Spin and Charge Transport in Dirty Superconductors

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Abstract

We consider a hybrid superconductor/ferromagnet system and calculate the transport equations for spin and charge in a superconductor with high concentration of impurities for the stationary case. The calculations are made with the Keldysh formalism, and the quasiclassical approximation is used. We find that the physical charge current is not conserved at each energy upon entering the superconductor, but is transformed in energy to accommodate for the superconducting energy gap. The physical spin-current is conserved only in absence of spin-flip scattering.

Preface

This thesis is submitted as the conclusion of my studies for the degree “Sivilingeniør” at the Norwegian University of Science and Technology (NTNU). The work started in February 2003 and the thesis was submitted on June 25$^{\text{th}}$ 2003. During this period my supervisor, Arne Brataas, has provided me with great help and guidance. I look forward to continue our collaboration. Also, I would like to express my gratitude to fellow student Martin S. Grønsleth for inspiring and helpful discussions throughout my study.

The field of non-equilibrium superconductivity was new to me as I started out on this thesis, and the final result reflects this fact. To gain thorough understanding of the subject I had to work out everything in detail, therefore the calculations presented here are quite elaborated.

Tools

My most important tools in this study have certainly been pencil and paper. Some of the tedious matrix calculations of Chapter 4 were done using Maple 8. All figures are made with Xfig, and the document is typeset using LaTeX2ε.

Conventions

Mathematical expressions are mostly typeset according to the standard of the American Physical Society[1]. Some limits on sums and integrals are omitted when there is no risk of confusion. Integrals are taken over the entire space when nothing else is indicated. The electronic charge is $e = -|e|$. Natural units will be used, so that $\hbar = c = k_B = 1$. Note: In BCS Hamiltonian my λ should be made negative in order to make contact to most other authors - where there is *attraction* between electrons.[2]

Jan Petter Morten — Trondheim, 2003-06-25

[1] `http://publish.aps.org/STYLE/math.pdf`
[2] Note added 2005-05-12

Contents

Chapter 1

Introduction

In this chapter we will first discuss quantitatively some general aspects of ferromagnetic and superconducting phenomena in solids. Then we will address the application of such properties, examining some recent experiments and theoretical studies. Motivated by the findings of these studies, the model which is studied in this thesis will be described. In the last section the organization of the following chapters is explained.

1.1 Ferromagnetism

In some solids, the individual magnetic moments of the constituents can organize so that the average magnetic moment is nonzero, even in zero magnetic field. This ordered state is described as ferromagnetic, and the magnetic moment is described by the magnetization vector, $\boldsymbol{M}$. Above a certain temperature, the Curie temperature T_{C}, this spontaneous magnetization will vanish. A variety of metals exhibit such behavior, like Fe, Co, Ni and Gd. The ferromagnetic ordering occurs when the inter-moment interaction is such that the state in which magnetic moments are aligned parallel to one another has lower energy than anti-parallel alignment. This leads to an imbalance of the spin populations at the Fermi level. The unequal filling of the energy bands is the source of the nonzero magnetic moment.

When a current is passed through a solid in the ferromagnetic state, the electrons with spin direction parallel to the magnetization will experience a higher conductance than electrons with spin aligned anti-parallel to the magnetization. Therefore the current will be polarized, so that in a current where there was initially equal amounts of spin-up and spin-down electrons there builds up an excess of electrons with spins parallel to $\boldsymbol{M}$. This property is very important in *spintronics*, where one exploits the properties of the electron spin in electronic devices. For a review of the prospects of spintronics see [1].

1.2 Superconductivity

Superconductivity is a phenomenon which occurs in some materials for temperatures below a certain critical temperature, T_{c}. In the superconducting state the electrical DC resistivity is zero, and the magnetic properties are dramatically different from the normal state. The zero resistivity can lead to a current flowing without any energy dissipation at all. These currents are called supercurrents, and there have been experiments where such supercurrents have been established and in the absence of any driving field persisted without discernible decay. A bulk superconductor behaves like a perfect diamagnet, i.e. the inductance in the interior of the superconductor vanishes. If a specimen is placed in a magnetic field and then cooled below the critical temperature for superconductivity, the magnetic field initially present is ejected from the specimen. This is known as the Meissner effect. Superconductivity occurs in many metallic elements like Al, Ti, Nb, Hg and Cd and in certain alloys and intermetallic compounds. The critical temperature can vary from 1.140 K for Al to 90.0 K for the compound $YBa_2Cu_3O_{0.69}$. The phenomenology of superconductivity is discussed in detail by Kittel [2].

The theory which describes superconductivity is due to Bardeen, Cooper and Schrieffer (BCS) [3] and Bogoliubov [4] and Valatin [5]. A clue as to the nature of superconductivity is offered by the experimental fact that the critical temperature is different for various isotopes of the same material. This means that the motion of the nuclei plays a role. The electron-lattice-electron interaction in superconductors leads to an effective attractive interaction between electrons. This causes the ground state to be very different from a free fermion gas. The free electron gas ground state is a filled Fermi sea of non-interacting electrons (all states up to energy E_{F} occupied according to the Pauli exclusion principle). This state allows for small excitations of electrons with an energy close to the Fermi energy. The BCS theory shows that the effective attraction between the electrons promotes the formation of pairs of electrons of opposite spin and momentum, i.e a pair of electrons in the states $(\boldsymbol{p}\uparrow, -\boldsymbol{p}\downarrow)$. Such a pair is called a Cooper pair. Because of the exclusion principle, the pair of electrons cannot be scattered into the Fermi sphere, but is confined to an effectively two-dimensional layer around it. Generalizing to the many-body case we must also take into account the quasiparticles (the quasiparticle concept is described in Section 2.2) residing below the Fermi surface, namely the holes. The total energy of the resulting state will for some conditions be lower than the Fermi state, and the system becomes superconducting.

In BCS theory [6] the effective electron-electron attractive interaction is taken into account by adding a two-particle operator term to the Hamiltonian. This operator is often treated in the mean field approximation, where one introduces the so-called anomalous averages. These are averages of two creation or annihilation operators[1] which should be zero in a state with a fixed number of particles. However, the nonzero anomalous averages are the fundamental feature of the superconducting state. They imply the existence of a long-range correlation between quasiparticle states, i.e. the superconductor is an ordered state. The apparent paradox of the creation and annihilation of quasiparticles in pairs is actually just a consequence of the mean field description we have chosen. An observable quantity of the system is always described by a composition of the anomalous averages which corresponds to an operator which is nonzero even if the number of particles is fixed.

The superconductor usually behaves as if there were a gap in energy of width 2Δ centered about the Fermi energy in the set of allowed one-electron levels. The allowed energy of an electron in a superconductor is therefore restricted by the condition $|E - E_{\mathrm{F}}| > \Delta$. The superconducting energy gap Δ increases in size as the temperature drops, and above the critical temperature it is zero. The gap in the energy spectrum is a very

[1] For the reader not familiar with the language of second quantization, I refer to Chapter 2 in which a short introduction is given.

important property of the superconducting state which allows us to understand many aspects of superconducting behavior.

1.3 Magneto-Electronics

Magneto-electronics is an approach to electronics in which one focuses more on the spin properties of the carriers than on charge properties of electrons and holes as in traditional semiconductor electronics. Research in magneto-electronics has lead to numerous technological applications, especially in the field of information storage [7]. The discovery of the "Giant Magneto Resistance" (GMR) effect was made in 1988 [8] and today it forms the basis of the leading technology for information storage by magnetic disc drives [9]. GMR is a quantum mechanical effect observed in layered magnetic thin-film structures that are composed of alternating ferromagnetic and non-magnetic layers. When the magnetization directions of the ferromagnetic layers are parallel, the spin dependent scattering of the carriers is minimized, and the material has low resistance. When the ferromagnetic layers are anti-aligned, the spin dependent resistance is maximized, and the material has its highest resistance. The directions of the magnetic moments are manipulated by external magnetic fields. Structures can now be fabricated which produce significant changes in resistance in response to a relatively small magnetic field and operate at room temperature.

A simple device based on the GMR effect is the so-called spin-valve. This is a simple three-layer system where two magnetic layers are separated by a non-magnetic. The magnetization of one of the ferromagnetic layers is very difficult to reverse in an applied magnetic field, whereas the magnetization of the other layer is very easy to reverse. The easily reversed layer acts a the "valve control" and is sensitive to manipulation by an external field. Such devices are the used in the "read" heads of most hard disk drives. There are numerous other applications of such devices, some are mentioned below.

Since the current through a ferromagnet will be spin polarized parallel to the magnetization direction, the injection of a anti-aligned spin polarized current into a ferromagnet should also cause a torque on the magnetization direction. This follows from an action-reaction argument. The spin-current induced magnetization torque arises from an interaction between conduction electron spins and the net magnetic moment of the ferromagnet, transferring angular momentum [10]. This effect is promising for applications by the ability to excite and probe the dynamics of magnetic moments at small length scales, and can be utilized in magnetic memory elements.

The utilization of spin-valves for magnetic memory elements is a very active research area, and companies like IBM, Motorola, Honeywell and Hewlett Packard are researching devices commonly known as MRAM (Magnetic Random Access Memory). MRAM depends on the polarity of spin-valves to store data, in contrast to DRAM (Dynamic Random Access Memory) chips which use electricity. In DRAM, a memory bit is stored as an electrical charge on a capacitor. Because the charge on a DRAM chip constantly leaks, it needs to be supplied with a near-continuous electrical current to retain the memory. When the power is turned off, DRAM chips lose their data. DRAM memory chips are used in current generation computers, and it is the loss of information in absence of current flow which necessitates the rather long boot-up time when a computer is turned on. Magnetic storage of information does not require power to retain its data, thus consuming much less power. Prospects of producing inexpensive MRAM chips with comparable or even better performance as current DRAM makes it a very promising technology. For a review of the state of MRAM technology see [11].

Recent studies of the effect of a superconducting contact to a GMR device has shown that the properties of the device will be dramatically changed [12, 13]. If spin mixing is allowed in the system, the GMR effect is enhanced by the presence of superconducting contacts. In a system with no spin mixing the GMR effect is effectively suppressed. Studies of how superconducting elements can be used to make very efficient spin-valves have recently appeared [14]. These results call for further studies of devices combining GMR and superconductivity.

1.4 Spin Transport in Superconductors

As we have seen, layered devices with ferromagnetic components give rise to imbalance between the number of spin-up and spin-down carriers. In superconductors, on the other hand, the unusual properties arise because of an interaction between pairs of spin-up and spin-down electrons. Therefore, ferromagnetism and superconductivity are very different phenomena, and new features arise in devices where both these properties are present.

Andreev reflection [15] is the elementary process which enables electron transport across a boundary between a non-superconducting and a superconducting material for energies below the superconducting energy gap. The incoming electron with spin e.g. up takes another electron with spin down to enter the superconductor as a Cooper pair with zero spin. This corresponds to the reflection of a positively charged hole with reversed spin direction. If the non-superconducting material is a ferromagnet, the reflection process is affected by the imbalance of number of spin-up and spin-down electrons. The result is that an excess spin density will arise close to the ferromagnet/superconductor interface which leads to a spin contact resistance [16, 17, 18, 19]. This is known as spin-accumulation. The resistance arising can be either enhanced or lowered in comparison to the normal case. Experiments by Pratt et al. have given information about the dynamics of this process, which is closely related to the spin-flip length in the superconductor [20, 21]. In these experiments the conductance of a spin-valve where the middle, nonmagnetic layer is superconducting, has been measured. Theoretical studies of this process [22] calls for further experiments.

When a superconductor is placed nearby a non-superconducting metal, there is the possibility of inducing superconductive properties in the non-superconducting metal. This is known as the proximity effect. It has been known for a long time [23], but has recently been studied in samples of very small size with ferromagnetic components. This has lead to the observation of unexpected transport properties [24]. Theoretical models to explain the proximity effect in the presence of splitting of energy levels for spin-up and spin-down states is currently heavily investigated [25, 26]. The question of coexistence of ferromagnetism and superconductivity is not just a theoretical one, but is motivated by the possible application to quantum computers [27].

1.5 Model

The experimental and theoretical work summarized above provides motivation to study the transport of spin and charge in hybrid superconductor/ferromagnet structures. We will consider a model where a mesoscopic[2] superconductor/ferromagnet sample is placed between a superconducting and a ferromagnetic reservoir. See Figure 1.1.

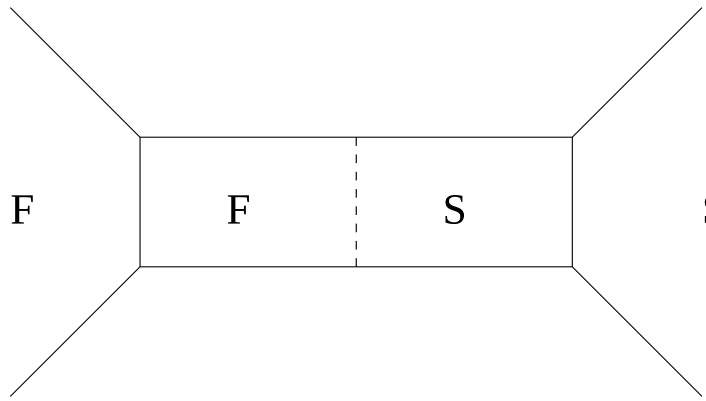


Figure 1.1: Geometry of the system we will consider. The left- and rightmost parts are Ferromagnetic and Superconducting reservoirs, and the middle two parts are the mesoscopic sample for which we will find kinetic equations. Since we will consider a system with high impurity scattering, the boundary surface inside the sample will be irrelevant.

We will assume the reservoir/sample interfaces to be transparent so that we can ignore the interface resistance. Furthermore, the ferromagnet is assumed to be monodomain with a well-defined direction of magnetization.

Because of time limitations, I had to focus only on the superconducting part of the sample in this thesis. The aim of the calculations is to derive transport equations which determine the distribution functions of quasiparticles in the mesoscopic superconductor.

1.6 Organization of Chapters

This thesis is organized in the following way: In Chapter 2 we will recapitulate some of the fundamental concepts of quantum theory which will be used in this thesis. There is also a short discussion of the quasiparticle concept and the main ideas of quasiclassical theory. A reader familiar with these topics can skip to Chapter 3. Here we will derive the Keldysh non-equilibrium formalism to describe superconductors. This results in equations of motion for the Green's functions. A gauge transformation will be introduced in order to make the superconducting gap enter only as a real, positive quantity. This will simplify the calculations, but demands us to include the complex phase of the gap order parameter explicitly in the equations. In this chapter we also derive some relations to express observable quantities by the Green's functions. In Chapter 4 we first introduce the Wigner

[2]The term mesoscopic derives from the word "mesos" meaning something in between. Small systems whose dimensions are intermediate between the microscopic and the macroscopic are called mesoscopic. This means that quantum phenomena are essential to the behavior of macroscopic quantities like electrical current.

distribution functions, which includes a shift into relative- and center of mass-coordinates as well as a Fourier transformation. Various approximations are then introduced to simplify the equations of motion. This includes the quasiclassical approximation mentioned above, and an expansion of the Green's function in spherical harmonics valid when scattering from impurities is dominant. This leads us to a diffusion equation for the superconductor and a parameterization of the Green's functions. Inserting the parameterized Green's functions into the diffusion equation yields kinetic equations which can be solved for the quasiparticle distribution functions. A conclusion and discussion of further prospects is given in Chapter 5. Notes on notation, equilibrium solutions and formulas for the quasiclassical formalism is gathered in appendices.

Chapter 2

Fundamental Concepts

In this chapter we will briefly recapitulate some of the essential quantum mechanical theory used in this thesis. Then we will give a quantitative introduction to the quasiclassical theory.

2.1 Quantum Theory

A necessary prerequisite to read this thesis is a general understanding of basic quantum theory, which is covered in textbooks by Hemmer [28] (Norwegian) or Schiff [29]. We will be using the second quantization description, which is covered by [30]. Also, the Green's function approach is described in this book.

2.1.1 Second Quantization

In order to describe the quantum mechanical state of a many-particle system, the number representation is convenient. In this description one assumes the existence of a vacuum state, $|0\rangle$. Particles are added and subtracted from this state by applying creation and annihilation operators. For example, the creation operator which adds an electron of momentum $\boldsymbol{p}$ and spin σ ($\sigma =\uparrow,\downarrow$) could be called $c^\dagger_{\boldsymbol{p}\sigma}$, and a one-particle state is given by

$$|\boldsymbol{p}\sigma\rangle = c^\dagger_{\boldsymbol{p}\sigma}|0\rangle. \tag{2.1}$$

The notation $|\boldsymbol{p},\sigma\rangle$ now means there is one electron present in the quantum state characterized by $\boldsymbol{p},\sigma$. The annihilation operator which removes an electron of momentum $\boldsymbol{p}$ and spin σ could be called $c_{\boldsymbol{p}\sigma}$, and when acting on the state in Equation (2.1) it gives back the empty vacuum state,

$$c_{\boldsymbol{p}\sigma}|\boldsymbol{p}\sigma\rangle = |0\rangle. \tag{2.2}$$

Acting on the empty state by the annihilation operator gives zero,

$$c_{\boldsymbol{p}\sigma}|0\rangle = 0. \tag{2.3}$$

The Pauli principle is incorporated in the theory by $(c^\dagger_{\boldsymbol{p}\sigma})^2 = 0$, which simply states that two particles can not be in the same single-particle state. Necessarily we must also have that $(c_{\boldsymbol{p}\sigma})^2 = 0$. A may-particle state is built up from the vacuum state as linear superpositions of states of the form

$$(c^\dagger_{r_1})^{n_1}(c^\dagger_{r_2})^{n_2}\cdots|0\rangle, \tag{2.4}$$

where r_i denotes a quantum state and n_i is an integer. Electrons are fermions, and thus the state is antisymmetric under interchange of particle labels. If two particles occupy different states characterized by $\boldsymbol{p}\sigma$ and $\boldsymbol{p}'\sigma'$ this means that

$$|\boldsymbol{p}\sigma,\boldsymbol{p}'\sigma'\rangle = c^\dagger_{\boldsymbol{p}\sigma}c^\dagger_{\boldsymbol{p}'\sigma'}|0\rangle = -c^\dagger_{\boldsymbol{p}'\sigma'}c^\dagger_{\boldsymbol{p}\sigma}|0\rangle = -|\boldsymbol{p}'\sigma',\boldsymbol{p}\sigma\rangle. \tag{2.5}$$

The relations we have mentioned so far could also have been derived by letting the creation and annihilation operators satisfy an anticommutation relation by definition. I.e. for two states r and s we demand that

$$\left[c_r, c^\dagger_s\right]_+ = \delta_{rs},\ \ [c_r, c_s]_+ = \left[c^\dagger_r, c^\dagger_s\right]_+ = 0. \tag{2.6}$$

We use the notation $[A,B]_+ = AB+BA$ to denote anticommutators[1]. Physical observables are in quantum mechanics represented as operators. In second quantization representation these operators are expressed in terms of the creation and annihilation operators. It can be shown [30] that for single-particle operators, the expression in second quantization is

$$F = \sum_{\boldsymbol{p}\boldsymbol{p}'}\sum_{\sigma\sigma'}\langle\boldsymbol{p}'\sigma'|f|\boldsymbol{p}\sigma\rangle c^\dagger_{\boldsymbol{p}'\sigma'}c_{\boldsymbol{p}\sigma}, \tag{2.7}$$

where $\langle\boldsymbol{p}'\sigma'|f|\boldsymbol{p}\sigma\rangle$ is the expectation value of the physical operator f (where f is the operator of "usual" quantum mechanics, i.e. not the second quantized operator).

Instead of the momentum-spin eigenfuction basis for quantum-mechanical states, we could use eigenfunctions of the position operators in position-spin representation. The transformation to this basis leads to a description in terms of the creation and annihilation operators $\psi^\dagger_\sigma(\boldsymbol{r},t)$ and $\psi_\sigma(\boldsymbol{r},t)$. These operators are traditionally called *field operators*. The interpretation of these is that $\psi^\dagger_\sigma(\boldsymbol{r},t)$ creates a particle localized at the space-time point $(\boldsymbol{r},t)$ in spin state σ, and $\psi_\sigma(\boldsymbol{r},t)$ annihilates a particle at space-time point $(\boldsymbol{r},t)$ in spin state σ. An important point about these operators is that at equal times they satisfy the same anticommutation relation as $c_{\boldsymbol{p}\sigma}, c^\dagger_{\boldsymbol{p}\sigma}$, i.e.

$$\begin{aligned}\left[\psi_\sigma(\boldsymbol{r},t),\psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\right]_+ &= \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}'),\\ \left[\psi_\sigma(\boldsymbol{r},t),\psi_{\sigma'}(\boldsymbol{r}',t)\right]_+ &= \left[\psi^\dagger_\sigma(\boldsymbol{r},t),\psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\right]_+ = 0.\end{aligned} \tag{2.8}$$

This means that the generalizations of relations (2.2)-(2.5) hold also for the field operators. The representation of single-particle operators by the field operators is

$$F = \sum_{\sigma\sigma'}\int \mathrm{d}\boldsymbol{r}\psi^\dagger_\sigma(\boldsymbol{r},t)f(\boldsymbol{r})\psi_{\sigma'}(\boldsymbol{r},t), \tag{2.9}$$

where $f(\boldsymbol{r})$ is the operator as in ordinary quantum mechanics in the position representation. In this thesis we will use the field operator description exclusively.

[1]See Appendix A for more about the definition of commutator and anticommutator.

2.1.2 Pictures

The observables of a quantum mechanical system are characterized by operators, but only the *average value* of such an operator represents a measurable quantity. This is crucial to the definition of the so-called pictures in quantum mechanics[2]. The Schrödinger picture is the most common. Here the time dependence of the system is carried by the quantum states, and the operators are constant in time. The time evolution of the states is given by a differential equation, namely the Scrhödinger equation,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle_{\mathrm{S}} = H|\Psi(t)\rangle_{\mathrm{S}}, \tag{2.10}$$

where H is the Hamilton operator and subscript S denotes Schrödinger picture. However, quantum mechanics can equally well be described in the Heisenberg picture. The time dependence is then carried by the operators themselves, and the quantum state is constant in time. Formally, the transition from the Schrödinger to the Heisenberg picture is performed by a unitary transformation. In the Heisenberg picture the time evolution of the system is given by the Heisenberg equation of motion, which states that when the Hamilton operator does not carry explicit time dependence,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{O}(t) = [\mathcal{O}(t), H]_{-}\,, \tag{2.11}$$

where $\mathcal{O}(t)$ denotes an operator in the Heisenberg picture. The commutation relations in the Schrödinger picture are also valid for the corresponding operators in the Heisenberg picture. When doing perturbation theory the interaction picture is used. As we will not consider perturbation theory rigorously, this picture will not be discussed further. We will use the Heisenberg picture exclusively in this thesis.

2.1.3 Free Electron Gas

As an example of the formalism discussed above, we will consider a system of non-interacting fermions in an electromagnetic field. Using (2.9) the Hamiltonian of this system is in the Heisenberg picture

$$H_0 = \sum_{\sigma}\int \mathrm{d}\boldsymbol{r}\psi_{\sigma}^{\dagger}(\boldsymbol{r},t)\left[\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\nabla - e\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + e\varphi(\boldsymbol{r},t)\right]\psi_{\sigma}(\boldsymbol{r},t). \tag{2.12}$$

This operator is diagonal in spin. In the next chapter we will add terms to the Hamiltonian to account for interactions and scattering.

2.1.4 Average Values

The measurable quantity for a quantum mechanical system is the average value of an operator. The definition of the average value of the physical observable operator $\mathcal{O}(t)$ in the Heisenberg picture is[3]

$$\langle\mathcal{O}(t)\rangle = \mathrm{Tr}\left\{\rho(H)\mathcal{O}(t)\right\}. \tag{2.13}$$

[2] For a short introduction to the concept of pictures in quantum mechanics, see Chapter 1.5 in the book by Mandl and Shaw [31].

[3] Sometimes we will use the angular brackets $\langle\cdots\rangle$ to denote other kinds of averaging. In these cases this is described in the text.

Here the trace denotes a sum over all possible states of the system, i.e.

$$\mathrm{Tr}\,\{\cdots\} = \sum_n \langle n|\cdots|n\rangle, \tag{2.14}$$

and ρ is the statistical operator. In equilibrium state at finite temperature this operator is [32]

$$\rho = \mathrm{e}^{-\beta(H-\Omega)} = \frac{\sum_n \mathrm{e}^{-\beta E_n}|n\rangle\langle n|}{\mathrm{Tr}\,\{\mathrm{e}^{-\beta E_n}\}}, \tag{2.15}$$

where $\beta = \frac{1}{k_\mathrm{B}T}$ is inverse temperature and E_n is the n-th energy eigenvalue of the Hamilton operator H. In the non-equilibrium situation the probability of a certain state is not given by simple Boltzmann-factors. We then have

$$\rho = \sum_m |\Phi_m\rangle W_m \langle\Phi_m|, \tag{2.16}$$

where W_m is the probability of finding the system in the quantum state $|\Phi_m\rangle$. These probabilities must add up to one, $\sum_m W_m = 1$.

2.2 Green's Functions

We will use Green's functions to describe the electrons in the superconductor. These functions are related to the *un*equal time anticommutator relation of the field operators (cf. Equation (2.8)). The one-particle Green's functions which we will employ are functions of two space-time coordinates, and can usually be interpreted as the transition amplitude for propagation of electrons between the two positions in a time interval. However, we will use several types of Green's functions, so that sometimes they describe propagation of other entities. They may be holes, i.e. the absence of an electron, or more generally quasiparticles. This means that instead of describing a number of interacting electrons in a process we model independent quasiparticles. For example, if we investigate the electrons in the periodic potential of a crystal lattice, we could approximate by neglecting the dynamics of the nuclei and fixate their positions at the equilibrium positions. We now model the electrons moving through the "frozen" lattice as "quasielectrons" with a mass and charge different from conventional electrons. The mass of the quasiparticles may now be anisotropic, the charge positive etc., leading us to the familiar concepts of effective mass and charge.

