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Introduction to Odd-Frequency Superconductivity in Josephson Junctions with Spin-Active Interfaces

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Preface

This paper was produced during the fall 2014 as a project in the 9th semester of the Master of Science education at the Norwegian University of Science and Technology. It was written for the Department of Physics, within the direction of theoretical physics. The project was supervised by Professor Jacob Linder. I am truly grateful for his patience with me, and for his willingness to share so much of his knowledge.

Abstract

We present the theory needed in order to study the odd-frequency triplet state in a superconductor/normal metal/superconductor junction. Thin layers of insulating ferromagnets are inserted at the interfaces, with the possibility of misaligned magnetizations. The superconductors are conventional BCS superconductors, and the extent of this paper is limited to the equilibrium state in the diffusive limit. We investigate the origin of the odd-frequency, and extend the Usadel equation for the normal Josephson junction to include triplet pairing. The spin-active interfaces are responsible for a phase shift of reflected Cooper pairs. With misaligned magnetizations, we expect to generate spin-polarization of electrons. The spin-active interfaces are taken into account by adding terms to the Kupriyanov-Lukichev boundary conditions. We employ the Riccati parameterization for the quasiclassical retarded Green's function, which will provide a good starting point for further numerical calculations.

Contents

| | | |
|----------|------------------------------------------------------------|-----------|
| 1 | Introduction | 1 |
| 1.1 | Motivation | 1 |
| 1.2 | Josephson Junction | 2 |
| 2 | Theory | 5 |
| 2.1 | Superconductivity | 5 |
| 2.1.1 | Meissner Effect | 5 |
| 2.1.2 | Andreev Reflection | 7 |
| 2.1.3 | Classification of Superconductors | 7 |
| 2.1.4 | Heisenberg Picture | 8 |
| 2.1.5 | Field Theory | 9 |
| 2.1.6 | BSC Theory and Mean Field Approximation | 10 |
| 2.2 | Ferromagnetism | 13 |
| 2.2.1 | Heisenberg Model | 14 |
| 2.2.2 | Mean Field Approximation | 15 |
| 2.2.3 | Magnetic Insulator | 15 |
| 2.3 | Green's Function Description for Superconductors | 16 |
| 2.3.1 | Equation of Motion and Keldysh Formalism | 16 |
| 2.3.2 | Energy Gap Function and Current Matrix | 17 |
| 2.3.3 | Mixed Representation | 18 |
| 2.3.4 | Kinetic Equation | 19 |
| 2.3.5 | Quasiclassical Theory | 19 |
| 2.3.6 | Usadel Equation | 20 |
| 2.4 | Riccati Parameterization | 21 |
| 2.4.1 | Riccati Parameterization for the Usadel Equation | 21 |
| 2.4.2 | Boundary Conditions for Normal Interfaces | 29 |
| 3 | Interplay Between FM and SC Order | 33 |
| 3.1 | Spin-Active Interfaces | 33 |
| 3.2 | Odd-Frequency Pairing | 37 |
| 3.3 | Numerical Solution of the Usadel Equation | 39 |
| 4 | Outlook | 41 |

| | | |
|----------|--------------------------|-----------|
| A | Notation | 45 |
| B | Green's Functions | 49 |

Chapter 1

Introduction

1.1 Motivation

The interplay between ferromagnetism and superconductivity has attracted a lot of interest over the past years. For a long time the two phenomena were considered incompatible, due to their seemingly mutual destruction of the other. However, from a quantum mechanical point of view, new effects arise in hybrid structures of these materials. The combination of conventional superconductors and ferromagnetic materials is expected to generate a type of odd-frequency superconductivity that is insensitive to impurity scattering. In the presence of noncollinear magnetization, the odd-frequency triplet state will be able to penetrate a ferromagnet at distances comparable to the penetration length of singlet components in normal metals. A review of odd-frequency pairing is given in [8].

Closely related to ferromagnetism is the concept of spintronics, where the idea is to detect and manipulate the spin property of electrons and use this to represent the information transfer. An electron can not be separated from its spin, and with a stable spin configuration, the information will not be lost when energy supply is cut off. A huge challenge of spintronics is to control and detect these spins properly. A spin dependent scattering, known as the GMR (giant magnetoresistance) effect [2], was already in the nineties utilized in hard drives, to read information. This is a good example of a successful appliance of spintronics in common technology.

In this paper, we focus on superconducting spintronics. The aim is to extract the benefits of two worlds, by combining the zero resistance of superconductors with magnetic properties of ferromagnets in a constructive matter. The field of superconducting spintronics is today under constant development, and opens the gate to new interesting quantum physics.

Recommended Pre-Knowledge

In this paper we assume that the reader has a basic understanding of quantum mechanics and is familiar with the concept of second quantization. The book by David J. Griffiths

[15] offers an introduction to general quantum mechanics. It would also be of advantage for the reader to be acquainted with the usage of Green's functions as probability amplitudes, applied in quantum mechanics concerning many-particle problems. There are many sources on this subject, where one of them is the book by Gerald. D. Mahan [20].

1.2 Josephson Junction

The specific junction we are going to look at, consists of two superconductors (S_1 , S_2) separated a normal metal (N). At each interface thin layers of insulating ferromagnetic material, with magnetization directions \mathbf{m}_1 and \mathbf{m}_2 , have been added. This will make the interfaces spin-active, as illustrated in Figure 1.1. The Josephson junction is known

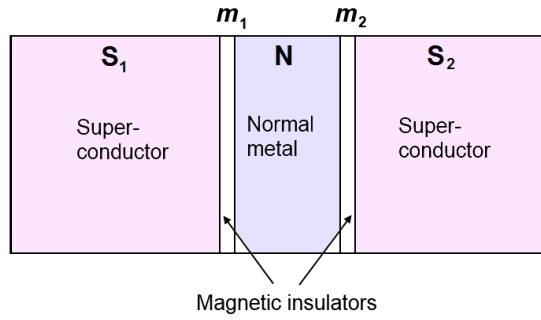


Figure 1.1: A junction of superconductor / normal metal / superconductor, with spin-active interfaces.

for the phenomenon of electrons tunneling through the junction without applied voltage. It has been shown that it is not single electrons but Cooper pairs, that tunnel through the junction [16]. The Cooper pairs are loosely linked electrons that behave in a boson like matter. This will allow super-current to flow through the junction, where the super-current is a current of Cooper pairs.

Diffusive Limit

We will operate in the diffusive limit, where the electrons are scattered in all directions by elastic collisions with impurities. This is the most realistic scenario, in contrast to the ballistic limit which would require really clean materials, illustrated in Figure 1.2. In the diffusive limit, the impurity scattering requires an averaging over the momentum direction, which will give us the Usadel equation as is to be shown in section 2.3.6.

For simplicity we will use natural units, such that we define $\hbar = 1$ and $c = 1$. This allows us to compare values of variables in a simple way. For instance, we could measure energy in kelvin, or mass in electron volt. This is done by dividing and multiplying with the correct natural constant. Natural units will also simplify numerical calculations, which are to be performed in a later project. The charge of an electron is defined as $q = e = -|e|$, and m is the electron mass.

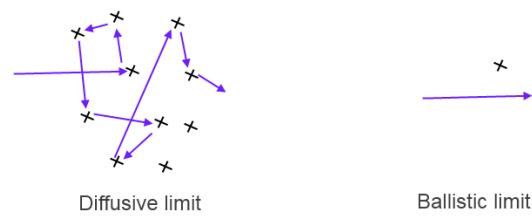


Figure 1.2: Diffusive limit vs. ballistic limit. The arrows are the trajectory of an electron propagating through a material, and the crosses are impurities.

Chapter 2

Theory

The theory chapter is divided into three main sections: one about superconductors, one on ferromagnets, and one concerning the quasiclassical theory. These are all essential parts for the Josephson junction in question. Each section addresses the fundamental theory behind its topic.

2.1 Superconductivity

The first superconductor was discovered in 1911 by a Dutch physicist with name Heike K. Onnes. Superconductivity is today commonly known as the phenomenon of a material having zero DC-resistance. This property occurs in some material below a certain critical temperature T_c , which varies for the different materials. There are also limitations on how much current a superconductor can conduct, before the superconductivity breaks down.

To have superconductivity we need to fulfill two criteria. First, the material needs to have a band in the energy distribution. This will prevent single particle states to enter this region, which in turn will shield the paired electrons that in fact are able to exist there. Second, the paired electrons in the energy gap have to be phase-coherent, not to create resistance. These paired electrons are the Cooper pairs.

The theory in section 2.1.1 and 2.1.6 is mostly based on chapter 1 and 3 in [13].

2.1.1 Meissner Effect

In addition to having zero resistance, a superconductor will also experience a magnetic susceptibility $\chi = -1$ below T_c , which is the value for an ideal diamagnet. The susceptibility is defined as $\chi = \frac{|\mathbf{M}|}{|\mathbf{H}|}$, where \mathbf{M} is the magnetization and \mathbf{H} is the applied magnetic field. A diamagnet is characterized by having negative χ . This means that a diamagnet will produce a magnetization in the opposite direction of an applied magnetic field. For a superconductor, this magnetization is produced by currents running at the surface of the superconductor, see Figure 2.1. If the external field is weak enough, the magnetization will manage to fully cancel the applied magnetic field inside the super-

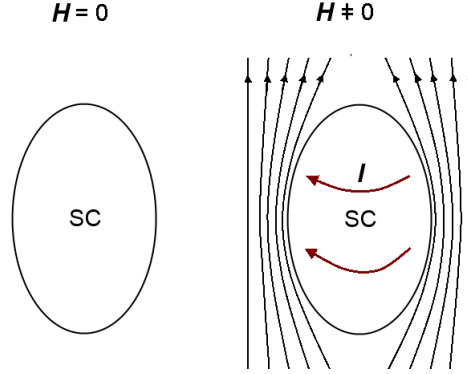


Figure 2.1: The Meissner effect. Left: a superconductor in absence of magnetic fields. Right: after applying a magnetic field, surface currents I will set up a magnetic field that expels the applied field from the superconducting core.

conductor. This is known as the Meissner effect, and was discovered by W. Meissner and R. Ochsenfeld in 1933 [21] (English translation). We can imagine this effect as if the superconductor pushes the magnetic flux lines outside itself, which also means that the field outside the superconductor will be amplified.¹

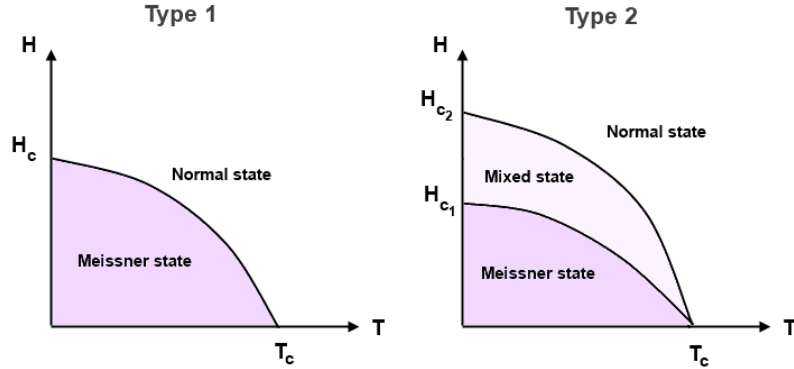


Figure 2.2: Qualitative sketches of magnetic field as function of temperature. Left: type 1 superconductors have only two states, Meissner state or normal state. Right: type 2 superconductors have in addition a mixed state.

Some superconductors have a well-defined critical temperature for where the expelling of \mathbf{H} vanishes; these are called type 1 superconductors. The remaining superconductors are called type 2 and have an upper and lower critical temperature, where

¹The applied field actually decays exponentially in the superconductor over a short distance from the surface. The decay depth is called the London penetration depth after the brothers Fritz and Heinz London. The brothers published in 1935 what was to be called the London equations [19], relating surface current to the electromagnetic fields.

the expelling gradually diminishes. Below the lower critical temperature, type 2 superconductors behave like type 1. In addition, these effects are dependent of the strength of the applied field. If the field is too strong, it will overcome the Meissner effect and penetrate the superconductor, which destroys the superconductivity. Type 1 superconductors show either full Meissner effect or none at all, while type 2 have an interval in $|\mathbf{H}|$ with partially expelling of the field, called a mixed state. The appearance of the mixed state is illustrated in Figure 2.2.

2.1.2 Andreev Reflection

The superconducting state is connected to the so-called energy band gap Δ in the energy spectrum. This band gap makes single particle states forbidden within the band gap. Electrons from a normal metal with energy less than the band gap are not allowed to enter the superconductor alone. But there is a way for electrons to circumvent this restriction. If two electrons enter together they can form what is known as a Cooper pair. This happens through a phonon-mediated interaction, and will allow the Cooper pairs to live in the energy gap. Figure 2.3 shows that when an electron at the Fermi surface of a normal metal hits the superconductor, it can be absorbed together with another electron and reflect a hole of opposite spin. This is the Andreev reflection [1]. The reflected holes will make the normal metal behave weakly as a superconductor near the interface, known as the proximity effect². Momentum, energy, charge and spin is conserved by the Andreev reflection [5].

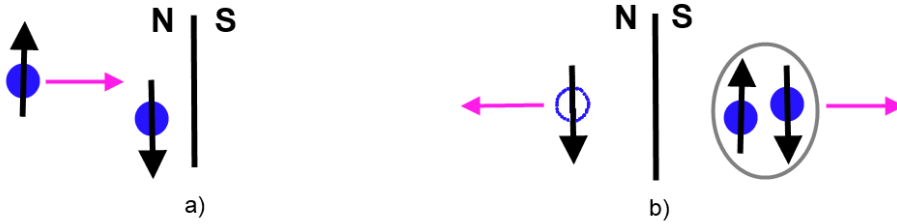


Figure 2.3: Andreev reflection. a) An incoming electron meets another electron near the surface. b) They form a Cooper pair and a hole is reflected in the normal metal.

2.1.3 Classification of Superconductors

In addition to the classification of type 1 and type 2 superconductors, we can classify the superconductors by symmetry. The Pauli Exclusion Principle states that a specific quantum state only can be occupied by one fermion at a time. To satisfy the Pauli principle we need the anomalous Green's function³ $F(1, 2) \propto \langle \{\psi_{\sigma_1}(\mathbf{r}_1, t_1), \psi_{\sigma_2}(\mathbf{r}_2, t_2)\} \rangle$

²There is also an inverse proximity effect that reduces the superconducting order near the interface in the superconductor.

³The Green's functions are given in Appendix B

to be anti-symmetric when interchanging particle 1 and 2 at equal times. We have here introduced the anti-commutator⁴ and the field annihilation operator $\psi_\sigma(\mathbf{r}, t)$. The 1 and 2 are respectively short for $\mathbf{r}_1, t_1, \sigma_1$ and $\mathbf{r}_2, t_2, \sigma_2$. As usual, we have \mathbf{r} as the real space coordinate, t is the time and σ denotes the spin configuration. By Fourier transforming in space and time⁵, the symmetry requirement is equivalent to having an anti-symmetric symmetry multiplication of momentum, frequency and spin.

The symmetry possibilities for spin- $\frac{1}{2}$ particles, such as electrons, are the anti-symmetric spin singlet $\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$ and the symmetric spin triplet $|\uparrow\uparrow\rangle, \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle], |\downarrow\downarrow\rangle$. The mean value of spin is zero for the singlet and one for the triplet. The momentum symmetry, called parity, is given by $(-1)^l$, where l is a quantum number. $l = 0, 1, 2$ represent in that order the s-wave, p-wave, d-wave. This gives us symmetric s- or d-wave or an anti-symmetric p-wave. The possible combinations of symmetry are listed in table 2.1. We label the frequency symmetry as either even or odd.

Table 2.1: Possible symmetry combinations to satisfy the Pauli Principle.

| | Frequency | Spin | Momentum |
|-----------------------------|-----------|------|----------|
| Even frequency spin singlet | +1 | -1 | +1 |
| Even frequency spin triplet | +1 | +1 | -1 |
| Odd frequency spin singlet | -1 | -1 | -1 |
| Odd frequency spin triplet | -1 | +1 | +1 |

For the p- and d-waves we have equal parts of negative and positive momentum ($k = |\mathbf{k}|$) in \mathbf{k} -space, leaving us with the average value of zero momentum. To have a visible state in a dirty superconductor, we need to have an s-wave. The s-wave has a spherical symmetry in \mathbf{k} -space, and is the only orbital with exclusively positive momentum values. When electrons are scattered in all directions, we will still have a finite average of momentum in the s-wave. This is supported by Anderson's theorem from mathematics.

