obtained in step 6 it can be seen that the solution to the problem is

$$H_{RKKY} = -S_1 \left( \frac{i}{2\pi} \frac{\det^2(\mathbf{M})}{16} \int_\Gamma dE\mathbf{\Phi} \right) S_2.$$

(6.48)

In this step the integrals over the components of $\mathbf{\Phi}$ are therefore simplified.

From 6.45 it can be seen that there is four integrals that needs to be evaluated, these are

$$\int_\Gamma dE K_0^2, \int_\Gamma dE(E - C)^2 K_0^2, \int_\Gamma dE(E - C)K_0K_1, \int_\Gamma dE K_1^2.$$

(6.49)

First these integrals are divided into their two parts along $\Gamma_1$ in the upper complex

plane, and along $\Gamma_2$ in the lower complex plane.[12]

$$
\begin{aligned}
\int_\Gamma dE K_0^2 &= \int_{\Gamma_1} \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_0^{(1)2}(\tilde{E}\tilde{R}) + \\
&\quad + \int_{\Gamma_2} \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_0^{(1)2}(-\tilde{E}\tilde{R}), \\
\int_\Gamma dE(E - C)^2 K_0^2 &= \int_{\Gamma_1} d\tilde{E}\tilde{E}\sqrt{\tilde{E}^2 + \tilde{k}_0^2}\,\mathbf{sgn}(E - C) H_0^{(1)2}(\tilde{E}\tilde{R}) + \\
&\quad + \int_{\Gamma_2} d\tilde{E}\tilde{E}\sqrt{\tilde{E}^2 + \tilde{k}_0^2}\,\mathbf{sgn}(E - C) H_0^{(1)2}(-\tilde{E}\tilde{R}), \\
\int_\Gamma dE(E - C) K_0 K_1 &= -\int_{\Gamma_1} d\tilde{E}\tilde{E}^2 H_0^{(1)}(\tilde{E}) H_1^{(1)}(\tilde{E}\tilde{R}) + \\
&\quad + \int_{\Gamma_2} d\tilde{E}\tilde{E}^2 H_0^{(1)}(-\tilde{E}\tilde{R}) H_1^{(1)}(-\tilde{E}\tilde{R}), \\
\int_\Gamma dE K_1^2 &= \int_{\Gamma_1} \frac{d\tilde{E}\tilde{E}^3}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_1^{(1)2}(\tilde{E}\tilde{R}) + \\
&\quad + \int_{\Gamma_2} \frac{d\tilde{E}\tilde{E}^3}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_1^{(1)2}(-\tilde{E}\tilde{R}),
\end{aligned}
\tag{6.50}
$$

where for notational convenience the abbreviation[13]

$$
\tilde{E} = \sqrt[*]{(E - C)^2 - \tilde{k}_0^2},
\tag{6.51}
$$

has been introduced.

Next, the earlier stated relation

$$
H_m^{(2)}(-\tilde{E}\tilde{R}) = (-1)^{1+m} H_m^{(1)}(\tilde{E}\tilde{R}),
\tag{6.52}
$$

---

[12]Strictly these are equalities in the limit $\delta \to 0$. Compare with the definition of $\int_{\tilde{\Gamma}_i}$ and the corresponding footnote below.

[13]Note that this almost is a change of variables, but not quite. The reason for this is that the sign of $E - C$ still is important, and the paths $\Gamma_1$ and $\Gamma_2$ has sections on both sides of $E = C$ that maps onto the same $\tilde{E}$ values.