The Green's functions will be represented by matrices in spin- and particle-hole space. Both spaces have a twofold freedom, resulting in 4×4 matrices in the general case. In addition we will use retarded, advanced and Keldysh time ordering of the Green's functions. The complete set of Green's functions can be gathered in an 8×8 matrix structure in "Keldysh space". This matrix will contain all relevant quantum mechanical information about the static and dynamic properties of superconductors. This formalism is due to Keldysh [33], and is widely used to describe non-equilibrium processes. A review was given by Rammer and Smith [34].

2.3 Quasiclassical Theory

The Green's function oscillates as a function of the relative coordinate on a scale of the Fermi wavelength λ_F. This is much shorter than the other characteristic length scales in the problem. Moreover, it is important to study the phase of the two-electron wavefunction, which depends on the center of mass coordinate. For these reasons it is possible to integrate out the dependence of the absolute value of the relative coordinate [35]. In momentum space this corresponds to obtaining a quantity integrated over quasiparticle momentum. In this approximation we assume that only particles with momentum close to the Fermi momentum will participate in physical processes, so that the *direction* of the Fermi momentum is the relevant quantity. But as a consequence all physical quantities are confined to the Fermi surface and a variety of effects can not be accounted for any more. Examples are weak localization and persistent currents which are controlled by the phase coherence of the single-electron wavefunction contained in the relative coordinate.

The quasiclassical theory consists furthermore of a transport-like differential equation for the 8×8 Green's function matrix. Various symmetries and conditions on this matrix makes a simple parameterization of the matrix possible. Gathering specific components of the matrix transport equation in scalar equations gives kinetic equations which determine the quasiparticle distribution functions for the non-equilibrium situation. Such equations are sometimes called "quantum Boltzmann equations" to emphasize the relation to classical transport theory. The distribution functions describe the spatial probability of a quasiparticle occupying a quantum state. The Boltzmann equation description of superconductors is used also in the framework of other formalisms, a review was given by Aronov et al. [36].

Chapter 3

Field Theory of Superconductors

In this chapter we will develop formalism to describe a superconductor. We will start from the Hamiltonians and derive equations of motion for 4-vector field operators. Then we define the normal and anomalous Green's functions which will be gathered in a matrix structure. Using the equations of motion for the 4-vectors we can find equations of motions for the matrix Green's functions.

3.1 Hamiltonian

We consider a hybrid system composed of ferromagnetic and superconductor elements. The Hamiltonians for ferromagnet and superconductor differ, so we will discuss them separately. We will take into account spin correlations and electron-hole correlations. We also include elastic scattering processes between electrons and impurities and elastic spin-flip scattering with magnetic impurities. Spin-orbit scattering will be neglected. We assume that since we have included magnetic impurity scattering, which is a mechanism also causing spin-flip, this approximation does not affect the transport-properties. Neglect of spin-orbit scattering is formally valid in materials where the spin-orbit coupling is weak and spin-flip scattering is dominated by the magnetic impurities present. The spin-orbit scattering time (i.e. the time an electron can diffuse before its spin direction is randomized), τ_{so}, scales linearly with the elastic scattering time, τ, approximately as [18]

$$\tau/\tau_{\mathrm{so}} \sim (\alpha Z)^4, \tag{3.1}$$

where α is the fine structure constant and Z is the atomic number of the impurity atoms. In a hybrid structure of a superconductor and a ferromagnet it is plausible that some magnetic impurities will be present as a consequence of the fabrication process. This means that our assumption is valid for a system with a superconductor of low atomic number, e. g. aluminum.

3.1.1 Ferromagnet

The purely ferromagnetic system is described by the following Hamiltonian,

$$H = H_0 + H_{\boldsymbol{M}} + H_{\mathrm{sf}} + H_{\mathrm{imp}}, \tag{3.2a}$$

$$H_0 = \sum_{\sigma} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) \left[\frac{1}{2m} \left(\frac{\hbar}{\mathrm{i}} \nabla - e\boldsymbol{A}(\boldsymbol{r},t) \right)^2 + e\varphi(\boldsymbol{r},t) - \mu \right] \psi_\sigma(\boldsymbol{r},t), \tag{3.2b}$$

$$H_{\boldsymbol{M}} = \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) \left[\bar{\tau}_3\right]_{\sigma\sigma'} M_z(\boldsymbol{r},t) \psi_{\sigma'}(\boldsymbol{r},t), \tag{3.2c}$$

$$H_{\mathrm{imp}} = \sum_{\sigma} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) V_{\mathrm{imp}}(\boldsymbol{r}) \psi_\sigma(\boldsymbol{r},t), \tag{3.2d}$$

$$H_{\mathrm{sf}} = \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) \left[\bar{\boldsymbol{\tau}} \cdot \boldsymbol{S}(\boldsymbol{r})\right]_{\sigma\sigma'} V_{\mathrm{sf}}(\boldsymbol{r}) \psi_{\sigma'}(\boldsymbol{r},t). \tag{3.2e}$$

Here $\psi_\sigma(\boldsymbol{r},t)$ is the Heisenberg field operator for spin $\sigma = \uparrow, \downarrow$ and $\psi_\sigma^\dagger(\boldsymbol{r},t)$ is the adjoint operator. The fermion operators satisfy the equal time anticommutation relation

$$\left[\psi_\sigma(\boldsymbol{r},t), \psi_{\sigma'}^\dagger(\boldsymbol{r}',t)\right]_+ = \psi_\sigma(\boldsymbol{r},t)\psi_{\sigma'}^\dagger(\boldsymbol{r}',t) + \psi_{\sigma'}^\dagger(\boldsymbol{r}',t)\psi_\sigma(\boldsymbol{r},t) = \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{3.3}$$

H_0 is the Hamiltonian for noninteracting particles, where $\varphi(\boldsymbol{r},t)$ and $\boldsymbol{A}(\boldsymbol{r},t)$ are the usual electromagnetic potentials, and μ is the chemical potential. $H_{\boldsymbol{M}}$ describes the effect of the magnetization, $\boldsymbol{M}$,[1] in the ferromagnet. In this case we have assumed it to be directed along the z-axis. The electron spin operator for z-direction is represented by the third Pauli matrix, $\bar{\tau}_3$, (more about the Pauli matrices in section 3.2). Impurity scattering is governed by H_{imp}, and spin-flip scattering by magnetic impurities is governed by H_{sf}. $\bar{\boldsymbol{\tau}} \cdot \boldsymbol{S}$ is a product of the Pauli spin matrices and spin operators $\boldsymbol{S}$ for the localized magnetic impurities. Note that we use the convention where the electron charge is $e = -|e|$.

3.1.2 Superconductor

The superconductor is described by the following Hamiltonian,

$$H = H_0 + H_{\mathrm{int}} + H_{\mathrm{sf}} + H_{\mathrm{imp}}, \tag{3.4a}$$

$$H_0 = \sum_{\sigma} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) \left[\frac{1}{2m} \left(\frac{\hbar}{\mathrm{i}} \nabla - e\boldsymbol{A}(\boldsymbol{r},t) \right)^2 + e\varphi(\boldsymbol{r},t) - \mu \right] \psi_\sigma(\boldsymbol{r},t), \tag{3.4b}$$

$$H_{\mathrm{int}} = \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}' V(\boldsymbol{r},t,\boldsymbol{r}',t) \psi_\uparrow^\dagger(\boldsymbol{r},t) \psi_\downarrow^\dagger(\boldsymbol{r}',t) \psi_\downarrow(\boldsymbol{r}',t) \psi_\uparrow(\boldsymbol{r},t), \tag{3.4c}$$

$$H_{\mathrm{imp}} = \sum_{\sigma} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) V_{\mathrm{imp}}(\boldsymbol{r}) \psi_\sigma(\boldsymbol{r},t), \tag{3.4d}$$

$$H_{\mathrm{sf}} = \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r},t) \left[\bar{\boldsymbol{\tau}} \cdot \boldsymbol{S}(\boldsymbol{r})\right]_{\sigma\sigma'} V_{\mathrm{sf}}(\boldsymbol{r}) \psi_{\sigma'}(\boldsymbol{r},t). \tag{3.4e}$$

Compared to the Hamiltonian describing a ferromagnetic system, the only difference is the absence of magnetization, $H_{\boldsymbol{M}}$, and the addition of H_{int} which is the BCS interaction

[1] Any prefactors are also included in this quantity.

term for a superconductor. Note that this term is a two-particle operator, and causes Cooper pairing inside the superconductor as discussed in the introduction (Section 1.2). This term will be treated in the mean field approximation.

Our focus in the calculations will be to derive transport equations for the superconducting part of the metal placed between ferromagnetic and superconducting reservoirs. Thus there will be no permanent magnetization present and we neglect the term $H_{\boldsymbol{M}}$ in the calculations ahead. We will use natural units so that $\hbar = c = k_B = 1$ in the following (see Chapter 6.1 in the book by Mandl and Shaw [31]).

BCS Mean Field Approximation

We use a mean field approximation to the BCS interaction (see page 134 in [30]). We also assume that the interaction is of a very short range, $V(\boldsymbol{r}, \boldsymbol{r}') = \lambda(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}')$ so that

$$H_{\text{int}} = \int \mathrm{d}\boldsymbol{r} \lambda(\boldsymbol{r}) \psi_\uparrow^\dagger(\boldsymbol{r}, t) \psi_\downarrow^\dagger(\boldsymbol{r}, t) \psi_\downarrow(\boldsymbol{r}, t) \psi_\uparrow(\boldsymbol{r}, t). \tag{3.5}$$

Inside a bulk superconductor $\lambda(\boldsymbol{r}) = \lambda_0$ is a constant, whereas in the normal metal and the ferromagnet the interaction strength vanishes, $\lambda(\boldsymbol{r}) = 0$. We introduce the quantity

$$\tilde{\Delta}(\boldsymbol{r}, t) = \langle \psi_\downarrow(\boldsymbol{r}, t) \psi_\uparrow(\boldsymbol{r}, t) \rangle \tag{3.6}$$

describing electron-hole correlations, where $\langle \cdots \rangle$ denotes average value. Consequently

$$\psi_\downarrow(\boldsymbol{r}, t)\psi_\uparrow(\boldsymbol{r}, t) = \tilde{\Delta}(\boldsymbol{r}, t) + \Big(\psi_\downarrow(\boldsymbol{r}, t)\psi_\uparrow(\boldsymbol{r}, t) - \tilde{\Delta}(\boldsymbol{r}, t) \Big) = \tilde{\Delta}(\boldsymbol{r}, t) + \delta_{\tilde{\Delta}}(\boldsymbol{r}, t), \tag{3.7a}$$

$$\psi_\uparrow^\dagger(\boldsymbol{r}, t)\psi_\downarrow^\dagger(\boldsymbol{r}, t) = \tilde{\Delta}^*(\boldsymbol{r}, t) + \Big(\psi_\uparrow^\dagger(\boldsymbol{r}, t)\psi_\downarrow^\dagger(\boldsymbol{r}, t) - \tilde{\Delta}^*(\boldsymbol{r}, t) \Big) = \tilde{\Delta}^*(\boldsymbol{r}, t) + \delta_{\tilde{\Delta}}^*(\boldsymbol{r}, t), \tag{3.7b}$$

where the deviation from the average value, $\delta_{\tilde{\Delta}}(\boldsymbol{r}, t)$, has been introduced. By inserting these expressions into (3.5) and disregarding second order terms of $\delta_{\tilde{\Delta}}$, we find

$$\begin{aligned}
H_{\text{int}} &= \int \mathrm{d}\boldsymbol{r} \lambda(\boldsymbol{r}) \Big[\tilde{\Delta}^*(\boldsymbol{r}, t) + \delta_{\tilde{\Delta}}^*(\boldsymbol{r}, t) \Big] \Big[\tilde{\Delta}(\boldsymbol{r}, t) + \delta_{\tilde{\Delta}}(\boldsymbol{r}, t) \Big] \\
&\approx \int \mathrm{d}\boldsymbol{r} \lambda(\boldsymbol{r}) \Big[\tilde{\Delta}^*(\boldsymbol{r}, t)\tilde{\Delta}(\boldsymbol{r}, t) + \tilde{\Delta}^*(\boldsymbol{r}, t)\delta_{\tilde{\Delta}}(\boldsymbol{r}, t) + \delta_{\tilde{\Delta}}^*(\boldsymbol{r}, t)\tilde{\Delta}(\boldsymbol{r}, t) \Big] \\
&= \int \mathrm{d}\boldsymbol{r} \lambda(\boldsymbol{r}) \Big[\tilde{\Delta}^*(\boldsymbol{r}, t)\psi_\downarrow(\boldsymbol{r}, t)\psi_\uparrow(\boldsymbol{r}, t) + \tilde{\Delta}(\boldsymbol{r}, t)\psi_\uparrow^\dagger(\boldsymbol{r}, t)\psi_\downarrow^\dagger(\boldsymbol{r}, t) \Big] + \text{constant}.
\end{aligned} \tag{3.8}$$

In the last step we have substituted the expression for $\delta_{\tilde{\Delta}}(\boldsymbol{r}, t)$. The constant term is independent of the operator $\psi_\sigma(\boldsymbol{r}, t)$ and can be disregarded. Now, we define the order parameter of the superconductor, or the gap function,

$$\Delta(\boldsymbol{r}, t) = \lambda(\boldsymbol{r}) \langle \psi_\downarrow(\boldsymbol{r}, t)\psi_\uparrow(\boldsymbol{r}, t) \rangle, \tag{3.9}$$

which brings the expression for H_{int} to the usual BCS mean field form

$$H_{\text{int}} = \int \mathrm{d}\boldsymbol{r} \Big[\Delta^*(\boldsymbol{r}, t)\psi_\downarrow(\boldsymbol{r}, t)\psi_\uparrow(\boldsymbol{r}, t) + \Delta(\boldsymbol{r}, t)\psi_\uparrow^\dagger(\boldsymbol{r}, t)\psi_\downarrow^\dagger(\boldsymbol{r}, t) \Big]. \tag{3.10}$$

Note that in this approximation we have reduced H_{int} from a two-particle operator to a one-particle operator, which is essential to our calculations.

3.2 4-Vector Notation

The BCS mean field interaction term introduces correlations between electrons and holes. Similarly the magnetization in the ferromagnet breaks the symmetry between spin-up and spin-down states. A convenient 4-vector notation for such a system was introduced by Maki [37] by defining

$$\psi^\dagger(\boldsymbol{r},t) = \begin{pmatrix} \psi^\dagger_\uparrow(\boldsymbol{r},t) & \psi^\dagger_\downarrow(\boldsymbol{r},t) & \psi_\uparrow(\boldsymbol{r},t) & \psi_\downarrow(\boldsymbol{r},t) \end{pmatrix}, \quad \psi(\boldsymbol{r},t) = \begin{pmatrix} \psi_\uparrow(\boldsymbol{r},t) \\ \psi_\downarrow(\boldsymbol{r},t) \\ \psi^\dagger_\uparrow(\boldsymbol{r},t) \\ \psi^\dagger_\downarrow(\boldsymbol{r},t) \end{pmatrix}. \tag{3.11}$$

Physical quantities can be represented in terms of matrices and vectors in this basis. Before we proceed, let us outline the representation we use for the matrices.

We will be working with matrices of different dimensions, so we adopt the following notation to distinguish 2×2, 4×4 and 8×8 matrices. Consider a matrix A:

- $\bar{A}$ denotes a 2×2 matrix,
- $\hat{A}$ denotes a 4×4 matrix,
- $\check{A}$ denotes a 8×8 matrix.

Note that complex conjugation is denoted by "*", since we have reserved the "bar" to emphasize matrix structure. Coordinate 3-vectors will be written in boldface, e.g. $\boldsymbol{r}$. The 2×2 Pauli-matrices will be designated $\bar{\tau}_i$, where

$$\bar{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \bar{\tau}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \bar{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.12}$$

A "4-dimensional Pauli-matrix" can be constructed by

$$\hat{\tau}_i = \begin{pmatrix} \bar{\tau}_i & 0 \\ 0 & \bar{\tau}_i \end{pmatrix}. \tag{3.13}$$

We will also be using the following 4×4 matrices $\hat{\rho}_i$

$$\hat{\rho}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \hat{\rho}_2 = \begin{pmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \end{pmatrix} \quad \hat{\rho}_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{3.14}$$

These are generalizations of the Pauli matrices to 4×4 dimensional basis. The matrices $\bar{\tau}_i$ and $\hat{\rho}_i$ are all traceless and the square of each matrix equals the identity matrix, i.e.

$$\mathrm{Tr}\{\bar{\tau}_i\} = 0,\ \mathrm{Tr}\{\hat{\rho}_i\} = 0, \tag{3.15a}$$

$$\bar{\tau}_i^2 = \bar{1},\ \hat{\rho}_i^2 = \hat{1}. \tag{3.15b}$$

Here $\bar{1}$ denotes the 2×2 identity matrix and $\hat{1}$ denotes the 4×4 identity matrix.

Some of the defined 4×4 operator matrices will subsequently be applied to 8×8 matrix objects in Keldysh space. To take this into account we adopt a convention for constructing a 8×8 operator matrix from a 4×4. The idea is the same as we used to find the 4×4 Pauli matrices in (3.13). We will simply repeat the 4×4 matrix on the diagonal block of a 8×8 matrix, i.e. a 4×4 operator matrix $\hat{\mathcal{O}}$ applied to a 8×8 matrix $\check{F}$ is to be understood as

$$\hat{\mathcal{O}}\check{F} = \begin{pmatrix} \hat{\mathcal{O}} & 0 \\ 0 & \hat{\mathcal{O}} \end{pmatrix} \check{F}, \tag{3.16}$$

where the zero elements in this equation are 4×4 zero matrices.

3.3 Equation of Motion

In this section we will derive an equation of motion for the 4-vector ψ and its adjoint $\psi^\dagger$. These relations will be useful for finding the equation of motion for the Green's functions to be introduced later.

The Heisenberg equation of motion for the field operator is

$$\begin{aligned} \mathrm{i}\frac{\partial\psi_\sigma(\boldsymbol{r},t)}{\partial t} &= [\psi_\sigma(\boldsymbol{r},t), H]_- \\ &= [\psi_\sigma(\boldsymbol{r},t), H_0 + H_{\mathrm{imp}}]_- + [\psi_\sigma(\boldsymbol{r},t), H_{\mathrm{sf}}]_- + [\psi_\sigma(\boldsymbol{r},t), H_{\mathrm{int}}]_- . \end{aligned} \tag{3.17}$$

We will consider the three terms on the right of this equation independently, starting with $[\psi_\sigma(\boldsymbol{r},t), H_0 + H_{\mathrm{imp}}]_-$ which is diagonal in the basis we have chosen. The noninteracting particle part H_0 is

$$H_0 = \sum_\sigma \int \mathrm{d}\boldsymbol{r}\psi_\sigma^\dagger(\boldsymbol{r},t)\left[-\frac{1}{2m}\left(\nabla - \mathrm{i}e\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + e\varphi(\boldsymbol{r},t) - \mu\right]\psi_\sigma(\boldsymbol{r},t), \tag{3.18}$$

where we have moved the imaginary unit from the denominator and set $\hbar = 1$. To simplify the notation we will write

$$H_{\mathrm{diag}}(\boldsymbol{r},t) = -\frac{1}{2m}\left(\nabla - \mathrm{i}e\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + e\varphi(\boldsymbol{r},t) - \mu + V_{\mathrm{imp}}(\boldsymbol{r}).$$

This gives

$$\begin{aligned} [\psi_\sigma(\boldsymbol{r},t), H_0 + H_{\mathrm{imp}}]_- &= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}'\left[\psi_\sigma(\boldsymbol{r},t), \psi_{\sigma'}^\dagger(\boldsymbol{r}',t)H_{\mathrm{diag}}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t)\right]_- \\ &= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}'\left\{\left[\psi_\sigma(\boldsymbol{r},t), \psi_{\sigma'}^\dagger(\boldsymbol{r}',t)\right]_+ H_{\mathrm{diag}}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t)\right. \\ &\quad \left. -\psi_{\sigma'}^\dagger(\boldsymbol{r}',t)\left[\psi_\sigma(\boldsymbol{r},t), H_{\mathrm{diag}}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t)\right]_+\right\} \\ &= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}'\left\{\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')H_{\mathrm{diag}}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t)\right. \\ &\quad \left. -\,\psi_{\sigma'}^\dagger(\boldsymbol{r}',t)H_{\mathrm{diag}}(\boldsymbol{r}',t)\underbrace{\left[\psi_\sigma(\boldsymbol{r},t), \psi_{\sigma'}(\boldsymbol{r}',t)\right]_+}_{=0}\right\} \\ &= H_{\mathrm{diag}}(\boldsymbol{r},t)\psi_\sigma(\boldsymbol{r},t). \end{aligned} \tag{3.19}$$

Here we have used the operator identity

$$[A, BC]_- = [A,B]_+ C - B[A,C]_+$$

and the anticommutator relation (3.3).

Next we consider the spin-flip scattering term.

$$\begin{aligned}
[\psi_\sigma(\boldsymbol{r},t), H_{\mathrm{sf}}]_- &= \sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}' \left[\psi_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''} V_{\mathrm{sf}}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t)\right]_- \\
&= \sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}' \Big\{ \left[\psi_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\right]_+ \left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''} V_{\mathrm{sf}}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t) \\
&\quad - \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\psi_\sigma(\boldsymbol{r},t), \left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''} V_{\mathrm{sf}}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t)\right]_+ \Big\} \\
&= \sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}' \big\{ \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''} V_{\mathrm{sf}}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t) \\
&\quad - \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''} V_{\mathrm{sf}}(\boldsymbol{r}') \underbrace{\left[\psi_\sigma(\boldsymbol{r},t), \psi_{\sigma'}(\boldsymbol{r}',t)\right]_+}_{=0} \big\} \\
&= \sum_{\sigma''}\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r})\right]_{\sigma\sigma''} V_{\mathrm{sf}}(\boldsymbol{r})\psi_{\sigma''}(\boldsymbol{r},t).
\end{aligned} \tag{3.20}$$

We now move on to the last term in (3.17). It involves H_{int} for which we will use the form obtained in (3.10).

$$\begin{aligned}
[\psi_\sigma(\boldsymbol{r},t), H_{\mathrm{int}}]_- &= \int \mathrm{d}\boldsymbol{r}' \left[\psi_\sigma(\boldsymbol{r},t), \Delta^*(\boldsymbol{r}',t)\psi_\downarrow(\boldsymbol{r}',t)\psi_\uparrow(\boldsymbol{r}',t) + \Delta(\boldsymbol{r}',t)\psi^\dagger_\uparrow(\boldsymbol{r}',t)\psi^\dagger_\downarrow(\boldsymbol{r}',t)\right]_- \\
&= \int \mathrm{d}\boldsymbol{r}' \{ \underbrace{\left[\psi_\sigma(\boldsymbol{r},t), \psi_\downarrow(\boldsymbol{r}',t)\right]_+}_{=0} \Delta^*(\boldsymbol{r}',t)\psi_\uparrow(\boldsymbol{r}',t) \\
&\quad - \psi_\downarrow(\boldsymbol{r}',t)\Delta^*(\boldsymbol{r}',t) \underbrace{\left[\psi_\sigma(\boldsymbol{r},t), \psi_\uparrow(\boldsymbol{r}',t)\right]_+}_{=0} \\
&\quad + \left[\psi_\sigma(\boldsymbol{r},t), \psi^\dagger_\uparrow(\boldsymbol{r}',t)\right]_+ \Delta(\boldsymbol{r}',t)\psi^\dagger_\downarrow(\boldsymbol{r}',t) \\
&\quad - \psi^\dagger_\uparrow(\boldsymbol{r}',t)\Delta(\boldsymbol{r}',t)\left[\psi_\sigma(\boldsymbol{r},t), \psi^\dagger_\downarrow(\boldsymbol{r}',t)\right]_+ \} \\
&= \int \mathrm{d}\boldsymbol{r}' \left\{ \delta_{\sigma\uparrow}\delta(\boldsymbol{r}-\boldsymbol{r}')\Delta(\boldsymbol{r}',t)\psi^\dagger_\downarrow(\boldsymbol{r}',t) - \psi^\dagger_\uparrow(\boldsymbol{r}',t)\Delta(\boldsymbol{r}',t)\delta_{\sigma\downarrow}\delta(\boldsymbol{r}-\boldsymbol{r}') \right\} \\
&= \delta_{\sigma\uparrow}\Delta(\boldsymbol{r},t)\psi^\dagger_\downarrow(\boldsymbol{r},t) - \delta_{\sigma\downarrow}\Delta(\boldsymbol{r},t)\psi^\dagger_\uparrow(\boldsymbol{r},t).
\end{aligned} \tag{3.21}$$

We have now found all terms in the right-hand side of (3.17) and thus obtained the equation of motion for ψ_σ. Next, we will find the equation of motion for the adjoint field operator $\psi^\dagger_\sigma$. We start as before by considering the Heisenberg equation of motion,[2]

$$\begin{aligned}
\mathrm{i}\frac{\partial\psi^\dagger_\sigma(\boldsymbol{r},t)}{\partial t} &= \left[\psi^\dagger_\sigma(\boldsymbol{r},t), H\right]_- \\
&= \left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_0 + H_{\mathrm{imp}}\right]_- + \left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_{\mathrm{sf}}\right]_- + \left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_{\mathrm{int}}\right]_- .
\end{aligned} \tag{3.22}$$

The calculations of the commutators on the last line are similar to those we needed for

[2] Another way to calculate the equation of motion for the adjoint field operator would be to simply perform the adjungation operation on the previous results. This leads to the same relations as here, but the calculation gives rise to terms involving Dirac delta functions which can be neglected.