2.1.4 Heisenberg Picture

We will use the Heisenberg picture as our quantum mechanical working space. In this picture the operators are time-dependent and the quantum states are constant in time. Other possibilities would be the Schrödinger picture with time-dependence in the quantum states and time constant operators, or the interaction picture which has time-dependence in both. None of the last two will be treated in this paper.

The equation of motion in the Heisenberg picture, with natural unites, reads

$$i \frac{d}{dt} O(t) = [O(t), H], \quad (2.1)$$

where $O(t)$ denotes an operator in this picture, and H is the Hamiltonian. On the left hand side we have introduced the commutator⁶.

⁴The anti-commutator is defined by $\{A, B\} = AB + BA$

⁵Even if we set $t_1 = t_2$ the Fourier transform will still depend on the frequency.

⁶The commutator is defined by $[A, B] = AB - BA$

A measurable physical quantity is represented by the average value of the associated operator, and may be written

$$\langle O(t) \rangle = \text{Tr}\{\rho(H)O(t)\}. \quad (2.2)$$

$\rho(H)$ is a statistical weighing operator and $\text{Tr}\{A\}$ is the trace of matrix A , equal to the sum over all spin states.

2.1.5 Field Theory

The field operators $\psi_\sigma^\dagger(\mathbf{r}, t)$ and $\psi_\sigma(\mathbf{r}, t)$, are respectively equal to the creation and the annihilation of an electron at (spin, position, time) = (σ, \mathbf{r}, t) . The field operators obey the anti-commutation relations at equal times

$$\begin{aligned} \{\psi_\sigma(\mathbf{r}, t), \psi_{\sigma'}(\mathbf{r}', t)\} &= 0, \\ \{\psi_\sigma^\dagger(\mathbf{r}, t), \psi_{\sigma'}^\dagger(\mathbf{r}', t)\} &= 0, \\ \{\psi_\sigma(\mathbf{r}, t), \psi_{\sigma'}^\dagger(\mathbf{r}', t)\} &= \delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (2.3)$$

The single-particle field representation in second quantization is given by

$$h = \sum_{\sigma\sigma'} \int d\mathbf{r} \psi_\sigma^\dagger(\mathbf{r}, t) h(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}, t), \quad (2.4)$$

where $h(\mathbf{r})$ is the operator in normal position representation in first quantization.

From classical mechanics we recognize that the Hamiltonian H is the sum of kinetic and potential energy. For a superconductor, the Hamiltonian can be split into four terms

$$H = H_0 + H_{\text{int}} + H_{\text{sf}} + H_{\text{imp}}. \quad (2.5)$$

Here H_0 is the non-interacting particle term, H_{int} represents the contribution from the pairing interactions, H_{sf} is the spin-flip term, which is important in the presence of magnetic impurities, and H_{imp} arises from scattering by non-magnetic impurities. We have not included the spin-orbit coupling, which is a valid assumption for atoms with low atomic numbers. We will assume that we can neglect the spin-orbit coupling due to the materials used in the junction. The expressions of the four terms in (2.5) are given in (2.6a) - (2.6d).

$$H_0 = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \left[\frac{1}{2m} \left(\frac{1}{i} \nabla - e\mathbf{A}(\mathbf{r}, t) \right)^2 + e\varphi(\mathbf{r}, t) - \mu \right] \psi_{\sigma}(\mathbf{r}, t) \quad (2.6a)$$

$$H_{\text{int}} = \int d\mathbf{r} \int d\mathbf{r}' V_{\text{int}}(\mathbf{r}, \mathbf{r}', t) \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}', t) \psi_{\downarrow}(\mathbf{r}', t) \psi_{\uparrow}(\mathbf{r}, t) \quad (2.6b)$$

$$H_{\text{sf}} = \sum_{\sigma\sigma'} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) [\bar{\boldsymbol{\tau}} \cdot \mathbf{S}(\mathbf{r})]_{\sigma\sigma'} V_{\text{sf}}(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}, t) \quad (2.6c)$$

$$H_{\text{imp}} = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) V_{\text{imp}}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}, t) \quad (2.6d)$$

In H_0 we have taken into account the possibility of an external electromagnetic field by the familiar scalar- and vector-potential $\varphi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$. The energy reference point is set to the chemical potential μ .⁷ V_{imp} is the scattering potential for impurities, and will in section 2.3.6 be replaced by a term averaged over all impurities, the self-energy representation. $[\bar{\boldsymbol{\tau}} \cdot \mathbf{S}(\mathbf{r})]_{\sigma\sigma'}$ $V_{\text{sf}}(\mathbf{r})$ is the spin-flip potential that includes the possibility for an electron to flip from σ' to σ at position \mathbf{r} . The Pauli matrices τ_i is given in Appendix A. The interaction term (2.6b) will be justified in the following section.

2.1.6 BSC Theory and Mean Field Approximation

In superconductors we observe an attractive electron-electron interaction, despite the strong repulsive Coulomb potential, between electrons. This originates from a phonon-mediated interaction of electrons at the Fermi surface with momenta in opposite directions. When an electron travels through a lattice, positively charged ions at lattice points feel the attractive Coulomb potential from the electron, and fall out of their stable equilibrium positions. This disturbance generates a wave in the material, a phonon. A second electron, entering the region at a later time, will be influenced by this wave and interact attractively relative to the first electron. This leads to an effectively attractive interaction between electrons.

The interaction will most likely occur when the strong Coulomb potential between the electrons is minimized. This happens when the distance between the electrons increases the most per time unit. Naturally, this is the case for electrons travelling in opposite directions. Another way to see this is by using the fact that all interactions of electrons in low temperature metals are limited to a thin shell at the Fermi surface, due to the Pauli principle. At low temperatures, all the low energy states in a spherical orbital are filled up to the Fermi surface in \mathbf{k} -space. The thermal energy for an electron far from the surface, is not large enough to excite electrons up to unoccupied states. If two electrons were to interact, the exchanged momentum has to keep both electrons at the Fermi surface, and therefore the total momentum of both electrons has to be zero, as in Figure 2.4.

⁷The chemical potential is the energy required to add one more particle to the system. It is a function of temperature, but at $T = 0$ K the chemical potential is equal to the Fermi energy E_F .

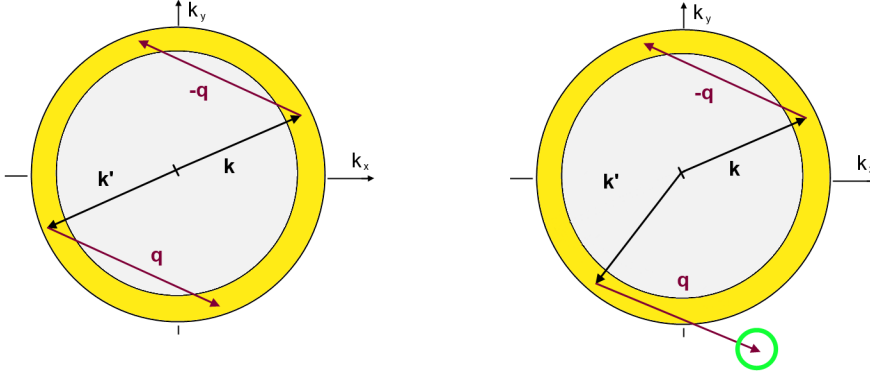


Figure 2.4: Phonon-mediated momentum exchange between two electrons, with initial momentum \mathbf{k} and \mathbf{k}' , in an s-wave superconductor. A sectional view in the $k_x k_y$ -plane. Electrons with momenta that differs from the opposite of each other, will not match the Fermi surface after the exchange of momentum \mathbf{q} .

We now write the interaction Hamiltonian as a sum of the repulsive Coulomb interaction and the attractive phonon-mediated interaction.

$$H_{\text{int}} = H_{\text{Coul}} + H_{\text{e-ph-e}}. \quad (2.7)$$

Here the Coulomb Hamiltonian H_{Coul} is given in the two-particle field representation as

$$H_{\text{Coul}} = \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma'}^{\dagger}(\mathbf{r}', t) \psi_{\sigma'}(\mathbf{r}', t) \psi_{\sigma}(\mathbf{r}, t). \quad (2.8)$$

The phonon-mediated Hamiltonian is the sum of the first and second electron-phonon interaction

$$\begin{aligned} H_{\text{e-ph-e}} = & \sum_{i\sigma} \int d\mathbf{r} V_{e-ph}(\mathbf{r} - \mathbf{R}_i) \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma}(\mathbf{r}, t) \\ & + \sum_{i\sigma'} \int d\mathbf{r}' V_{ph-e}(\mathbf{r}' - \mathbf{R}_i) \psi_{\sigma'}^{\dagger}(\mathbf{r}', t) \psi_{\sigma'}(\mathbf{r}', t). \end{aligned} \quad (2.9)$$

By considering the Feynman diagrams in Figure 2.5, the two belonging electron scattering events can be replaced by a higher order diagram with a phonon propagator.

We can write this coupled diagram as

$$H_{\text{e-ph-e}} \approx \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' V_{\text{eff}}(\mathbf{r}, \mathbf{r}', t) \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma'}^{\dagger}(\mathbf{r}', t) \psi_{\sigma'}(\mathbf{r}', t) \psi_{\sigma}(\mathbf{r}, t). \quad (2.10)$$

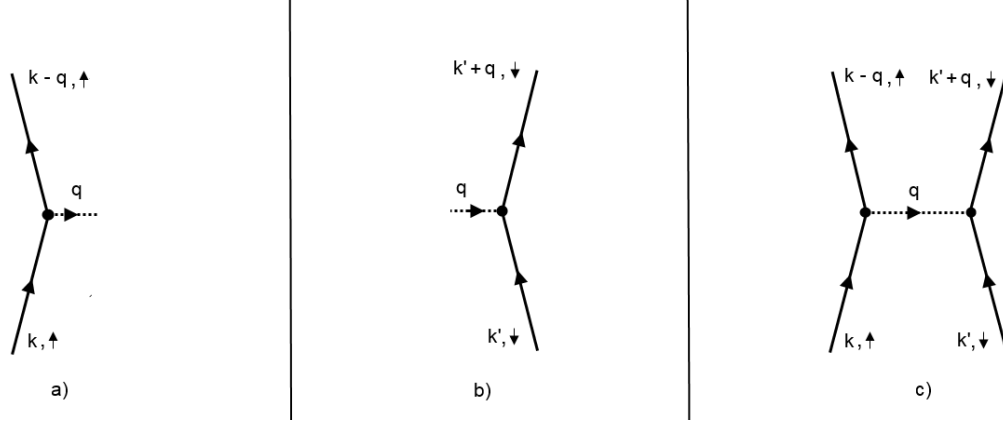


Figure 2.5: a) First electron-phonon scattering. b) Second electron-phonon scattering. c) Coupled diagram, representing the effective attractive two-particle scattering.

Equation (2.7) will now take the form

$$\begin{aligned}
 H_{\text{int}} &= \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' [V_{\text{Coul}}(\mathbf{r}, \mathbf{r}', t) + V_{\text{eff}}(\mathbf{r}, \mathbf{r}', t)] \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma'}^{\dagger}(\mathbf{r}', t) \psi_{\sigma'}(\mathbf{r}', t) \psi_{\sigma}(\mathbf{r}, t) \\
 &= \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}' V_{\text{int}}(\mathbf{r}, \mathbf{r}', t) \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma'}^{\dagger}(\mathbf{r}', t) \psi_{\sigma'}(\mathbf{r}', t) \psi_{\sigma}(\mathbf{r}, t).
 \end{aligned} \tag{2.11}$$

This is a general expression for a two particle scattering by the potential $V_{\text{int}}(\mathbf{r}, \mathbf{r}', t)$. Due to the spin singlet symmetry for the BCS superconductors, we set $\sigma = \uparrow$ and $\sigma' = \downarrow$, which leads to the form in (2.6b), as we wanted to show. The Coulomb potential is positive (repelling) and the effective phonon-mediated potential is negative (attractive). If $V_{\text{eff}} > V_{\text{Coul}}$, then the whole interaction potential is attractive.

If we now apply the mean-field approximation to the interaction Hamiltonian it transforms from a two-particle problem to a one-particle problem. We assume that we can set $V_{\text{int}}(\mathbf{r}, \mathbf{r}', t) = \lambda(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')$, where the interaction strength $\lambda(\mathbf{r})$ is a negative, real constant inside the superconductor and zero elsewhere. We choose to express $\psi_{\downarrow}(\mathbf{r}, t)\psi_{\uparrow}(\mathbf{r}, t)$, and its conjugated, as the mean value plus derivation,

$$\psi_{\downarrow}(\mathbf{r}, t)\psi_{\uparrow}(\mathbf{r}, t) = \langle \psi_{\downarrow}(\mathbf{r}, t)\psi_{\uparrow}(\mathbf{r}, t) \rangle + \delta(\mathbf{r}, t), \tag{2.12a}$$

$$\psi_{\uparrow}^{\dagger}(\mathbf{r}, t)\psi_{\downarrow}^{\dagger}(\mathbf{r}, t) = \langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t)\psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \rangle + \delta^{\dagger}(\mathbf{r}, t). \tag{2.12b}$$

In the first approximation, we remove constant terms and neglected all second order terms. After reinstating the expression for $\delta(\mathbf{r}, t)$ and $\delta^{\dagger}(\mathbf{r}, t)$, we approximate in the same way again.

$$\begin{aligned}
H_{\text{int}} &= \int d\mathbf{r} \int d\mathbf{r}' \lambda(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}', t) \psi_{\downarrow}(\mathbf{r}', t) \psi_{\uparrow}(\mathbf{r}, t) \\
&= \int d\mathbf{r} \lambda(\mathbf{r}) \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \\
&= \int d\mathbf{r} \lambda(\mathbf{r}) \left[\left\langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right\rangle + \delta^{\dagger}(\mathbf{r}, t) \right] [\langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle + \delta(\mathbf{r}, t)] \\
&\approx \int d\mathbf{r} \lambda(\mathbf{r}) \left[\left\langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right\rangle \delta(\mathbf{r}, t) + \delta^{\dagger}(\mathbf{r}, t) \langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle \right] \\
&= \int d\mathbf{r} \lambda(\mathbf{r}) \left[\left\langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right\rangle \{ \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) - \langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle \} \right. \\
&\quad \left. + \left\{ \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) - \left\langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right\rangle \right\} \langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle \right] \\
&\approx \int d\mathbf{r} \lambda(\mathbf{r}) \left[\left\langle \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right\rangle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) + \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle \right]
\end{aligned} \tag{2.13}$$

This can be written as

$$H_{\text{int}} \approx \int d\mathbf{r} \left[\Delta^*(\mathbf{r}, t) \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) + \Delta(\mathbf{r}, t) \psi_{\uparrow}^{\dagger}(\mathbf{r}, t) \psi_{\downarrow}^{\dagger}(\mathbf{r}, t) \right], \tag{2.14}$$

where we have defined the energy gap function

$$\Delta(\mathbf{r}, t) = \lambda(\mathbf{r}) \langle \psi_{\downarrow}(\mathbf{r}, t) \psi_{\uparrow}(\mathbf{r}, t) \rangle. \tag{2.15}$$

Equation (2.14) is the BCS Hamiltonian found by Bardeen, Cooper and Schrieffer [4]. The energy gap function can be considered as the superconducting order parameter. If the order parameter has a non-zero value, we have superconductivity, and if it is zero we do not. This means that above the critical temperature the gap function goes to zero. Notice that even if the energy gap function is zero in the normal metal in a superconductor/normal metal bilayer, we may still have superconducting correlations in the normal metal due to the proximity effect.

The energy gap function is a complex number, and may be written as $\Delta = |\Delta|e^{i\phi_s}$, where ϕ_s is the phase of the superconductor. If we only had one superconductor in the system, we could have transformed all equations to the situation where Δ is a real parameter. However, since we have two superconductors, as in Figure 1.1, we have the possibility of a phase difference (the Josephson phase) between the superconductors [17]. For this reason, we will in the following will treat Δ as a complex number.

2.2 Ferromagnetism

Ferromagnetism appears in ferromagnetic materials below the Curie temperature T_C . For these materials the energetically favorable structure is to have the spin of valence

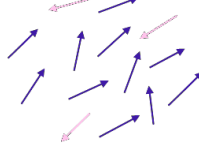


Figure 2.6: Example of spin-orientations in a ferromagnet. The majority of spin tends to point in a specific direction. The blue (dark gray) arrows contribute constructively to the magnetization, and the pink (light gray) arrows weaken the magnetization.

electrons point towards a common direction, illustrated in Figure 2.6. The Pauli principle states that only one electron is allowed to be in a specific quantum state. This means that we could have two electrons with opposite spins in the same k -state. In ferromagnetic materials we see an absence of overlap in the wave functions. This indicates that the Coulomb potential between such two electrons will increase the energy sufficiently to make this an undesirable effect. When keeping spins in the same direction, the Pauli principle ensures a stable low energy for the system.