is used to rewrite the expressions as

$$
\int_\Gamma dE K_0^2 = \int_{\Gamma_1} \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_0^{(1)2}(\tilde{E}\tilde{R}) +
$$

$$
+ \int_{\Gamma_2} \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_0^{(2)2}(\tilde{E}\tilde{R}),
$$

$$
\int_\Gamma dE(E - C)^2 K_0^2 = \int_{\Gamma_1} d\tilde{E}\tilde{E}\sqrt{\tilde{E}^2 + \tilde{k}_0^2} \mathbf{sgn}(E - C) H_0^{(1)2}(\tilde{E}\tilde{R}) +
$$

$$
+ \int_{\Gamma_2} d\tilde{E}\tilde{E}\sqrt{\tilde{E}^2 + \tilde{k}_0^2} \mathbf{sgn}(E - C) H_0^{(2)2}(\tilde{E}\tilde{R}),
$$

$$
\int_\Gamma dE(E - C) K_0 K_1 = -\int_{\Gamma_1} d\tilde{E}\tilde{E}^2 H_0^{(1)}(\tilde{E}\tilde{R}) H_1^{(1)}(\tilde{E}\tilde{R}) -
$$

$$
- \int_{\Gamma_2} d\tilde{E}\tilde{E}^2 H_0^{(2)}(\tilde{E}\tilde{R}) H_1^{(2)}(\tilde{E}\tilde{R}),
$$

$$
\int_\Gamma dE K_1^2 = \int_{\Gamma_1} \frac{d\tilde{E}\tilde{E}^3}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_1^{(1)2}(\tilde{E}\tilde{R}) +
$$

$$
+ \int_{\Gamma_2} \frac{d\tilde{E}\tilde{E}^3}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} \mathbf{sgn}(E - C) H_1^{(2)2}(\tilde{E}\tilde{R}).
$$

(6.53)

Taking the limit $i\delta \to 0$, and using the relations

$$
H_m^{(1)}(\tilde{E}\tilde{R}) = J_m(\tilde{E}\tilde{R}) + iY_m(\tilde{E}\tilde{R}),
$$
$$
H_m^{(2)}(\tilde{E}\tilde{R}) = J_m(\tilde{E}\tilde{R}) - iY_m(\tilde{E}\tilde{R}),
$$

(6.54)

some algebra gives that these can be written as

$$
\int_\Gamma dE K_0^2 = 4i \int_A \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0}} J_0(\tilde{E}\tilde{R}) Y_0(\tilde{E}\tilde{R}) + 2 \int_B \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} H_0^{(1)2}(\tilde{E}\tilde{R})
$$

(6.55)

Turning back the branch cut for $H_m^{(2)}$ to the negative real axis and taking the limit of

$\Gamma_i \to \mathrm{Re}(\Gamma_i)$, this can further be written

$$\int_\Gamma dE K_0^2 = \int_{\tilde\Gamma_1} \frac{d\tilde E \tilde E}{\sqrt{\tilde E^2 + \tilde k_0^2}} H_0^{(1)2}(\tilde E \tilde R) - \int_{\tilde\Gamma_2} \frac{d\tilde E \tilde E}{\sqrt{\tilde E^2 + \tilde k_0^2}} H_0^{(2)2}(\tilde E \tilde R),$$

$$\int_\Gamma dE (E - C)^2 K_0^2 = \int_{\tilde\Gamma_1} d\tilde E \tilde E \sqrt{\tilde E^2 + \tilde k_0^2} H_0^{(1)2}(\tilde E \tilde R) -$$

$$- \int_{\tilde\Gamma_2} d\tilde E \tilde E \sqrt{\tilde E^2 + \tilde k_0^2} H_0^{(2)2}(\tilde E \tilde R)$$

$$\int_\Gamma dE (E - C) K_0 K_1 =$$

$$= - \int_{\sqrt{(E_c+C)^2 - \tilde k_0}}^{\sqrt{C^2 - \tilde k_0^2}} d\tilde E \tilde E^2 \left( H_0^{(1)}(\tilde E \tilde R) H_1^{(1)}(\tilde E \tilde R) - H_0^{(2)}(\tilde E \tilde R) H_1^{(2)}(\tilde E \tilde R) \right),$$

$$\int_\Gamma dE K_1^2 = \int_{\tilde\Gamma_1} \frac{d\tilde E \tilde E^3}{\sqrt{\tilde E^2 + \tilde k_0^2}} H_1^{(1)2}(\tilde E \tilde R) - \int_{\tilde\Gamma_2} \frac{d\tilde E \tilde E^3}{\sqrt{\tilde E^2 + \tilde k_0^2}} H_1^{(2)2}(\tilde E \tilde R).$$