Equation (3.17).

$$
\begin{aligned}
\left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_0+H_\text{imp}\right]_- &= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}' \left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t) H_\text{diag}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t)\right]_- \\
&= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}' \{ \underbrace{\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\right]_+}_{=0} H_\text{diag}(\boldsymbol{r}',t)\psi_{\sigma'}(\boldsymbol{r}',t) \\
&\quad - \psi^\dagger_{\sigma'}(\boldsymbol{r}',t) H_\text{diag}(\boldsymbol{r}',t) \underbrace{\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi_{\sigma'}(\boldsymbol{r}',t)\right]_+}_{=\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')} \} \\
&= \sum_{\sigma'}\int \mathrm{d}\boldsymbol{r}' \left\{-\psi^\dagger_{\sigma'}(\boldsymbol{r}',t) H_\text{diag}(\boldsymbol{r}',t)\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')\right\}
\end{aligned}
$$

The operator H_0 in H_diag contains differentiation operators, so that we need to perform partial integrations in order to move these operations to the field operator in the last line. We consider the terms involving differentiation separately,

$$
\begin{aligned}
&\int \mathrm{d}\boldsymbol{r}'\psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[-\frac{1}{2m}\left(\nabla'^2 - \mathrm{i}e\nabla'\boldsymbol{A}(\boldsymbol{r}',t) - \mathrm{i}e\boldsymbol{A}(\boldsymbol{r}',t)\nabla' - e^2\boldsymbol{A}^2(\boldsymbol{r}',t)\right)\right]\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&= \int \mathrm{d}\boldsymbol{r}'\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')\left[-\frac{1}{2m}\left(\nabla'^2 + \mathrm{i}e\nabla'\boldsymbol{A}(\boldsymbol{r}',t) + \mathrm{i}e\boldsymbol{A}(\boldsymbol{r}',t)\nabla' - e^2\boldsymbol{A}^2(\boldsymbol{r}',t)\right)\right]\psi^\dagger_{\sigma'}(\boldsymbol{r}',t) \\
&= \int \mathrm{d}\boldsymbol{r}'\delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')\left[-\frac{1}{2m}\left(\nabla' + \mathrm{i}e\boldsymbol{A}(\boldsymbol{r}',t)\right)^2\right]\psi^\dagger_{\sigma'}(\boldsymbol{r}',t) \qquad (3.23)
\end{aligned}
$$

Thus we see that a change of sign in front of the vector potential $\boldsymbol{A}$ is introduced (this is in correspondence with Equation (4.64) in the textbook by Zagoskin [32]), and the result is

$$
\left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_0+H_\text{imp}\right]_- = -\left[-\frac{1}{2m}\left(\nabla + \mathrm{i}e\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + e\varphi(\boldsymbol{r},t) - \mu + V_\text{imp}(\boldsymbol{r})\right]\psi^\dagger_\sigma(\boldsymbol{r},t). \qquad (3.24)
$$

The next term in (3.22) is

$$
\begin{aligned}
\left[\psi^\dagger_\sigma(\boldsymbol{r},t), H_\text{sf}\right]_- &= \sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}'\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''}V_\text{sf}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t)\right]_- \\
&= \sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}'\{ \underbrace{\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\right]_+}_{=0}\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''}V_\text{sf}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t) \\
&\quad - \psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''}V_\text{sf}(\boldsymbol{r}')\psi_{\sigma''}(\boldsymbol{r}',t)\right]_+ \} \\
&= -\sum_{\sigma'\sigma''}\int \mathrm{d}\boldsymbol{r}'\psi^\dagger_{\sigma'}(\boldsymbol{r}',t)\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r}')\right]_{\sigma'\sigma''}V_\text{sf}(\boldsymbol{r}')\underbrace{\left[\psi^\dagger_\sigma(\boldsymbol{r},t), \psi_{\sigma''}(\boldsymbol{r}',t)\right]_+}_{=\delta_{\sigma\sigma''}\delta(\boldsymbol{r}-\boldsymbol{r}')} \\
&= -\sum_{\sigma'}\psi^\dagger_{\sigma'}(\boldsymbol{r},t)\left[\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S}(\boldsymbol{r})\right]^T_{\sigma\sigma'}V_\text{sf}(\boldsymbol{r}). \qquad (3.25)
\end{aligned}
$$

The last commutator in (3.22) involves the interaction part of the Hamiltonian,

$$\begin{aligned}
\left[\psi_\sigma^\dagger(\boldsymbol{r},t), H_{\text{int}}\right]_- =& \int \mathrm{d}\boldsymbol{r}' \left[\psi_\sigma^\dagger(\boldsymbol{r},t), \Delta^*(\boldsymbol{r}',t)\psi_\downarrow(\boldsymbol{r}',t)\psi_\uparrow(\boldsymbol{r}',t) + \Delta(\boldsymbol{r}',t)\psi_\uparrow^\dagger(\boldsymbol{r}',t)\psi_\downarrow^\dagger(\boldsymbol{r}',t)\right]_- \\
=& \int \mathrm{d}\boldsymbol{r}' \Big\{ \left[\psi_\sigma^\dagger(\boldsymbol{r},t), \psi_\downarrow(\boldsymbol{r}',t)\right]_+ \Delta^*(\boldsymbol{r}',t)\psi_\uparrow(\boldsymbol{r}',t) \\
& - \psi_\downarrow(\boldsymbol{r}',t)\Delta^*(\boldsymbol{r}',t) \left[\psi_\sigma^\dagger(\boldsymbol{r},t), \psi_\uparrow(\boldsymbol{r}',t)\right]_+ \\
& + \underbrace{\left[\psi_\sigma^\dagger(\boldsymbol{r},t), \psi_\uparrow^\dagger(\boldsymbol{r}',t)\right]_+}_{=0} \Delta(\boldsymbol{r}',t)\psi_\downarrow^\dagger(\boldsymbol{r}',t) \\
& - \psi_\uparrow^\dagger(\boldsymbol{r}',t)\Delta(\boldsymbol{r}',t) \underbrace{\left[\psi_\sigma^\dagger(\boldsymbol{r},t), \psi_\downarrow^\dagger(\boldsymbol{r}',t)\right]_+}_{=0} \Big\} \\
=& \int \mathrm{d}\boldsymbol{r}' \left\{\delta_{\sigma\downarrow}\delta(\boldsymbol{r}-\boldsymbol{r}')\Delta^*(\boldsymbol{r}',t)\psi_\downarrow(\boldsymbol{r}',t) - \psi_\downarrow(\boldsymbol{r}',t)\Delta^*(\boldsymbol{r}',t)\delta_{\sigma\uparrow}\delta(\boldsymbol{r}-\boldsymbol{r}')\right\} \\
=& \delta_{\sigma\downarrow}\Delta^*(\boldsymbol{r},t)\psi_\uparrow(\boldsymbol{r},t) - \delta_{\sigma\uparrow}\Delta^*(\boldsymbol{r},t)\psi_\downarrow(\boldsymbol{r},t).
\end{aligned} \tag{3.26}$$

We have now obtained the Heisenberg equation of motion for each of the elements of the 4-vector ψ and our results can be written compactly

$$\boxed{\mathrm{i}\frac{\partial}{\partial t}\hat{\rho}_3\psi(\boldsymbol{r},t) = \hat{H}(\boldsymbol{r},t)\psi(\boldsymbol{r},t),} \tag{3.27}$$

which defines the matrix $\hat{H}$ consisting of the terms

$$\hat{H} = \hat{\xi} + V_{\text{imp}}\hat{1} + \hat{S} + \hat{\Delta}, \tag{3.28}$$

$$\hat{\xi} = -\frac{1}{2m}\left(\nabla - \mathrm{i}e\boldsymbol{A}\hat{\rho}_3\right)^2 + e\varphi\hat{1} - \mu\hat{1}, \tag{3.29}$$

$$\hat{S} = V_{\text{sf}} \begin{pmatrix} \overline{\boldsymbol{\tau}}\cdot\boldsymbol{S} & 0 \\ 0 & [\overline{\boldsymbol{\tau}}\cdot\boldsymbol{S}]^T \end{pmatrix}, \tag{3.30}$$

$$\hat{\Delta} = \begin{pmatrix} 0 & 0 & 0 & \Delta \\ 0 & 0 & -\Delta & 0 \\ 0 & \Delta^* & 0 & 0 \\ -\Delta^* & 0 & 0 & 0 \end{pmatrix}. \tag{3.31}$$

Here we have introduced the matrices $\hat{\xi}$ (diagonal matrix), $\hat{S}$ and $\hat{\Delta}$. The matrix $\hat{\Delta}$ is anti-Hermitean, i.e. $\hat{\Delta}^\dagger = -\hat{\Delta}$.

The vector $\psi^\dagger$ contains the same elements as ψ and we can also write down the equation of motion in this basis. Using the symbols defined above we get

$$\psi^\dagger(\boldsymbol{r},t)\left(-\mathrm{i}\frac{\partial}{\partial t}\hat{\rho}_3\right) = \psi^\dagger(\boldsymbol{r},t)\left(\hat{\xi}^*(\boldsymbol{r},t) + V_{\text{imp}}(\boldsymbol{r},t)\hat{1} + \hat{S}(\boldsymbol{r}) - \hat{\Delta}(\boldsymbol{r},t)\right). \tag{3.32}$$

Care is needed when reading (3.32), because here the differentiation-operators work toward the *left*. To simplify the notation we will use the symbol $\hat{H}^\dagger$ to represent the operator on the right in (3.32), i.e.

$$\hat{H}^\dagger(\boldsymbol{r},t) = \hat{\xi}^*(\boldsymbol{r},t) + V_{\text{imp}}(\boldsymbol{r})\hat{1} + \hat{S}(\boldsymbol{r},t) - \hat{\Delta}(\boldsymbol{r},t), \tag{3.33}$$

so that (3.32) now can be written

$$\boxed{\psi^\dagger(\boldsymbol{r},t)\left(-\mathrm{i}\frac{\partial}{\partial t}\hat{\rho}_3\right) = \psi^\dagger(\boldsymbol{r},t)\hat{H}^\dagger(\boldsymbol{r},t).} \tag{3.34}$$

We have thus found that the equations of motion for $\psi(\boldsymbol{r},t)$ and $\psi^\dagger(\boldsymbol{r},t)$.

3.4 Keldysh Formalism

We will now introduce the Keldysh formalism and define matrices of Green's functions, or more generally one-particle correlation functions in particle-hole space. To simplify the notation we will write $(\boldsymbol{r}_1,t_1) = 1$ etc.

The Green's functions of the Keldysh formalism are defined by the following 2×2 matrices in spin space,

$$\bar{G}^{\mathrm{R}}_{\sigma\sigma'}(1,2) = -\mathrm{i}\Theta(t_1-t_2)\left\langle\left[\psi_\sigma(1),\psi^\dagger_{\sigma'}(2)\right]_+\right\rangle, \tag{3.35a}$$

$$\bar{G}^{\mathrm{A}}_{\sigma\sigma'}(1,2) = \mathrm{i}\Theta(t_2-t_1)\left\langle\left[\psi_\sigma(1),\psi^\dagger_{\sigma'}(2)\right]_+\right\rangle, \tag{3.35b}$$

$$\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(1,2) = -\mathrm{i}\left\langle\left[\psi_\sigma(1),\psi^\dagger_{\sigma'}(2)\right]_-\right\rangle. \tag{3.35c}$$

We have here introduced the Heaviside step function

$$\Theta(t) = \begin{cases} 0 & t<0 \\ 1 & t>0. \end{cases} \tag{3.36}$$

We will refer to the functions (3.35) as the retarded ($\bar{G}^{\mathrm{R}}$), advanced ($\bar{G}^{\mathrm{A}}$) and Keldysh components ($\bar{G}^{\mathrm{K}}$). Note that there is an anticommutator in the retarded and advanced components, but a commutator in the Keldysh component. Likewise we will define the anomalous Green's functions as

$$\bar{F}^{\mathrm{R}}_{\sigma\sigma'}(1,2) = -\mathrm{i}\Theta(t_1-t_2)\left\langle[\psi_\sigma(1),\psi_{\sigma'}(2)]_+\right\rangle, \tag{3.37a}$$

$$\bar{F}^{\mathrm{A}}_{\sigma\sigma'}(1,2) = \mathrm{i}\Theta(t_2-t_1)\left\langle[\psi_\sigma(1),\psi_{\sigma'}(2)]_+\right\rangle, \tag{3.37b}$$

$$\bar{F}^{\mathrm{K}}_{\sigma\sigma'}(1,2) = -\mathrm{i}\left\langle[\psi_\sigma(1),\psi_{\sigma'}(2)]_-\right\rangle. \tag{3.37c}$$

From these functions we may construct 4×4 Green's function matrices in the following way,

$$\hat{G}^{\mathrm{R}}(1,2) = \begin{pmatrix} \bar{G}^{\mathrm{R}}(1,2) & \bar{F}^{\mathrm{R}}(1,2) \\ \left(\bar{F}^{R}\right)^*(1,2) & \left(\bar{G}^{R}\right)^*(1,2) \end{pmatrix}, \tag{3.38a}$$

$$\hat{G}^{\mathrm{A}}(1,2) = \begin{pmatrix} \bar{G}^{\mathrm{A}}(1,2) & \bar{F}^{\mathrm{A}}(1,2) \\ \left(\bar{F}^{A}\right)^*(1,2) & \left(\bar{G}^{A}\right)^*(1,2) \end{pmatrix}, \tag{3.38b}$$

$$\hat{G}^{\mathrm{K}}(1,2) = \begin{pmatrix} \bar{G}^{\mathrm{K}}(1,2) & \bar{F}^{\mathrm{K}}(1,2) \\ -\left(\bar{F}^{K}\right)^*(1,2) & -\left(\bar{G}^{K}\right)^*(1,2) \end{pmatrix}. \tag{3.38c}$$

The detailed structure of these matrices can be found in Appendix B for reference. To make the notation more compact we will collect all of these quantities in one 8×8 Green's function matrix

$$\check{G}(1,2) = \begin{pmatrix} \hat{G}^{\mathrm{R}}(1,2) & \hat{G}^{\mathrm{K}}(1,2) \\ 0 & \hat{G}^{\mathrm{A}}(1,2) \end{pmatrix}. \tag{3.39}$$

This is known as a matrix in Keldysh space.

We will now find an equation of motion which will later be used to determine the Green's functions. Consider first the retarded component using a matrix element representation (see Appendix B),

$$\begin{aligned}
\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3\hat{G}^{\mathrm{R}}(1,2)\right)_{ij} =& \sum_k \mathrm{i}\frac{\partial}{\partial t_1}\left(\hat{\rho}_3\right)_{ik}\left(\hat{G}^{\mathrm{R}}(1,2)\right)_{kj} \\
=& \sum_{kl} \mathrm{i}\frac{\partial}{\partial t_1}\left(\hat{\rho}_3\right)_{ik}\left(-\mathrm{i}\Theta(t_1-t_2)\right)\left(\hat{\rho}_3\right)_{kl}\left\langle\left[\left(\psi(1)\right)_l, \left(\psi^\dagger(2)\right)_j\right]_+\right\rangle \\
=& \sum_{kl} \delta(t_1-t_2)\left(\hat{\rho}_3\right)_{ik}\left(\hat{\rho}_3\right)_{kl}\left\langle\left[\left(\psi(1)\right)_l, \left(\psi^\dagger(2)\right)_j\right]_+\right\rangle \\
&+ \sum_{kl}\left(-\mathrm{i}\Theta(t_1-t_2)\right)\left(\hat{\rho}_3\right)_{kl}\left\langle\left[\mathrm{i}\frac{\partial}{\partial t_1}\left(\hat{\rho}_3\right)_{ik}\left(\psi(1)\right)_l, \left(\psi^\dagger(2)\right)_j\right]_+\right\rangle \\
=& \sum_l \delta(t_1-t_2)\delta_{il}\delta_{lj}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2) \\
&+ \sum_l\left(-\mathrm{i}\Theta(t_1-t_2)\right)\left(\hat{\rho}_3\right)_{ll}\left\langle\left[\left(\hat{H}(1)\right)_{il}\left(\psi(1)\right)_l, \left(\psi^\dagger(2)\right)_j\right]_+\right\rangle \\
=& \delta_{ij}\delta(1-2) + \sum_l\left(\hat{H}(1)\right)_{il}\left(-\mathrm{i}\Theta(t_1-t_2)\right)\left(\hat{\rho}_3\right)_{ll}\left\langle\left[\left(\psi(1)\right)_l, \left(\psi^\dagger(2)\right)_j\right]_+\right\rangle \\
=& \delta_{ij}\delta(1-2) + \left(\hat{H}(1)\hat{G}^{\mathrm{R}}(1,2)\right)_{ij}.
\end{aligned} \tag{3.40}$$

Here we have used the anticommutator relation (3.3), that the matrix $\hat{\rho}_3$ is diagonal and the equation of motion for the 4-vector in (3.27) which in matrix element representation states

$$\sum_l \mathrm{i}\frac{\partial}{\partial t}\left(\hat{\rho}_3\right)_{il}\left(\psi(1)\right)_l = \sum_l\left(\hat{H}(1)\right)_{il}\left(\psi(1)\right)_l. \tag{3.41}$$

The resulting equation of motion is

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1)\right)\hat{G}^{\mathrm{R}}(1,2) = \delta(1-2)\hat{1}. \tag{3.42}$$

$\hat{G}^{\mathrm{A}}(1,2)$ satisfies the same equation. The derivation of this result is similar as for $\hat{G}^{\mathrm{R}}(1,2)$, only the differentiation of the time dependent prefactor differs

$$\mathrm{i}\frac{\partial}{\partial t_1}\mathrm{i}\Theta(t_2-t_1) = -\frac{\partial}{\partial t_1}\left(1-\Theta(t_1-t_2)\right) = \delta(t_1-t_2).$$

This gives

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1)\right)\hat{G}^{\mathrm{A}}(1,2) = \delta(1-2)\hat{1}. \tag{3.43}$$

For the Keldysh component we find by a similar calculation

$$
\begin{aligned}
\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3\hat{G}^{\mathrm{K}}(1,2)\right)_{ij} &= \sum_k \mathrm{i}\frac{\partial}{\partial t_1}(\hat{\rho}_3)_{ik}\left(\hat{G}^{\mathrm{K}}(1,2)\right)_{kj} \\
&= \sum_{kl} \mathrm{i}\frac{\partial}{\partial t_1}(\hat{\rho}_3)_{ik}(-\mathrm{i})(\hat{\rho}_3)_{kl}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_j\right]_-\right\rangle \\
&= \sum_{kl}(-\mathrm{i})(\hat{\rho}_3)_{kl}\left\langle\left[\mathrm{i}\frac{\partial}{\partial t_1}(\hat{\rho}_3)_{ik}\,(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_j\right]_-\right\rangle \\
&= \sum_{l}(-\mathrm{i})(\hat{\rho}_3)_{ll}\left\langle\left[\left(\hat{H}(1)\right)_{il}(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_j\right]_-\right\rangle \\
&= \sum_{l}\left(\hat{H}(1)\right)_{il}(-\mathrm{i})(\hat{\rho}_3)_{ll}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_j\right]_-\right\rangle \\
&= \left(\hat{H}(1)\hat{G}^k(1,2)\right)_{ij},
\end{aligned}
\tag{3.44}
$$

so that the equation of motion becomes

$$
\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1)\right)\hat{G}^{\mathrm{K}}(1,2) = 0. \tag{3.45}
$$

Using these results we can now write down the equation of motion for the Green's functions compactly as (remember that a 4×4 matrix operating on a 8×8 matrix should be understood as an 8×8 matrix with the 4×4 matrix repeated along the diagonal)

$$
\boxed{\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1)\right)\check{G}(1,2) = \delta(1-2)\check{1}.} \tag{3.46}
$$

We will now find the "left-hand" equation of motion for the Green's function. Let operators work toward the *left* and consider

$$
\begin{aligned}
&\left(\hat{G}^{\mathrm{R}}(1,2)\left(-\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3\right)\right)_{ij} = \sum_k\left(\hat{G}^{\mathrm{R}}(1,2)\right)_{ik}(-\mathrm{i})\frac{\partial}{\partial t_2}(\hat{\rho}_3)_{kj} \\
&= \sum_{kl}(-\mathrm{i}\Theta(t_1-t_2))(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_k\right]_+\right\rangle(-\mathrm{i})\frac{\partial}{\partial t_2}(\hat{\rho}_3)_{kj} \\
&= \sum_{kl}\delta(t_2-t_1)(\hat{\rho}_3)_{il}(\hat{\rho}_3)_{kj}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_k\right]_+\right\rangle \\
&\quad+\sum_{kl}(-\mathrm{i}\Theta(t_1-t_2))(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,(-\mathrm{i})\left(\frac{\partial\psi^\dagger(2)}{\partial t_2}\right)_k(\hat{\rho}_3)_{kj}\right]_+\right\rangle \\
&= \sum_{kl}\delta(t_1-t_2)\delta_{ij}\delta_{lk}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2) \\
&\quad+\sum_{kl}(-\mathrm{i}\Theta(t_1-t_2))(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_k\left(\hat{H}^\dagger(2)\right)_{kj}\right]_+\right\rangle \\
&= \delta_{ij}\delta(1-2)+\sum_{kl}(-\mathrm{i}\Theta(t_1-t_2))(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^\dagger(2)\right)_k\right]_+\right\rangle\left(\hat{H}^\dagger(2)\right)_{kj} \\
&= \delta_{ij}\delta(1-2)+\left(\hat{G}^{\mathrm{R}}(1,2)\hat{H}^\dagger(2)\right)_{ij}.
\end{aligned}
\tag{3.47}
$$

The resulting equation of motion is

$$\hat{G}^{\mathrm{R}}(1,2)\left(\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3-\hat{H}(2)\right)^{\dagger}=\delta(1-2)\hat{1}. \tag{3.48}$$

Once again we have used the equal time anticommutator relation and the result (3.32). For the advanced component a similar calculation gives

$$\hat{G}^{\mathrm{A}}(1,2)\left(\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3-\hat{H}(2)\right)^{\dagger}=\delta(1-2)\hat{1}. \tag{3.49}$$

The Keldysh component is a little different since there is no step function. The calculation gives

$$\begin{aligned}\left(\hat{G}^{\mathrm{K}}(1,2)\left(-\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3\right)\right)_{ij} &=\sum_k\left(\hat{G}^{\mathrm{K}}(1,2)\right)_{ik}(-\mathrm{i})\frac{\partial}{\partial t_2}(\hat{\rho}_3)_{kj}\\ &=\sum_{kl}(-\mathrm{i})(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^{\dagger}(2)\right)_k\right]_-\right\rangle(-\mathrm{i})\frac{\partial}{\partial t_2}(\hat{\rho}_3)_{kj}\\ &=\sum_{kl}(-\mathrm{i})(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,(-\mathrm{i})\left(\frac{\partial\psi^{\dagger}(2)}{\partial t_2}\right)_k(\hat{\rho}_3)_{kj}\right]_-\right\rangle\\ &=\sum_{kl}(-\mathrm{i})(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^{\dagger}(2)\right)_k\left(\hat{H}^{\dagger}(2)\right)_{kj}\right]_-\right\rangle\\ &=\sum_{kl}(-\mathrm{i})(\hat{\rho}_3)_{il}\left\langle\left[(\psi(1))_l\,,\left(\psi^{\dagger}(2)\right)_k\right]_-\right\rangle\left(\hat{H}^{\dagger}(2)\right)_{kj}\\ &=\left(\hat{G}^{\mathrm{K}}(1,2)\hat{H}^{\dagger}(2)\right)_{ij},\end{aligned} \tag{3.50}$$

which gives the equation of motion

$$\hat{G}^{\mathrm{K}}(1,2)\left(\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3-\hat{H}(2)\right)^{\dagger}=0. \tag{3.51}$$

These results can be expressed compactly

$$\boxed{\check{G}(1,2)\left(\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3-\hat{H}(2)\right)^{\dagger}=\delta(1-2)\check{1}.} \tag{3.52}$$

The equations of motion for the Green's functions which we have obtained ((3.46) and (3.52)) will in the next chapter be used to find a transport equation.