However, if the region of ferromagnetism becomes large, the long-range magnetostatic energy potential for the magnetic field may make it preferable to construct specific domains in the material. These domains are individually ferromagnetic, but as seen from a macroscopic point of view, the material has no total magnetization. By applying an external magnetic field of some minimum strength, we can orient these domains to prefer the direction of the applied field, which would make a permanent magnet. The permanent magnetization can in turn be destroyed by, for instance, other applied fields or heating above T_C .

2.2.1 Heisenberg Model

The field Hamiltonian for a ferromagnet differs from the superconductor by one of the four terms in equation (2.5). The interaction term is replaced by a magnetization term H_M . This term originates from the Heisenberg model, which in position representation is given by

$$H'_M = \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2.16)$$

The one half factor in front compensates for that the summation is preformed over each spin pair twice. In the ferromagnetic case we have the constant $J_{ij} < 0$. This can be understood by thinking that the ground state should minimize the energy. In a ferromagnetic ground state the dot-product of neighboring spins should be positive and maximized, leaving us in need of a negative constant in (2.16).

2.2.2 Mean Field Approximation

Analogously to what we did to the interaction Hamiltonian in (2.13), we perform a mean field approximation to the Heisenberg model (2.16). We write $\mathbf{S}_i = \mathbf{m} + \delta\mathbf{S}_i$, where $\mathbf{m} = \langle \mathbf{S}_i \rangle$ is the mean field of the nearest neighbors, and considered to be constant⁸. In the first approximation we remove the constant term and neglect second order terms. In the second approximation we again neglect second order terms and only include nearest neighbor sites. The δ notation includes the next site in x-, y- and z-direction, which means that we only include each pair once, and we remove the one half factor in (2.16). We assume the strength J_{ij} to be equal between all nearest neighbors and rename it J .

$$\begin{aligned}
H'_M &= \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} J_{ij} (\mathbf{m} + \delta\mathbf{S}_i) \cdot (\mathbf{m} + \delta\mathbf{S}_j) \\
&= \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} J_{ij} \mathbf{m} \cdot \mathbf{m} + \mathbf{m} \cdot \delta\mathbf{S}_j + \delta\mathbf{S}_i \cdot \mathbf{m} + \delta\mathbf{S}_i \cdot \delta\mathbf{S}_j \\
&\approx \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} J_{ij} \mathbf{m} \cdot \delta\mathbf{S}_j + \delta\mathbf{S}_i \cdot \mathbf{m} \\
&= \frac{1}{2} \sum_{\substack{ij \\ i \neq j}} J_{ij} \mathbf{m} \cdot (\mathbf{S}_j - \mathbf{m}) + (\mathbf{S}_i - \mathbf{m}) \cdot \mathbf{m} \\
&\approx J\mathbf{m} \sum_{i,\delta} \mathbf{S}_{i+\delta} + \mathbf{S}_i \\
&= 6J\mathbf{m} \sum_i \mathbf{S}_i
\end{aligned} \tag{2.17}$$

This Hamiltonian has now been transformed into a single particle problem, where the factor 6 is the number of nearest neighbors. The operator for \mathbf{S} is $\frac{1}{2}\bar{\tau}$. Represented by field operators, defined in equation (2.4), the Hamiltonian is written

$$H_M = \sum_{\sigma\sigma'} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) [\bar{\tau} \cdot \mathbf{M}(\mathbf{r}, t)]_{\sigma\sigma'} \psi_{\sigma'}(\mathbf{r}, t). \tag{2.18}$$

Here the $\mathbf{M} = -\frac{6|J|}{2}\mathbf{m}$, so that it contains all the constants. In our Josephson junction $M = 0$ except from at the interfaces.

2.2.3 Magnetic Insulator

A magnetic insulator is a magnetic material with no current carriers. If we only have a thin layer of such a material, some electrons are able to tunnel through the barrier. The

⁸We will have uniform magnetization at each interface in our junction, but the two interfaces may have different magnetizations.

likelihood of tunneling will depend on the electron spin direction relative to the magnetic field of the insulator. This produces a difference in the scattering potential for spin-up and spin-down electrons, illustrated in Figure 2.7. The purpose of create this difference is to investigate properties connected to the superconductor wave function with total spin not equal to zero.

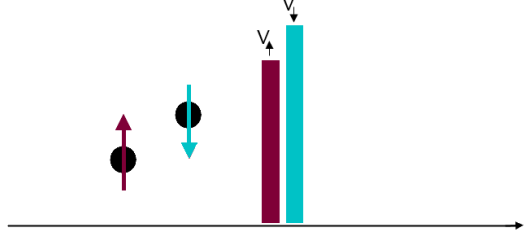


Figure 2.7: The spin-up and spin-down electrons experience different tunneling barrier when hitting a magnetic insulator. The magnetization of the insulator in this picture is aligned with the spin-up.

If an electron gets reflected from the magnetic insulator it will pick up a phase, which is dependent on the spin direction. This gives rise to a modification of the wave function, which we will come back to in section 3.1.

2.3 Green's Function Description for Superconductors

In section 2.3 we will base our theory on the work of J. P. Morten in [22]. An alternative review is given in [6].

2.3.1 Equation of Motion and Keldysh Formalism

We insert the field 4-vectors, in electron-hole space,

$$\psi^\dagger(\mathbf{r}, t) = \begin{pmatrix} \psi^\dagger_\uparrow(\mathbf{r}, t) & \psi^\dagger_\downarrow(\mathbf{r}, t) & \psi_\uparrow(\mathbf{r}, t) & \psi_\downarrow(\mathbf{r}, t) \end{pmatrix}, \quad \psi(\mathbf{r}, t) = \begin{pmatrix} \psi_\uparrow(\mathbf{r}, t) \\ \psi_\downarrow(\mathbf{r}, t) \\ \psi^\dagger_\uparrow(\mathbf{r}, t) \\ \psi^\dagger_\downarrow(\mathbf{r}, t) \end{pmatrix}, \quad (2.19)$$

as the operators in Heisenberg equation of motion (2.1), and use the Hamiltonian given in (2.5). When evaluated, the equations of motion becomes compactly

$$i \frac{\partial}{\partial t} \hat{\rho}_3 \psi(\mathbf{r}, t) = \hat{H}(\mathbf{r}, t) \psi(\mathbf{r}, t), \quad (2.20)$$

$$\psi^\dagger(\mathbf{r}, t) (-i \frac{\partial}{\partial t} \hat{\rho}_3) = \psi^\dagger(\mathbf{r}, t) \hat{H}^\dagger(\mathbf{r}, t). \quad (2.21)$$

Notice that the $(-i\frac{\partial}{\partial t}\hat{\rho}_3)$ and $\hat{H}^\dagger(\mathbf{r}, t)$ in (2.21) work to the left, in contrasts to the similar terms in (2.20) that as usual work to the right. We have in this way gathered all the information in the matrices \hat{H} and \hat{H}^\dagger defined as

$$\begin{aligned}\hat{H} &= \hat{\xi} + V_{\text{imp}}\hat{1} + \hat{S} + \hat{\Delta}, \\ \hat{H}^\dagger &= \hat{\xi}^* + V_{\text{imp}}\hat{1} + \hat{S} - \hat{\Delta},\end{aligned}\tag{2.22}$$

where $\hat{\xi}$, \hat{S} and $\hat{\Delta}$ are given by

$$\hat{\xi} = -\frac{1}{2m}(\nabla - ie\mathbf{A}\hat{\rho}_3)^2 + e\varphi\hat{1} - \mu\hat{1},\tag{2.23}$$

$$\hat{S} = V_{\text{sf}} \begin{pmatrix} \bar{\boldsymbol{\tau}} \cdot \mathbf{S} & 0 \\ 0 & [\bar{\boldsymbol{\tau}} \cdot \mathbf{S}]^T \end{pmatrix},\tag{2.24}$$

$$\hat{\Delta} = \begin{pmatrix} 0 & i\Delta\tau_2 \\ i\Delta^*\tau_2 & 0 \end{pmatrix}.\tag{2.25}$$

From Appendix B, we interpret the normal Green's function $\bar{G}(1, 2)$ as a matrix of probability amplitudes for an electron to jump from one state to another within a specific time interval, meanwhile the anomalous Green's function $\bar{F}(1, 2)$ contains the probability amplitudes for having Cooper pairs. By examining how the 8×8 Green's function in Keldysh space \check{G} would work as the state of the left hand sides in (2.20) and (2.21), we end up with the equation of motion for the Green's function in Keldysh space

$$\left(i\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1)\right)\check{G}(1, 2) = \delta(1 - 2)\check{1},\tag{2.26}$$

$$\check{G}(1, 2)\left(i\frac{\partial}{\partial t_2}\hat{\rho}_3 - \hat{H}(2)\right)^\dagger = \delta(1 - 2)\check{1}.\tag{2.27}$$

2.3.2 Energy Gap Function and Current Matrix

The superconducting order parameter in equation (2.15) can be expressed with the Keldysh Green's function as

$$\Delta(1) = -\frac{i}{4}\lambda\text{Tr}\left\{\frac{\hat{\rho}_1 - i\hat{\rho}_2}{2}\hat{\tau}_3\hat{G}^{\text{K}}(1, 1)\right\}.\tag{2.28}$$

λ is the negative, constant interaction strength from (2.15). The trace expression is equivalent to subtracting element 23 from 14 in $\hat{G}^{\text{K}}(1, 1)$ (see Appendix A). Equation (2.28) can be justified by writing out element 23 and 14 (equal to element 12 and 21 in (B.10)) for equal times, and using the commutation relation of the field operators in (2.3). This leads back to the expression in (2.15).

Quantum mechanically, normal charge current is given by

$$\mathbf{j} = \frac{e}{m} \text{Re} \left\{ \psi^\dagger (\mathbf{p} - e\mathbf{A}) \psi \right\}, \quad (2.29)$$

where we have the momentum operator in position representation with natural units $\mathbf{p} = -i\nabla$. The charge current is equal to the sum over all the charge current contributions, where these contributions are expressed by exchanging the wave function ψ in (2.29), by the field operator $\psi_\sigma(1)$. This gives us

$$\mathbf{j}(1) = \sum_\sigma \frac{e}{m} \text{Re} \left\{ \psi_\sigma^\dagger(1) [\mathbf{p}(1) - e\mathbf{A}(1)] \psi_\sigma(1) \right\}. \quad (2.30)$$

Notice that even if the total charge-current is zero, the current of each spin does not necessarily have to be zero. It can be shown that (2.30) may be written

$$\hat{\mathbf{j}}(1) = -\frac{e}{4m} \text{Tr} \left\{ \lim_{1 \rightarrow 2} [(\nabla_1 - ie\mathbf{A}(1)) - (\nabla_2 - ie\mathbf{A}(2))] \bar{G}^K(1, 2) \right\}. \quad (2.31)$$

The charge current is then expressed by element 11 and 22 in the Keldysh Green's function (B.9), which makes sense because these elements are related to the propagation of spin-up and spin-down electrons. If we remove the trace in (2.31) and exchange $\bar{G}^K(1, 2)$ with $\hat{G}^K(1, 2)$, we get the current matrix.

$$\hat{\mathbf{j}}(1) = -\frac{e}{4m} \lim_{1 \rightarrow 2} [(\nabla_1 - ie\mathbf{A}(1)) - (\nabla_2 - ie\mathbf{A}(2))] \hat{G}^K(1, 2). \quad (2.32)$$

We would get back our normal charge current by summing element 11 and 22 in $\hat{\mathbf{j}}(1)$. As shown in Appendix A, this is mathematically expressed as

$$\mathbf{j}(1) = \text{Tr} \left\{ \frac{\hat{1} + \hat{\rho}_3}{2} \hat{\mathbf{j}}(1) \right\}. \quad (2.33)$$

2.3.3 Mixed Representation

Analogously to the center of mass representation, we introduce the mixed representation.

$$\begin{aligned} \mathbf{r}_1 &= \mathbf{R} + \frac{\mathbf{r}}{2}, & t_1 &= T + \frac{t}{2} \\ \mathbf{r}_2 &= \mathbf{R} - \frac{\mathbf{r}}{2}, & t_2 &= T - \frac{t}{2} \end{aligned} \quad (2.34)$$

T and \mathbf{R} are the mean value coordinates, and the \mathbf{r} and t are the relative coordinates from the mean values. The associated 4-vectors are then written

$$X = (\mathbf{R}, T), \quad x = (\mathbf{r}, t). \quad (2.35)$$

We also have the 4-momentum $p = (\mathbf{p}, E)$, where \mathbf{p} is the momentum space vector, making $px = \mathbf{p} \cdot \mathbf{r} - Et$. The Fourier transform over the relative coordinate is given by

$$\check{G}(X, p) = \int d\mathbf{x} e^{-ipx} \check{G}(X + \frac{x}{2}, X - \frac{x}{2}). \quad (2.36)$$

When we are working with the wave function of Cooper pairs, we are mostly interested in the mean coordinate of the two-particle wave function. The relative coordinate will oscillate at lengths in the order of the Fermi wavelength, which is much smaller than the system we are looking at. For our purposes, it is a valid assumption that we may integrate out this rapid oscillation, without losing important information.

2.3.4 Kinetic Equation

By subtracting (2.27) from (2.26) and Fourier transforming as in (2.36) over the relative coordinate, we obtain the kinetic equation⁹

$$\begin{aligned} & \left[E\hat{\rho}_3 + i\frac{\mathbf{p}}{m}\hat{\boldsymbol{\theta}} - e\varphi\hat{1} - V_{\text{imp}}\hat{1} - \hat{S} - \hat{\Delta} \circledast \check{G}(X, p) \right] \\ & - \frac{1}{2m} \left[e^2 \mathbf{A}^2 + ie(\nabla_{\mathbf{R}} \mathbf{A})\hat{\rho}_3 \circledast \check{G}(X, p) \right] - \frac{1}{2m} \left\{ ie\mathbf{A}\hat{\rho}_3 \circledast (\nabla_{\mathbf{R}} \check{G})(X, p) \right\} = 0. \end{aligned} \quad (2.37)$$

This equation will be simplified in section 2.3.5. We have introduced $\hat{\boldsymbol{\theta}} = \nabla\hat{1} - ie\mathbf{A}\hat{\rho}_3$, and the notation $[\hat{\boldsymbol{\theta}} \circledast \check{G}] = \nabla_{\mathbf{R}}\check{G} - ie[\mathbf{A}\hat{\rho}_3 \circledast \check{G}]$. When not considering time dependence, the star product \circledast reduces to normal multiplication. Later we will set $\mathbf{A} = 0$, and the two last terms in (2.37) would vanish, but we will show in section 2.3.5 that in the quasiclassical case these terms disappear anyway.

2.3.5 Quasiclassical Theory

At low temperatures, electrons will fill the energy states up to the Fermi surface, as discussed in section 2.1.6. The conducting electrons will then have momenta close to the Fermi momentum \mathbf{p}_F . We have that $|\mathbf{p}| = \frac{2\pi}{\lambda}$, meaning that these electrons have wavelengths in the order of the Fermi wavelength λ_F . The conducting electrons therefore have the smallest wavelengths of all the electrons in the system.

We now assume that all physical quantities of interest are much larger than the Fermi wavelength λ_F , and denote L as the typical size of our system. Notice that $\hat{\boldsymbol{\theta}}$ is in the order of $\sim \frac{1}{L}$, which means that $e\mathbf{A} \sim \frac{1}{L}$ and $\nabla \sim \frac{1}{L}$. We already know that $\mathbf{p} \sim \frac{1}{\lambda_F}$, which makes the term $i\frac{\mathbf{p}}{m}\hat{\boldsymbol{\theta}}$ in (2.37) much larger than all the terms in second commutator and in the anti-commutator. We then neglect these terms.