$$(6.56)$$

where

$$\tilde\Gamma_1 = \left[ E_C, \mathrm{Re}(\sqrt{E_F^2 - \tilde k_0^2}) \right] \cup [0, ia] \cup \left[ ib, |\tilde k_0| \right],$$

$$\begin{array}{ll} a = |\tilde k_0| & \text{if } E_F > 0, \\ a = -\sqrt{E_F^2 - \tilde k_0^2} & \text{if } -|\tilde k_0| < E_F < 0, \\ a = 0 & \text{if } E_F < |\tilde k_0|, \\ b = i|\tilde k_0| & \text{if } E_F < 0, \\ b = \sqrt{E_F^2 - \tilde k_0^2} & \text{if } 0 < E_F < |\tilde k_0|, \\ b = 0 & \text{if } E_F > |\tilde k_0|, \end{array}$$

$$\int_{\tilde\Gamma_1} = \int_0^{\sqrt{E_c - \tilde k_0^2}} + \int_{\sqrt{C^2 - \tilde k_0^2}}^{E_F} + 2 \int_{i|\tilde k_0|}^0,$$

$$\int_{\tilde\Gamma_1} = 2 \int_0^{\sqrt{C^2 - \tilde k_0^2}} + \int_{\sqrt{C^2 - \tilde k_0^2}}^{E_F} + 2 \int_{-i|\tilde k_0|}^0.$$

$$\int_{\tilde\Gamma_1} = 2 \int_0^{\sqrt{C^2 - \tilde k_0^2}} + \int_{\sqrt{C^2 - \tilde k_0^2}}^{E_F} + 2 \int_{i|\tilde k_0|}^0,$$

$$\int_{\tilde\Gamma_1} = 2 \int_0^{\sqrt{C^2 - \tilde k_0^2}} + \int_{\sqrt{C^2 - \tilde k_0^2}}^{E_F} + 2 \int_{-i|\tilde k_0|}^0.$$

$$(6.57)$$

Finally, by using the expressions

$$H_m^{(1)}(\tilde E \tilde R) = J_m(\tilde E \tilde R) + i Y_m(\tilde E \tilde R),$$

$$H_m^{(2)}(\tilde E \tilde R) = J_m(\tilde E \tilde R) - i Y_m(\tilde E \tilde R),$$

$$(6.58)$$

the integrals becomes

$$\int_\Gamma dE K_0^2 = 4i \int_{\tilde\Gamma} \frac{d\tilde E \tilde E}{\sqrt{\tilde E^2 + \tilde k_0^2}} J_0(\tilde E \tilde R) Y_0(\tilde E \tilde R),$$

$$\int_\Gamma dE (E-C)^2 K_0^2 = 4i \int_{\tilde\Gamma} d\tilde E \tilde E \sqrt{\tilde E^2 + \tilde k_0^2} J_0(\tilde E \tilde R) Y_0(\tilde E \tilde R),$$

$$\int_\Gamma dE (E-C) K_0 K_1 = \qquad (6.59)$$

$$= -2i \int_{\sqrt{C^2 - \tilde k_0^2}}^{\sqrt{(E_F - C)^2 - \tilde k_0^2}} d\tilde E \tilde E^2 \left( J_0(\tilde E \tilde R) Y_1(\tilde E \tilde R) + J_1(\tilde E \tilde R) Y_0(\tilde E \tilde R) \right),$$

$$\int_\Gamma dE K_1^2 = 4i \int_{\tilde\Gamma} \frac{d\tilde E \tilde E^3}{\sqrt{\tilde E^2 + \tilde k_0^2}} J_1(\tilde E \tilde R) Y_1(\tilde E \tilde R).$$

where

$$\int_{\tilde\Gamma} = 2 \int_0^{\sqrt{C^2 - \tilde k_0^2}} + \int_{\sqrt{C^2 - \tilde k_0^2}}^{\sqrt{(\tilde E - C)^2 - \tilde k_0^2}}. \qquad (6.60)$$