3.5 Observables

We will now express the superconducting order parameter, Δ, and the (spin) current in terms of the Green's functions. The definition of the order parameter was introduced in Eq. (3.9),

$$\Delta(\boldsymbol{r})=\lambda\left\langle\psi_{\downarrow}(\boldsymbol{r},t)\psi_{\uparrow}(\boldsymbol{r},t)\right\rangle.$$

The Keldysh anomalous Green's function was defined as (3.37c)

$$\bar{F}^{\mathrm{K}}_{\sigma\sigma'}(1,2)=-\mathrm{i}\left\langle\left[\psi_{\sigma}(1),\psi_{\sigma'}(2)\right]_-\right\rangle.$$

Consider the diagonal terms with respect to coordinates (and off-diagonal with respect to spin indexes) of this function

$$\bar{F}^{\mathrm{K}}_{\downarrow\uparrow}(1,1) = -\,\mathrm{i}\left\langle \psi_\downarrow(1)\psi_\uparrow(1) - \psi_\uparrow(1)\psi_\downarrow(1)\right\rangle = -2\mathrm{i}\left\langle \psi_\downarrow(1)\psi_\uparrow(1)\right\rangle, \tag{3.53a}$$

$$\bar{F}^{\mathrm{K}}_{\uparrow\downarrow}(1,1) = -\,\mathrm{i}\left\langle \psi_\uparrow(1)\psi_\downarrow(1) - \psi_\downarrow(1)\psi_\uparrow(1)\right\rangle = 2\mathrm{i}\left\langle \psi_\downarrow(1)\psi_\uparrow(1)\right\rangle. \tag{3.53b}$$

These are the (2,3) and (1,4) components of the 4×4 Keldysh Green's function matrix $\hat{G}^{\mathrm{K}}$ (see Appendix B). We can therefore express the expectation value in (3.9) by[3]

$$-\frac{\mathrm{i}}{4}\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\hat{G}^{\mathrm{K}}(1,1)\right\} = -\frac{\mathrm{i}}{4}\left(-\hat{G}^{\mathrm{K}}_{2,3} + \hat{G}^{\mathrm{K}}_{1,4}\right) = \left\langle \psi_\downarrow(1)\psi_\uparrow(1)\right\rangle, \tag{3.54}$$

so that our expression for the order parameter is

$$\boxed{\Delta(1) = -\frac{\mathrm{i}}{4}\lambda\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\hat{G}^{\mathrm{K}}(1,1)\right\}.} \tag{3.55}$$

We will now consider the electrical current. In quantum mechanics, the current is expressed by

$$\boldsymbol{j} = \frac{e}{m}\Re\left\langle \psi^\dagger\left(\boldsymbol{p} - e\boldsymbol{A}\right)\psi\right\rangle, \tag{3.56}$$

where $\boldsymbol{p}$ is the momentum operator (hermitean). We will now generalize this expression to a spin dependent representation, defining

$$\begin{aligned}
\boldsymbol{j}(1) =& \sum_\sigma \boldsymbol{j}_\sigma(1) = \sum_\sigma \frac{e}{m}\Re\left\langle \psi^\dagger_\sigma(1)\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right]\psi_\sigma(1)\right\rangle \\
=& \sum_\sigma \frac{e}{2m}\left\{\left\langle \psi^\dagger_\sigma(1)\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right]\psi_\sigma(1)\right\rangle + \left\langle \psi^\dagger_\sigma(1)\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right]\psi_\sigma(1)\right\rangle^*\right\} \\
=& \sum_\sigma \frac{e}{2m}\left\{\left\langle \psi^\dagger_\sigma(1)\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right]\psi_\sigma(1)\right\rangle + \left\langle \psi^\dagger_\sigma(1)\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right]^*\psi_\sigma(1)\right\rangle\right\} \\
=& \sum_\sigma \frac{e}{2m}\lim_{1\to 2}\left(\left[\boldsymbol{p}(1) - e\boldsymbol{A}(1)\right] + \left[\boldsymbol{p}(2) - e\boldsymbol{A}(2)\right]^*\right)\left\langle \psi^\dagger_\sigma(2)\psi_\sigma(1)\right\rangle \\
&+ \sum_\sigma \frac{e}{2m}\lim_{1\to 2}\left\langle \left[\boldsymbol{p}(2) - e\boldsymbol{A}(2)\right]\delta(1-2)\right\rangle.
\end{aligned} \tag{3.57}$$

In this calculation we have used the hermitean property of the momentum operator and the anticommutation relation. The term on the last line does not depend on the state of the system and will be neglected. Consider the expectation value on the second last line. It will now be written as an expression involving the Green's functions,

$$\begin{aligned}
\left\langle \psi^\dagger_\sigma(2)\psi_\sigma(1)\right\rangle =& \frac{1}{2}\left\langle \psi^\dagger_\sigma(2)\psi_\sigma(1)\right\rangle + \frac{1}{2}\left\langle \psi^\dagger_\sigma(2)\psi_\sigma(1)\right\rangle \\
=& -\frac{1}{2}\left\langle \psi_\sigma(1)\psi^\dagger_\sigma(2)\right\rangle + \frac{1}{2}\left\langle \delta(1-2)\right\rangle + \frac{1}{2}\left\langle \psi^\dagger_\sigma(2)\psi_\sigma(1)\right\rangle \\
=& \frac{1}{2\mathrm{i}}\bar{G}^{\mathrm{K}}_{\sigma\sigma} + \frac{1}{2}\left\langle \delta(1-2)\right\rangle.
\end{aligned} \tag{3.58}$$

The last term in the result on the lower line will be neglected. Writing out the expression for the impulse operator in coordinate representation and rearranging gives

$$\boldsymbol{j}(1) = -\frac{e}{4m}\mathrm{Tr}\left\{\lim_{1\to 2}\left[\left(\nabla_1 - \mathrm{i}e\boldsymbol{A}(1)\right) - \left(\nabla_2 + \mathrm{i}e\boldsymbol{A}(2)\right)\right]\bar{G}^{\mathrm{K}}(1,2)\right\}. \tag{3.59}$$

[3]The choice of matrices to project out the correct components of $\hat{G}^{\mathrm{K}}$ is of course not unique.

This result can be extended to spin space by omitting the Tr$\{\ldots\}$ operation. The off-diagonal components in the "current matrix" will account for spin-currents. Generalizing also to particle-hole space gives us a 4×4 current matrix with vectors as components,

$$\boxed{\hat{\boldsymbol{\jmath}}(1) = -\frac{e}{4m}\lim_{1\to 2}\left[(\nabla_1 - \mathrm{i}e\boldsymbol{A}(1)) - (\nabla_2 - \mathrm{i}e\boldsymbol{A}(2))\right]\hat{G}^{\mathrm{K}}(1,2).} \tag{3.60}$$

In order to obtain the electronic current from this expression we must multiply with a matrix to extract the components in the upper left block. The electrical current is then given by

$$\boldsymbol{j}(1) = \mathrm{Tr}\left\{\frac{\hat{1}+\hat{\rho}_3}{2}\hat{\boldsymbol{\jmath}}(1)\right\}. \tag{3.61}$$

The expressions obtained here for observables will be extended to the quasiclassical formalism in section 4.3.2.

3.6 Gauge Invariance

We will in this section introduce a gauge transformation which makes the gap of a superconductor (Δ) a real quantity. We will perform a simultaneous $U(1)$ gauge transformation on the field operators ($\psi, \psi^\dagger$) and the electromagnetic fields ($\varphi, \boldsymbol{A}$). The description of our system in terms of these new fields should be completely equivalent since physically observable quantities remain unchanged. Because of the transformations, additional terms will arise in the Hamiltonian. The only terms of the Hamiltonian that are nontrivially changed by the transformations are

$$H_0 = \sum_\sigma \int \mathrm{d}\boldsymbol{r}\psi_\sigma^\dagger(\boldsymbol{r},t)\left[-\frac{1}{2m}\left(\nabla - \mathrm{i}e\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + e\varphi(\boldsymbol{r},t) - \mu\right]\psi_\sigma(\boldsymbol{r},t), \tag{3.62}$$

and

$$H_{\mathrm{int}} = \int \mathrm{d}\boldsymbol{r}\left[\Delta^*(\boldsymbol{r},t)\psi_\downarrow(\boldsymbol{r},t)\psi_\uparrow(\boldsymbol{r},t) + \Delta(\boldsymbol{r},t)\psi_\uparrow^\dagger(\boldsymbol{r},t)\psi_\downarrow^\dagger(\boldsymbol{r},t)\right]. \tag{3.63}$$

The gap can be written

$$\Delta = |\Delta|\mathrm{e}^{\mathrm{i}\phi}, \tag{3.64}$$

where $|\Delta|$ is the absolute value and $\mathrm{e}^{\mathrm{i}\phi}$ the complex phase of Δ. Both quantities may depend on space and time. The transformations we will now consider will remove the phase ϕ leaving Δ as a purely real quantity in the Hamiltonian.

3.6.1 Field Operators

Consider the transformation

$$\begin{aligned}\psi_\sigma &\to \psi'_\sigma = \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}}\psi_\sigma \\ \psi_\sigma^\dagger &\to \psi'^\dagger_\sigma = \mathrm{e}^{\mathrm{i}\frac{\phi}{2}}\psi_\sigma^\dagger.\end{aligned} \tag{3.65}$$

In terms of the 4-vectors this is

$$\begin{aligned}\psi \rightarrow \psi' &= \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\phi}{2}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\phi}{2}} & 0 \\ 0 & 0 & 0 & e^{i\frac{\phi}{2}} \end{pmatrix} \psi \\ \psi^\dagger \rightarrow \psi'^\dagger &= \begin{pmatrix} e^{i\frac{\phi}{2}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\phi}{2}} & 0 & 0 \\ 0 & 0 & e^{-i\frac{\phi}{2}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\phi}{2}} \end{pmatrix} \psi^\dagger.\end{aligned} \tag{3.66}$$

We will now introduce the transformed quantities into the Hamiltonian, starting with the BCS mean field interaction part H_{int},

$$\begin{aligned} H_{\text{int}} &= \int d\boldsymbol{r} \left\{ |\Delta| e^{-i\phi} e^{i\frac{\phi}{2}} \psi'_\downarrow e^{i\frac{\phi}{2}} \psi'_\uparrow + |\Delta| e^{i\phi} e^{-i\frac{\phi}{2}} \psi'^\dagger_\downarrow e^{-i\frac{\phi}{2}} \psi'^\dagger_\uparrow \right\} \\ &= \int d\boldsymbol{r} \left\{ |\Delta| \psi'_\downarrow \psi'_\uparrow + |\Delta| \psi'^\dagger_\uparrow \psi'^\dagger_\downarrow \right\}. \end{aligned} \tag{3.67}$$

This calculation also shows how the complex part of Δ is removed from the calculations, making the gap purely real and positive in the Hamiltonian.

When we substitute the transformed quantities into the noninteracting particle part H_0 we will get additional terms in the Hamiltonian because of the derivatives with respect to ψ. For these calculations we will need the relations

$$\nabla \left(e^{i\frac{\phi}{2}} \psi'_\sigma \right) = e^{i\frac{\phi}{2}} \left[\frac{i}{2}(\nabla\phi) + \nabla \right] \psi'_\sigma, \tag{3.68}$$

$$\nabla^2 \left(e^{i\frac{\phi}{2}} \psi'_\sigma \right) = e^{i\frac{\phi}{2}} \left[-\frac{1}{4} (\nabla\phi)^2 + i(\nabla\phi)\cdot\nabla + \frac{i}{2} \left(\nabla^2\phi\right) + \nabla^2 \right] \psi'_\sigma. \tag{3.69}$$

The momentum operator part in (3.62) is

$$(\nabla - ie\boldsymbol{A})^2 = \nabla^2 - ie\nabla\cdot\boldsymbol{A} - ie\boldsymbol{A}\cdot\nabla - e^2\boldsymbol{A}^2. \tag{3.70}$$

We will now calculate the expressions involving these operators in the transformed fields. Consider first the term containing the operator ∇^2 (the factor $-\frac{1}{2m}$ has been omitted here)

$$\sum_\sigma \int d\boldsymbol{r} \psi^\dagger_\sigma \nabla^2 \psi_\sigma = \sum_\sigma \int d\boldsymbol{r} e^{-i\frac{\phi}{2}} \psi'^\dagger_\sigma \nabla^2 e^{i\frac{\phi}{2}} \psi'_\sigma \tag{3.71}$$

$$= \sum_\sigma \int d\boldsymbol{r} \psi'^\dagger_\sigma \left[-\frac{1}{4} (\nabla\phi)^2 + i(\nabla\phi)\cdot\nabla + \frac{i}{2} \left(\nabla^2\phi\right) + \nabla^2 \right] \psi'_\sigma. \tag{3.72}$$

Consider next the second and third terms in (3.70).

$$
\begin{aligned}
&\sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi^\dagger_\sigma \left[-\mathrm{i}e\nabla\cdot\boldsymbol{A} - \mathrm{i}e\boldsymbol{A}\cdot\nabla\right]\psi_\sigma \\
&= \sum_\sigma \int \mathrm{d}\boldsymbol{r} \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}} \psi'^\dagger_\sigma \left[-\mathrm{i}e\nabla\cdot\boldsymbol{A} - \mathrm{i}e\boldsymbol{A}\cdot\nabla\right] \mathrm{e}^{\mathrm{i}\frac{\phi}{2}} \psi'_\sigma \\
&= \sum_\sigma \int \mathrm{d}\boldsymbol{r} \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}} \psi'^\dagger_\sigma \left[-\mathrm{i}e(\nabla\cdot\boldsymbol{A}) - 2\mathrm{i}e\boldsymbol{A}\cdot\nabla\right] \mathrm{e}^{\mathrm{i}\frac{\phi}{2}} \psi'_\sigma \\
&= \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi'^\dagger_\sigma \left[-\mathrm{i}e(\nabla\cdot\boldsymbol{A}) - 2\mathrm{i}e\boldsymbol{A}\left(\frac{\mathrm{i}}{2}(\nabla\phi) + \nabla\right)\right] \psi'_\sigma \\
&= \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi'^\dagger_\sigma \left[-\mathrm{i}e\nabla\cdot\boldsymbol{A} - \mathrm{i}e\boldsymbol{A}\cdot\nabla\right]\psi'_\sigma + \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi'^\dagger_\sigma e\boldsymbol{A}\cdot(\nabla\phi)\psi'_\sigma.
\end{aligned}
\tag{3.73}
$$

The last term here is introduced by the transformation. The last term in (3.70) will not give rise to new terms in the transformed basis because it is a scalar and commutes with the phase prefactors giving immediate cancellation.

We can now write down the Hamiltonian in the transformed basis

$$
H_0 + H_{\mathrm{int}} = \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi'^\dagger_\sigma \left[-\frac{1}{2m}\left(\nabla - \mathrm{i}e\boldsymbol{A}\right)^2 + e\varphi - \mu\right]\psi'_\sigma + \int \mathrm{d}\boldsymbol{r} \left[|\Delta|\psi'_\downarrow\psi'_\uparrow + |\Delta|\psi'^\dagger_\uparrow\psi'^\dagger_\downarrow\right] \tag{3.74a}
$$

$$
+ \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi'^\dagger_\sigma \left[-\frac{1}{2m}\left\{-\frac{1}{4}(\nabla\phi)^2 + \mathrm{i}(\nabla\phi)\cdot\nabla + \frac{\mathrm{i}}{2}\left(\nabla^2\phi\right) + e\boldsymbol{A}\cdot(\nabla\phi)\right\}\right]\psi'_\sigma. \tag{3.74b}
$$

The last line contains the new terms introduced by the gauge transformation. These terms will be canceled when we also transform the electromagnetic field, which is done in the next section.

3.6.2 Electromagnetic Field

We will make use of the gauge invariance of the electromagnetic fields. This allows us to introduce new fields according to

$$
\begin{aligned}
e\varphi \to & e\varphi' = e\varphi + \frac{1}{2}\dot{\phi}, \\
e\boldsymbol{A} \to & e\boldsymbol{A}' = e\boldsymbol{A} - \frac{1}{2}(\nabla\phi).
\end{aligned}
\tag{3.75}
$$

The terms in the Hamiltonian that will be changed by this transformation is H_0 and some of the terms in (3.74b). Let us first see what happens to the original expression for H_0,

$$\begin{aligned}
H_0 =& \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger \left[-\frac{1}{2m} \left(\nabla - \mathrm{i}e\boldsymbol{A}\right)^2 + e\varphi - \mu \right] \psi_\sigma \\
=& \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger \left\{ -\frac{1}{2m} \left(\nabla - \mathrm{i} \left[\frac{1}{2}(\nabla\phi) + e\boldsymbol{A}' \right] \right)^2 - \frac{1}{2}\dot{\phi} + e\varphi' - \mu \right\} \psi_\sigma \\
=& \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger \left[-\frac{1}{2m} \left(\nabla - \mathrm{i}e\boldsymbol{A}'\right)^2 + e\varphi' - \mu \right] \psi_\sigma \\
&+ \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma^\dagger \left[-\frac{1}{2m} \left(-\mathrm{i}(\nabla\phi)\cdot\nabla - \frac{\mathrm{i}}{2}\left(\nabla^2\phi\right) - \frac{1}{4}(\nabla\phi)^2 - e\boldsymbol{A}'\cdot(\nabla\phi) \right) - \frac{1}{2}\dot{\phi} \right] \psi_\sigma .
\end{aligned} \tag{3.76}$$

The last line are new terms introduced by the transformation, and comparison with (3.74b) reveals that most of them will cancel out of the total expression. But we must also introduce the transformed electromagnetic fields in the new terms from transformation of the electron fields,

$$\begin{aligned}
&\sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma'^\dagger \left[-\frac{1}{2m} \left\{ -\frac{1}{4}(\nabla\phi)^2 + \mathrm{i}(\nabla\phi)\cdot\nabla + \frac{\mathrm{i}}{2}\left(\nabla^2\phi\right) + e\boldsymbol{A}\cdot(\nabla\phi) \right\} \right] \psi_\sigma' \\
=& \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma'^\dagger \left[-\frac{1}{2m} \left\{ -\frac{1}{4}(\nabla\phi)^2 + \mathrm{i}(\nabla\phi)\cdot\nabla + \frac{\mathrm{i}}{2}\left(\nabla^2\phi\right) + (e\boldsymbol{A}' + \frac{1}{2}(\nabla\phi))\cdot(\nabla\phi) \right\} \right] \psi_\sigma' .
\end{aligned} \tag{3.77}$$

We have now first transformed the field operators and then the electromagnetic fields. The order of these transformations is of course irrelevant, as a small calculation would show. The results of the transformations are collected in the next section.

3.6.3 Transformed Hamiltonian

The Hamiltonian given by the transformed field operators (3.65) and electromagnetic fields (3.75) can now be found by collecting the results from the last two sections. Most of the new terms will cancel, and now the gap enters as a real quantity

$$H_0 + H_{\mathrm{int}} = \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma'^\dagger \left[-\frac{1}{2m} \left(\nabla - \mathrm{i}e\boldsymbol{A}'\right)^2 + e\varphi' - \frac{1}{2}\dot{\phi} - \mu \right] \psi' \tag{3.78}$$

$$+ \int \mathrm{d}\boldsymbol{r} \left\{ |\Delta| \psi_\downarrow' \psi_\uparrow' + |\Delta| \psi_\uparrow'^\dagger \psi_\downarrow'^\dagger \right\} . \tag{3.79}$$

The combinations of potentials and derivatives of phase which appear here accommodates a physical interpretation. Following Schmid [38] we can define the quantity $\boldsymbol{v}_\mathrm{s}$ by

$$m\boldsymbol{v}_\mathrm{s} = -e\boldsymbol{A}' = \frac{1}{2}(\nabla\phi) - e\boldsymbol{A}, \tag{3.80}$$

which allows us to write the two terms of the Hamiltonian we have been discussing as

$$\begin{aligned}
H_0 + H_{\mathrm{int}} =& \sum_\sigma \int \mathrm{d}\boldsymbol{r} \psi_\sigma'^\dagger \left[-\frac{1}{2m} \left(\nabla + \mathrm{i}m\boldsymbol{v}_s\right)^2 + e\varphi' - \left(\mu + \frac{1}{2}\dot{\phi} \right) \right] \psi' \\
&+ \int \mathrm{d}\boldsymbol{r} \left\{ |\Delta| \psi_\downarrow' \psi_\uparrow' + |\Delta| \psi_\uparrow'^\dagger \psi_\downarrow'^\dagger \right\} .
\end{aligned} \tag{3.81}$$

Comparison with Ginzburg-Landau theory shows that $\boldsymbol{v}_\mathrm{s}$ is the superfluid velocity [39]. The quantity $-\dot{\phi}/2$ can be considered as the chemical potential of the Cooper pairs (per particle) (see Equation (6-45a) in the book by Tinkham [6]).

In the following we will use the gauge which has been introduced in this section, i.e. the gap is a real quantity. The relations obtained earlier in this chapter are then valid by putting $e\varphi \to e\varphi' - \frac{1}{2}\dot{\phi}$, $e\boldsymbol{A} \to -m\boldsymbol{v}_s$ (the validity of the expression for current is checked below). We will not always use this notation, but instead continue using the original expression for the Hamiltonian where the mentioned substitutions are to be understood implicitly.

Current in Transformed Fields

The electrical current was defined in (3.56). Let us now introduce the transformations (3.65) and (3.75) in the expression for current carried by spins σ,

$$\begin{aligned}
\boldsymbol{j}_\sigma =& \frac{e}{m}\Re\left\langle \psi_\sigma^\dagger \left(\frac{\nabla}{\mathrm{i}} - e\boldsymbol{A}\right)\psi_\sigma \right\rangle \\
=& \frac{e}{m}\Re\left\langle \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}}\psi_\sigma'^\dagger \left(\frac{\nabla}{\mathrm{i}} - e\boldsymbol{A}'\right)\mathrm{e}^{\mathrm{i}\frac{\phi}{2}}\psi_\sigma' - \frac{1}{2}(\nabla\phi)\psi_\sigma'^\dagger\psi_\sigma' \right\rangle \\
=& \frac{e}{m}\Re\left\langle \psi_\sigma'^\dagger \left(\frac{\nabla}{\mathrm{i}} - e\boldsymbol{A}'\right)\psi_\sigma' + \frac{1}{2}(\nabla\phi)\psi_\sigma'^\dagger\psi_\sigma' - \frac{1}{2}(\nabla\phi)\psi_\sigma'^\dagger\psi_\sigma' \right\rangle \\
=& \frac{e}{m}\Re\left\langle \psi_\sigma'^\dagger \left(\frac{\nabla}{\mathrm{i}} - e\boldsymbol{A}'\right)\psi_\sigma' \right\rangle .
\end{aligned} \tag{3.82}$$

Thus we see that the expression for the current is invariant since it looks completely similar in the transformed fields. However, the quantity $\boldsymbol{A}'$ now has special meaning and carries the contribution from supercurrent.

Chapter 4

Transport Equations

Using the formalism developed so far we will derive transport equations for the system we are considering. We will use the quasiclassical approximation and consider the limit of high impurity concentration. These steps will simplify the diffusion equation considerably, and allows for a simpler parameterization of the Green's functions. Substituting the parameterized Green's function into the diffusion equations gives transport equations.

4.1 Mixed Representation

We will in this section introduce the mixed or Wigner representation. This means that we shift the frame of reference to the center-of-mass system defined by variables

$$\begin{aligned} \boldsymbol{R} &= \tfrac{1}{2}\left(\boldsymbol{r}_1 + \boldsymbol{r}_2\right), \qquad & T &= \tfrac{1}{2}\left(t_1 + t_2\right) \\ \boldsymbol{r} &= \boldsymbol{r}_1 - \boldsymbol{r}_2, & t &= t_1 - t_2. \end{aligned} \tag{4.1}$$

In the original coordinates we have

$$\begin{aligned} \boldsymbol{r}_1 &= \boldsymbol{R} + \tfrac{\boldsymbol{r}}{2} \quad ; \quad t_1 = T + \tfrac{t}{2} \\ \boldsymbol{r}_2 &= \boldsymbol{R} - \tfrac{\boldsymbol{r}}{2} \quad ; \quad t_2 = T - \tfrac{t}{2}, \end{aligned} \tag{4.2}$$

so that the Green's function can be written

$$\check{G}(1,2) = \check{G}(\boldsymbol{r}_1, t_1, \boldsymbol{r}_2, t_2) = \check{G}(\boldsymbol{R} + \frac{\boldsymbol{r}}{2}, T + \frac{t}{2}, \boldsymbol{R} - \frac{\boldsymbol{r}}{2}, T - \frac{t}{2}). \tag{4.3}$$

Fourier transforming with respect to the relative coordinates $\boldsymbol{r}$ and t gives

$$\check{G}(\boldsymbol{R}, T, \boldsymbol{p}, E) = \int \mathrm{d}\boldsymbol{r} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} \int \mathrm{d}t \mathrm{e}^{+\mathrm{i}tE} \check{G}(\boldsymbol{R} + \frac{\boldsymbol{r}}{2}, T + \frac{t}{2}, \boldsymbol{R} - \frac{\boldsymbol{r}}{2}, T - \frac{t}{2}). \tag{4.4a}$$

The inverse transformation is

$$\check{G}(\boldsymbol{R} + \frac{\boldsymbol{r}}{2}, T + \frac{t}{2}, \boldsymbol{R} - \frac{\boldsymbol{r}}{2}, T - \frac{t}{2}) = \frac{1}{(2\pi)^4} \int \mathrm{d}\boldsymbol{p} \mathrm{e}^{+\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{p}} \int \mathrm{d}t \mathrm{e}^{-\mathrm{i}Et} \check{G}(\boldsymbol{R}, T, \boldsymbol{p}, E). \tag{4.4b}$$

To make the notation more compact we will also introduce a space-time 4-vector notation by

$$\begin{aligned} X &= (\boldsymbol{R}, T), \qquad x = (\boldsymbol{r}, t) \\ p &= (\boldsymbol{p}, E). \end{aligned} \tag{4.5}$$

We will also write

$$px = -Et + \boldsymbol{p} \cdot \boldsymbol{r} \tag{4.6}$$

in close analogy to the covariant/contravariant vector formulation of field theory. The Fourier transform (4.4) can now be written

$$\check{G}(X,p) = \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \check{G}(X + \frac{x}{2}, X - \frac{x}{2}), \tag{4.7a}$$

with inverse transformation

$$\check{G}(X + \frac{x}{2}, X - \frac{x}{2}) = \frac{1}{(2\pi)^4} \int \mathrm{d}p \mathrm{e}^{+\mathrm{i}px} \check{G}(X,p). \tag{4.7b}$$

The mixed representation allows us integrate out the rapidly oscillating part of the Green's functions, as we will see later in this chapter.