If we apply the gradient approximation to the remaining part of (2.37), only keeping the derivatives to the first order in space, we get

$$\begin{aligned} & \left[E\hat{\rho}_3 + i\frac{\mathbf{p}}{m}\hat{\boldsymbol{\theta}} - e\varphi\hat{1} - V_{\text{imp}}\hat{1} - \hat{S} - \hat{\Delta} \circledast \check{G} \right] \approx \left[E\hat{\rho}_3 + i\frac{\mathbf{p}}{m}\hat{\boldsymbol{\theta}} - e\varphi\hat{1} - V_{\text{imp}}\hat{1} - \hat{S} - \hat{\Delta} \circledast \check{G} \right] \\ & - \frac{i}{2} \left\{ \nabla_{\mathbf{R}} \left(e\varphi\hat{1} + V_{\text{imp}}\hat{1} + \hat{S} + \hat{\Delta} \right), \nabla_{\mathbf{p}} \check{G} \right\}. \end{aligned} \quad (2.38)$$

⁹The star product is defined as $A(X, p) \otimes B(X, p) = e^{\frac{i}{2}(\partial_{X_A} \partial_{p_B} - \partial_{p_A} \partial_{X_B})} A(X, p) B(X, p)$, and we will also use $A(X, p) \circ B(X, p) = e^{\frac{i}{2}(\partial_{T_A} \partial_{E_B} - \partial_{E_A} \partial_{T_B})} A(X, p) B(X, p)$. Remember that we can write $e^u = \sum_{n=0}^{\infty} \frac{u^n}{n!}$.

The last term goes to zero if we set $\mathbf{p} = \mathbf{p}_F$, since \mathbf{p}_F has a constant absolute value.

The quasiclassical Green's function was introduced by Eilenberger [11] and is defined as

$$\check{g}(X, \mathbf{p}_F, E) = \frac{i}{\pi} \int_{-\infty}^{\infty} d\xi_p \check{G}(X, p), \quad (2.39)$$

where $\xi_p = \frac{p^2}{2m}$. Equation (2.39) will then average over the square of the absolute value of momentum, only keeping the direction dependence of the Fermi momentum. The Green's function $\check{G}(X, p)$ has values that peaks around \mathbf{p}_F , which means that we do not lose that much information by averaging over the momentum value. The integral from $-\infty$ to ∞ can be replaced by integration in the complex plane, and when we neglect the high energy integral parts we are left with contour integration for the low-energy contribution.

After applying the gradient approximation and the quasiclassical approximation, we arrive at the simpler form

$$\left[E\hat{\rho}_3 + i\mathbf{v}_F\hat{\boldsymbol{\theta}} - e\varphi\hat{1} - V_{\text{imp}}\hat{1} - \hat{S} - \hat{\Delta} \circ \check{g} \right] = 0. \quad (2.40)$$

We use the notation $[\hat{\boldsymbol{\theta}} \circ \check{g}] = \nabla_{\mathbf{R}}\check{g} - ie[\mathbf{A}\hat{\rho}_3 \circ \check{g}]$, and have defined the Fermi velocity $\mathbf{v}_F = \frac{\mathbf{p}_F}{m}$.

2.3.6 Usadel Equation

The diffusive limit refers to the situation where the particle in question is scattered in many different directions, on its way through the material. The superconductor is then considered dirty. The opposite situation is ballistic scattering, where the material is so clean that particle scattering is minimal. Experimentally we have higher demands when making such clean materials, which make them difficult and expensive to produce. In our calculation, we will focus on the diffusive limit.

In the diffusive limit we replace the quasiclassical Green's function by its approximate, only expanding in the spherical s- and p-waves, like suggested by Usadel [25].

$$\check{g}(X, \mathbf{p}_F, E) \approx \check{g}_s(X, E) + \mathbf{e}_F \cdot \check{\mathbf{g}}_p(X, E) \quad (2.41)$$

We have here named the unit vector of the Fermi momentum \mathbf{e}_F .

Next, we replace the impurity scattering potential with the self-energy in the Born approximation ($V_{\text{imp}}\hat{1} \rightarrow \check{\sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}_F, E)$). This gives us

$$\check{\sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}_F, E) \approx -\frac{i}{2\tau}\check{g}_s, \quad (2.42)$$

where τ is the relaxation time¹⁰.

¹⁰The relaxation time is the mean time interval between two scattering events. It describes the mean time a particle can "relax" before it hits an impurity again.

After replacing \check{g} by the expression in (2.40) and including (2.42) in (2.41), we get

$$\left[E\hat{\rho}_3 + iv_F\hat{\boldsymbol{\theta}} - e\varphi\hat{1} + \frac{i}{2\tau}\check{g}_s - \hat{S} - \hat{\Delta} \circ \check{g}_s + \mathbf{e}_F \cdot \check{\mathbf{g}}_p \right] = 0. \quad (2.43)$$

If we now average over all angles in (2.43), we are left with

$$\left[E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta} \circ \check{g}_s \right] + \frac{i}{3}v_F \left[\hat{\boldsymbol{\theta}} \circ \check{\mathbf{g}}_p \right] = 0. \quad (2.44)$$

And the in the same way, if we multiply with \mathbf{e}_F before averaging, we get

$$\frac{i}{2\tau} [\check{g}_s \circ \check{\mathbf{g}}_p] + iv_F [\hat{\boldsymbol{\theta}} \circ \check{g}_s] = 0. \quad (2.45)$$

The normalization condition for the quasiclassical Green's function is $\check{g} \circ \check{g} = \hat{1}$. To the first order, this gives us

$$\check{g}_s \circ \check{g}_s = \hat{1} \quad \text{and} \quad \check{g}_s \circ \check{\mathbf{g}}_p + \check{\mathbf{g}}_p \circ \check{g}_s = 0. \quad (2.46)$$

After multiplying (2.45) with $\check{g}_s \circ$ from the left, we get

$$\begin{aligned} \check{g}_s \circ \frac{i}{2\tau} [\check{g}_s \circ \check{\mathbf{g}}_p] + \check{g}_s \circ iv_F [\hat{\boldsymbol{\theta}} \circ \check{g}_s] &= 0 \\ \check{g}_s \circ \check{g}_s \circ \check{\mathbf{g}}_p - \check{g}_s \circ \check{\mathbf{g}}_p \circ \check{g}_s + 2\tau v_F \check{g}_s \circ [\hat{\boldsymbol{\theta}} \circ \check{g}_s] &= 0 \\ \check{\mathbf{g}}_p + \check{g}_s \circ \check{g}_s \circ \check{\mathbf{g}}_p + 2\tau v_F \check{g}_s \circ [\hat{\boldsymbol{\theta}} \circ \check{g}_s] &= 0 \\ \check{\mathbf{g}}_p &= -\tau v_F \check{g}_s \circ [\hat{\boldsymbol{\theta}} \circ \check{g}_s] \end{aligned} \quad (2.47)$$

By putting this expression into (2.44), we have managed to reduce the problem to only depend on \check{g}_s , which has elements independent of direction \mathbf{e}_F .

$$\boxed{D_s \left[\hat{\boldsymbol{\theta}} \circ \check{g}_s \circ [\hat{\boldsymbol{\theta}} \circ \check{g}_s] \right] + i \left[E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta} \circ \check{g}_s \right] = 0.} \quad (2.48)$$

We have defined the constant $D_s = \frac{1}{3}\tau v_F^2$, called the diffusion constant. Equation (2.48) is the Usadel equation. If we solve this equation, we will get the Green's function, which in turn can be used to calculate physical observables. From the different components of the Green's function matrix, we are able to analyze what kind of superconductivity the system generated.

2.4 Riccati Parameterization

2.4.1 Riccati Parameterization for the Usadel Equation

At this point we will go further than the work of J. P. Morten. The Usadel equation (2.48) can be presented in a way that is convenient for numerical calculations. We now apply the Riccati parameterization [24] and [23] to the Usadel equation.

For simplicity we define

$$\hat{K} = E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (2.49)$$

where we get the 2×2 -matrices¹¹ in (2.50) by retrieving terms from (2.24), (2.25) and (A.8).

$$\begin{aligned} a &= (E - e\varphi) - \boldsymbol{\tau} \cdot \mathbf{S} \\ b &= -i\Delta\tau_2 \\ c &= -i\Delta^*\tau_2 \\ d &= -E - e\varphi - [\boldsymbol{\tau} \cdot \mathbf{S}]^T \end{aligned} \quad (2.50)$$

When $\mathbf{A} = 0$, and we only consider the x-direction, equation (2.48) reduces to

$$D_s (\partial_x \check{g}_s (\partial_x \check{g}_s)) + i [\hat{K}, \check{g}_s] = 0. \quad (2.51)$$

We want to solve this equation for the quasiclassical Green's function \check{g}_s . At this point we drop the subtext $_s$ for the quasiclassical Green's function ($\check{g}_s = \check{g}$). We also drop the bar notation \sim for the 2×2 -matrices in order to keep the expressions readable. The Usadel equation (2.51) consists of 8×8 -matrices and can be split into three equations¹² of 4×4 -matrices by applying (B.11). The equation for the retarded Green's function then becomes

$$D_s (\partial_x \hat{g}^R (\partial_x \hat{g}^R)) + i [\hat{K}, \hat{g}^R] = 0, \quad (2.52)$$

which is on the same form as (2.51). We also get an equation on this form for the advanced quasiclassical Green's function \hat{g}^A , but we can use the relation $\hat{g}^A = -[\hat{\rho}_3 \hat{g}^R \hat{\rho}_3]^\dagger$ (see Appendix B) to find \hat{g}^A , if we already have \hat{g}^R . This allows us to concentrate on only one of the Green's functions¹³. We choose to continue with \hat{g}^R .

By looking at the quasiclassical retarded Green's function in (B.12), we can write

$$\hat{g}^R = \begin{pmatrix} g^R & f^R \\ -\tilde{f}^R & -\tilde{g}^R \end{pmatrix}. \quad (2.53)$$

The $\tilde{}$ notation equals replacing E by $-E$ and complex conjugate, meaning that $\tilde{f}(E) = f^*(-E)$. To ensure the required symmetry in (2.53), we use the Riccati parameterization

$$\hat{g}^R = \begin{pmatrix} N(1 + \gamma\tilde{\gamma}) & 2N\gamma \\ -2\tilde{N}\tilde{\gamma} & -\tilde{N}(1 + \tilde{\gamma}\gamma) \end{pmatrix}. \quad (2.54)$$

Here γ is a 2×2 -matrix, and we have defined the normalization matrices as

¹¹In principle, these matrices can be modified to represent other materials, as long as we know the content of \hat{K} , and that all the approximations up til now are valid.

¹²We would also get a trivial equation, zero equal zero, but that does not give us much.

¹³The Keldysh Green's function \hat{g}^K can be found from \hat{g}^R and \hat{g}^A together with a function \hat{h} .

$$\begin{aligned} N &= (1 - \gamma\tilde{\gamma})^{-1}, \\ \tilde{N} &= (1 - \tilde{\gamma}\gamma)^{-1}. \end{aligned} \quad (2.55)$$

Useful properties of the Riccati parameterization are:

$$\begin{aligned} N\gamma &= \gamma\tilde{N} \\ \tilde{N}\tilde{\gamma} &= \tilde{\gamma}N \end{aligned} \quad (2.56)$$

$$\begin{aligned} \partial_x N &= NDN \\ \partial_x \tilde{N} &= \tilde{N}\tilde{D}\tilde{N} \end{aligned} \quad (2.57)$$

Here we have defined the D and \tilde{D} as

$$\begin{aligned} D &= \partial_x(\gamma\tilde{\gamma}) = (\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma}), \\ \tilde{D} &= \partial_x(\tilde{\gamma}\gamma) = (\partial_x\tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x\gamma). \end{aligned} \quad (2.58)$$

By using (2.56), we are free to write the Riccati parameterization in a slightly different way

$$\hat{g}^R = \begin{pmatrix} (1 + \gamma\tilde{\gamma})N & 2\gamma\tilde{N} \\ -2\tilde{\gamma}N & -(1 + \tilde{\gamma}\gamma)\tilde{N} \end{pmatrix}. \quad (2.59)$$

In the forthcoming derivations, it will often be of advantage to push the N -matrices as close to the "edges" as possible, making it easier to manipulate the expressions. This is done by alternating between (2.54) and (2.59), in a sensible way.

Our first goal is to express the left side of the Usadel equation (2.52) with the Riccati parameterization. Using equation (2.59), we start by calculating $\partial_x \hat{g}^R$.

$$\begin{aligned} \partial_x \hat{g}^R &= \partial_x \begin{pmatrix} (1 + \gamma\tilde{\gamma})N & 2\gamma\tilde{N} \\ -2\tilde{\gamma}N & -(1 + \tilde{\gamma}\gamma)\tilde{N} \end{pmatrix} \\ &= \begin{pmatrix} DN + NDN + \gamma\tilde{\gamma}NDN & 2(\partial_x\gamma)\tilde{N} + 2\gamma\tilde{N}\tilde{D}\tilde{N} \\ -2(\partial_x\tilde{\gamma})N - 2\tilde{\gamma}NDN & -\tilde{D}\tilde{N} - \tilde{N}\tilde{D}\tilde{N} - \tilde{\gamma}\gamma\tilde{N}\tilde{D}\tilde{N} \end{pmatrix} \\ &= \begin{pmatrix} DN - NDN + \gamma\tilde{\gamma}NDN + 2NDN & 2(\partial_x\gamma)\tilde{N} + 2\gamma\tilde{N}\tilde{D}\tilde{N} \\ -2(\partial_x\tilde{\gamma})N - 2\tilde{\gamma}NDN & -\tilde{D}\tilde{N} + \tilde{N}\tilde{D}\tilde{N} - \tilde{\gamma}\gamma\tilde{N}\tilde{D}\tilde{N} - 2\tilde{N}\tilde{D}\tilde{N} \end{pmatrix} \\ &= \begin{pmatrix} DN - (1 - \gamma\tilde{\gamma})NDN + 2NDN & 2(\partial_x\gamma)\tilde{N} + 2\gamma\tilde{N}\tilde{D}\tilde{N} \\ -2(\partial_x\tilde{\gamma})N - 2\tilde{\gamma}NDN & -\tilde{D}\tilde{N} + (1 - \tilde{\gamma}\gamma)\tilde{N}\tilde{D}\tilde{N} - 2\tilde{N}\tilde{D}\tilde{N} \end{pmatrix} \\ &= 2 \begin{pmatrix} NDN & (\partial_x\gamma)\tilde{N} + \gamma\tilde{N}\tilde{D}\tilde{N} \\ -(\partial_x\tilde{\gamma})N - \tilde{\gamma}NDN & -\tilde{N}\tilde{D}\tilde{N} \end{pmatrix} \end{aligned} \quad (2.60)$$

We have used the definition of the normalization matrices (2.55) to simplify in the next last step. Further, we derive $\hat{g}^R(\partial_x \hat{g}^R)$ by multiplying (2.60) with (2.54) from the left.

$$\begin{aligned} \hat{g}^R(\partial_x \hat{g}^R) &= 2 \begin{pmatrix} N(1 + \gamma\tilde{\gamma}) & 2N\gamma \\ -2\tilde{N}\tilde{\gamma} & -\tilde{N}(1 + \tilde{\gamma}\gamma) \end{pmatrix} \begin{pmatrix} NDN & (\partial_x \gamma)\tilde{N} + \gamma\tilde{N}\tilde{D}\tilde{N} \\ -(\partial_x \tilde{\gamma})N - \tilde{\gamma}NDN & -\tilde{N}\tilde{D}\tilde{N} \end{pmatrix} \\ &= \begin{pmatrix} [\hat{g}^R(\partial_x \hat{g}^R)]_{11} & [\hat{g}^R(\partial_x \hat{g}^R)]_{12} \\ [\hat{g}^R(\partial_x \hat{g}^R)]_{21} & [\hat{g}^R(\partial_x \hat{g}^R)]_{22} \end{pmatrix} \end{aligned} \quad (2.61)$$

It will be helpful to notice the symmetry

$$\begin{aligned} \hat{g}^R(\partial_x \hat{g}^R) &= \begin{pmatrix} g^R & f^R \\ -\tilde{f}^R & -\tilde{g}^R \end{pmatrix} \begin{pmatrix} \partial_x g^R & \partial_x f^R \\ -\partial_x \tilde{f}^R & -\partial_x \tilde{g}^R \end{pmatrix} \\ &= \begin{pmatrix} g^R(\partial_x g^R) - f^R(\partial_x \tilde{f}^R) & g^R(\partial_x f^R) - f^R(\partial_x \tilde{g}^R) \\ \tilde{g}^R(\partial_x \tilde{f}^R) - \tilde{f}^R(\partial_x g^R) & \tilde{g}^R(\partial_x \tilde{g}^R) - \tilde{f}^R(\partial_x f^R) \end{pmatrix}, \end{aligned} \quad (2.62)$$

where we will get element 22 from 11, and 21 from 12, by exchanging all matrices by their tilde-version. We choose to write out the elements $[\hat{g}^R(\partial_x \hat{g}^R)]_{11}$ and $[\hat{g}^R(\partial_x \hat{g}^R)]_{12}$ separately, and find $[\hat{g}^R(\partial_x \hat{g}^R)]_{21}$ and $[\hat{g}^R(\partial_x \hat{g}^R)]_{22}$ from this symmetry. If we look for terms with the structure $vNw - v\gamma\tilde{\gamma}Nw$, this can be shortened to vw by the definition of N in (2.55).