For one of these integrals further integration has been found to be possible. This is for

$$\int_\Gamma dE (E-C) K_0 K_1. \qquad (6.61)$$

Using the relations[14]

$$\frac{\partial}{\partial x}(x^m J_m(x)) = x^m J_{m-1}(x),$$

$$\frac{\partial}{\partial x}(x^m Y_m(x)) = x^m Y_{m-1}(x), \qquad (6.62)$$

the integral becomes

$$\int_\Gamma dE (E-C) K_0 K_1 = -2i \left[ \frac{\tilde E^2}{\tilde R} J_1(\tilde E \tilde R) Y_1(\tilde E \tilde R) \right]_{\sqrt{C^2 - \tilde k_0^2}}^{\sqrt{(E_F - C)^2 - \tilde k_0^2}}. \qquad (6.63)$$

## 6.9   Summary of the method

Due to that each step was explained and justified at the same place above, the method seems a bit lengthy. Therefore the important steps and results are collected and summarized here in an algorithmic way that should be enough for carrying out the actual computations.

Find the constant $C$ and matrix $\mathbf{A}$ that allows the Hamiltonian to be written as

$$H = C + \boldsymbol{\sigma}^T \mathbf{A} \mathbf{K}, \qquad (6.64)$$

---

[14]???

where $\mathbf{K} = (1, \mathbf{k})$.

Find the rotation matrix $\mathbf{T}$ that makes $\mathbf{TA}$ lower triangular and define

$$\tilde{\mathbf{K}} = \mathbf{TAK}, \tag{6.65}$$

and label the entries in $\tilde{\mathbf{K}}$ by $\tilde{\mathbf{K}}^T = (\tilde{k}_0, \tilde{\mathbf{k}})$.

Find the matrix $\mathbf{M}$ and vector $\mathbf{n}$ that gives

$$\mathbf{k} = \mathbf{M}\tilde{\mathbf{k}} + \mathbf{n}. \tag{6.66}$$

Define

$$\tilde{\mathbf{R}}^T = \mathbf{R}^T\mathbf{M}. \tag{6.67}$$

The Hamiltonian describing the two interacting spins are now given by

$$H_{RKKY} = \frac{i}{2\pi} \frac{\det^2(\mathbf{M})}{16} \mathbf{J} \left( \mathbf{\Psi}_\alpha \alpha + \mathbf{\Psi}_\beta \beta + \mathbf{\Psi}_\gamma \gamma + \mathbf{\Psi}_\delta \delta \right) \mathbf{J} \tag{6.68}$$

where

$$\mathbf{J} = \begin{bmatrix} J_x & 0 & 0 \\ 0 & J_y & 0 \\ 0 & 0 & J_z \end{bmatrix},$$

$$\mathbf{\Psi}_\alpha = 4 \begin{bmatrix} \phi_1^2 - \phi_S & 2\phi_1\phi_2 & 2\phi_1\phi_3 \\ 2\phi_1\phi_2 & \phi_2^2 - \phi_S & 2\phi_2\phi_3 \\ 2\phi_1\phi_3 & 2\phi_2\phi_3 & \phi_3^2 - \phi_S \end{bmatrix},$$

$$\mathbf{\Psi}_\beta = 4 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{6.69}$$

$$\mathbf{\Psi}_\gamma = 8 \begin{bmatrix} 0 & -\varphi_3 & \varphi_2 \\ \varphi_3 & 0 & -\varphi_1 \\ -\varphi_2 & \varphi_1 & 0 \end{bmatrix},$$

$$\mathbf{\Psi}_\delta = 4 \begin{bmatrix} 2\varphi_1^2 - \varphi_S & 2\varphi_1\varphi_2 & 2\varphi_1\varphi_3 \\ 2\varphi_1\varphi_2 & 2\varphi_2^2 - \varphi_S) & 2\varphi_2\varphi_3 \\ 2\varphi_1\varphi_3 & 2\varphi_2\varphi_3 & 2\varphi_3^2 - \varphi_S \end{bmatrix},$$