4.2 Kinetic Equations

We will in this chapter obtain the kinetic equation for the superconductor. To this end we now form the difference between the equations of motion for the Green's functions. Some of the momentum-dependent terms will then cancel. The resulting equation is

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{H}(1) \right) \check{G}(1,2) - \check{G}(1,2) \left(\mathrm{i}\frac{\partial}{\partial t_2}\hat{\rho}_3 - \hat{H}(2) \right)^{\dagger} = 0, \tag{4.8a}$$

where the terms on the left side will be treated separately,

$$\begin{aligned}
&\mathrm{i}\hat{\rho}_3 \frac{\partial \check{G}(1,2)}{\partial t_1} + \frac{\partial \check{G}(1,2)}{\partial t_2} \mathrm{i}\hat{\rho}_3, && (4.8b)\\
&- \hat{\xi}(1)\check{G}(1,2) + \check{G}(1,2)\hat{\xi}^*(2), && (4.8c)\\
&- V_{\mathrm{imp}}(1)\check{G}(1,2) + \check{G}(1,2)V_{\mathrm{imp}}(2), && (4.8d)\\
&- \hat{S}(1)\check{G}(1,2) + \check{G}(1,2)\hat{S}(2), && (4.8e)\\
&- \hat{\Delta}(1)\check{G}(1,2) - \check{G}(1,2)\hat{\Delta}(2). && (4.8f)
\end{aligned}$$

The differentiations with respect to time are contained in (4.8b). In the mixed representation the differentiations become

$$\begin{aligned}
\frac{\partial}{\partial t_1} &= \frac{\partial}{\partial t} + \frac{1}{2}\frac{\partial}{\partial T}, \\
\frac{\partial}{\partial t_2} &= -\frac{\partial}{\partial t} + \frac{1}{2}\frac{\partial}{\partial T}
\end{aligned} \tag{4.9}$$

Using these results and Fourier transforming, this term becomes

$$\begin{aligned}
&\int \mathrm{d}x\mathrm{e}^{-\mathrm{i}px}\left\{\mathrm{i}\hat{\rho}_3\left(\frac{\partial}{\partial t}+\frac{1}{2}\frac{\partial}{\partial T}\right)\check{G}(1,2)+\left(-\frac{\partial}{\partial t}+\frac{1}{2}\frac{\partial}{\partial T}\right)\check{G}(1,2)\mathrm{i}\hat{\rho}_3\right\}\\
=&-(\mathrm{i}E)\mathrm{i}\hat{\rho}_3\int \mathrm{d}x\mathrm{e}^{-\mathrm{i}px}\check{G}(1,2)+\frac{1}{2}\frac{\partial}{\partial T}\mathrm{i}\hat{\rho}_3\int \mathrm{d}x\mathrm{e}^{-\mathrm{i}px}\check{G}(1,2)\\
&+(\mathrm{i}E)\int \mathrm{d}x\mathrm{e}^{-\mathrm{i}px}\check{G}(1,2)\mathrm{i}\hat{\rho}_3+\frac{1}{2}\frac{\partial}{\partial T}\int \mathrm{d}x\mathrm{e}^{-\mathrm{i}px}\check{G}(1,2)\mathrm{i}\hat{\rho}_3\\
=&E\hat{\rho}_3\check{G}(X,p)+\frac{1}{2}\frac{\partial}{\partial T}\mathrm{i}\hat{\rho}_3\check{G}(X,p)-\check{G}(X,p)E\hat{\rho}_3+\frac{1}{2}\frac{\partial}{\partial T}\check{G}(X,p)\mathrm{i}\hat{\rho}_3\\
=&\left[E\hat{\rho}_3,\check{G}(X,p)\right]_-+\frac{1}{2}\mathrm{i}\left[\hat{\rho}_3,\frac{\partial\check{G}(X,p)}{\partial T}\right]_+ .
\end{aligned}\tag{4.10}$$

We will now introduce the "star product" of two functions A and B,

$$A\otimes B(X,p)=\mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B}-\partial_{p_A}\partial_{X_B}\right)/2}A(X,p)B(X,p).\tag{4.11}$$

This formalism will simplify the notation considerably, and the star-product is discussed in more detail in Appendix D. The terms in (4.10) can now be rewritten as

$$\left[E\hat{\rho}_3,\check{G}(X,p)\right]_-+\frac{1}{2}\mathrm{i}\left[\hat{\rho}_3,\frac{\partial\check{G}(X,p)}{\partial T}\right]_+=\left[E\hat{\rho}_3\stackrel{\otimes}{,}\check{G}\right]_- .\tag{4.12}$$

Here we have introduced notation for commutator involving star product, $\left[A\stackrel{\otimes}{,}B\right]_-=A\otimes B-B\otimes A$ etc.

When considering (4.8c) we must keep in mind that the operators in ξ^* are meant to work toward the left, i.e.

$$\begin{aligned}
\check{G}(1,2)\xi^*(2)=-\frac{1}{2m}&\left[\left(\nabla_2^2\check{G}(1,2)\right)+\mathrm{i}e\left(\nabla_2\check{G}(1,2)\right)\boldsymbol{A}(2)\hat{\rho}_3+\mathrm{i}e\nabla_2\left(\check{G}(1,2)\boldsymbol{A}(2)\right)\hat{\rho}_3\right.\\
&\left.-e^2\boldsymbol{A}^2(2)\check{G}(1,2)\right]+e\varphi(2)\check{G}(1,2)-\mu\check{G}(1,2).
\end{aligned}\tag{4.13}$$

The terms in (4.8c) now become

$$\frac{1}{2m}\left(\nabla_1^2-\nabla_2^2\right)\check{G}(1,2)\tag{4.14a}$$

$$+\frac{1}{2m}\left(-e^2\boldsymbol{A}^2(1)+e^2\boldsymbol{A}^2(2)\right)\check{G}(1,2)+\left(-e\varphi(1)+e\varphi(2)\right)\check{G}(1,2)\tag{4.14b}$$

$$+\frac{1}{2m}\left[-\mathrm{i}e\nabla_1\left(\boldsymbol{A}(1)\hat{\rho}_3\check{G}(1,2)\right)-\mathrm{i}e\nabla_2\left(\check{G}(1,2)\hat{\rho}_3\boldsymbol{A}(2)\right)\right]\tag{4.14c}$$

$$+\frac{1}{2m}\left[-\mathrm{i}e\boldsymbol{A}(1)\left(\nabla_1\hat{\rho}_3\check{G}(1,2)\right)-\mathrm{i}e\boldsymbol{A}(2)\left(\nabla_2\check{G}(1,2)\hat{\rho}_3\right)\right]\tag{4.14d}$$

The differentiation operators in the mixed representation are

$$\begin{aligned}
\nabla_1&=\nabla_{\boldsymbol{r}}+\frac{1}{2}\nabla_{\boldsymbol{R}}\\
\nabla_2&=-\nabla_{\boldsymbol{r}}+\frac{1}{2}\nabla_{\boldsymbol{R}},
\end{aligned}$$

so that the Fourier transform of the terms in (4.14a) becomes

$$
\begin{aligned}
&\frac{1}{2m}\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px}\left(\nabla_1^2-\nabla_2^2\right)\check{G}(1,2) \\
&=\frac{1}{2m}\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px}\left[\left(\nabla_{\boldsymbol{r}}+\frac{1}{2}\nabla_{\boldsymbol{R}}\right)^2-\left(-\nabla_{\boldsymbol{r}}+\frac{1}{2}\nabla_{\boldsymbol{R}}\right)^2\right]\check{G}(1,2) \\
&=\frac{1}{2m}\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px}\left[2\nabla_{\boldsymbol{R}}\nabla_{\boldsymbol{r}}\right]\check{G}(1,2) \\
&=\frac{1}{m}\nabla_{\boldsymbol{R}}\mathrm{i}\boldsymbol{p}\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px}\check{G}\left(X+\frac{x}{2},X-\frac{x}{2}\right) \\
&=\mathrm{i}\frac{\boldsymbol{p}}{m}\nabla_{\boldsymbol{R}}\check{G}(X,p), \qquad (4.15)
\end{aligned}
$$

where we have performed a partial integration in the $\boldsymbol{r}$ variable.

When we Fourier transform the remaining terms we may rewrite to the form of star-products and use the formulas derived in Appendix D. The terms in (4.14b) become

$$
\begin{aligned}
&\frac{e^2}{2m}\left(-\boldsymbol{A}^2\otimes\check{G}(X,p)+\check{G}\otimes\boldsymbol{A}^2(X,p)\right) \\
&=\frac{e^2}{2m}\left(-\mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_G}\right)/2}\boldsymbol{A}^2(X)\check{G}(X,p)+\mathrm{e}^{-\mathrm{i}\left(\partial_{p_G}\partial_{X_A}\right)/2}\check{G}(X,p)\boldsymbol{A}^2(X)\right), \qquad (4.16)
\end{aligned}
$$

and

$$
\begin{aligned}
&-e\varphi\otimes\check{G}(X,p)+\check{G}\otimes e\varphi(X,p) \\
&=-e\mathrm{e}^{\mathrm{i}\left(\partial_{X_\varphi}\partial_{p_G}\right)/2}\varphi(X)\check{G}(X,p)+e\mathrm{e}^{-\mathrm{i}\left(\partial_{p_G}\partial_{X_\varphi}\right)/2}\check{G}(X,p)\varphi(X), \qquad (4.17)
\end{aligned}
$$

and for clarity we will keep the star product notation. Terms containing divergences of $\boldsymbol{A}$ are covered by special cases of the star product (see Appendix D). Fourier transforming the terms in (4.14c) we get the following forms

$$
\begin{aligned}
\left[\nabla\cdot\boldsymbol{A}\right]\otimes\left[\hat{\rho}_3\check{G}\right](X,p) &=\mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_G}\right)/2}\left[\nabla_{\boldsymbol{R}}\cdot\boldsymbol{A}(X)\right]\hat{\rho}_3\check{G}(X,p), \qquad (4.18)\\
\left[\check{G}\hat{\rho}_3\right]\otimes\left[\nabla\cdot\boldsymbol{A}\right](X,p) &=\mathrm{e}^{-\mathrm{i}\left(\partial_{p_G}\partial_{X_A}\right)/2}\check{G}(X,p)\hat{\rho}_3\left[\nabla_{\boldsymbol{R}}\cdot\boldsymbol{A}(X)\right]. \qquad (4.19)
\end{aligned}
$$

Derivatives with respect to $\check{G}$ are of the following form,

$$
\begin{aligned}
\boldsymbol{A}\otimes\left[\hat{\rho}_3\nabla_1\check{G}\right](X,p) &=\mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_G}\right)/2}\boldsymbol{A}(X)\left(\mathrm{i}\boldsymbol{p}\hat{\rho}_3\check{G}(X,p)+\frac{1}{2}\nabla_{\boldsymbol{R}}\hat{\rho}_3\check{G}(X,p)\right) \\
&=\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{A}\hat{\rho}_3\otimes\check{G}+\frac{1}{2}\boldsymbol{A}\hat{\rho}_3\otimes\nabla_{\boldsymbol{R}}\check{G}, \qquad (4.20)
\end{aligned}
$$

$$
\begin{aligned}
\left[\nabla_2\check{G}\hat{\rho}_3\right]\otimes\boldsymbol{A}(X,p) &=\mathrm{e}^{-\mathrm{i}\left(\partial_{p_G}\partial_{X_A}\right)/2}\left(-\mathrm{i}\boldsymbol{p}\check{G}(X,p)\hat{\rho}_3+\frac{1}{2}\nabla_{\boldsymbol{R}}\check{G}(X,p)\hat{\rho}_3\right)A(X) \\
&=-\mathrm{i}\boldsymbol{p}\check{G}\otimes\boldsymbol{A}\hat{\rho}_3+\frac{1}{2}\nabla_{\boldsymbol{R}}\check{G}\otimes\boldsymbol{A}\hat{\rho}_3. \qquad (4.21)
\end{aligned}
$$

Altogether the terms in (4.8c) become

$$
\begin{aligned}
&\mathrm{i}\frac{\boldsymbol{p}}{m}\nabla_{\boldsymbol{R}}\check{G}(X,p)-\mathrm{i}\frac{\boldsymbol{p}}{m}\left[\mathrm{i}e\boldsymbol{A}\hat{\rho}_3\overset{\otimes}{,}\check{G}\right]_- -\left[e\varphi\overset{\otimes}{,}\check{G}\right]_- -\frac{1}{2m}\left[e^2\boldsymbol{A}^2\overset{\otimes}{,}\check{G}\right]_- \\
&\quad-\frac{1}{2m}\left[\mathrm{i}e\left(\nabla_{\boldsymbol{R}}\boldsymbol{A}\right)\hat{\rho}_3\overset{\otimes}{,}\check{G}\right]_- -\frac{1}{2m}\left[\mathrm{i}e\boldsymbol{A}\hat{\rho}_3\overset{\otimes}{,}\left(\nabla_{\boldsymbol{R}}\check{G}\right)\right]_+. \qquad (4.22)
\end{aligned}
$$

The remaining terms (4.8d)-(4.8f) are (star product is associative)

$$-\left[V_{\text{imp}} + \hat{S} + \hat{\Delta} \overset{\otimes}{,} \check{G}\right]_{-}. \tag{4.23}$$

Now we define the symbol $\hat{\boldsymbol{\partial}} = \nabla_{\boldsymbol{R}}\hat{1} - \mathrm{i}e\boldsymbol{A}(X)\hat{\rho}_3$[1] for the gauge-invariant derivative. We can then write (4.8a) compactly[2,3]

$$\left[E\hat{\rho}_3 + \mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_{\text{imp}}\hat{1} - \hat{S} - \hat{\Delta} \overset{\otimes}{,} \check{G}\right]_{-} \tag{4.24a}$$

$$-\frac{1}{2m}\left[e^2\boldsymbol{A}^2 + \mathrm{i}e\left(\nabla_{\boldsymbol{R}}\boldsymbol{A}\right)\hat{\rho}_3 \overset{\otimes}{,} \check{G}\right]_{-} - \frac{1}{2m}\left[\mathrm{i}e\boldsymbol{A}\hat{\rho}_3 \overset{\otimes}{,} \left(\nabla_{\boldsymbol{R}}\check{G}\right)\right]_{+} = 0. \tag{4.24b}$$

We have now obtained an equation of motion for the Green's function in terms of star products. This equation is sometimes named the Eilenberger equation in the literature. It is a convenient starting point for approximations.

4.3 Approximations

In the last section we obtained an equation of motion for the Green's function matrix in the form of star-products[4]. No approximations have been introduced so far, so this equation is exact although very complicated. We will now perform some approximations to bring the equation to a form better suited for calculations.

The occurrence of the operator $\hat{\boldsymbol{\partial}} = \nabla\hat{1} - \mathrm{i}e\boldsymbol{A}\hat{\rho}_3$ in (4.24) implies that ∇ and $e\boldsymbol{A}$ are terms of the same order $\sim \frac{1}{L}$, where L is some length scale. This means that the order of the term $\frac{e^2\boldsymbol{A}^2}{2m} \sim \frac{1}{m}\frac{1}{L^2}$. The order of the term $\mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}} \sim \frac{1}{\lambda_{\mathrm{F}} m}\frac{1}{L}$ in the quasiclassical approximation[5]. Here we are considering systems where $\lambda_{\mathrm{F}} \ll L$, therefore $\frac{e^2\boldsymbol{A}^2}{2m} \ll \mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}}$. The terms $\frac{\mathrm{i}e}{2m}\nabla\boldsymbol{A}\hat{\rho}_3$ and $-\frac{\mathrm{i}e}{2m}\boldsymbol{A}\hat{\rho}_3\nabla$ are both of the order $\sim \frac{1}{m}\frac{1}{L^2}$, and thus also much smaller than $\mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}} \sim \frac{1}{\lambda_{\mathrm{F}} m}\frac{1}{L}$ for the same reason. This means that we can neglect all terms in (4.24b) since the dominating terms are all in (4.24a).

4.3.1 Gradient Approximation

The star-products in Equation (4.24a) are defined as expansions in powers of derivatives, and in conventional units it means expansions in powers of $\hbar$. In the gradient approximation one neglects short-range oscillations in space, or in other words, one assumes that all quantities vary slowly in comparison to the Fermi wavelength. This is taken into

[1] Remember that we are working in a particular gauge, cf section 3.6, so that in fact $e\boldsymbol{A} = -m\boldsymbol{v}_s$ where $\boldsymbol{v}_s$ is the superfluid velocity.

[2] Note that in this expression we must interpret $\left[\hat{\boldsymbol{\partial}} \overset{\otimes}{,} \check{G}\right]_{-} = \nabla_{\boldsymbol{R}}\check{G} - \mathrm{i}e\left[\boldsymbol{A}\hat{\rho}_3 \overset{\otimes}{,} \check{G}\right]_{-}$, i.e. the result is not an operator.

[3] In the term $\mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}}$ the variable $\boldsymbol{p}$ is not a part of the star product, i.e. $\left[\mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}} \overset{\otimes}{,} \check{G}\right]_{-} = \mathrm{i}\frac{\boldsymbol{p}}{m}\left[\hat{\boldsymbol{\partial}} \overset{\otimes}{,} \check{G}\right]_{-}$.

[4] See Appendix D for more about the star-product

[5] In the quasiclassical approximation one only considers momentum of the order of Fermi momentum, thus $\boldsymbol{p} \to \boldsymbol{p}_{\mathrm{F}} \propto \boldsymbol{k}_{\mathrm{F}} \propto \frac{1}{\lambda_{\mathrm{F}}}$. Remember also that because of the Pauli principle, all processes will involve only electrons with momentum at the Fermi level.

account by keeping only derivatives up to first order in space in the equation of motion (note that we are keeping all terms with derivatives with respect to time), i.e.

$$\begin{aligned}
A \otimes B \approx & A \cdot B + \frac{\mathrm{i}}{2}\left[-\frac{\partial A}{\partial T}\frac{\partial B}{\partial E} + \nabla_{\boldsymbol{R}} A \nabla_{\boldsymbol{p}} B + \frac{\partial A}{\partial E}\frac{\partial B}{\partial T} - \nabla_{\boldsymbol{p}} A \nabla_{\boldsymbol{R}} B\right] \\
& - \frac{1}{8}\left[\frac{\partial^2 A}{\partial t^2}\frac{\partial^2 B}{\partial E^2} - 2\frac{\partial^2 A}{\partial t\, \partial E}\frac{\partial^2 B}{\partial E\, \partial t} + \frac{\partial^2 A}{\partial E^2}\frac{\partial^2 B}{\partial t^2}\right] + \cdots \\
= & A \circ B + \frac{i}{2}\left[\nabla_{\boldsymbol{R}} A \nabla_{\boldsymbol{p}} B - \nabla_{\boldsymbol{p}} A \nabla_{\boldsymbol{R}} B\right].
\end{aligned} \tag{4.25}$$

In the last step we have introduced a convenient notation for the infinite series of differentiations with respect to time[6].

With this approximation we may write (4.24a) as

$$\begin{aligned}
& \left[E\hat{\rho}_3 + \mathrm{i}\frac{\boldsymbol{p}}{m}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_{\mathrm{imp}}\hat{1} - \hat{S} - \hat{\Delta} \circ\!\!, \check{G}\right]_- \\
& -\frac{\mathrm{i}}{2}\left[\nabla_R\left(e\varphi\hat{1} + V_{\mathrm{imp}}\hat{1} + \hat{S} + \hat{\Delta}\right), \nabla_{\boldsymbol{p}}\check{G}\right]_+ = 0.
\end{aligned} \tag{4.26}$$

This equation is considerably more simple than (4.24) since there is now no infinite series of differentiations with respect to the spatial variables.

4.3.2 Quasiclassical Approximation

The starting point for the quasiclassical approximation is to assume that the range of spatial variation of the physical quantities is much larger than the Fermi wavelength λ_{F}. This means that the Green's function depends weakly on the quantity

$$\xi_{\boldsymbol{p}} = \frac{\boldsymbol{p}^2}{2m}. \tag{4.27}$$

The only important information contained in $\boldsymbol{p}$ is the direction at the Fermi surface since only particles with momentum close to the Fermi momentum will participate in physical processes (in other words we assume that all the particles are moving in the vicinity of the Fermi surface and have approximately the same momenta, this is a consequence of the Pauli principle). Therefore we will integrate $\check{G}(X,p)$ with respect to $\xi_{\boldsymbol{p}}$ and retain only the variable $\boldsymbol{p}_{\mathrm{F}}$ which is a vector at the Fermi surface. We thus define the quasiclassical Green's function[7]

$$\check{g}(X, \boldsymbol{p}_{\mathrm{F}}, E) = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \check{G}(X,p). \tag{4.28}$$

The integrand in this equation is not well behaved for large values of $\xi_{\boldsymbol{p}}$ since it falls off as $\frac{1}{\xi_{\boldsymbol{p}}}$. To ensure convergence of the integral we will use a decomposition introduced by Eilenberger [40] and discussed in [34]. The integration from $-\infty$ to ∞ is replaced by two closed semicircles in the upper and lower half-plane corresponding to the low energy contribution and a high energy contribution, see Figure 4.1. The low energy contribution is the term of physical interest, and the high energy contribution contains terms that do not depend on the non-equilibrium state and can therefore be dropped in the equation of motion.

[6] $A \circ B = \mathrm{e}^{\mathrm{i}\left(\partial_{T_A}\partial_{E_B} - \partial_{E_A}\partial_{T_B}\right)/2} A \cdot B$.

[7] This function is sometimes also named “The ξ-integrated Green's function” in the literature.

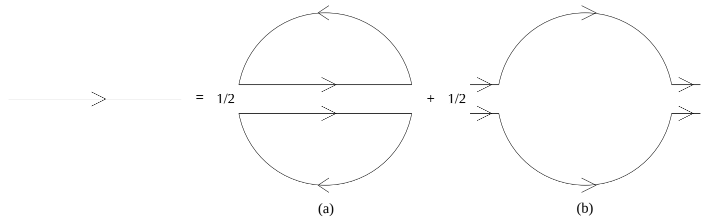


Figure 4.1: The high- and low-energy integration decomposition. The contour in (a) is denoted Γ, and the contour (b) will be neglected.

We will now introduce the quasiclassical Green's function in (4.26) as described and let $\boldsymbol{p} \to \boldsymbol{p}_\mathrm{F}$ since we are considering processes at the Fermi-level. This gives

$$\left[E\hat{\rho}_3 + \mathrm{i}\frac{\boldsymbol{p}_\mathrm{F}}{m}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_\mathrm{imp}\hat{1} - \hat{S} - \hat{\Delta} \circ\!\!, \check{g}\right]_- = 0. \tag{4.29}$$

The anticommutator in (4.26) has dropped out of the equation as a consequence of fixing the momentum variable. We will write $\frac{\boldsymbol{p}_\mathrm{F}}{m} = \boldsymbol{v}_\mathrm{F}$ which is simply the Fermi velocity. The final equation becomes

$$\boxed{\left[E\hat{\rho}_3 + \mathrm{i}\boldsymbol{v}_\mathrm{F}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_\mathrm{imp}\hat{1} - \hat{S} - \hat{\Delta} \circ\!\!, \check{g}\right]_- = 0.} \tag{4.30}$$

This is an important result, since it is the starting point for obtaining kinetic equations for the system we are considering.

Observables

We will now show how we can express physical quantities in terms of the quasiclassical Green's functions. In section 3.5 we found that the order parameter can be obtained from the Keldysh Green's function. Inserting the Fourier representation in Equation (3.55) we get

$$\Delta(1) = -\frac{\mathrm{i}}{4}\lambda\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3 \lim_{\substack{\boldsymbol{r}\to 0\\ t\to 0}} \int \frac{\mathrm{d}E}{2\pi}\mathrm{e}^{-\mathrm{i}Et}\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\hat{G}^\mathrm{K}(\boldsymbol{R},T,\boldsymbol{p},E)\right\}. \tag{4.31}$$

The limit must be taken since the Green's function should be evaluated at coordinates $(1,1)$. The following approximation is valid in the quasiclassical formalism when particle-hole symmetry applies,

$$\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \to N_0\int\mathrm{d}\xi_{\boldsymbol{p}}\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}. \tag{4.32}$$

Here N_0 is the density of states per spin at the Fermi level, and $\boldsymbol{e}_F$ is a unit vector in the $\boldsymbol{p}$ direction. The last integral represents angular averaging over the Fermi surface. Letting the relative variables approach zero and using this approximation we get

$$\Delta(1) = -\frac{1}{8}N_0\lambda\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\int\mathrm{d}E\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}\hat{g}^\mathrm{K}(X,\boldsymbol{p}_\mathrm{F},E)\right\}\bigg|_{X=(\boldsymbol{r}_1,t_1)}, \tag{4.33}$$

where the definition of the quasiclassical Green's function (4.28) has been used. In Appendix C it is shown how this equation leads to the usual BCS gap equation in the case of equilibrium.

Now we will find the current in the quasiclassical approximation, starting with the expression obtained in (3.60). Inserting the Fourier representation of the Green's function gives

$$\begin{aligned}\hat{\boldsymbol{\jmath}}(1) &= -\frac{e}{4m}\lim_{1\to 2}\left[(\nabla_1 - \mathrm{i}e\boldsymbol{A}(1)) - (\nabla_2 + \mathrm{i}e\boldsymbol{A}(2))\right]\int\frac{\mathrm{d}E}{2\pi}\mathrm{e}^{-\mathrm{i}Et}\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\hat{G}^{\mathrm{K}}(\boldsymbol{R},T,\boldsymbol{p},E)\\ &= -\frac{e}{4m}\lim_{\substack{\boldsymbol{r}\to 0\\ t\to 0}}\int\frac{\mathrm{d}E}{2\pi}\mathrm{e}^{-\mathrm{i}Et}\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\left(2\mathrm{i}\boldsymbol{p} - \mathrm{i}e\boldsymbol{A}(1) - \mathrm{i}e\boldsymbol{A}(2)\right)\hat{G}^{\mathrm{K}}(\boldsymbol{R},T,\boldsymbol{p},E).\end{aligned} \tag{4.34}$$

The following approximation is valid in the quasiclassical formalism when particle-hole symmetry applies,

$$\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}\boldsymbol{p} \to N_0 p_{\mathrm{F}}\int\mathrm{d}\xi_{\boldsymbol{p}}\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}\boldsymbol{e}_{\mathrm{F}}, \tag{4.35}$$

where p_{F} is the magnitude of the Fermi momentum. Letting the relative variables approach zero and using this approximation we get

$$\begin{aligned}\hat{\boldsymbol{\jmath}}(1) &= \frac{e}{2\mathrm{i}m}\int\frac{\mathrm{d}E}{2\pi}N_0 p_{\mathrm{F}}\int\mathrm{d}\xi_{\boldsymbol{p}}\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}\boldsymbol{e}_{\mathrm{F}}\hat{G}^{\mathrm{K}}(X,p)\Big|_{X=(\boldsymbol{r_1},t_1)}\\ &= -\frac{N_0 e v_{\mathrm{F}}}{4}\int\mathrm{d}E\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}\boldsymbol{e}_{\mathrm{F}}\hat{g}^{\mathrm{K}}(X,\boldsymbol{p}_{\mathrm{F}},E)\Big|_{X=(\boldsymbol{r_1},t_1)}.\end{aligned} \tag{4.36}$$

Here v_{F} is the magnitude of the Fermi velocity. We will later expand the Green's function in spherical harmonics, which causes the expression for the current to change also. This is discussed in Section 4.5.4. The diamagnetic term is cancelled by normal state contribution of contour (b) in Figure 4.1 (see Kopnin (2001) page 83).