$$\begin{aligned} [\hat{g}^R(\partial_x \hat{g}^R)]_{11} &= 2N(1 + \gamma\tilde{\gamma})NDN - 4N\gamma(\partial_x \tilde{\gamma})N - 4N\gamma\tilde{\gamma}NDN \\ &= 2N[ND + \gamma\tilde{\gamma}]ND - 2\gamma(\partial_x \tilde{\gamma})N - \gamma\tilde{\gamma}ND - \gamma\tilde{\gamma}ND]N \\ &= 2N[N(1 - \gamma\tilde{\gamma})D - 2\gamma(\partial_x \tilde{\gamma})]N \\ &= 2N[D - 2\gamma(\partial_x \tilde{\gamma})]N \\ &= 2N[(\partial_x \gamma)\tilde{\gamma} - \gamma(\partial_x \tilde{\gamma})]N \end{aligned} \quad (2.63)$$

$$\begin{aligned} [\hat{g}^R(\partial_x \hat{g}^R)]_{12} &= 2N(1 + \gamma\tilde{\gamma})(\partial_x \gamma)\tilde{N} + 2N(1 + \gamma\tilde{\gamma})\gamma\tilde{N}\tilde{D}\tilde{N} - 4N\gamma\tilde{N}\tilde{D}\tilde{N} \\ &= 2N[(\partial_x \gamma) + \gamma\tilde{\gamma}(\partial_x \gamma) + \gamma\tilde{N}\tilde{D} + \gamma\tilde{\gamma}\gamma\tilde{N}\tilde{D} - 2\gamma\tilde{N}\tilde{D}]\tilde{N} \\ &= 2N[(\partial_x \gamma) + \gamma\tilde{\gamma}(\partial_x \gamma) - \gamma(1 - \tilde{\gamma}\gamma)\tilde{N}\tilde{D}]\tilde{N} \\ &= 2N[(\partial_x \gamma) + \gamma\tilde{\gamma}(\partial_x \gamma) - \gamma\{(\partial_x \tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x \gamma)\}]\tilde{N} \\ &= 2N[(\partial_x \gamma) - \gamma(\partial_x \tilde{\gamma})\gamma]\tilde{N} \end{aligned} \quad (2.64)$$

From symmetry, we then also have

$$[\hat{g}^R(\partial_x \hat{g}^R)]_{21} = 2\tilde{N} [(\partial_x \tilde{\gamma}) - \tilde{\gamma}(\partial_x \gamma) \tilde{\gamma}] N, \quad (2.65)$$

$$[\hat{g}^R(\partial_x \hat{g}^R)]_{22} = 2\tilde{N} [(\partial_x \tilde{\gamma}) \gamma - \tilde{\gamma}(\partial_x \gamma)] \tilde{N}. \quad (2.66)$$

We now differentiate these terms in order to obtain the same form as for the first term in equation (2.52).

$$\begin{aligned} [\partial_x(\hat{g}^R(\partial_x \hat{g}^R))]_{11} &= \partial_x(2N [(\partial_x \gamma) \tilde{\gamma} - \gamma(\partial_x \tilde{\gamma})] N) \\ &= 2NDN [(\partial_x \gamma) \tilde{\gamma} - \gamma(\partial_x \tilde{\gamma})] N \\ &\quad + 2N(\partial_x [(\partial_x \gamma) \tilde{\gamma} - \gamma(\partial_x \tilde{\gamma})]) N \\ &\quad + 2N [(\partial_x \gamma) \tilde{\gamma} - \gamma(\partial_x \tilde{\gamma})] NDN \\ &= 2N[DN(\partial_x \gamma) \tilde{\gamma} - DN\gamma(\partial_x \tilde{\gamma}) + (\partial_x^2 \gamma) \tilde{\gamma} + (\partial_x \gamma)(\partial_x \tilde{\gamma}) - (\partial_x \gamma)(\partial_x \tilde{\gamma}) \\ &\quad - \gamma(\partial_x^2 \tilde{\gamma}) + (\partial_x \gamma) \tilde{\gamma} ND - \gamma(\partial_x \tilde{\gamma}) ND] N \\ &= 2N[DN(\partial_x \gamma) \tilde{\gamma} - DN\gamma(\partial_x \tilde{\gamma}) + (\partial_x^2 \gamma) \tilde{\gamma} - \gamma(\partial_x^2 \tilde{\gamma}) \\ &\quad + (\partial_x \gamma) \tilde{\gamma} ND - \gamma(\partial_x \tilde{\gamma}) ND] N \\ &= 2N[\{(\partial_x \gamma) \tilde{\gamma} + \gamma(\partial_x \tilde{\gamma})\} N(\partial_x \gamma) \tilde{\gamma} - \{(\partial_x \gamma) \tilde{\gamma} + \gamma(\partial_x \tilde{\gamma})\} N\gamma(\partial_x \tilde{\gamma}) \\ &\quad + (\partial_x^2 \gamma) \tilde{\gamma} - \gamma(\partial_x^2 \tilde{\gamma}) + (\partial_x \gamma) \tilde{\gamma} N \{(\partial_x \gamma) \tilde{\gamma} + \gamma(\partial_x \tilde{\gamma})\} \\ &\quad - \gamma(\partial_x \tilde{\gamma}) N \{(\partial_x \gamma) \tilde{\gamma} + \gamma(\partial_x \tilde{\gamma})\}] N \\ &= 2N[(\partial_x \gamma) \tilde{\gamma} N(\partial_x \gamma) \tilde{\gamma} + \gamma(\partial_x \tilde{\gamma}) N(\partial_x \gamma) \tilde{\gamma} - (\partial_x \gamma) \tilde{\gamma} N\gamma(\partial_x \tilde{\gamma}) \\ &\quad - \gamma(\partial_x \tilde{\gamma}) N\gamma(\partial_x \tilde{\gamma}) + (\partial_x^2 \gamma) \tilde{\gamma} - \gamma(\partial_x^2 \tilde{\gamma}) + (\partial_x \gamma) \tilde{\gamma} N(\partial_x \gamma) \tilde{\gamma} \\ &\quad + (\partial_x \gamma) \tilde{\gamma} N\gamma(\partial_x \tilde{\gamma}) - \gamma(\partial_x \tilde{\gamma}) N(\partial_x \gamma) \tilde{\gamma} - \gamma(\partial_x \tilde{\gamma}) N\gamma(\partial_x \tilde{\gamma})] N \\ &= 2N[2(\partial_x \gamma) \tilde{\gamma} N(\partial_x \gamma) \tilde{\gamma} - 2\gamma(\partial_x \tilde{\gamma}) N\gamma(\partial_x \tilde{\gamma}) + (\partial_x^2 \gamma) \tilde{\gamma} - \gamma(\partial_x^2 \tilde{\gamma})] N \end{aligned} \quad (2.67)$$

$$\begin{aligned}
[\partial_x(\hat{g}^R(\partial_x\hat{g}^R))]_{12} &= \partial_x(2N[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{N}) \\
&= 2NDN[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{N} \\
&\quad + 2N(\partial_x[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma])\tilde{N} \\
&\quad + 2N[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{N}\tilde{D}\tilde{N} \\
&= 2N[DN(\partial_x\gamma) - DN\gamma(\partial_x\tilde{\gamma})\gamma + (\partial_x^2\gamma) - (\partial_x\gamma)(\partial_x\tilde{\gamma})\gamma \\
&\quad - \gamma(\partial_x^2\tilde{\gamma})\gamma - \gamma(\partial_x\tilde{\gamma})(\partial_x\gamma) + (\partial_x\gamma)\tilde{N}\tilde{D} - \gamma(\partial_x\tilde{\gamma})\gamma\tilde{N}\tilde{D}]\tilde{N} \\
&= 2N[\{(\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma})\}N(\partial_x\gamma) - \{(\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma})\}N\gamma(\partial_x\tilde{\gamma})\gamma \\
&\quad + (\partial_x^2\gamma) - (\partial_x\gamma)(\partial_x\tilde{\gamma})\gamma - \gamma(\partial_x^2\tilde{\gamma})\gamma - \gamma(\partial_x\tilde{\gamma})(\partial_x\gamma) \\
&\quad + (\partial_x\gamma)\tilde{N}\{(\partial_x\tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x\gamma)\} - \gamma(\partial_x\tilde{\gamma})\gamma\tilde{N}\{(\partial_x\tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x\gamma)\}]\tilde{N} \\
&= 2N[(\partial_x\gamma)\tilde{\gamma}N(\partial_x\gamma) + \gamma(\partial_x\tilde{\gamma})N(\partial_x\gamma) - (\partial_x\gamma)\tilde{\gamma}N\gamma(\partial_x\tilde{\gamma})\gamma \\
&\quad - \gamma(\partial_x\tilde{\gamma})N\gamma(\partial_x\tilde{\gamma})\gamma + (\partial_x^2\gamma) - (\partial_x\gamma)(\partial_x\tilde{\gamma})\gamma \\
&\quad - \gamma(\partial_x^2\tilde{\gamma})\gamma - \gamma(\partial_x\tilde{\gamma})(\partial_x\gamma) + (\partial_x\gamma)\tilde{N}(\partial_x\tilde{\gamma})\gamma \\
&\quad + (\partial_x\gamma)\tilde{N}\tilde{\gamma}(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma\tilde{N}(\partial_x\tilde{\gamma})\gamma - \gamma(\partial_x\tilde{\gamma})\gamma\tilde{N}\tilde{\gamma}(\partial_x\gamma)]\tilde{N} \\
&= 2N[2(\partial_x\gamma)\tilde{\gamma}N(\partial_x\gamma) + \gamma(\partial_x\tilde{\gamma})\{N - 1 - \gamma\tilde{N}\tilde{\gamma}\}(\partial_x\gamma) \\
&\quad + (\partial_x\gamma)\{-\tilde{\gamma}N\gamma - 1 + \tilde{N}\}(\partial_x\tilde{\gamma})\gamma - 2\gamma(\partial_x\tilde{\gamma})N\gamma(\partial_x\tilde{\gamma})\gamma \\
&\quad + (\partial_x^2\gamma) - \gamma(\partial_x^2\tilde{\gamma})\gamma]\tilde{N} \\
&= 2N[2(\partial_x\gamma)\tilde{\gamma}N(\partial_x\gamma) - 2\gamma(\partial_x\tilde{\gamma})N\gamma(\partial_x\tilde{\gamma})\gamma + (\partial_x^2\gamma) - \gamma(\partial_x^2\tilde{\gamma})\gamma]\tilde{N}
\end{aligned} \tag{2.68}$$

By looking at the results from (2.67) and (2.68), we see that there are some almost similar terms. Part of these terms will cancel out by calculating $N^{-1}[(12) - (11)N^{-1}\gamma\tilde{N}]$.

$$\begin{aligned}
& N^{-1} \left[[\partial_x(\hat{g}^R(\partial_x \hat{g}^R))]_{12} - [\partial_x(\hat{g}^R(\partial_x \hat{g}^R))]_{11} N^{-1} \gamma \tilde{N} \right] \\
&= 4(\partial_x \gamma) \tilde{\gamma} N (\partial_x \gamma) \tilde{N} - 4\gamma (\partial_x \tilde{\gamma}) N \gamma (\partial_x \tilde{\gamma}) \gamma \tilde{N} + 2(\partial_x^2 \gamma) \tilde{N} - 2\gamma (\partial_x^2 \tilde{\gamma}) \gamma \tilde{N} \\
&\quad - 4(\partial_x \gamma) \tilde{\gamma} N (\partial_x \gamma) \tilde{\gamma} \gamma \tilde{N} + 4\gamma (\partial_x \tilde{\gamma}) N \gamma (\partial_x \tilde{\gamma}) \gamma \tilde{N} - 2(\partial_x^2 \gamma) \tilde{\gamma} \gamma \tilde{N} + 2\gamma (\partial_x^2 \tilde{\gamma}) \gamma \tilde{N} \quad (2.69) \\
&= 4(\partial_x \gamma) \tilde{\gamma} N (\partial_x \gamma) (1 - \tilde{\gamma} \gamma) \tilde{N} + 2(\partial_x^2 \gamma) (1 - \tilde{\gamma} \gamma) \tilde{N} \\
&= 4(\partial_x \gamma) \tilde{\gamma} N (\partial_x \gamma) + 2(\partial_x^2 \gamma)
\end{aligned}$$

Equivalently we get

$$\tilde{N}^{-1} \left[[\partial_x(\hat{g}^R(\partial_x \hat{g}^R))]_{21} - [\partial_x(\hat{g}^R(\partial_x \hat{g}^R))]_{22} \tilde{N}^{-1} \tilde{\gamma} N \right] = 4(\partial_x \tilde{\gamma}) \gamma \tilde{N} (\partial_x \tilde{\gamma}) + 2(\partial_x^2 \tilde{\gamma}). \quad (2.70)$$

Next, we need the remaining part the Usadel equation¹⁴ in (2.52).

$$\begin{aligned}
[\hat{K}, \hat{g}^R] &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} (1 + \gamma \tilde{\gamma}) N & 2\gamma \tilde{N} \\ -2\tilde{\gamma} N & -(1 + \tilde{\gamma} \gamma) \tilde{N} \end{pmatrix} \\
&\quad - \begin{pmatrix} (1 + \gamma \tilde{\gamma}) N & 2\gamma \tilde{N} \\ -2\tilde{\gamma} N & -(1 + \tilde{\gamma} \gamma) \tilde{N} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (2.71)
\end{aligned}$$

First we write the elements of (2.71)

$$[\hat{K}, \hat{g}^R]_{11} = a(1 + \gamma \tilde{\gamma}) N - 2b\tilde{\gamma} N - (1 + \gamma \tilde{\gamma}) Na - 2\gamma \tilde{N} c \quad (2.72a)$$

$$[\hat{K}, \hat{g}^R]_{12} = 2a\gamma \tilde{N} - b(1 + \tilde{\gamma} \gamma) \tilde{N} - (1 + \gamma \tilde{\gamma}) Nb - 2\gamma \tilde{N} d \quad (2.72b)$$

$$[\hat{K}, \hat{g}^R]_{21} = -2d\tilde{\gamma} N + c(1 + \gamma \tilde{\gamma}) N + (1 + \tilde{\gamma} \gamma) \tilde{N} c + 2\tilde{\gamma} Na \quad (2.72c)$$

$$[\hat{K}, \hat{g}^R]_{22} = -d(1 + \tilde{\gamma} \gamma) \tilde{N} + 2c\gamma \tilde{N} + (1 + \tilde{\gamma} \gamma) \tilde{N} d + 2\tilde{\gamma} Nb \quad (2.72d)$$

We notice that we get (2.72c) from (2.72b) and (2.72d) from (2.72a) by interchanging $\gamma \leftrightarrow \tilde{\gamma}$, $N \leftrightarrow \tilde{N}$, $a \leftrightarrow -d$ and $b \leftrightarrow -c$. Next, we have to perform the same calculations as for (2.69) and (2.70). Again we only have to do the actual calculation for element 11 and 12. We use that $N^{-1} \gamma \tilde{N} = \gamma$ from the property (2.56) and the fact that $N^{-1} N = 1$. We also keep in mind that $N^{-1} = (1 - \gamma \tilde{\gamma})$.