$$\phi_i = a_{i1} + a_{i2}n_x + a_{i3}n_y,$$

$$\phi_S = \sum_{i=1}^{3} \phi_i^2,$$

$$\varphi_i = a_{i2}\frac{\partial \tilde{R}}{\partial x} + a_{i3}\frac{\partial \tilde{R}}{\partial y}, \tag{6.70}$$

$$\varphi_S = \sum_{i=1}^{3} \varphi_i^2.s$$

and

$$\alpha = 4i \int_{\tilde{\Gamma}} \frac{d\tilde{E}\tilde{E}}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} J_0(\tilde{E}\tilde{R})Y_0(\tilde{E}\tilde{R}),$$

$$\beta = 4i \int_{\tilde{\Gamma}} d\tilde{E}\tilde{E}\sqrt{\tilde{E}^2 + \tilde{k}_0^2} J_0(\tilde{E}\tilde{R})Y_0(\tilde{E}\tilde{R}),$$

$$\gamma = -2i \left[ \frac{\tilde{E}^2}{\tilde{R}} J_1(\tilde{E}\tilde{R})Y_1(\tilde{E}\tilde{R}) \right]_{\tilde{E}=\sqrt{C^2-\tilde{k}_0^2}}^{\sqrt{(E_F-C)^2-\tilde{k}_0^2}}, \qquad (6.71)$$

$$\delta = 4i \int_{\tilde{\Gamma}} \frac{d\tilde{E}\tilde{E}^3}{\sqrt{\tilde{E}^2 + \tilde{k}_0^2}} J_1(\tilde{E}\tilde{R})Y_1(\tilde{E}\tilde{R}),$$

$$\int_{\tilde{\Gamma}} = 2 \int_0^{\sqrt{C^2-\tilde{k}_0^2}} + \int_{\sqrt{C^2-\tilde{k}_0^2}}^{\sqrt{(E-C)^2-\tilde{k}_0^2}}.$$

# Appendix A

# Appendix

## A.1 Evaluation of commutation relation in spin-orbit derivation

$$[\boldsymbol{\sigma} \cdot \mathbf{p}, \boldsymbol{\sigma} \cdot \mathbf{E}] = -i\hbar \left( \nabla \cdot \mathbf{E} + \sigma_x \sigma_y \left( \partial_x E_y + E_y \partial_x - E_x \partial_y \right) + \right.$$
$$+ \sigma_x \sigma_z \left( \partial_x E_z + E_z \partial_x - E_x \partial_z \right) + \sigma_y \sigma_z \left( \partial_y E_z + E_z \partial_y - E_y \partial_z \right) +$$
$$+ \sigma_y \sigma_x \left( \partial_y E_x + E_x \partial_y - E_y \partial_x \right) + \sigma_z \sigma_x \left( \partial_z E_x + E_x \partial_z - E_z \partial_x \right) +$$
$$\left. + \sigma_z \sigma_y \left( \partial_z E_y + E_y \partial_z - E_z \partial_y \right) \right) =$$
$$= -i\hbar \left( \nabla \cdot \mathbf{E} + i\sigma_z \left( \partial_x E_y - \partial_y E_x + 2 E_y \partial_x - 2 E_x \partial_y \right) + \right. \tag{A.1}$$
$$+ i\sigma_y \left( \partial_z E_x - \partial_x E_z - 2 E_z \partial_x + 2 E_x \partial_z \right) +$$
$$\left. + i\sigma_x \left( \partial_y E_z - \partial_z E_y + 2 E_z \partial_y - 2 E_y \partial_z \right) \right) =$$
$$= -i\hbar \left( \nabla \cdot \mathbf{E} + i\boldsymbol{\sigma} \cdot \left( \nabla \times \mathbf{E} \right) - 2i\boldsymbol{\sigma} \cdot \left( \mathbf{E} \times \nabla \right) \right) =$$
$$= -i\hbar \nabla \cdot \mathbf{E} - 2i\boldsymbol{\sigma} \cdot \left( \mathbf{E} \times \mathbf{p} \right)$$

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