4.4 Normalization Condition

Equation (4.30) is homogeneous in the function $\check{g}$ and does not determine the quasiclassical Green's function completely. We can remedy this by applying the following normalization condition

$$\check{g}\circ\check{g} = \check{1}. \tag{4.37}$$

This relation is valid for the following reasons [38]:

- In the limiting case of thermal equilibrium and in a spatially homogeneous state, we can calculate this result explicitly. The calculation is shown in Appendix C.
- In the general case we can derive from (4.30) an equation of the same form, but where $\check{g}\circ\check{g}$ replaces $\check{g}$. Multiplying (4.30) with $\check{g}$ from the right and then adding and subtracting suitable terms we can write

$$\begin{aligned}&\left[E\hat{\rho}_3 + \mathrm{i}\frac{\boldsymbol{p}_{\mathrm{F}}}{m}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_{\mathrm{imp}}\hat{1} - \hat{S} - \hat{\Delta} \,\overset{\circ}{,}\, \check{g}\circ\check{g}\right]_-\\ &- \check{g}\circ\left(\left[E\hat{\rho}_3 + \mathrm{i}\frac{\boldsymbol{p}_{\mathrm{F}}}{m}\hat{\boldsymbol{\partial}} - e\varphi\hat{1} - V_{\mathrm{imp}}\hat{1} - \hat{S} - \hat{\Delta} \,\overset{\circ}{,}\, \check{g}\right]_-\right) = 0.\end{aligned} \tag{4.38}$$

  The last parenthesis is zero by the original equation, giving the desired result. Using (4.37) as an ansatz solution we find that this is a solution of the equation, and since it joins up smoothly to the equilibrium solution, it is the only possible solution.

Various other discussions of the normalization condition can be found in [41], [35] and [42].

4.5 Dirty Limit

We will in the following consider only systems with strong impurity scattering, which is known as the "dirty limit" in the literature. In this case the elastic scattering self-energy dominates all other terms in the equation of motion for the Green's function[8]. This corresponds to the case of quasiparticle *diffusion*.

4.5.1 Expansion

The frequent scattering will make $\check{g}$ predominantly isotropic, and the dependence on the direction of the Fermi momentum is small. The geometry of the sample is also not important in this case. We may thus expand the Green's function in spherical harmonics up to first order,

$$\check{g}(X, E, \boldsymbol{p}_\mathrm{F}) \approx \check{g}_s(X, E) + \boldsymbol{e}_\mathrm{F} \cdot \check{\boldsymbol{g}}_p(X, E), \tag{4.39}$$

where $\boldsymbol{e}_\mathrm{F} = \frac{\boldsymbol{p}_\mathrm{F}}{|\boldsymbol{p}_\mathrm{F}|}$ is a unit vector parallel to the Fermi momentum vector. This expansion was first used by Usadel [43], and defines the s- and p-wave expansion terms of our Green's function.

4.5.2 Impurity Scattering

Elastic impurity scattering will be treated self-consistently in the Born approximation. The effect of scattering is then taken into account by the self-energy term (replacing the term $V_\mathrm{imp}\hat{1}$) (see Mahan [44]) defined by

$$\check{\Sigma}_\mathrm{imp}(1, 2) = \left\langle V(1)\check{G}(1, 2)V(2)\right\rangle_\mathrm{imp}. \tag{4.40}$$

The notation $\langle \cdots \rangle_\mathrm{imp}$ denotes average over positions of impurities. V is an impurity potential given by a sum over positions of impurities

$$V(\boldsymbol{r}) = \sum_{\boldsymbol{r}_i} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}} v(\boldsymbol{q}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)}, \tag{4.41}$$

where $v(\boldsymbol{q})$ is the Fourier transformed potential and $\mathcal{V}$ is volume. Inserted into (4.40) this gives

$$\begin{aligned}
\check{\Sigma}_\mathrm{imp}(1, 2) &= \left\langle \sum_{\boldsymbol{r}_i} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{r}_j} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}'} v(\boldsymbol{q}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_i)} v(\boldsymbol{q}') \mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}_2-\boldsymbol{r}_j)} \check{G}(1, 2) \right\rangle_\mathrm{imp} \\
&= \left\langle \sum_{\boldsymbol{r}_i} \frac{1}{\mathcal{V}^2} \sum_{\boldsymbol{q},\boldsymbol{q}'} v(\boldsymbol{q}) v(\boldsymbol{q}') \mathrm{e}^{-\mathrm{i}\boldsymbol{r}_i\cdot(\boldsymbol{q}+\boldsymbol{q}')} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_1} \mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}_2} \check{G}(1, 2) \right\rangle_\mathrm{imp} \\
&\quad + \left\langle \sum_{\boldsymbol{r}_i \neq \boldsymbol{r}_j} \frac{1}{\mathcal{V}^2} \sum_{\boldsymbol{q},\boldsymbol{q}'} v(\boldsymbol{q}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_i)} v(\boldsymbol{q}') \mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}_2-\boldsymbol{r}_j)} \check{G}(1, 2) \right\rangle_\mathrm{imp}.
\end{aligned} \tag{4.42}$$

[8]More specifically we will have $\frac{1}{\tau_\mathrm{imp}} \gg \Delta, T$ and $l_\mathrm{imp} \ll L$, where τ_imp is the impurity scattering time, l_imp is the elastic impurity scattering length and L is of the order of sample size.

We assume the impurities to be randomly located with no correlation in position. The term on the lower line here will then be zero unless both $\boldsymbol{q}$ and $\boldsymbol{q'}$ are zero because of the random fluctuations in the phase as we perform the average. We will therefore disregard this term. The other term is zero unless $\boldsymbol{q}+\boldsymbol{q'}=0$ in which case the exponential is 1 and averaging gives a factor $N_i = n_i\mathcal{V}$ where N_i is the number of impurities and n_i is the concentration. We now get

$$\check{\Sigma}_{\text{imp}}(1,2) = n_i\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}'} v(\boldsymbol{q}')v(-\boldsymbol{q}')\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}\check{G}(1,2) \approx n_i\int\frac{\mathrm{d}\boldsymbol{q}'}{(2\pi)^3}|v(\boldsymbol{q}')|^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}\check{G}(1,2), \tag{4.43}$$

where we have assumed $V(\boldsymbol{r})$ to be a real quantity (so that $v(-\boldsymbol{q}') = v^*(\boldsymbol{q}')$). It is the Fourier transform of this expression that enters into our equations, we thus calculate

$$\begin{aligned}\check{\Sigma}_{\text{imp}}(\boldsymbol{R},T,\boldsymbol{p},E) &= \int\mathrm{d}\boldsymbol{r}\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\int\mathrm{d}t\mathrm{e}^{\mathrm{i}Et}n_i\int\frac{\mathrm{d}\boldsymbol{q}'}{(2\pi)^3}|v(\boldsymbol{q}')|^2\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\check{G}(1,2)\\ &= n_i\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}|v(\boldsymbol{p}-\boldsymbol{q})|^2\check{G}(\boldsymbol{R},T,\boldsymbol{q},E),\end{aligned} \tag{4.44}$$

where we performed a change of variable in the last step. We now need to express this through the quasiclassical Green's function. v is assumed to depend weakly on $|\boldsymbol{p}|$, and in the range where $\check{G}$ is non-negligible we approximate $v(\boldsymbol{p}-\boldsymbol{q}) \approx v(\boldsymbol{p}_{\mathrm{F}}-\boldsymbol{q})$. Using the approximation (4.32) we get

$$\begin{aligned}\check{\sigma}_{\text{imp}}(\boldsymbol{R},T,\boldsymbol{p}_{\mathrm{F}},E) &= n_iN_0\int\mathrm{d}\xi_{\boldsymbol{q}}\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}|v(\boldsymbol{p}_{\mathrm{F}}-\boldsymbol{q})|^2\check{G}(\boldsymbol{R},T,\boldsymbol{q},E)\\ &= -\mathrm{i}\pi n_iN_0\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}|v(\boldsymbol{p}_{\mathrm{F}}-\boldsymbol{q})|^2\check{g}(\boldsymbol{R},T,\boldsymbol{p}_{\mathrm{F}},E).\end{aligned} \tag{4.45}$$

Note that in this expression $\boldsymbol{e}_{\mathrm{F}}$ is a unit vector pointing in the $\boldsymbol{q}$ direction. We have changed the symbol $\check{\Sigma}$ into $\check{\sigma}$ to reflect the fact that we now have a functional of $\check{g}$ instead of $\check{G}$. We are considering cases where the angular dependence of $\check{g}$ is small, therefore we assume the scattering to be isotropic and neglect any terms arising containing $\check{\boldsymbol{g}}_p$,

$$\check{\sigma}_{\text{imp}}(\boldsymbol{R},T,\boldsymbol{p}_{\mathrm{F}},E) \approx -\frac{\mathrm{i}}{2\tau}\check{g}_s. \tag{4.46}$$

Here we have defined the constant relaxation-time

$$\frac{1}{\tau} = 2\pi n_iN_0\int\frac{\mathrm{d}\boldsymbol{e}_F}{4\pi}|v(\boldsymbol{p}_{\mathrm{F}}-\boldsymbol{q})|^2. \tag{4.47}$$

This procedure has simplified the term governing impurity scattering considerably, and it is now possible to perform an angular average of the equation of motion (4.30).

4.5.3 Odd and Even Splitting

The expansion of the Green's function in spherical harmonics defines the s- and p-wave terms of our Green's function. The equation of motion can now be split into an even and an odd part with respect to $\boldsymbol{p}_{\mathrm{F}}$. The even part is separated by averaging over all directions of $\boldsymbol{p}_{\mathrm{F}}$, and the odd part is separated by the same averaging after multiplying the equation by $\boldsymbol{e}_\mathrm{F}$. In (4.30) we write $\boldsymbol{v}_\mathrm{F} = v_\mathrm{F}\boldsymbol{e}_\mathrm{F}$ where $v_\mathrm{F} = |\boldsymbol{v}_\mathrm{F}|$. For a spherical Fermi surface the unit vector can be parametrized by

$$\boldsymbol{e}_\mathrm{F} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\,, \tag{4.48}$$

and the angular average is performed by integrating $\frac{1}{4\pi}\int \mathrm{d}\Omega$. Substituting (4.39) into (4.30) and averaging yields

$$\left[E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta} \,\overset{\circ}{,}\, \check{g}_s\right]_- + \frac{\mathrm{i}}{3}v_\mathrm{F}\left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{\boldsymbol{g}}_p\right]_- = 0. \tag{4.49}$$

The odd part of (4.30) is obtained by averaging after first multiplying by $\boldsymbol{e}_\mathrm{F}$ as explained above. This gives

$$\frac{\mathrm{i}}{2\tau}\left[\check{g}_s \,\overset{\circ}{,}\, \check{\boldsymbol{g}}_p\right]_- + \mathrm{i}v_\mathrm{F}\left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{g}_s\right]_- = 0. \tag{4.50}$$

Because of the normalization condition (4.37) we must have (neglecting second order terms in $\check{\boldsymbol{g}}_p$ in accordance with expansion (4.39))

$$\check{g}_s \circ \check{g}_s = \check{1}, \qquad \check{g}_s \circ \check{\boldsymbol{g}}_p + \check{\boldsymbol{g}}_p \circ \check{g}_s = 0. \tag{4.51}$$

These conditions can be used to decouple the "even" and "odd" equations. Multiplying (4.50) by $\check{g}_s\circ$ from the left allows us now to separate

$$\check{\boldsymbol{g}}_p = -\tau v_\mathrm{F}\check{g}_s \circ \left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{g}_s\right]_- . \tag{4.52}$$

Substituting this result back into (4.49) gives

$$\boxed{D\left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{g}_s \circ \left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{g}_s\right]_-\right]_- + \mathrm{i}\left[E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta} \,\overset{\circ}{,}\, \check{g}_s\right]_- = 0,} \tag{4.53}$$

where we have defined the diffusion constant $D = \frac{1}{3}\tau v_\mathrm{F}^2$. This equation is much simpler than the original (4.30) because it is completely independent of the direction of the Fermi momentum.

4.5.4 Observables

For the formalism we have derived so far to be self contained, we will need expressions for gap and current in terms of $\check{g}_s$. Starting with expression (4.33) we can substitute the expansion of the Green's function and perform the angular average which gives

$$\Delta(1) = -\frac{1}{8}N_0\lambda\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\int \mathrm{d}E\hat{g}_s^\mathrm{K}(X,E)\right\}\Bigg|_{X=(\boldsymbol{r}_1,t_1)} . \tag{4.54}$$

We can also find the current from (4.36) following the same procedure,

$$\begin{aligned}\hat{\boldsymbol{\jmath}}(1) &= -\frac{N_0 e v_\mathrm{F}}{4}\int \mathrm{d}E\frac{1}{3}\hat{\boldsymbol{g}}_p^\mathrm{K}(X,E)\Bigg|_{X=(\boldsymbol{r}_1,t_1)} \\ &= \frac{N_0 e D}{4}\int \mathrm{d}E\left(\check{g}_s(X,E) \circ \left[\hat{\boldsymbol{\partial}} \,\overset{\circ}{,}\, \check{g}_s(X,E)\right]_-\right)_\mathrm{K}\Bigg|_{X=(\boldsymbol{r}_1,t_1)} ,\end{aligned} \tag{4.55}$$

where the notation $(\cdots)_{\mathrm{K}}$ denotes Keldysh component of the matrix (i.e. upper left block). We will now define some quantities which will be useful and have a direct physical interpretation. We define the energy dependent current matrix as

$$\hat{\boldsymbol{\jmath}}(X,E) = \left(\check{g}_s(X,E) \circ \left[\hat{\boldsymbol{\partial}} \overset{\circ}{,} \check{g}_s(X,E)\right]_-\right)_{\mathrm{K}}. \tag{4.56}$$

The following quantities are derived from the spectral current,

$$\begin{aligned} \boldsymbol{j}_{\mathrm{L}} &= \frac{1}{4}\operatorname{Tr}\{\hat{\boldsymbol{\jmath}}\}, && (4.57a)\\ \boldsymbol{j}_{\mathrm{T}} &= \frac{1}{4}\operatorname{Tr}\{\hat{\rho}_3\hat{\boldsymbol{\jmath}}\}, && (4.57b)\\ \boldsymbol{j}_{\mathrm{LS}} &= \frac{1}{4}\operatorname{Tr}\{\hat{\tau}_3\hat{\boldsymbol{\jmath}}\}, && (4.57c)\\ \boldsymbol{j}_{\mathrm{TS}} &= \frac{1}{4}\operatorname{Tr}\{\hat{\rho}_3\hat{\tau}_3\hat{\boldsymbol{\jmath}}\}. && (4.57d) \end{aligned}$$

These quantities have direct physical interpretations as we will see. The L,T,S index notation is explained in Section 4.8.1. If we can solve Equation (4.53) we may extract information about physical quantities using the expressions given in this section.

4.6 Symmetries and Parameterizations

From the redundancies in the definitions of the Green's functions and the normalization condition there follows symmetries which allows us to reduce the complexity of our system. We will also apply some of the symmetries of the equilibrium system, and together this allows for a parametrization of the Green's function that will simplify the calculations.

4.6.1 General Symmetries

Because of the normalization condition we have the following symmetries

$$\hat{g}^{\mathrm{R}} \circ \hat{g}^{\mathrm{R}} = \hat{g}^{\mathrm{A}} \circ \hat{g}^{\mathrm{A}} = \hat{1}, \tag{4.58}$$

$$\hat{g}^{\mathrm{R}} \circ \hat{g}^{\mathrm{K}} + \hat{g}^{\mathrm{K}} \circ \hat{g}^{\mathrm{A}} = 0. \tag{4.59}$$

These relations also apply to $\hat{g}_s$, which is independent of $\boldsymbol{p}_{\mathrm{F}}$. The last equation can be solved by the ansatz

$$\hat{g}^{\mathrm{K}} = \hat{g}^{\mathrm{R}} \circ \hat{h} - \hat{h} \circ \hat{g}^{\mathrm{A}}. \tag{4.60}$$

In addition we may derive from the definitions (see Appendix B) that

$$\hat{g}^{\mathrm{A}}(X,\boldsymbol{p}_{\mathrm{F}},E) = -\left[\hat{\rho}_3 \hat{g}^{\mathrm{R}}(X,\boldsymbol{p}_{\mathrm{F}},E)\hat{\rho}_3\right]^{\dagger}. \tag{4.61}$$

Therefore if we know $\hat{g}^{\mathrm{A}}$ we can calculate $\hat{g}^{\mathrm{R}}$.

4.6.2 Equilibrium Properties

It is calculated in Appendix C that the equilibrium solution for the BCS state is given by

$$\begin{aligned}\hat{g}^{\mathrm{R}}(E) =&\hat{\rho}_3\left[\frac{|E|}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2)-\frac{\mathrm{i}E}{\sqrt{|\Delta|^2-E^2}}\Theta(|\Delta|^2-E^2)\right]\\ &-\hat{\Delta}\left[\frac{\mathrm{sgn}(E)}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2)-\frac{\mathrm{i}}{\sqrt{|\Delta|^2-E^2}}\Theta(|\Delta|^2-E^2)\right],\end{aligned} \tag{4.62}$$

and that the symmetries of the quasiclassical Green's function are

$$\hat{g}^{\mathrm{R}}(X,\boldsymbol{p}_{\mathrm{F}},E)=\begin{pmatrix}\bar{g}^{\mathrm{R}}(X,\boldsymbol{p}_{\mathrm{F}},E) & \bar{f}^{\mathrm{R}}(X,\boldsymbol{p}_{\mathrm{F}},E)\\ -\left[\bar{f}(X,-\boldsymbol{p}_{\mathrm{F}},-E)\right]^* & -\left[\bar{g}(X,-\boldsymbol{p}_{\mathrm{F}},-E)\right]^*\end{pmatrix}. \tag{4.63}$$

Here $\bar{g}^{\mathrm{R}}$, $\bar{f}^{\mathrm{R}}$ denote the quasiclassical counterpart of the normal and anomalous 2×2 retarded Green's functions $\bar{G}^{\mathrm{R}}$, $\bar{F}^{\mathrm{R}}$. For the equilibrium solution we have that

$$\left[\bar{g}^{\mathrm{R}}(-E)\right]^*=\bar{g}^{\mathrm{R}}(E). \tag{4.64}$$

The matrix structure for equilibrium system is also simplified by

$$\bar{g}^{\mathrm{R}}(E)=\bar{1}g^{\mathrm{R}}(E),\qquad \bar{f}^{\mathrm{R}}(E)=\mathrm{i}\bar{\tau}_2 f^{\mathrm{R}}(E). \tag{4.65}$$

We will *assume* that these symmetries are also valid for the non-equilibrium system. It should be checked that this is indeed self-consistently satisfied. However, this assumption also has a physical interpretation. If $\bar{g}^{\mathrm{R}}$ were to have off-diagonal components this would for Keldysh component (obtained from (4.60)) imply that there existed spin-accumulation which was not quantized along the z-axis, i.e. spin-accumulation in the x- or y-directions. For co-linear magnetization this is not the case. Diagonal components in $\bar{f}^{\mathrm{R}}$ would imply correlations between electrons and holes with equal spin. Since we are considering the singlet superconducting state, this cannot be the case[9].

We will now consider only the isotropic part of the Green's function, $\hat{g}_s^{\mathrm{R}}(X,E)$. Because of the symmetries it can be written

$$\hat{g}_s^{\mathrm{R}}(X,E)=\begin{pmatrix} g_s^{\mathrm{R}}(X,E) & 0 & 0 & f_s^{\mathrm{R}}(X,E)\\ 0 & g_s^{\mathrm{R}}(X,E) & -f_s^{\mathrm{R}}(X,E) & 0\\ 0 & -\left[f_s^{\mathrm{R}}(X,-E)\right]^* & -g_s^{\mathrm{R}}(X,E) & 0\\ \left[f_s^{\mathrm{R}}(X,-E)\right]^* & 0 & 0 & -g_s^{\mathrm{R}}(X,E)\end{pmatrix}. \tag{4.66}$$

The normalization condition now implies that

$$g_s^{\mathrm{R}}(X,E)\circ g_s^{\mathrm{R}}(X,E)+f_s^{\mathrm{R}}(X,E)\circ\left[f_s^{\mathrm{R}}(X,-E)\right]^*=1. \tag{4.67}$$

[9]The Cooper-pair superconducting state which we are considering is not the only possible pairing mechanism. What we described was pairing of electrons in singlet states (i.e. the spin part of the wave-function is antisymmetric with respect to particle label interchange). However, there is also the possibility of pairing of electrons in triplet states where the spin part of the wave function is symmetric. In this case there will occur diagonal components in $\bar{f}^{\mathrm{R}}$.

4.6.3 Parametrization

The symmetries we have now found will be satisfied by the following parameterization

$$g_s^{\mathrm{R}}(X,E) = \cosh\{\theta(X,E)\}\,, \tag{4.68}$$
$$f_s^{\mathrm{R}}(X,E) = \sinh\{\theta(X,E)\}\,\mathrm{e}^{\mathrm{i}\chi(X,E)}. \tag{4.69}$$

There are additional symmetry relations for the complex functions $\theta(X,E)$ and $\chi(X,E)$ which we have now introduced. These relations are imposed by (4.64) and (4.67) and can be easily verified by substituting the given ansatz. One then obtains

$$\boxed{\begin{aligned}\theta^*(X,-E) &= -\theta(X,E),\\ \chi^*(X,-E) &= \chi(X,E).\end{aligned}} \tag{4.70}$$

The isotropic part of the quasiclassical retarded Green's function is now

$$\boxed{\hat{g}_s^{\mathrm{R}}(X,E) = \begin{pmatrix} \bar{1}\cosh\{\theta(X,E)\} & \mathrm{i}\bar{\tau}_2\sinh\{\theta(X,E)\}\,\mathrm{e}^{\mathrm{i}\chi(X,E)} \\ \mathrm{i}\bar{\tau}_2\sinh\{\theta(X,E)\}\,\mathrm{e}^{-\mathrm{i}\chi(X,E)} & -\bar{1}\cosh\{\theta(X,E)\}\end{pmatrix}.} \tag{4.71}$$

This ansatz will be substituted into the equation of motion for the Green's function, i.e. Equation (4.53).

4.6.4 Self-Consistency

We can now substitute the parametrization into the gap-equation (4.33) to see what relations hold for a general non-BCS state[10]. We will consider the equilibrium situation, and in this case we may use the following relation to obtain an expression for the Keldysh component of the Green's function matrix

$$\hat{g}_s^{\mathrm{K}}(X,\boldsymbol{p}_{\mathrm{F}},E) = \left\{\hat{g}_s^{\mathrm{R}}(X,\boldsymbol{p}_{\mathrm{F}},E) - \hat{g}_s^{\mathrm{A}}(X,\boldsymbol{p}_{\mathrm{F}},E)\right\}\tanh\left(\frac{\beta E}{2}\right). \tag{4.72}$$

This relation is discussed in Appendix C and is a special case of (4.60). Thus we need to calculate $\hat{g}^{\mathrm{A}}$ which is done easily by using the identity (4.61) together with the parameterization of $\hat{g}^{\mathrm{R}}$ giving

$$\hat{g}_s^{\mathrm{A}}(X,E) = \begin{pmatrix} -\bar{1}\cosh\{\theta^*(X,E)\} & -\mathrm{i}\bar{\tau}_2\sinh\{\theta^*(X,E)\}\,\mathrm{e}^{\mathrm{i}\chi^*(X,E)} \\ -\mathrm{i}\bar{\tau}_2\sinh\{\theta^*(X,E)\}\,\mathrm{e}^{-\mathrm{i}\chi^*(X,E)} & \bar{1}\cosh\{\theta^*(X,E)\}\end{pmatrix}. \tag{4.73}$$

The star denotes complex conjugation. We can now find that

$$\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\left(\hat{g}_s^{\mathrm{R}} - \hat{g}_s^{\mathrm{A}}\right)\right\} = 2\left(\sinh(\theta)\,\mathrm{e}^{\mathrm{i}\chi} + \sinh(\theta^*)\,\mathrm{e}^{\mathrm{i}\chi^*}\right), \tag{4.74}$$

and the gap equation is

$$\Delta = -\frac{1}{4}N_0\lambda\int \mathrm{d}E\left(\sinh(\theta)\,\mathrm{e}^{\mathrm{i}\chi} + \sinh(\theta^*)\,\mathrm{e}^{\mathrm{i}\chi^*}\right)\tanh\left(\frac{\beta E}{2}\right). \tag{4.75}$$

[10]The result for BCS is found in Appendix C.