¹⁴We have derived the parameterization for the first term of the Usadel equation without the constant D_s . At the moment, we will also ignore the complex i . These constants will be taken back when we sew it all together.

$$\begin{aligned}
& N^{-1} \left[[\hat{K}, \hat{g}^R]_{12} - [\hat{K}, \hat{g}^R]_{11} N^{-1} \gamma \tilde{N} \right] \\
&= N^{-1} [2a\gamma\tilde{N} - b(1 + \tilde{\gamma}\gamma)\tilde{N} - (1 + \gamma\tilde{\gamma})Nb - 2\gamma\tilde{N}d \\
&\quad - \{a(1 + \gamma\tilde{\gamma})N - 2b\tilde{\gamma}N - (1 + \gamma\tilde{\gamma})Na - 2\gamma\tilde{N}c\} N^{-1} \gamma \tilde{N}] \\
&= (1 - \gamma\tilde{\gamma})2a\gamma\tilde{N} - (1 - \gamma\tilde{\gamma})b(1 + \tilde{\gamma}\gamma)\tilde{N} - (1 + \gamma\tilde{\gamma})b - 2\gamma d \\
&\quad - (1 - \gamma\tilde{\gamma})a(1 + \gamma\tilde{\gamma})\gamma\tilde{N} + (1 - \gamma\tilde{\gamma})2b\tilde{\gamma}\gamma\tilde{N} + (1 + \gamma\tilde{\gamma})a\gamma + 2\gamma c\gamma \\
&= 2a\gamma\tilde{N} - 2\gamma\tilde{\gamma}a\gamma\tilde{N} - b\tilde{N} - b\tilde{\gamma}\gamma\tilde{N} + \gamma\tilde{\gamma}b\tilde{N} + \gamma\tilde{\gamma}b\tilde{\gamma}\gamma\tilde{N} - b - \gamma\tilde{\gamma}b - 2\gamma d \\
&\quad - a\gamma\tilde{N} - a\gamma\tilde{\gamma}\gamma\tilde{N} + \gamma\tilde{\gamma}a\gamma\tilde{N} + \gamma\tilde{\gamma}a\gamma\tilde{\gamma}\gamma\tilde{N} + 2b\tilde{\gamma}\gamma\tilde{N} - 2\gamma\tilde{\gamma}b\tilde{\gamma}\gamma\tilde{N} + a\gamma + \gamma\tilde{\gamma}a\gamma + 2\gamma c\gamma \\
&= a\gamma\tilde{N} - \gamma\tilde{\gamma}a\gamma\tilde{N} - b\tilde{N} + b\tilde{\gamma}\gamma\tilde{N} + \gamma\tilde{\gamma}b\tilde{N} - \gamma\tilde{\gamma}b\tilde{\gamma}\gamma\tilde{N} - b - \gamma\tilde{\gamma}b - 2\gamma d \\
&\quad - a\gamma\tilde{\gamma}\gamma\tilde{N} + \gamma\tilde{\gamma}a\gamma\tilde{\gamma}\gamma\tilde{N} + a\gamma + \gamma\tilde{\gamma}a\gamma + 2\gamma c\gamma \\
&= a\gamma(1 - \tilde{\gamma}\gamma)\tilde{N} + a\gamma - 2\gamma d + 2\gamma c\gamma - b(1 - \tilde{\gamma}\gamma)\tilde{N} - b \\
&\quad - \gamma\tilde{\gamma}a(1 - \tilde{\gamma}\gamma)N\gamma + \gamma\tilde{\gamma}a\gamma + \gamma\tilde{\gamma}b(1 - \tilde{\gamma}\gamma)\tilde{N} - \gamma\tilde{\gamma}b \\
&= a\gamma + a\gamma - 2\gamma d + 2\gamma c\gamma - b - b - \gamma\tilde{\gamma}a\gamma + \gamma\tilde{\gamma}a\gamma + \gamma\tilde{\gamma}b - \gamma\tilde{\gamma}b \\
&= 2[a\gamma - \gamma d + \gamma c\gamma - b]
\end{aligned} \tag{2.73}$$

In the same way we get

$$\tilde{N}^{-1} \left[[\hat{K}, \hat{g}^R]_{21} - [\hat{K}, \hat{g}^R]_{22} \tilde{N}^{-1} \tilde{\gamma} N \right] = 2[-d\tilde{\gamma} + \tilde{\gamma}a - \tilde{\gamma}b\tilde{\gamma} + c]. \tag{2.74}$$

If we now connect the results from (2.69) and (2.73) in the way needed to fulfill (2.52) (and divide by 2), our parameterized equation becomes

$$D_s[2(\partial_x \gamma)\tilde{\gamma}N(\partial_x \gamma) + (\partial_x^2 \gamma)] + i[a\gamma - \gamma d + \gamma c\gamma - b] = 0. \tag{2.75}$$

And equivalently, we get from (2.70) and (2.74) the corresponding equation

$$D_s[2(\partial_x \tilde{\gamma})\gamma\tilde{N}(\partial_x \tilde{\gamma}) + (\partial_x^2 \tilde{\gamma})] + i[\tilde{\gamma}a - d\tilde{\gamma} - \tilde{\gamma}b\tilde{\gamma} + c] = 0. \tag{2.76}$$

Notice that the scalar potential φ times the identity matrix in (2.50) commutes with γ and $\tilde{\gamma}$, and cancels out in (2.75) and (2.76). We see that these are coupled second order differential equations. In order to solve them, we need complementary boundary conditions and initial conditions, as we would have with ordinary scalar equations.

2.4.2 Boundary Conditions for Normal Interfaces

The normal boundary conditions in the diffusive limit for low transparency, are derived by Kupriyanov-Lukichev [18], and can be written as

$$2L_j\zeta_j\check{g}_j\partial_x\check{g}_j = [\check{g}_l, \check{g}_r]. \quad (2.77)$$

The subscripts l and r correspond respectively to the left and right side of the interface¹⁵, and $j = l, r$ means that equation (2.77) actually is two equations. L_j is the length of material j and $\zeta_j = \frac{R_B}{R_j}$ is the relative resistance of the interface barrier and the bulk material on side j . To have low transparency we need $R_B > R_j$, which often is the case due to interatomic mismatch of the materials.¹⁶ This is called the tunneling limit, which we will have when using ferromagnetic insulators at the interfaces.

We now apply the definition of \check{g} (B.11) to (2.77)

$$2L_j\zeta_j \begin{pmatrix} \hat{g}_j^R & \hat{g}_j^K \\ 0 & \hat{g}_j^A \end{pmatrix} \begin{pmatrix} \partial_x \hat{g}_j^R & \partial_x \hat{g}_j^K \\ 0 & \partial_x \hat{g}_j^A \end{pmatrix} = \begin{pmatrix} \hat{g}_l^R & \hat{g}_l^K \\ 0 & \hat{g}_l^A \end{pmatrix} \begin{pmatrix} \hat{g}_r^R & \hat{g}_r^K \\ 0 & \hat{g}_r^A \end{pmatrix} - \begin{pmatrix} \hat{g}_r^R & \hat{g}_r^K \\ 0 & \hat{g}_r^A \end{pmatrix} \begin{pmatrix} \hat{g}_l^R & \hat{g}_l^K \\ 0 & \hat{g}_l^A \end{pmatrix}, \quad (2.78)$$

and by fundamental matrix multiplication we get

$$2L_j\zeta_j \begin{pmatrix} \hat{g}_j^R(\partial_x \hat{g}_j^R) & \hat{g}_j^R(\partial_x \hat{g}_j^K) + \hat{g}_j^K(\partial_x \hat{g}_j^A) \\ 0 & \hat{g}_j^A(\partial_x \hat{g}_j^A) \end{pmatrix} = \begin{pmatrix} \hat{g}_l^R \hat{g}_r^R - \hat{g}_r^R \hat{g}_l^R & \hat{g}_l^R \hat{g}_r^K + \hat{g}_l^K \hat{g}_r^A - \hat{g}_r^R \hat{g}_l^K - \hat{g}_r^K \hat{g}_l^A \\ 0 & \hat{g}_l^A \hat{g}_r^A - \hat{g}_r^A \hat{g}_l^A \end{pmatrix}. \quad (2.79)$$

This is now the same as three non-trivial equations. The upper left part of (2.79) gives us the equations for the quasiclassical retarded Green's function

$$2L_j\zeta_j\hat{g}_j^R(\partial_x \hat{g}_j^R) = [\hat{g}_l^R, \hat{g}_r^R]. \quad (2.80)$$

The left side of (2.80) is already found with the Riccati parameterization in section 2.4.1. We borrow our results from (2.63)-(2.66).

$$[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{11} = 2N_j[(\partial_x \gamma_j)\tilde{\gamma}_j - \gamma_j(\partial_x \tilde{\gamma}_j)]N_j \quad (2.81)$$

$$[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{12} = 2N_j[(\partial_x \gamma_j) - \gamma_j(\partial_x \tilde{\gamma}_j)\gamma_j]\tilde{N}_j \quad (2.82)$$

$$[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{21} = 2\tilde{N}_j[(\partial_x \tilde{\gamma}_j) - \tilde{\gamma}_j(\partial_x \gamma_j)\tilde{\gamma}_j]N_j \quad (2.83)$$

$$[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{22} = 2\tilde{N}_j[(\partial_x \tilde{\gamma}_j)\gamma_j - \tilde{\gamma}_j(\partial_x \gamma_j)]\tilde{N}_j \quad (2.84)$$

After inserting the Riccati parameterizations (2.54) and (2.59) for the matrices on the right side of (2.80), we split it into four elements, like we have for the left side.

¹⁵This is analogous to the discontinuity relation for a delta function in quantum mechanics.

¹⁶Some heterostructures, where the lattice constant is almost the same for the materials involved, will have high transparency, meaning that $\zeta_j \rightarrow 1$.

$$[\hat{g}_l^R, \hat{g}_r^R]_{11} = N_l(1 + \gamma_l \tilde{\gamma}_l)(1 + \gamma_r \tilde{\gamma}_r)N_r - 4N_l \gamma_l \tilde{\gamma}_r N_r - N_r(1 + \gamma_r \tilde{\gamma}_r)(1 + \gamma_l \tilde{\gamma}_l)N_l + 4N_r \gamma_r \tilde{\gamma}_l N_l \quad (2.85)$$

$$[\hat{g}_l^R, \hat{g}_r^R]_{12} = 2N_l(1 + \gamma_l \tilde{\gamma}_l)\gamma_r \tilde{N}_r - 2N_l \gamma_l(1 + \tilde{\gamma}_r \gamma_r)\tilde{N}_r - 2N_r(1 + \gamma_r \tilde{\gamma}_r)\gamma_l \tilde{N}_l + 2N_r \gamma_r(1 + \tilde{\gamma}_l \gamma_l)\tilde{N}_l \quad (2.86)$$

$$[\hat{g}_l^R, \hat{g}_r^R]_{21} = -2\tilde{N}_l \tilde{\gamma}_l(1 + \gamma_r \tilde{\gamma}_r)N_r + 2\tilde{N}_l(1 + \tilde{\gamma}_l \gamma_l)\tilde{\gamma}_r N_r + 2\tilde{N}_r \tilde{\gamma}_r(1 + \gamma_l \tilde{\gamma}_l)N_l - 2\tilde{N}_r(1 + \tilde{\gamma}_r \gamma_r)\tilde{\gamma}_l N_l \quad (2.87)$$

$$[\hat{g}_l^R, \hat{g}_r^R]_{22} = -4\tilde{N}_l \tilde{\gamma}_l \gamma_r \tilde{N}_r + \tilde{N}_l(1 + \tilde{\gamma}_l \gamma_l)(1 + \tilde{\gamma}_r \gamma_r)\tilde{N}_r + 4\tilde{N}_r \tilde{\gamma}_r \gamma_l \tilde{N}_l - \tilde{N}_r(1 + \tilde{\gamma}_r \gamma_r)(1 + \tilde{\gamma}_l \gamma_l)\tilde{N}_l \quad (2.88)$$

Notice that we also here get element 21 from 12, and 22 from 11 by tilde all the matrices. To isolate $\partial_x \gamma_j$ we calculate

$$N_j^{-1} \left[[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{12} - [\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{11} N_j^{-1} \gamma_j \tilde{N}_j \right] \quad (2.89)$$

$$= N_j^{-1} \left[2N_j[(\partial_x \gamma_j) - \gamma_j(\partial_x \tilde{\gamma}_j)\gamma_j]\tilde{N}_j - 2N_j[(\partial_x \gamma_j)\tilde{\gamma}_j - \gamma_j(\partial_x \tilde{\gamma}_j)]N_j N_j^{-1} \gamma_j \tilde{N}_j \right] \quad (2.90)$$

$$= 2 \left[[(\partial_x \gamma_j) - \gamma_j(\partial_x \tilde{\gamma}_j)\gamma_j]\tilde{N}_j - [(\partial_x \gamma_j)\tilde{\gamma}_j - \gamma_j(\partial_x \tilde{\gamma}_j)]\gamma_j \tilde{N}_j \right] \quad (2.91)$$

$$= 2 \left[(\partial_x \gamma_j)\tilde{N}_j - \gamma_j(\partial_x \tilde{\gamma}_j)\gamma_j \tilde{N}_j - (\partial_x \gamma_j)\tilde{\gamma}_j \gamma_j \tilde{N}_j + \gamma_j(\partial_x \tilde{\gamma}_j)\gamma_j \tilde{N}_j \right] \quad (2.92)$$

$$= 2(\partial_x \gamma_j)(1 - \tilde{\gamma}_j \gamma_j)\tilde{N}_j \quad (2.93)$$

$$= 2(\partial_x \gamma_j) \quad (2.94)$$

$$(2.95)$$

And in the same way, we have

$$\tilde{N}_j^{-1} \left[[\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{21} - [\hat{g}_j^R(\partial_x \hat{g}_j^R)]_{22} \tilde{N}_j^{-1} \tilde{\gamma}_j N_j \right] = 2(\partial_x \tilde{\gamma}_j) \quad (2.96)$$

$$(2.97)$$

This is the same kind of calculation as we did for the Usadel equation to obtain (2.75) and (2.76). Doing this calculation for both sides of (2.80), we end up with

$$4L_j \zeta_j(\partial_x \gamma_j) = \Gamma, \quad (2.98)$$

$$4L_j \zeta_j(\partial_x \tilde{\gamma}_j) = \tilde{\Gamma}. \quad (2.99)$$

We have defined Γ and $\tilde{\Gamma}$

$$\Gamma = N_j^{-1} \left[[\hat{g}_l^R, \hat{g}_r^R]_{12} - [\hat{g}_l^R, \hat{g}_r^R]_{11} N_j^{-1} \gamma_j \tilde{N}_j \right], \quad (2.100)$$

$$\tilde{\Gamma} = \tilde{N}_j^{-1} \left[[\hat{g}_l^R, \hat{g}_r^R]_{21} - [\hat{g}_l^R, \hat{g}_r^R]_{22} \tilde{N}_j^{-1} \tilde{\gamma}_j N_j \right], \quad (2.101)$$

since it at this point is more disturbing than helpful to write out the full expressions. The important thing is that they are matrices consisting of $\gamma_l, \tilde{\gamma}_l, \gamma_r$ and $\tilde{\gamma}_r$ without any derivatives. We see that equation (2.99) is equal to (2.98), if we change all the matrices to their tilde-versions.

Chapter 3

Interplay Between FM and SC Order

In this chapter we will study the interplay between ferromagnetic and superconducting order in the Josephson junction from Figure 1.1. We will see that the presence of spin-active interfaces gives rise to exotic states in the junction.

3.1 Spin-Active Interfaces

Until now we have left out the spin-active interfaces in the equations. The effect of a spin-active interface enters the boundary conditions through additional terms. The full boundary conditions are derived in [10]. In our notation the boundary conditions become

$$2L_l\zeta_l\check{g}_l(\partial_x\check{g}_l) = [\check{g}_l, \check{g}_r] + G_{MR}R_B [\check{g}_l, \{\check{A}, \check{g}_r\}] + iG_\theta^l R_B [\check{g}_l, \check{A}], \quad (3.1)$$

$$2L_r\zeta_r\check{g}_r(\partial_x\check{g}_r) = [\check{g}_l, \check{g}_r] - G_{MR}R_B [\check{g}_r, \{\check{A}, \check{g}_l\}] - iG_\theta^r R_B [\check{g}_r, \check{A}]. \quad (3.2)$$

We have introduced the conductance parameters G_{MR} and $G_\theta^{l(r)}$, which respectively represent the magnetoresistance and the interfacial scattering phase shift. For an arbitrary spin reference frame we have

$$\check{A} = \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{A} \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} \mathbf{m} \cdot \bar{\boldsymbol{\tau}} & 0 \\ 0 & \mathbf{m} \cdot \bar{\boldsymbol{\tau}}^* \end{pmatrix} \quad (3.3)$$

where \mathbf{m} is the magnetization direction of the interface. If the magnetization was set to be in the z-direction ($\mathbf{m} = \mathbf{e}_z$) then \hat{A} would have taken the form $\hat{\tau}_3$, which is the third 4×4 Pauli matrix (Appendix A). If we only have spin-active interfaces with collinear magnetization, we can always choose the coordinate system so that the magnetization is in the z-direction. This means that \hat{A} only has elements on the diagonal. On the other

hand, if we have noncollinear magnetization, take for instance two magnetic interfaces with different magnetization directions ($\mathbf{m}_1 \neq \mathbf{m}_2$), then only one of the magnetization directions can be chosen as the z-direction. This means that the other magnetization direction is forced to have a displacement angle $\phi = \arccos(\mathbf{m}_1 \cdot \mathbf{m}_2)$ from the first. This can lead to spin-flip, which we will briefly discuss in the next section.