Because of the gauge-transformations we made in section 3.6 the gap is a real quantity, and we demand the imaginary part of the right hand side of the equation above to be zero,

$$\begin{aligned}0 = \Im\{\Delta\} &= -\frac{1}{2\mathrm{i}}\frac{1}{4}N_0\lambda \int \mathrm{d}E \left(\sinh(\theta)\left[\mathrm{e}^{\mathrm{i}\chi} - \mathrm{e}^{-\mathrm{i}\chi}\right] + \sinh(\theta^*)\left[\mathrm{e}^{\mathrm{i}\chi^*} - \mathrm{e}^{-\mathrm{i}\chi^*}\right]\right) \tanh\left(\frac{\beta E}{2}\right) \\ &= -\frac{1}{4}N_0\lambda \int \mathrm{d}E \left[\sinh(\theta)\sin(\chi) + \sinh(\theta^*)\sin(\chi^*)\right] \tanh\left(\frac{\beta E}{2}\right). \end{aligned} \tag{4.76}$$

A nontrivial solution of this equation which satisfies the boundary conditions is

$$\Re\{\chi\} = (2n+1)\pi,\ n = 0, 1, 2, \cdots; \qquad \Im\{\chi\} = 0. \tag{4.77}$$

This means that the phase factor χ is a real constant, where we choose n so that the sign of Δ is correct. From this constraint follows drastic simplifications of the transport problem.

4.7 Retarded (Advanced) Component

In this section we will consider the upper left block of Equation (4.53) in the stationary case. In this limit all dependence on the variable T will be neglected and products involving infinite series of differentiations with respect to time ("$\circ$") simplify to "ordinary" products. The equation involves $\hat{g}_s^{\mathrm{R}}$ only,

$$D\left[\hat{\boldsymbol{\partial}}, \hat{g}_s^{\mathrm{R(A)}}\left[\hat{\boldsymbol{\partial}}, \hat{g}_s^{\mathrm{R(A)}}\right]_-\right]_- + \mathrm{i}\left[E\hat{\rho}_3 - e\varphi\hat{1} - \hat{S} - \hat{\Delta}, \hat{g}_s^{\mathrm{R(A)}}\right]_- = 0. \tag{4.78}$$

We have written (A) in parenthesis since if we consider instead the lower right block of Equation (4.53) we will find that the advanced Green's function obeys the same differential equation. Since the advanced Green's function is given by the retarded, the equation of motion for this component does not give any new information. We will substitute the parameterization of $\hat{g}_s^{\mathrm{R}}$ given in (4.71) into (4.78). The resulting relations are often called Usadel equations. The calculations in this section involve products of 4×4 matrices, and are thus most easily done using a symbolic computer algebra system. Therefore only a limited amount of the calculations are shown here.

4.7.1 Spin-Flip Scattering

Spin-flip scattering resulting from magnetic impurities has so far been accounted for by the term $\hat{S}$. We will approximate the contribution from such scattering by replacing $\hat{S}$ with a self-energy term

$$\check{\Sigma}_{\mathrm{sf}}(1,2) = \left\langle \hat{S}(1)\check{G}(1,2)\hat{S}(2)\right\rangle_{\mathrm{sf}}, \tag{4.79}$$

where $\langle\cdots\rangle_{\mathrm{sf}}$ denotes average over positions and spin states of the magnetic impurities. The matrix $\hat{S}$ is represented as

$$\hat{S}(\boldsymbol{r}) = \sum_{\boldsymbol{r}_i}\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}} v_{\mathrm{sf}}(\boldsymbol{q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_i)}\begin{pmatrix}\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S} & 0 \\ 0 & (\bar{\boldsymbol{\tau}}\cdot\boldsymbol{S})^T\end{pmatrix}. \tag{4.80}$$

Here $\boldsymbol{r}_i$ are the positions of the magnetic impurities, $v_{\rm sf}(\boldsymbol{q})$ is the Fourier transformed magnetic impurity potential and

$$\bar{\boldsymbol{\tau}} \cdot \boldsymbol{S} = \bar{\tau}_1 S_x + \bar{\tau}_2 S_y + \bar{\tau}_3 S_z, \tag{4.81}$$

where S_i are spin operators. Defining the matrices $\hat{\alpha}_i$

$$\hat{\alpha}_i = \begin{pmatrix} \bar{\tau}_i & 0 \\ 0 & \bar{\tau}_i^T \end{pmatrix}, \tag{4.82}$$

we can write the spin-flip self-energy as

$$\check{\Sigma}_{\rm sf}(1,2) = \left\langle \sum_{\boldsymbol{r}_i} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{r}_j} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}'} v_{\rm sf}(\boldsymbol{q}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_i)} v_{\rm sf}(\boldsymbol{q}') \mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}_2 - \boldsymbol{r}_j)} \sum_{l,m=1}^{3} \hat{\alpha}_l S_l \check{G}(1,2) \hat{\alpha}_m S_m \right\rangle_{\rm sf} . \tag{4.83}$$

We assume the spin states of the magnetic impurities to be random so that

$$\langle S_i S_j \rangle_{\rm sf} = \begin{cases} \frac{1}{3} S(S+1) & i = j \\ 0 & i \neq j, \end{cases} \tag{4.84}$$

where S is the spin quantum number. Proceeding in the same way as we did for impurity scattering in section 4.5.2 we obtain for the Fourier transformed self-energy in the quasiclassical limit

$$\check{\sigma}_{\rm sf}(\boldsymbol{R}, \boldsymbol{p}_F, E) = -\frac{\mathrm{i}}{2\tau_{\rm sf}} \left[\frac{1}{4} \sum_i \hat{\alpha}_i \check{g}_s(\boldsymbol{R}, \boldsymbol{p}_F, E) \hat{\alpha}_i \right], \tag{4.85}$$

where we have defined the spin-flip relaxation time as

$$\frac{1}{\tau_{\rm sf}} = \frac{4}{3} 2\pi n_{\rm sf} N_0 S(S+1) \int \frac{\mathrm{d}\boldsymbol{e}_F}{4\pi} |v_{\rm sf}(\boldsymbol{p}_F - \boldsymbol{q})|^2, \tag{4.86}$$

where $n_{\rm sf}$ is the concentration of magnetic impurities. Having specified all the terms in (4.78) we are now ready to calculate the kinetic equations, but first we will take a closer look at the retarded part (i.e. upper left matrix block) of spin-flip scattering. Using the matrix structure given in (4.71) we find that

$$\hat{\alpha}_i \hat{g}^{\rm R} \hat{\alpha}_i = \hat{\rho}_3 \hat{g}^{\rm R} \hat{\rho}_3 \,\mathrm{for}\, i = 1,2,3. \tag{4.87}$$

This means that we can simplify

$$\hat{\sigma}_{\rm sf}^{\rm R}(\boldsymbol{R}, \boldsymbol{p}_F, E) = -\frac{\mathrm{i}}{2\tau_{sf}} \frac{3}{4} \hat{\rho}_3 \hat{g}_s^{\rm R}(\boldsymbol{R}, \boldsymbol{p}_F, E) \hat{\rho}_3, \tag{4.88}$$

making the calculations below a little easier.

4.7.2 Usadel Equations

For a stationary system we find[11]

$$\mathrm{i}\left[E\hat{\rho}_3, \hat{g}_s^{\mathrm{R}}\right]_- = 2\mathrm{i}E\sinh(\theta)\begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\chi} \\ 0 & 0 & -\mathrm{e}^{\mathrm{i}\chi} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 \\ \mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 & 0 \end{pmatrix}, \tag{4.89}$$

$$\mathrm{i}\left[-e\varphi, \hat{g}_s^{\mathrm{R}}\right]_- = 0, \tag{4.90}$$

$$\mathrm{i}\left[\frac{\mathrm{i}}{2\tau_{sf}}\frac{3}{4}\hat{\rho}_3\hat{g}_s^{\mathrm{R}}\hat{\rho}_3, \hat{g}_s^{\mathrm{R}}\right]_- = -\frac{3}{4}\frac{1}{\tau_{sf}}\sinh(2\theta)\begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\chi} \\ 0 & 0 & -\mathrm{e}^{\mathrm{i}\chi} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 \\ \mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 & 0 \end{pmatrix}, \tag{4.91}$$

$$\mathrm{i}\left[-\hat{\Delta}, \hat{g}_s^{\mathrm{R}}\right]_- = -\mathrm{i}\sinh(\theta)\Delta\left(\mathrm{e}^{\mathrm{i}\chi} - \mathrm{e}^{-\mathrm{i}\chi}\right)\hat{\rho}_3 + 2\mathrm{i}\cosh(\theta)\Delta\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{4.92}$$

The term involving gauge-invariant derivative has a rather complicated structure. This is evident if one writes out the commutators. However, close inspection of all terms arising reveal high symmetry and we find that the vector potential always occurs in connection with χ as $\nabla\chi - 2e\boldsymbol{A}$. The derivatives in (4.53) become

$$\begin{aligned}\left[\hat{\boldsymbol{\partial}}, \hat{g}_s^{\mathrm{R}}\left[\hat{\boldsymbol{\partial}}, \hat{g}_s^{\mathrm{R}}\right]_-\right]_- &= \nabla\left[\mathrm{i}\sinh^2(\theta)(\nabla\chi - 2e\boldsymbol{A})\right]\hat{\rho}_3 \\ &+ \left[2\mathrm{i}\cosh^2(\theta)(\nabla\theta)(\nabla\chi - 2e\boldsymbol{A}) + \frac{1}{2}\mathrm{i}\sinh(2\theta)(\nabla(\nabla\chi - 2e\boldsymbol{A}))\right]\begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\chi} \\ 0 & 0 & -\mathrm{e}^{\mathrm{i}\chi} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 \\ -\mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 & 0 \end{pmatrix} \\ &+ \left[\nabla^2\theta - \frac{1}{2}\sinh(2\theta)(\nabla\chi - 2e\boldsymbol{A})^2\right]\begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\chi} \\ 0 & 0 & -\mathrm{e}^{\mathrm{i}\chi} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 \\ \mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 & 0 \end{pmatrix}.\end{aligned} \tag{4.93}$$

We define the spectral supercurrent by

$$\boldsymbol{j}_E = 2(\nabla\chi - 2e\boldsymbol{A})\sinh^2(\theta), \tag{4.94}$$

which can be recognized in the expression for the derivative. In our case χ is a constant, therefore the term $\nabla\chi = 0$. To obtain scalar equations from the matrix relations we will take the trace after multiplying with a suitable matrix. Performing the operation $\mathrm{Tr}\{\hat{\rho}_3\cdots\}$ on (4.78) gives

$$\boxed{\nabla\cdot\boldsymbol{j}_E = 0.} \tag{4.95}$$

[11] Remember that we are working in a gauge where Δ is a real quantity.

This equation expresses conservation of the quantity $\boldsymbol{j}_E$. The constraints on χ (4.77) have been used. Another equation can be found by performing the operation

$$\mathrm{Tr}\left\{\begin{pmatrix} 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\chi} \\ 0 & 0 & -\mathrm{e}^{\mathrm{i}\chi} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 \\ \mathrm{e}^{-\mathrm{i}\chi} & 0 & 0 & 0 \end{pmatrix} \dots \right\},$$

which gives

$$\boxed{D\left[\nabla^2\theta - 2\sinh(2\theta)\,(e\boldsymbol{A})^2\right] = -2\mathrm{i}E\sinh(\theta) - 2\mathrm{i}\cosh(\theta)\Delta\mathrm{e}^{\mathrm{i}\chi} + \frac{3}{4}\frac{1}{\tau_{sf}}\sinh(2\theta)}. \tag{4.96}$$

In this result we have used the constraints on χ (4.77). Equations (4.95) and (4.96) determine the retarded and advanced Green's function.

4.7.3 Boundary Condition

Comparing the parameterization of $\hat{g}^{\mathrm{R}}$ with the BCS state equilibrium solution (4.62) we may derive boundary conditions. In order for the two solutions to agree we must have

$$\sinh\left(\theta(X,E)\right)\mathrm{e}^{\mathrm{i}\chi(X,E)} = -\Delta\left[\frac{\mathrm{sgn}(E)}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2) - \frac{\mathrm{i}}{\sqrt{|\Delta|^2-E^2}}\Theta(|\Delta|^2-E^2)\right] \tag{4.97}$$

$$\cosh\left(\theta(X,E)\right) = \frac{|E|}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2) - \frac{\mathrm{i}E}{\sqrt{|\Delta|^2-E^2}}\Theta(|\Delta|^2-E^2). \tag{4.98}$$

Let us first consider the case $|E| > |\Delta|$. We can then find

$$\tanh(\theta)\mathrm{e}^{\mathrm{i}\chi} = \frac{\Delta}{E}, \tag{4.99}$$

and since for a superconducting reservoir $\Delta = |\Delta|\mathrm{e}^{\mathrm{i}\phi_0}$ this gives us the conditions

$$\chi = \phi_0, \tag{4.100}$$

$$\theta = \mathrm{arctanh}\left(\frac{|\Delta|}{E}\right). \tag{4.101}$$

If $|E| \gg |\Delta|$ we have the limit of no superconductivity which implies $\theta = 0$. This is the case inside the ferromagnetic lead. Examining the conditions when $|E| < |\Delta|$ shows that this gives us no new condition. Now we must remember that we are working in a gauge where the gap is a real quantity. This means that $\phi_0 = 0, \pi$. The boundary conditions for our system may therefore be summarized

$$\text{Ferromagnetic lead}: \begin{cases}\chi = \text{irrelevant} \\ \theta = 0,\end{cases} \quad \text{Superconducting lead}: \begin{cases}\chi = \phi_0 \\ \theta = \mathrm{arctan}\left(\frac{|\Delta|}{E}\right).\end{cases} \tag{4.102}$$

4.8 Keldysh Component

Having found the retarded and advanced kinetic equations in the last section, we turn now to the Keldysh kinetic equation. This is the upper right block of matrix equation (4.53) and determines the non-thermal distribution functions.

4.8.1 Distribution Function

The Keldysh Green's function was given an ansatz solution in (4.60), in the stationary case it is $\hat{g}^{\mathrm{K}} = \hat{g}^{\mathrm{R}}\hat{h} - \hat{h}\hat{g}^{\mathrm{A}}$. We will assume the distribution matrix $\hat{h}$ to be diagonal. This assumption does not violate the boundary conditions, and we will later check whether the resulting differential equation can be fulfilled. The diagonal distribution matrix can now be written as a linear combination of four linearly independent diagonal matrices,

$$\hat{h} = \hat{1}h_{\mathrm{L}} + \hat{\tau}_3 h_{\mathrm{LS}} + \hat{\rho}_3 h_{\mathrm{T}} + \hat{\rho}_3\hat{\tau}_3 h_{\mathrm{TS}}, \tag{4.103}$$

These components each have a physical interpretation. L and T indexes are abbreviations for longitudinal and transversal, and S is abbreviation for spin. The L, T terminology is due to Schmid and Schön [45]. h_{L} represents distribution of energy, and h_{T} distribution of charge (particles and holes). The terms h_{LS} and h_{TS} represent spin-accumulation. This terminology is also used for the current operators defined in (4.57).

A distribution function for electrons can be obtained by the transformation [38]

$$f_L = \tfrac{1-h_{\mathrm{L}}}{2}, \qquad f_T = -\tfrac{h_{\mathrm{T}}}{2}. \tag{4.104}$$

Comparing with (4.72) we see that f_{L} equals the Fermi-Dirac function and that f_{T} is zero in the equilibrium case.

4.8.2 Kinetic Equations

With the definition of the energy dependent current matrix in (4.56) the Keldysh part of the diffusion equation (4.53) can be written

$$D\left[\hat{\boldsymbol{\partial}}, \hat{\boldsymbol{\jmath}}\right]_- = \mathrm{i}\left\{-\left[E\hat{\rho}_3, \hat{g}_s^{\mathrm{K}}\right]_- + \left[e\varphi, \hat{g}_s^{\mathrm{K}}\right]_- + \left([\check{\sigma}_{\mathrm{sf}}, \check{g}_s]_-\right)_{\mathrm{K}} + \left[\hat{\Delta}, \hat{g}_s^{\mathrm{K}}\right]_-\right\}. \tag{4.105}$$

In the spin-flip term, subscript K denotes upper right block of the total matrix (Keldysh component). Explicitly

$$\left([\check{\sigma}_{\mathrm{sf}}, \check{g}]_-\right)_{\mathrm{K}} = \hat{\sigma}_{\mathrm{sf}}^{\mathrm{R}}\hat{g}^{\mathrm{K}} + \hat{\sigma}_{\mathrm{sf}}^{\mathrm{K}}\hat{g}^{\mathrm{A}} - \hat{g}^{\mathrm{R}}\hat{\sigma}_{\mathrm{sf}}^{\mathrm{K}} - \hat{g}^{\mathrm{K}}\hat{\sigma}_{\mathrm{sf}}^{\mathrm{A}}. \tag{4.106}$$

The calculation of the right-hand side of Equation (4.105) is well suited for computer algebra systems such as Maple. To obtain four linearly independent scalar equations we will perform the following operations on (4.105)

$$\mathrm{Tr}\left\{\cdots\right\}, \ \mathrm{Tr}\left\{\hat{\rho}_3\cdots\right\}, \ \mathrm{Tr}\left\{\hat{\tau}_3\ldots\right\}, \ \mathrm{Tr}\left\{\hat{\rho}_3\hat{\tau}_3\cdots\right\}. \tag{4.107}$$

When we take the trace, the term in the gauge invariant derivative proportional to the vector potential, $\boldsymbol{A}$, will cancel, i.e.

$$\mathrm{Tr}\left\{\left[\hat{\boldsymbol{\partial}}, \hat{\boldsymbol{\jmath}}\right]_-\right\} = \mathrm{Tr}\left\{\nabla\cdot\hat{\boldsymbol{\jmath}} - \mathrm{i}e\boldsymbol{A}\cdot[\hat{\rho}_3, \hat{\boldsymbol{\jmath}}]_-\right\} = \mathrm{Tr}\left\{\nabla\cdot\hat{\boldsymbol{\jmath}}\right\}. \tag{4.108}$$

This also happens for the three other trace operations in (4.107). Using the definitions (4.57) for the various currents, we can write the four scalar equations compactly[12] in matrix notation

$$\boxed{\nabla\cdot\begin{pmatrix} \boldsymbol{j}_{\mathrm{L}} \\ \boldsymbol{j}_{\mathrm{T}} \\ \boldsymbol{j}_{\mathrm{LS}} \\ \boldsymbol{j}_{\mathrm{TS}} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \alpha_{\mathrm{TL}} & \alpha_{\mathrm{TT}} & 0 & 0 \\ 0 & 0 & \alpha_{\mathrm{TT}} & \alpha_{\mathrm{TL}} \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} h_{\mathrm{L}} \\ h_{\mathrm{T}} \\ h_{\mathrm{LS}} \\ h_{\mathrm{TS}} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha_{\mathrm{LSLS}} & 0 \\ 0 & 0 & 0 & \alpha_{\mathrm{TSTS}} \end{pmatrix}\begin{pmatrix} h_{\mathrm{L}} \\ h_{\mathrm{T}} \\ h_{\mathrm{LS}} \\ h_{\mathrm{TS}} \end{pmatrix}}. \tag{4.109}$$

We have here defined the symbols

$$\alpha_{\mathrm{TL}} = -2\frac{1}{D}\Delta\Im\left\{\sinh(\theta)\left[\mathrm{e}^{\mathrm{i}\chi} - \mathrm{e}^{-\mathrm{i}\chi}\right]\right\}, \tag{4.110a}$$

$$\alpha_{\mathrm{TT}} = 2\frac{1}{D}\Delta\Im\left\{\sinh(\theta)\left[\mathrm{e}^{\mathrm{i}\chi} + \mathrm{e}^{-\mathrm{i}\chi}\right]\right\}, \tag{4.110b}$$

$$\alpha_{\mathrm{LSLS}} = 2\frac{1}{D\tau_{\mathrm{sf}}}\left[(\Re\{\cosh(\theta)\})^2 - (\Im\{\sinh(\theta)\})^2\right], \tag{4.110c}$$

$$\alpha_{\mathrm{TSTS}} = 2\frac{1}{D\tau_{\mathrm{sf}}}\left[(\Re\{\cosh(\theta)\})^2 + (\Re\{\sinh(\theta)\})^2\right]. \tag{4.110d}$$

Because of the constraints on χ we find that $\alpha_{\mathrm{TL}} = 0$. The first term on the right hand side in (4.109) comes from "gap" scattering due to the superconductor, and the second term is due to spin-flips. From the matrix structure of the spin-flip term we see that the physical energy and charge currents ($\boldsymbol{j}_{\mathrm{L}}$ and $\boldsymbol{j}_{\mathrm{T}}$) decouple from spin-flip scattering.

We can introduce the generalized diffusion coefficients (energy dependent)

$$D_{\mathrm{L}} = \frac{1}{4}\mathrm{Tr}\left\{\hat{1} - \hat{g}_s^{\mathrm{R}}\hat{g}_s^{\mathrm{A}}\right\} = 1 + |\cosh(\theta)|^2 - |\sinh(\theta)|^2, \tag{4.111}$$

$$D_{\mathrm{T}} = \frac{1}{4}\mathrm{Tr}\left\{\hat{1} - \hat{\tau}_3\hat{g}_s^{\mathrm{R}}\hat{\tau}_3\hat{g}_s^{\mathrm{A}}\right\} = 1 + |\cosh(\theta)|^2 + |\sinh(\theta)|^2, \tag{4.112}$$

and then the currents can be expressed as

$$\boldsymbol{j}_{\mathrm{L}} = D_{\mathrm{L}}\nabla h_{\mathrm{L}} - \Im\{\boldsymbol{j}_{\mathrm{E}}\}h_{\mathrm{T}}, \tag{4.113a}$$

$$\boldsymbol{j}_{\mathrm{T}} = D_{\mathrm{T}}\nabla h_{\mathrm{T}} - \Im\{\boldsymbol{j}_{\mathrm{E}}\}h_{\mathrm{L}}, \tag{4.113b}$$

$$\boldsymbol{j}_{\mathrm{LS}} = D_{\mathrm{T}}\nabla h_{\mathrm{LS}} - \Im\{\boldsymbol{j}_{\mathrm{E}}\}h_{\mathrm{TS}}, \tag{4.113c}$$

$$\boldsymbol{j}_{\mathrm{TS}} = D_{\mathrm{L}}\nabla h_{\mathrm{TS}} - \Im\{\boldsymbol{j}_{\mathrm{E}}\}h_{\mathrm{LS}}. \tag{4.113d}$$

Because of Equations (4.95) and (4.96) the coefficients in this equation are known, and we may use the kinetic equations (4.109) to calculate the distribution functions.

4.8.3 Boundary Condition

At the superconducting side, we can obtain boundary conditions from the BCS equilibrium solution. For $|E| > |\Delta|$ we have

$$\cosh(\theta) = \frac{|E|}{\sqrt{E^2 - |\Delta|^2}}, \quad \sinh(\theta) = -\mathrm{sgn}(E)\frac{\Delta}{\sqrt{E^2 - |\Delta|^2}}, \tag{4.114}$$

[12] We are using the constraints on χ obtained in Section 4.6.4, so that e.g. $\mathrm{e}^{\pm 2\mathrm{i}\chi} = 1$ etc.

which implies for the quantities in (4.110) that

$$\alpha_{\mathrm{TL}} = 0, \tag{4.115a}$$
$$\alpha_{\mathrm{TT}} = 0, \tag{4.115b}$$
$$\alpha_{\mathrm{LSLS}} = 2\frac{1}{\tau_{\mathrm{sf}}}\frac{E^2}{E^2 - |\Delta|^2}, \tag{4.115c}$$
$$\alpha_{\mathrm{TSTS}} = 2\frac{1}{\tau_{\mathrm{sf}}}\frac{E^2 + \Delta^2}{E^2 - |\Delta|^2}. \tag{4.115d}$$

Below the superconducting gap, i.e. for $|E| < |\Delta|$, the boundary conditions are

$$\cosh(\theta) = -\mathrm{i}\frac{E}{\sqrt{|\Delta|^2 - E^2}}, \ \sinh(\theta) = \mathrm{i}\frac{\Delta}{\sqrt{|\Delta|^2 - E^2}}. \tag{4.116}$$

With these conditions the quantities in (4.110) must be

$$\alpha_{\mathrm{TL}} = 0, \tag{4.117a}$$
$$\alpha_{\mathrm{TT}} = 4\frac{\Delta^2}{\sqrt{|\Delta|^2 - E^2}}\mathrm{e}^{\mathrm{i}\chi}, \tag{4.117b}$$
$$\alpha_{\mathrm{LSLS}} = -2\frac{1}{\tau_{\mathrm{sf}}}\frac{\Delta^2}{|\Delta|^2 - E^2}, \tag{4.117c}$$
$$\alpha_{\mathrm{TSTS}} = 0. \tag{4.117d}$$

The factor $\mathrm{e}^{\mathrm{i}\chi}$ is either 1 or -1, depending on the sign of Δ in the reservoir.

4.8.4 Physical Content of Kinetic Equation

From Equation (4.109) we can see that the physical charge current $\boldsymbol{j}_{\mathrm{T}}$ is not conserved at each energy, but let us check whether the total particle current, $\boldsymbol{j}_{\mathrm{p}}$ is conserved.

The argument in this sections is not valid due to a sign error. It has been censored in this version. 2005-05-12

As we have seen, the physical charge current is not conserved at each energy. This can be understood as follows. Inside the superconducting reservoir the supercurrent is solely carried by energies $E = \pm|\Delta|$. The dissipative charge current entering the superconductor must therefore be transformed with respect to energy, which is why it is not conserved. The kinetic equation also implies that the physical spin current ($\boldsymbol{j}_{\mathrm{TS}}$) is conserved in absence of spin-flip scattering (lower line of (4.109)). A transformation in energy is then not possible in which case spin-current into the superconductor must vanish.