Incoming electrons at the interface can either be reflected back into the superconductor, or tunnel through the thin insulator into the normal metal. The reflection is illustrated in Figure 3.1, and due to the spin-dependent phase shift, the wave function will be modified near the interface [12]. As already illustrated in Figure 2.7, the tunneling probability is also dependent on the spin orientation.

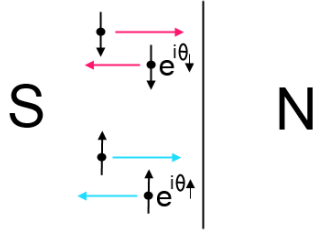


Figure 3.1: Spin-dependent interfacial phase shift. Electrons in the superconductor pick up a phase when reflected from a spin-active interface. The phase differs for spin-up and spin-down.

The boundary conditions look the same for \hat{g}^R as for \check{g} , we only change \check{A} to \hat{A} for the retarded Green's function. This can be checked by inserting the definition of the quasiclassical \check{g} in (B.11), as earlier. The boundary conditions for the retarded Green's function are then

$$2L_l \zeta_l \hat{g}_l^R (\partial_x \hat{g}_l^R) = [\hat{g}_l^R, \hat{g}_r^R] + \frac{G_{MR}}{G_T} [\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}] + i \frac{G_\theta^l}{G_T} [\hat{g}_l^R, \hat{A}], \quad (3.4)$$

$$2L_r \zeta_r \hat{g}_r^R (\partial_x \hat{g}_r^R) = [\hat{g}_l^R, \hat{g}_r^R] - \frac{G_{MR}}{G_T} [\hat{g}_r^R, \{\hat{A}, \hat{g}_l^R\}] - i \frac{G_\theta^r}{G_T} [\hat{g}_r^R, \hat{A}]. \quad (3.5)$$

We have used that conductance is the inverse of resistance¹, and defined $R_B = \frac{1}{G_T}$.

Next, we apply the Riccati parameterization to the added terms in the boundary conditions (3.4) and (3.5). It is sufficient to find the parameterized expression for one of these equations, then the other equation is easily found by interchanging $l \leftrightarrow r$, and add a minus sign in front of all terms coming from the commutators. We start by unravelling the commutator for the spin-dependent interfacial phase shift.

¹While the B in R_B stands barrier, the T in G_T stands for tunneling.

$$\begin{aligned}
\left[\hat{g}_l^R, \hat{A} \right] &= \begin{pmatrix} N_l(1 + \gamma_l \tilde{\gamma}_l) & 2N_l \gamma_l \\ -2\tilde{N}_l \tilde{\gamma}_l & -\tilde{N}_l(1 + \tilde{\gamma}_l \gamma_l) \end{pmatrix} \begin{pmatrix} \mathbf{m} \cdot \bar{\boldsymbol{\tau}} & 0 \\ 0 & \mathbf{m} \cdot \bar{\boldsymbol{\tau}}^* \end{pmatrix} \\
&\quad - \begin{pmatrix} \mathbf{m} \cdot \bar{\boldsymbol{\tau}} & 0 \\ 0 & \mathbf{m} \cdot \bar{\boldsymbol{\tau}}^* \end{pmatrix} \begin{pmatrix} (1 + \gamma_l \tilde{\gamma}_l)N_l & 2\gamma_l \tilde{N}_l \\ -2\tilde{\gamma}_l N_l & -(1 + \tilde{\gamma}_l \gamma_l)\tilde{N}_l \end{pmatrix}
\end{aligned} \tag{3.6}$$

We write out the elements.

$$\left[\hat{g}_l^R, \hat{A} \right]_{11} = N_l(1 + \gamma_l \tilde{\gamma}_l)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}})(1 + \gamma_l \tilde{\gamma}_l)N_l \tag{3.7}$$

$$\left[\hat{g}_l^R, \hat{A} \right]_{12} = 2N_l \gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) 2\gamma_l \tilde{N}_l \tag{3.8}$$

$$\left[\hat{g}_l^R, \hat{A} \right]_{21} = -2\tilde{N}_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) 2\tilde{\gamma}_l N_l \tag{3.9}$$

$$\left[\hat{g}_l^R, \hat{A} \right]_{22} = -\tilde{N}_l(1 + \tilde{\gamma}_l \gamma_l)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*)(1 + \tilde{\gamma}_l \gamma_l)\tilde{N}_l \tag{3.10}$$

In order to fit into the form in (2.98) and (2.99), we do the calculation in the same way.

$$\begin{aligned}
&N_l^{-1} \left[\left[\hat{g}_l^R, \hat{A} \right]_{12} - \left[\hat{g}_l^R, \hat{A} \right]_{11} N_l^{-1} \gamma_l \tilde{N}_l \right] \\
&= 2\gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - (1 - \gamma_l \tilde{\gamma}_l)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) 2\gamma_l \tilde{N}_l \\
&\quad - (1 + \gamma_l \tilde{\gamma}_l)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l + (1 - \gamma_l \tilde{\gamma}_l)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}})(1 + \gamma_l \tilde{\gamma}_l) \gamma_l \tilde{N}_l \\
&= 2\gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - 2(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{N}_l + 2\gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{N}_l - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l - \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \\
&\quad + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{N}_l + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{\gamma}_l \gamma_l \tilde{N}_l - \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{N}_l - \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \tilde{\gamma}_l \gamma_l \tilde{N}_l \\
&= 2\gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l - \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \\
&\quad - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l (1 - \tilde{\gamma}_l \gamma_l) \tilde{N}_l + \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l (1 - \tilde{\gamma}_l \gamma_l) \tilde{N}_l \\
&= 2\gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l - \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l + \gamma_l \tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l \\
&= 2\gamma_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - 2(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) \gamma_l
\end{aligned} \tag{3.11}$$

Then by considering the symmetry, we equivalently have

$$\tilde{N}_l^{-1} \left[\left[\hat{g}_l^R, \hat{A} \right]_{21} - \left[\hat{g}_l^R, \hat{A} \right]_{22} \tilde{N}_l^{-1} \tilde{\gamma}_l N_l \right] = -2\tilde{\gamma}_l (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) + 2(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) \tilde{\gamma}_l. \tag{3.12}$$

To get from (3.11) to (3.12), we have added a minus sign and tilded all the matrices, which is justified by studying (3.7) vs. (3.10), and (3.8) vs. (3.9).

This calculation could have been made easier by realizing that $[\hat{g}_l^R, \hat{A}]$ has the same structure as $[\hat{K}, \hat{g}^R]$ in (2.71) except from an overall minus sign. We would have gotten the same expressions as in (3.11) and (3.12) directly by using the results in (2.73) and (2.74), and redefining $a = -(\mathbf{m} \cdot \bar{\boldsymbol{\tau}})$, $b = c = 0$ and $d = -(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*)$. This method will be used to find the equations for the remaining term in (3.4). We have

$$[\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}], \quad (3.13)$$

and define the anti-commutator as

$$\{\hat{A}, \hat{g}_r^R\} = \begin{pmatrix} a_r & b_r \\ c_r & d_r \end{pmatrix}, \quad (3.14)$$

where the elements are given by

$$a_r = N_r(1 + \gamma_r \tilde{\gamma}_r)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}})(1 + \gamma_r \tilde{\gamma}_r)N_r, \quad (3.15)$$

$$b_r = 2N_r\gamma_r(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) + (\mathbf{m} \cdot \bar{\boldsymbol{\tau}})2\gamma_r\tilde{N}_r, \quad (3.16)$$

$$c_r = -2\tilde{N}_r\tilde{\gamma}_r(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*)2\tilde{\gamma}_rN_r, \quad (3.17)$$

$$d_r = -\tilde{N}_r(1 + \tilde{\gamma}_r\gamma_r)(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - (\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*)(1 + \tilde{\gamma}_r\gamma_r)\tilde{N}_r. \quad (3.18)$$

This gives us

$$N_l^{-1} \left[[\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}]_{12} - [\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}]_{11} N_l^{-1} \gamma_l \tilde{N}_l \right] \quad (3.19)$$

$$= -2[a_r\gamma_l - \gamma_l d_r + \gamma_l c_r\gamma_l - b_r],$$

$$\tilde{N}_l^{-1} \left[[\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}]_{21} - [\hat{g}_l^R, \{\hat{A}, \hat{g}_r^R\}]_{22} \tilde{N}_l^{-1} \tilde{\gamma}_l N_l \right] \quad (3.20)$$

$$= -2[-d_r\tilde{\gamma}_l + \tilde{\gamma}_l a_r - \tilde{\gamma}_l b_r\tilde{\gamma}_l + c_r].$$

Finally, we write out the total boundary conditions written with the Riccati parameterization.

$$4L_l\zeta_l(\partial_x\gamma_l) = \Gamma + i\frac{G_\phi^l}{G_T}(2\gamma_l(\mathbf{m} \cdot \bar{\boldsymbol{\tau}}^*) - 2(\mathbf{m} \cdot \bar{\boldsymbol{\tau}})\gamma_l) + \frac{G_{MR}}{G_T}(-2[a_r\gamma_l - \gamma_l d_r + \gamma_l c_r\gamma_l - b_r]) \quad (3.21)$$

$$4L_l\zeta_l(\partial_x\tilde{\gamma}_l) = \tilde{\Gamma} + i\frac{G_\phi^l}{G_T}(-2\tilde{\gamma}_l(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}) + 2(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}^*)\tilde{\gamma}_l) + \frac{G_{MR}}{G_T}(-2[-d_r\tilde{\gamma}_l + \tilde{\gamma}_la_r - \tilde{\gamma}_lb_r\tilde{\gamma}_l + c_r]) \quad (3.22)$$

$$4L_r\zeta_r(\partial_x\gamma_r) = \Gamma - i\frac{G_\phi^r}{G_T}(2\gamma_r(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}^*) - 2(\mathbf{m}\cdot\bar{\boldsymbol{\tau}})\gamma_r) - \frac{G_{MR}}{G_T}(-2[a_l\gamma_r - \gamma_rd_l + \gamma_rc_l\gamma_r - b_l]) \quad (3.23)$$

$$4L_r\zeta_r(\partial_x\tilde{\gamma}_r) = \tilde{\Gamma} - i\frac{G_\phi^r}{G_T}(-2\tilde{\gamma}_r(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}) + 2(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}^*)\tilde{\gamma}_r) - \frac{G_{MR}}{G_T}(-2[-d_l\tilde{\gamma}_r + \tilde{\gamma}_ra_l - \tilde{\gamma}_rb_l\tilde{\gamma}_r + c_l]) \quad (3.24)$$

Of course we can embellish these equations, dividing by two and gathering the signs. But in the way they are written now, the origin of different terms should be clear. If we want to, we can write $d_{l(r)} = -\tilde{a}_{l(r)}$, $c_{l(r)} = -\tilde{b}_{l(r)}$ from looking at (3.15)-(3.18), since $(\mathbf{m}\cdot\bar{\boldsymbol{\tau}})$ does not contain the energy E , and \mathbf{m} is a real space vector. The tilde-version of $(\mathbf{m}\cdot\bar{\boldsymbol{\tau}})$ is just the complex conjugated $(\mathbf{m}\cdot\bar{\boldsymbol{\tau}}^*)$. This way, we can reduce the notation.

3.2 Odd-Frequency Pairing

In section 2.1.3 we discussed the possible symmetries for the anomalous Green's function. This function is linked to the Cooper pairs, and thereby superconductivity. From table 2.1 we have two possibilities for having odd-frequency superconductivity, the odd-frequency spin-singlet and the odd-frequency spin triplet. The odd-frequency singlet, discussed in [3], needs to have parity of minus one, hence have equal parts of positive and negative momentum in \mathbf{k} -space. In our case we consider the diffusive limit. This means that the electrons will be scattered in all directions, due to collisions with impurities. The impurity scattering therefore suppresses the odd-frequency singlet. In contrast, the odd-frequency triplet is even in momentum, which makes it compatible to the only orbital structure insensitive to impurities, namely the s-wave.

The first to suggest this odd-frequency superconductivity was Berezinskii in 1974 [7]. The reasoning was that the anomalous Green's function may be written as a sum over frequencies with the Matsubara representation (3.25) as in section 3.1 in ref. [20], which makes it possible to have the sum equal to zero if the function is odd in frequency. We will need the anomalous Green's function to be zero, since the oddness of frequency demands a change of sign, when interchanging at equal times. This way, we avoid breaking the Pauli principle.

$$F(it) \propto \sum_{\omega} e^{-i\omega(it)} F(i\omega) \quad (3.25)$$

If we have a conventional BSC superconductor in contact with a spin-active interface, the singlet will make a mixed state of singlet and triplet near the interface due to the

spin-dependent phase shift, as illustrated in Figure 3.1. We know from the BCS theory in section 2.1.6 that electrons pair with another electrons of opposite \mathbf{k} . If we start with a singlet in the superconductor, it could have one electron labeled $|\uparrow, k\rangle_1$ travelling towards the interface, pairing with another $|\downarrow, -k\rangle_2$ travelling away from the interface. After the reflection, electron 1 changes to $|\uparrow, -k\rangle_1 e^{i\phi_\uparrow}$ and pairs with an new electron $|\downarrow, k\rangle_3$. We define the phase difference $\theta = \theta_\uparrow - \theta_\downarrow$.

Before reflection:

$$|\uparrow, k\rangle_1 |\downarrow, -k\rangle_2 - |\downarrow, k\rangle_1 |\uparrow, -k\rangle_2 \quad (3.26)$$

After reflection:

$$|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 e^{i\theta_\downarrow} - |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1 e^{i\theta_\uparrow} \quad (3.27)$$

$$= e^{i\theta_\downarrow} e^{i\frac{\theta}{2}} \left(|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 e^{-i\frac{\theta}{2}} - |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1 e^{i\frac{\theta}{2}} \right) \quad (3.28)$$

$$= e^{i\theta_\downarrow} e^{i\frac{\theta}{2}} \left(|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 \left(\cos \frac{\theta}{2} - i \sin \frac{\theta}{2} \right) - |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1 \left(\cos \frac{\theta}{2} + i \sin \frac{\theta}{2} \right) \right) \quad (3.29)$$

$$= e^{i\theta_\downarrow} e^{i\frac{\theta}{2}} \cos \frac{\theta}{2} (|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 - |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1) \quad (3.30)$$

$$- e^{i\theta_\downarrow} e^{i\frac{\theta}{2}} i \sin \frac{\theta}{2} (|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 + |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1) \quad (3.31)$$

$$\propto c_s (|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 - |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1) + c_t (|\uparrow, k\rangle_3 |\downarrow, -k\rangle_1 + |\downarrow, k\rangle_3 |\uparrow, -k\rangle_1) \quad (3.32)$$

This leads to a mix of singlet and triplet components. In [12] the corresponding expression for reflection of both electrons within the interface is given, which gives the same effect, only with a larger phase difference. If the triplet component keeps the s-wave orbital, it would not be destroyed in the diffusive limit². This is the odd-frequency triplet.

When we have noncollinear magnetizations of the two interfaces, the triplet state may be flipped and generate the long-range components $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, which gives us all the spin triplet components $S_z = 0, \pm 1$. This effect was experimentally measured in 1998 on a ferromagnetic cobalt wire attached to superconducting aluminum [14].

The long-range triplet pairing is discussed in [9] and [26]. We call them long-range because they penetrate a ferromagnet without being destroyed by the exchange field. The penetration length of the parallel triplet spin components ($S_z = \pm 1$) in a ferromagnet, is in order of $\sqrt{D/E}$, while the penetration length of the singlet component and triplet anti-parallel component ($S_z = 0$) is of the much shorter order $\sqrt{D/h}$. Here we have D as the diffusion constant in the ferromagnet and h as the strength of the exchange field. We see that the penetration length of parallel spins are independent of the exchange field, but that for anti-parallel spins, the penetration length decay as $h^{-\frac{1}{2}}$. We may think of this as if the exchange field tries to align the spins, to fit into the ferromagnetic

²If we by any chance manage to produce other kinds of superconductivity, they would die out within a short distance from the interface, due to impurity scattering.

structure. Since the parallel parts already are aligned, they do not get affected by the exchange field, meanwhile the anti-parallel parts are broken by the field.

3.3 Numerical Solution of the Usadel Equation

The parameterized transport equations are provided in (2.75) and (2.76). These equations, together with the boundary conditions (3.21), (3.22), (3.23) and (3.24), give us a good starting point for numerical calculations on a Josephson junction with spin-active interfaces. Since these equations correspond to two coupled second order differential equations, with four boundary conditions at each interface, we also need to know the initial conditions in the superconductors. We assume that the length of the normal metal is sufficiently small to make the inverse proximity effect negligible, like illustrated in Figure 3.2. Then the superconductivity is only weakly destroyed at the interfaces. We

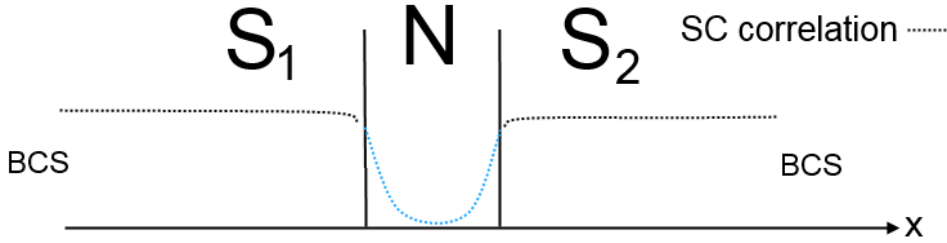


Figure 3.2: Qualitative sketch of the superconducting singlet correlation function. Near the interface, the function is approximately equal to the constant BCS value.

assume that we can approximate the Green's function solution in the superconductor near the interface, to the BCS solution. To find the corresponding BCS- γ -matrices, we compare the Riccati parameterization to the known θ -parameterization in equilibrium for the retarded BCS Green's function.

$$\hat{g}_{bcs}^R = \begin{pmatrix} N_{bcs}(1 + \gamma_{bcs}\tilde{\gamma}_{bcs}) & 2N_{bcs}\gamma_{bcs} \\ -2\tilde{N}_{bcs}\tilde{\gamma}_{bcs} & -\tilde{N}_{bcs}(1 + \tilde{\gamma}_{bcs}\gamma_{bcs}) \end{pmatrix} = \begin{pmatrix} \bar{1} \cosh \theta & i\bar{\tau}_2 \sinh \theta \\ i\bar{\tau}_2 \sinh \theta & -\bar{1} \cosh \theta \end{pmatrix} \quad (3.33)$$

Here $\theta = \tanh^{-1}(\frac{\Delta}{E})$.

Dropping the subscript, we get the equations

$$(1 + \gamma\tilde{\gamma}) = (1 - \gamma\tilde{\gamma}) \cosh(\theta), \quad (3.34)$$

$$2\gamma = (1 - \gamma\tilde{\gamma})i\bar{\tau}_2 \sinh(\theta), \quad (3.35)$$

$$2\tilde{\gamma} = -(1 - \tilde{\gamma}\gamma)i\bar{\tau}_2 \sinh(\theta), \quad (3.36)$$

$$(1 + \tilde{\gamma}\gamma) = (1 - \tilde{\gamma}\gamma) \cosh(\theta), \quad (3.37)$$

where we have multiplied from left with the proper inverse normalization matrix. Rearranging (3.34), we have

$$(1 + \gamma\tilde{\gamma}) = (1 - \gamma\tilde{\gamma}) \cosh(\theta) \quad (3.38)$$

$$\gamma\tilde{\gamma}(1 + \cosh(\theta)) = \cosh(\theta) - 1 \quad (3.39)$$

$$\gamma\tilde{\gamma} = \frac{(\cosh(\theta) - 1)}{(1 + \cosh(\theta))}. \quad (3.40)$$

Inserted into (3.35), we get the expression for the BCS- γ .

$$2\gamma = (1 - \frac{(\cosh(\theta) - 1)}{(1 + \cosh(\theta))})i\bar{\tau}_2 \sinh(\theta) \quad (3.41)$$

$$2\gamma = \frac{1 + \cosh(\theta) - \cosh(\theta) + 1}{(1 + \cosh(\theta))}i\bar{\tau}_2 \sinh(\theta) \quad (3.42)$$

$$\gamma = \frac{i\bar{\tau}_2 \sinh(\theta)}{(1 + \cosh(\theta))} \quad (3.43)$$

In a similar way we get from (3.37) and (3.36)

$$\tilde{\gamma} = -\frac{i\bar{\tau}_2 \sinh(\theta)}{(1 + \cosh(\theta))}. \quad (3.44)$$

Now the fully parameterized set of equations can be solved, giving numerical values of the γ - and $\tilde{\gamma}$ -matrices in the normal metal region. Each solution is a 2×2 -matrix where the elements are row-vectors giving the value of the element at a specific point at the x-axis in the junction. We may, for instance, set the interfaces at $x = -L_N/2$ and $x = L_N/2$, where L_N is the length of the normal metal.

In order to get numbers out of the calculation, we need to assign values to the tunable parameters $L_l, L_r, \zeta_l, \zeta_r, \frac{G_\phi^l}{G_T}, \frac{G_\phi^r}{G_T}, \frac{G_{MR}}{G_T}, \frac{\Delta}{E}, \frac{D_s}{E}$ and $\frac{\mathbf{S}}{E}$, where we have divided (2.75) and (2.76) by E to make them dimensionless. When assigning values to the parameters, we have to keep in mind the requirement of low transparency of the interfaces and other restrictions. The solution of γ and $\tilde{\gamma}$ will in turn be set back into retarded Green's function by (2.54). We then have solved the Usadel equation, and obtained the retarded Green's function for the normal region \hat{g}_N^R . From the retarded Green's function we can find physical observables, and investigate how these behave when tuning different parameters, such as the relative angle between the magnetizations at the two interfaces. The calculations may be performed with the computer program MATLAB, which has an integrated function (ode45) for solving this kind of equations.

If we only have nonmagnetic impurities $\mathbf{S} = 0$, and aligned magnetization $\mathbf{m}_1 = \mathbf{m}_2$, we expect to not generate the $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ ($S_z = 1$) components of the anomalous Green's function.

Chapter 4

Outlook

We have seen that the odd-frequency triplet superconductivity is expected to appear in a Josephson junction with spin-active interfaces, and that all the three triplet components may exist in the presence of inhomogeneous magnetization.

The equations needed in order to obtain the retarded Green's function from numerical calculations, are derived from the Usadel equation and the boundary condition for spin-active interfaces, by applying the Riccati parameterization. This can be used to find the retarded Green's function in the normal metal part if we assume that the inverse proximity effect is negligible. This way, we may set the BCS solution of the retarded Green's function at the superconducting side of the interfaces. From the retarded Green's function we can identify the triplet and singlet components. We can also find the advanced Green's function and the Keldysh Green's function from the retarded Green's function, which allows us to calculate the current-matrix and find the spin-current, or the energy gap function.

Further work, is to do the numerical calculations and investigate how different parameters, such as current and magnetization directions, influence the odd-frequency triplet components.

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Appendix A

Notation

Constants from Physical Data Group 2014:

$$e = 1.602176565(35) \cdot 10^{-19} \text{ C} \quad (\text{A.1})$$

$$m = 0.510998928(11) \text{ MeV} \quad (\text{A.2})$$

Bold symbols are vectors, for instance, the position vector $\mathbf{r} = r\hat{\mathbf{e}}_{\mathbf{r}}$.

For a matrix A we have used \bar{A} for 2×2 -matrices, \hat{A} for 4×4 -matrices and \check{A} for 8×8 -matrices.

Pauli Matrices

2×2 -version:

$$\bar{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} 1, \quad \bar{\tau}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \bar{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.3})$$

4×4 -version:

$$\hat{\tau}_i = \begin{pmatrix} \bar{\tau}_i & 0 \\ 0 & \bar{\tau}_i \end{pmatrix} \quad (\text{A.4})$$

We have $i = x, y, z$.

$$\bar{\boldsymbol{\tau}} = \bar{\tau}_1 \hat{\mathbf{e}}_x + \bar{\tau}_2 \hat{\mathbf{e}}_y + \bar{\tau}_3 \hat{\mathbf{e}}_z \quad (\text{A.5})$$

where $\hat{\mathbf{e}}_i$ is the unit vector in the i -direction.

Operators

These operators are obtained by replacing all elements in the Pauli matrices with the scalar times the identity 2×2 -matrix.

$$\hat{\rho}_1 = \begin{pmatrix} 0 & \bar{1} \\ \bar{1} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A.6})$$

$$\hat{\rho}_2 = \begin{pmatrix} 0 & -i\bar{1} \\ i\bar{1} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad (\text{A.7})$$

$$\hat{\rho}_3 = \begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (\text{A.8})$$

Trace Manipulation

If we have an arbitrary 4×4 -matrix \hat{A} , it may be written

$$\hat{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}. \quad (\text{A.9})$$

The trace of a matrix is the sum over all elements on the diagonal. To only sum over the elements a_{11} and a_{22} , we manipulate the matrix, so that we get the wanted elements alone on the diagonal. One way to do this is to write $\text{Tr}\{\frac{\hat{1}+\hat{\rho}_3}{2}\hat{A}\}$, where we have

$$\begin{aligned} & \frac{\hat{1} + \hat{\rho}_3}{2} \hat{A} \\ &= \frac{1}{2} \left[\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \right] \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \\ &= \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (\text{A.10})$$

We see that the trace of (A.10) equals $a_{11} + a_{22}$.

If we want to express $a_{14} - a_{23}$, we may calculate $\text{Tr}\{\frac{\hat{\rho}_1 - i\hat{\rho}_2}{2}\hat{\tau}_3\hat{A}\}$, where we have

$$\begin{aligned}
& \frac{\hat{\rho}_1 - i\hat{\rho}_2}{2}\hat{\tau}_3\hat{A} \\
&= \frac{1}{2} \left[\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} - i \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -a_{21} & -a_{22} & -a_{23} & -a_{24} \\ a_{11} & a_{12} & a_{13} & a_{14} \end{pmatrix}.
\end{aligned}
\tag{A.11}$$

Appendix B

Green's Functions

The Green's function in Keldysh space is defined as

$$\check{G}(1, 2) = \begin{pmatrix} \hat{G}^R(1, 2) & \hat{G}^K(1, 2) \\ 0 & \hat{G}^A(1, 2) \end{pmatrix}, \quad (\text{B.1})$$

where R stands for retarded, A for advanced, and K for Keldysh. The $(1, 2)$ stands for $(t_1, \mathbf{r}_1, \sigma_1; t_2, \mathbf{r}_2, \sigma_2)$

Retarded Green's Function

$$\hat{G}^R(1, 2) = \begin{pmatrix} \bar{G}^R(1, 2) & \bar{F}^R(1, 2) \\ (\bar{F}^R)^*(1, 2) & (\bar{G}^R)^*(1, 2) \end{pmatrix} \quad (\text{B.2})$$

$$\bar{G}^R(1, 2) = -i\Theta(t_1 - t_2) \left(\left\langle \left\{ \begin{matrix} \psi_\uparrow(1), \psi_\uparrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\uparrow^\dagger(2) \end{matrix} \right\} \right\rangle \left\langle \left\{ \begin{matrix} \psi_\uparrow(1), \psi_\downarrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\downarrow^\dagger(2) \end{matrix} \right\} \right\rangle \right) \quad (\text{B.3})$$

$$\bar{F}^R(1, 2) = -i\Theta(t_1 - t_2) \begin{pmatrix} \langle \{ \psi_\uparrow(1), \psi_\uparrow(2) \} \rangle & \langle \{ \psi_\uparrow(1), \psi_\downarrow(2) \} \rangle \\ \langle \{ \psi_\downarrow(1), \psi_\uparrow(2) \} \rangle & \langle \{ \psi_\downarrow(1), \psi_\downarrow(2) \} \rangle \end{pmatrix} \quad (\text{B.4})$$

Advanced Green's Function

$$\hat{G}^A(1, 2) = \begin{pmatrix} \bar{G}^A(1, 2) & \bar{F}^A(1, 2) \\ (\bar{F}^A)^*(1, 2) & (\bar{G}^A)^*(1, 2) \end{pmatrix} \quad (\text{B.5})$$

$$\bar{G}^A(1, 2) = i\Theta(t_2 - t_1) \left(\left\langle \left\{ \begin{matrix} \psi_\uparrow(1), \psi_\uparrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\uparrow^\dagger(2) \end{matrix} \right\} \right\rangle \left\langle \left\{ \begin{matrix} \psi_\uparrow(1), \psi_\downarrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\downarrow^\dagger(2) \end{matrix} \right\} \right\rangle \right) \quad (\text{B.6})$$

$$\bar{F}^A(1, 2) = i\Theta(t_2 - t_1) \begin{pmatrix} \langle \{ \psi_\uparrow(1), \psi_\uparrow(2) \} \rangle & \langle \{ \psi_\uparrow(1), \psi_\downarrow(2) \} \rangle \\ \langle \{ \psi_\downarrow(1), \psi_\uparrow(2) \} \rangle & \langle \{ \psi_\downarrow(1), \psi_\downarrow(2) \} \rangle \end{pmatrix} \quad (\text{B.7})$$

Keldysh Green's Function

$$\hat{G}^K(1, 2) = \begin{pmatrix} \bar{G}^K(1, 2) & \bar{F}^K(1, 2) \\ -(\bar{F}^K)^*(1, 2) & -(\bar{G}^K)^*(1, 2) \end{pmatrix} \quad (\text{B.8})$$

$$\bar{G}^K(1, 2) = -i \left(\left\langle \begin{bmatrix} \psi_\uparrow(1), \psi_\uparrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\downarrow^\dagger(2) \end{bmatrix} \right\rangle \quad \left\langle \begin{bmatrix} \psi_\uparrow(1), \psi_\downarrow^\dagger(2) \\ \psi_\downarrow(1), \psi_\downarrow^\dagger(2) \end{bmatrix} \right\rangle \right) \quad (\text{B.9})$$

$$\bar{F}^K(1, 2) = -i \begin{pmatrix} \langle [\psi_\uparrow(1), \psi_\uparrow(2)] \rangle & \langle [\psi_\uparrow(1), \psi_\downarrow(2)] \rangle \\ \langle [\psi_\downarrow(1), \psi_\uparrow(2)] \rangle & \langle [\psi_\downarrow(1), \psi_\downarrow(2)] \rangle \end{pmatrix} \quad (\text{B.10})$$

Quasiclassical Green's Function

The quasiclassical Green's function in Keldysh space

$$\check{g} = \begin{pmatrix} \hat{g}^R & \hat{g}^K \\ 0 & \hat{g}^A \end{pmatrix}, \quad (\text{B.11})$$

consisting of the 4×4 -matrices

$$\hat{g}^R(X, E) = \begin{pmatrix} \bar{g}^R(X, \mathbf{p}_F, E) & \bar{f}^R(X, \mathbf{p}_F, E) \\ -(\bar{f}^R(X, -\mathbf{p}_F, -E))^* & -(\bar{g}^R(X, -\mathbf{p}_F, -E))^* \end{pmatrix}, \quad (\text{B.12})$$

$$\hat{g}^A(X, E) = \begin{pmatrix} \bar{g}^A(X, \mathbf{p}_F, E) & \bar{f}^A(X, \mathbf{p}_F, E) \\ -(\bar{f}^A(X, -\mathbf{p}_F, -E))^* & -(\bar{g}^A(X, -\mathbf{p}_F, -E))^* \end{pmatrix}, \quad (\text{B.13})$$

$$\hat{g}^K(X, E) = \begin{pmatrix} \bar{g}^K(X, \mathbf{p}_F, E) & \bar{f}^K(X, \mathbf{p}_F, E) \\ (\bar{f}^K(X, -\mathbf{p}_F, -E))^* & (\bar{g}^K(X, -\mathbf{p}_F, -E))^* \end{pmatrix}. \quad (\text{B.14})$$

The first row in (B.12), (B.13) and (B.14) is just from the definition of the Green's function

$$\bar{g}(X, \mathbf{p}_F, E) = \frac{i}{\pi} \int d\xi_{\mathbf{p}} \hat{G}(X, p), \quad (\text{B.15})$$

with

$$\bar{G}(X, p) = \int dx e^{-ipx} \bar{G}(X + \frac{x}{2}, X - \frac{x}{2}). \quad (\text{B.16})$$

The second rows can be shown from

$$\frac{i}{\pi} \int d\xi_{\mathbf{p}} \int dx e^{-ipx} \left[\bar{G}(X + \frac{x}{2}, X - \frac{x}{2}) \right]^* = -(\bar{g}(X, -\mathbf{p}_F, -E))^*. \quad (\text{B.17})$$

Symmetries

The relation between the advanced and retarded Green's functions is

$$\hat{G}^{\text{A}}(1, 2) = \left[\hat{\rho}_3 \hat{G}^{\text{R}}(2, 1) \hat{\rho}_3 \right]^{\dagger}, \quad (\text{B.18})$$

which becomes in the quasiclassical case

$$\hat{g}^{\text{A}}(X, \boldsymbol{p}_{\text{F}}, E) = - \left[\hat{\rho}_3 \hat{g}^{\text{R}}(X, \boldsymbol{p}_{\text{F}}, E) \hat{\rho}_3 \right]^{\dagger}. \quad (\text{B.19})$$