Chapter 5

Conclusion

In this thesis we have investigated some of the properties of a hybrid superconductor/ferromagnet system. Equations of motion for the Green's function in the Keldysh formalism were derived. A gauge transformation was performed at this point, which caused a dramatic simplification of the calculations at a later stage. From the equations of motion we were able to obtain a transport-like equation. This equation was simplified considerably by the quasiclassical approximation and that we consider a stationary system in the dirty limit. Assumptions about the physical state of the system accommodated a parameterization of the Green's function which led to the desired kinetic equations. These equations were simplified considerably, since the gauge transformation ensures that the superconducting order parameter is a real quantity.

The most important findings are actually the equations themselves, which have yet to be solved in order to understand the properties of the system. Some insight is also offered by the structure of these equations alone. We found that a transformation in energy of the physical charge current entering the superconductor takes place because of the superconducting energy gap. If we neglect spin-flip scattering the physical spin current is conserved.

5.1 Prospects

The results obtained in this thesis forms the background for several further tasks. We have now obtained the kinetic equations for the dirty superconductor/ferromagnet system, but these have yet to be solved. This can be done numerically, and will provide a description of the behavior of the system. To make the derivation of the equations in this thesis more rigorous, the calculation of equations of motion for Green's functions in Chapter 3 should be rewritten using a perturbative approach. With this formalism we would also avoid the awkward introduction of self-energies in Chapter 4.

The kinetic equations were obtained by neglecting time dependence. When the properties of the stationary system have been revealed, one should try to find the time dependent equations which may show new behavior. One possibility is that since the superconducting gap depends on time and position we could see oscillating Josephson currents.

Appendix A

Notation

The following notation is used in this thesis:

Commutator

$$[A, B]_- = AB - BA.$$

Anticommutator

$$[A, B]_+ = AB + BA.$$

Real and imaginary part of complex number $z = x + \mathrm{i}y$

$$\Re\{z\} = x,\ \Im\{z\} = y.$$

Matrix dimensions

$$\dim\{\bar{A}\} = 2 \times 2,\ \dim\{\hat{A}\} = 4 \times 4,\ \dim\{\check{A}\} = 8 \times 8.$$

Pauli matrices are denoted $\bar{\tau}_i$ and their 4×4 generalization $\hat{\rho}_i$. See Section 3.2.

List of symbols:

Symbol	**Unit**	**Definition**
e	C	Electron charge, $e = -\lvert e\rvert$
$\hbar$	Js	Plack constant divided by 2π
k_B	J/K	Boltzmann constant
$\beta(T)$	J^{-1}	Inverse temperature
$\Theta(t)$	-	Heaviside step-function, see Equation (3.36)
$\delta(x)$	-	Dirac delta-function
δ_{ij}	-	Kronecker delta
$\varphi(\boldsymbol{r}, t)$	V	Electrostatic scalar potential
$\boldsymbol{A}(\boldsymbol{r}, t)$	Tm	Magnetic vector potential
$\boldsymbol{j}(\boldsymbol{r}, t)$	$\mathrm{C/m^2}$	Electrical current-density operator
$\psi(\boldsymbol{r}, t)$	-	Electron annihilation field operator
$\psi^\dagger(\boldsymbol{r}, t)$	-	Electron destruction field operator
H	J	Hamilton operator
N_0	J^{-1}	Density of states per spin at the Fermi level

Appendix B

Green's Function Matrices

For reference we will explicitly give the matrix elements of the Green's funtions. We will also see that there are redundancies which results in a symmetry relation between the retarded and advanced Green's functions.

B.1 Representations

$$\begin{aligned}\hat{G}^{\mathrm{R}}(1,2) &= \begin{pmatrix} \bar{G}^{\mathrm{R}}(1,2) & \bar{F}^{\mathrm{R}}(1,2) \\ \left(\bar{F}^{\mathrm{R}}\right)^{*}(1,2) & \left(\bar{G}^{\mathrm{R}}\right)^{*}(1,2) \end{pmatrix} = \sum_{j} \left(-\mathrm{i}\Theta(t_1-t_2)\right)(\hat{\rho}_3)_{ij} \left\langle \left[\left(\psi(1)\right)_j , \left(\psi^{\dagger}(2)\right)_k \right]_+ \right\rangle \\ &= -\mathrm{i}\Theta(t_1-t_2) \begin{pmatrix} \left\langle\left[\psi_\uparrow(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\uparrow(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow(2)\right]_+\right\rangle \\ \left\langle\left[\psi_\downarrow(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\uparrow(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow(2)\right]_+\right\rangle \\ -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow(2)\right]_+\right\rangle \\ -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow(2)\right]_+\right\rangle \end{pmatrix}\end{aligned} \tag{B.1a}$$

$$\begin{aligned}\hat{G}^{\mathrm{A}}(1,2) &= \begin{pmatrix} \bar{G}^{\mathrm{A}}(1,2) & \bar{F}^{\mathrm{A}}(1,2) \\ \left(\bar{F}^{\mathrm{A}}\right)^{*}(1,2) & \left(\bar{G}^{\mathrm{A}}\right)^{*}(1,2) \end{pmatrix} = \sum_{j} \mathrm{i}\Theta(t_2-t_1)(\hat{\rho}_3)_{ij} \left\langle \left[\left(\psi(1)\right)_j , \left(\psi^{\dagger}(2)\right)_k \right]_+ \right\rangle \\ &= \mathrm{i}\Theta(t_2-t_1) \begin{pmatrix} \left\langle\left[\psi_\uparrow(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\uparrow(2)\right]_+\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow(2)\right]_+\right\rangle \\ \left\langle\left[\psi_\downarrow(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\uparrow(2)\right]_+\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow(2)\right]_+\right\rangle \\ -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow(2)\right]_+\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow(2)\right]_+\right\rangle \\ -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow(2)\right]_+\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow(2)\right]_+\right\rangle \end{pmatrix}\end{aligned} \tag{B.1b}$$

$$\begin{aligned}\hat{G}^{\mathrm{K}}(1,2) &= \begin{pmatrix} \bar{G}^{\mathrm{K}}(1,2) & \bar{F}^{\mathrm{K}}(1,2) \\ -\left(\bar{F}^{\mathrm{K}}\right)^{*}(1,2) & -\left(\bar{G}^{\mathrm{K}}\right)^{*}(1,2) \end{pmatrix} = \sum_{j} (-\mathrm{i})(\hat{\rho}_3)_{ij} \left\langle \left[\left(\psi(1)\right)_j , \left(\psi^{\dagger}(2)\right)_k \right]_- \right\rangle \\ &= -\mathrm{i} \begin{pmatrix} \left\langle\left[\psi_\uparrow(1),\psi_\uparrow^\dagger(2)\right]_-\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow^\dagger(2)\right]_-\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\uparrow(2)\right]_-\right\rangle & \left\langle\left[\psi_\uparrow(1),\psi_\downarrow(2)\right]_-\right\rangle \\ \left\langle\left[\psi_\downarrow(1),\psi_\uparrow^\dagger(2)\right]_-\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow^\dagger(2)\right]_-\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\uparrow(2)\right]_-\right\rangle & \left\langle\left[\psi_\downarrow(1),\psi_\downarrow(2)\right]_-\right\rangle \\ -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_-\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_-\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\uparrow(2)\right]_-\right\rangle & -\left\langle\left[\psi_\uparrow^\dagger(1),\psi_\downarrow(2)\right]_-\right\rangle \\ -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow^\dagger(2)\right]_-\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow^\dagger(2)\right]_-\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\uparrow(2)\right]_-\right\rangle & -\left\langle\left[\psi_\downarrow^\dagger(1),\psi_\downarrow(2)\right]_-\right\rangle \end{pmatrix}\end{aligned} \tag{B.1c}$$

B.2 Symmetries

We will now derive some relations between the different Green's functions.

$$
\begin{aligned}
\left[\hat{\rho}_3\hat{G}^{\mathrm{R}}(2,1)\hat{\rho}_3\right]^\dagger_{hk} &= \sum_{ijl} (\hat{\rho}_3)_{hi}\, \mathrm{i}\Theta(t_2-t_1) \left[(\hat{\rho}_3)_{ij} \left\langle \left[(\psi(2))_j\,, \left(\psi^\dagger(1)\right)_l\right]_+ \right\rangle\right]^\dagger (\hat{\rho}_3)_{lk} \\
&= \sum_{ijl} (\hat{\rho}_3)_{hi}\, \mathrm{i}\Theta(t_2-t_1) \left\langle \left[(\psi(1))_i\,, \left(\psi^\dagger(2)\right)_j\right]_+ \right\rangle (\hat{\rho}_3)_{jl}\, (\hat{\rho}_3)_{lk} \\
&= \sum_{i} \mathrm{i}\Theta(t_2-t_1)\, (\hat{\rho}_3)_{hi} \left\langle \left[(\psi(1))_i\,, \left(\psi^\dagger(2)\right)_k\right]_+ \right\rangle \\
&= \left(\hat{G}^{\mathrm{A}}\right)_{hk}.
\end{aligned}
\tag{B.2}
$$

Let us now find the corresponding result for the quasiclassical Green's functions. Using the definitions we get

$$
\begin{aligned}
\hat{g}^{\mathrm{A}}(X,\boldsymbol{p}_F,E) =& \frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \hat{G}^{\mathrm{A}}\left(X+\frac{x}{2}, X-\frac{x}{2}\right) \\
=& \frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \left[\hat{\rho}_3\hat{G}^{\mathrm{R}}\left(X+\frac{-x}{2}, X-\frac{-x}{2}\right)\hat{\rho}_3\right]^\dagger \\
=& -\left[\frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{+\mathrm{i}px} \hat{\rho}_3\hat{G}^{\mathrm{R}}\left(X+\frac{-x}{2}, X-\frac{-x}{2}\right)\hat{\rho}_3\right]^\dagger \\
=& -\left[\frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \hat{\rho}_3\hat{G}^{\mathrm{R}}\left(X+\frac{x}{2}, X-\frac{x}{2}\right)\hat{\rho}_3\right]^\dagger \\
=& -\left[\hat{\rho}_3\hat{g}^{\mathrm{R}}(X,\boldsymbol{p}_F,E)\hat{\rho}_3\right]^\dagger.
\end{aligned}
\tag{B.3}
$$

This relation means that if we can calculate $\hat{g}^{\mathrm{R}}$ we also know $\hat{g}^{\mathrm{A}}$.

Let us consider in more detail the retarded quasiclassical Green's function. Denote the quasiclassical counterpart of $\bar{G}^{\mathrm{R}}$, $\bar{F}^{\mathrm{R}}$ by $\bar{g}^{\mathrm{R}}$, $\bar{f}^{\mathrm{R}}$. The symmetry between the diagonal blocks of $\hat{G}^{\mathrm{R}}$ in the quasiclassical case will now be calculated:

$$
\begin{aligned}
&\frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \left[\bar{G}^{R}\left(X+\frac{x}{2}, X-\frac{x}{2}\right)\right]^* \\
&= -\left[\frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}(-p)x} \bar{G}^{R}\left(X+\frac{x}{2}, X-\frac{x}{2}\right)\right]^* = -\left[\bar{g}^{\mathrm{R}}(X,-\boldsymbol{p}_F,-E)\right]^*,
\end{aligned}
\tag{B.4}
$$

and similarly for the anomalous component

$$
\frac{\mathrm{i}}{\pi}\int \mathrm{d}\xi_{\boldsymbol{p}} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \left[\bar{F}^{R}\left(X+\frac{x}{2}, X-\frac{x}{2}\right)\right]^* = -\left[\bar{f}^{\mathrm{R}}(X,-\boldsymbol{p}_F,-E)\right]^*.
\tag{B.5}
$$

Altogether, the quasiclassical Green's function is

$$
\hat{g}^{\mathrm{R}}(X,\boldsymbol{p}_F,E) = \begin{pmatrix} \bar{g}^{\mathrm{R}}(X,\boldsymbol{p}_F,E) & \bar{f}^{\mathrm{R}}(X,\boldsymbol{p}_F,E) \\ -\left[\bar{f}^{\mathrm{R}}(X,-\boldsymbol{p}_F,-E)\right]^* & -\left[\bar{g}^{\mathrm{R}}(X,-\boldsymbol{p}_F,-E)\right]^* \end{pmatrix}.
\tag{B.6}
$$

Appendix C

Equilibrium Solutions

In this appendix we will derive the quasiclassical Green's functions in the special case of equilibrium. Some important relations which are needed elsewhere will also be discussed here. Finally we consider the limit in which the superconducting gap disappears, that is we consider the case of normal metal.

C.1 Quasiclassical Green's Functions

The equation of motion for the Green's function in thermal equilibrium inside a superconductor without electromagnetic field (see Equation (3.46))

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}\hat{\rho}_3 - \hat{\xi} - \hat{\Delta}\right)\check{G}(1,2) = \delta(1-2)\check{1}, \tag{C.1}$$

where $\hat{\xi} = -\frac{1}{2m}\nabla_1^2\hat{1}$. For a homogeneous and isotropic system the Green's function only depends on the relative coordinates, i.e. $\check{G}(\boldsymbol{r}_1, t_1, \boldsymbol{r}_2, t_2) = \check{G}(\boldsymbol{r}_1 - \boldsymbol{r}_2, t_1 - t_2)$. Fourier transforming into the coordinates $(\boldsymbol{p}, E)$ we get

$$\left(E\hat{\rho}_3 - \hat{\xi}_{\boldsymbol{p}} - \hat{\Delta}\right)\check{G}(\boldsymbol{p}, E) = \check{1}. \tag{C.2}$$

We have now introduced the symbol $\hat{\xi}_{\boldsymbol{p}} = \xi_{\boldsymbol{p}}\hat{1} = \frac{\boldsymbol{p}^2}{2m}\hat{1}$. The upper left diagonal block determines the retarded component, $\hat{G}^{\mathrm{R}}$. The matrix equation in this block can be solved formally for

$$\hat{G}^{\mathrm{R}}(\boldsymbol{p}, E) = \left[E\hat{\rho}_3 - \hat{\xi}_{\boldsymbol{p}} - \hat{\Delta}\right]^{-1}. \tag{C.3}$$

The inverse Fourier transform will be performed by residue calculation in the complex plane. Since the integrand will contain a factor $\mathrm{e}^{-\mathrm{i}Et} = \mathrm{e}^{-\mathrm{i}t\Re\{E\}+t\Im\{E\}}$, we must now add a convergence factor. If $t > 0$ the contour must be closed in the lower half-plane where the factor $\mathrm{e}^{t\Im\{E\}}$ will ensure convergence, and if $t < 0$ we must close the contour in the upper half-plane. $t > 0$ also corresponds to a nonzero retarded Green's function. Thus in this case the pole in the E-integration must be shifted below the real axis. This can be done by writing $E \to E + \mathrm{i}\delta$, where δ is an infinitesimal positive number. Then for $t < 0$ the contour does not contain any singularity and the retarded Green's function, $\hat{G}^{\mathrm{R}}$, will be identically zero. Performing the matrix inversion we obtain for the retarded Green's function

$$\hat{G}^{\mathrm{R}}(\boldsymbol{p},E) = \left[(E+\mathrm{i}\delta)\hat{\rho}_3 - \hat{\xi}_{\boldsymbol{p}} - \hat{\Delta}\right]^{-1}$$
$$= \hat{\rho}_3 \frac{E}{(E+\mathrm{i}\delta)^2 - |\Delta|^2 - \xi_{\boldsymbol{p}}^2} + \hat{1}\frac{\hat{\xi}_{\boldsymbol{p}}}{(E+\mathrm{i}\delta)^2 - |\Delta|^2 - \xi_{\boldsymbol{p}}^2} - \hat{\Delta}\frac{1}{(E+\mathrm{i}\delta)^2 - |\Delta|^2 - \xi_{\boldsymbol{p}}^2}. \tag{C.4}$$

The quasiclassical Green's function was defined as

$$\hat{g}^{\mathrm{R}}(X,p) = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \hat{G}^{\mathrm{R}}(X,p). \tag{C.5}$$

The middle term in (C.4) is an odd function in $\xi_{\boldsymbol{p}}$ so that the integral will be zero. Only the terms proportional to $\hat{\rho}_3$ and $\hat{\Delta}$ give contributions, leading us to consider the integral

$$I = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \frac{1}{(E+\mathrm{i}\delta)^2 - |\Delta|^2 - \xi_{\boldsymbol{p}}^2} = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \frac{1}{E^2 - |\Delta|^2 - \xi_{\boldsymbol{p}}^2 + \mathrm{i}\delta'\mathrm{sgn}(E)}. \tag{C.6}$$

We have neglected higher order terms in δ, and $\delta' = 2\delta|E|$ is another infinitesimal. We will now distinguish between the two cases $E^2 > |\Delta|^2$ and $E^2 < |\Delta|^2$.

1) $E^2 > |\Delta|^2$

$$I = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \left[\frac{1}{\sqrt{E^2 - |\Delta|^2 + \mathrm{i}\delta''\mathrm{sgn}(E)} - \xi_{\boldsymbol{p}}} \times \frac{1}{\sqrt{E^2 - |\Delta|^2 + \mathrm{i}\delta''\mathrm{sgn}(E)} + \xi_{\boldsymbol{p}}}\right]$$
$$= \frac{\mathrm{i}}{\pi}(-2\pi\mathrm{i})\mathrm{sgn}(E) \lim_{\xi_{\boldsymbol{p}} \to -\sqrt{E^2-|\Delta|^2}} \left[(\xi_{\boldsymbol{p}} + \sqrt{E^2 - |\Delta|^2})\frac{1}{\sqrt{E^2 - |\Delta|^2} - \xi_{\boldsymbol{p}}} \times \frac{1}{\sqrt{E^2 - |\Delta|^2} + \xi_{\boldsymbol{p}}}\right]$$
$$= \frac{\mathrm{sgn}(E)}{\sqrt{E^2 - |\Delta|^2}} \tag{C.7}$$

Here we have used the integration contour in Figure C.1 (an extra negative sign has been introduced since the contour is traversed in the negative direction), and the factor sgn(E) corresponds to different locations of the poles as indicated in the figure. $\delta'' = \frac{1}{2}\frac{1}{\sqrt{E^2-|\Delta|^2}}\delta'$ is yet another infinitesimal.

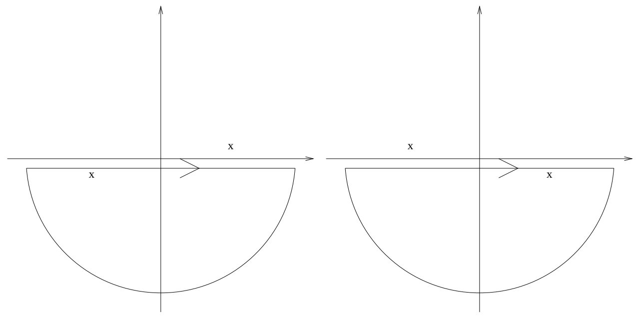
2) $E^2 < |\Delta|^2$

If we first rewrite the integral to

$$I = -\frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi_{\boldsymbol{p}} \frac{1}{|\Delta|^2 - E^2 + \xi_{\boldsymbol{p}}^2 - \mathrm{i}\delta'\mathrm{sgn}(E)}, \tag{C.8}$$

we can easily see that the poles are now on the imaginary axis, $\xi_{\boldsymbol{p}} = \pm\mathrm{i}\sqrt{|\Delta|^2 - E^2}$, and the infinitesimal is irrelevant. We use the integration contour in Figure C.2 and obtain

$$I = -\frac{\mathrm{i}}{\pi} 2\pi\mathrm{i}\,\frac{1}{2\xi_{\boldsymbol{p}}}\bigg|_{\xi_{\boldsymbol{p}}=\mathrm{i}\sqrt{|\Delta|^2-E^2}} = -\frac{\mathrm{i}}{\sqrt{|\Delta|^2 - E^2}}. \tag{C.9}$$



(a) Location of poles for $\mathrm{sgn}(E) = +1$.

(b) Location of poles for $\mathrm{sgn}(E) = -1$.

Figure C.1: The "x" mark the poles at $\xi_{\boldsymbol{p}} = \pm\sqrt{E^2 - |\Delta|^2}$. The residue for the the two different situations differ only by sign.

Our result for the quasiclassical, retarded propagator is

$$
\begin{aligned}
\hat{g}^{\mathrm{R}}(E) =& \hat{\rho}_3 \left[\frac{|E|}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}E}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2) \right] \\
&- \hat{\Delta} \left[\frac{\mathrm{sgn}(E)}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2) \right].
\end{aligned} \tag{C.10}
$$

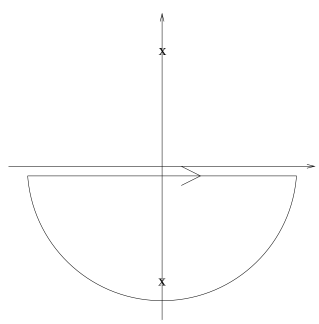


Figure C.2: The "x" mark the poles at $\xi_{\boldsymbol{p}} = \pm \mathrm{i}\sqrt{|\Delta|^2 - E^2}$.

To get the advanced propagator we must shift the pole to the upper half-plane by writing $E \to E - \mathrm{i}\delta$, and a similar calculation as for the retarded propagator gives

$$
\begin{aligned}
\hat{g}^{\mathrm{A}}(E) =& \hat{\rho}_3 \left[-\frac{|E|}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}E}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2) \right] \\
&- \hat{\Delta} \left[-\frac{\mathrm{sgn}(E)}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2) \right].
\end{aligned} \tag{C.11}
$$

C.2 Properties of Equilibrium Solutions

We will now derive the result $(\hat{g}^{\mathrm{R}})^2 = (\hat{g}^{\mathrm{A}})^2 = 1$. From the definitions we have $(\hat{\rho}_3)^2 = \hat{1}$ and $(\hat{\Delta})^2 = -|\Delta|^2\hat{1}$. Cross terms will be of the form $(\hat{\rho}_3\hat{\Delta} + \hat{\Delta}\hat{\rho}_3)[...] = 0$ which is seen by performing the matrix multiplications. Products like $\Theta(E^2 - |\Delta|^2)\Theta(|\Delta|^2 - E^2) = 0$ by the properties of the Heaviside step function. For the retarded propagator we now find

$$\begin{aligned}(\hat{g}^{\mathrm{R}})^2 =& \hat{1}\left[\frac{|E|}{\sqrt{E^2 - |\Delta|^2}}\Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}E}{\sqrt{|\Delta|^2 - E^2}}\Theta(|\Delta|^2 - E^2)\right]^2 \\ &- |\Delta|^2\hat{1}\left[\frac{\mathrm{sgn}(E)}{\sqrt{E^2 - |\Delta|^2}}\Theta(E^2 - |\Delta|^2) - \frac{\mathrm{i}}{\sqrt{|\Delta|^2 - E^2}}\Theta(|\Delta|^2 - E^2)\right]^2 \\ =& \hat{1}\frac{E^2}{E^2 - |\Delta|^2} - |\Delta|^2\hat{1}\frac{1}{E^2 - |\Delta|^2} = \hat{1}. \end{aligned} \tag{C.12}$$

The calculation for the advanced propagator is similar.

In the homogeneous, stationary case there is a relation between the average value of the commutator and anticommutator. This result is derived in Chapter 3.3.2 in the textbook by Zagoskin [32] and states that for some operator $\mathcal{A}(t)$,

$$\int \mathrm{d}t e^{\mathrm{i}\omega t}\left\langle [\mathcal{A}(t), \mathcal{A}(0)]_- \right\rangle = \int \mathrm{d}t e^{\mathrm{i}\omega t}\left\langle [\mathcal{A}(t), \mathcal{A}(0)]_+ \right\rangle \tanh\left(\frac{\beta\omega}{2}\right). \tag{C.13}$$

We can use this result to obtain a definite connection between $\hat{G}^{\mathrm{K}}$ and $\hat{G}^{\mathrm{R}}$, $\hat{G}^{\mathrm{A}}$. Using the matrix element representation of the Green's functions given in Appendix B and Fourier transforming we get

$$\begin{aligned}&\int \mathrm{d}x e^{-\mathrm{i}px}\left\{\mathrm{i}\left(\hat{G}^{\mathrm{R}}(X + \frac{x}{2}, X - \frac{x}{2})\right)_{ik} - \mathrm{i}\left(\hat{G}^{\mathrm{A}}(X + \frac{x}{2}, X - \frac{x}{2})\right)_{ik}\right\}\tanh\left(\frac{\beta E}{2}\right) \\ &= \int \mathrm{d}x e^{-\mathrm{i}px}\left\{\Theta(t_1 - t_2) + \Theta(t_2 - t_1)\right\}\sum_j (\hat{\rho}_3)_{ij}\left\langle\left[(\psi(1))_j, \left(\psi^\dagger(2)\right)_k\right]_+\right\rangle\tanh\left(\frac{\beta E}{2}\right) \\ &= \int \mathrm{d}x e^{-\mathrm{i}px}\sum_j (\hat{\rho}_3)_{ij}\left\langle\left[(\psi(1))_j, \left(\psi^\dagger(2)\right)_k\right]_+\right\rangle\tanh\left(\frac{\beta E}{2}\right) \\ &= \int \mathrm{d}x e^{-\mathrm{i}px}\sum_j (\hat{\rho}_3)_{ij}\left\langle\left[(\psi(1))_j, \left(\psi^\dagger(2)\right)_k\right]_-\right\rangle = \int \mathrm{d}x e^{-\mathrm{i}px}\mathrm{i}\left(\hat{G}^{\mathrm{K}}(X + \frac{x}{2}, X - \frac{x}{2})\right)_{ik},\end{aligned} \tag{C.14}$$

where (C.13) was used in the third step. In another notation we may write this result as

$$\boxed{\hat{G}^{\mathrm{K}}(X, p) = \left\{\hat{G}^{\mathrm{R}}(X, p) - \hat{G}^{\mathrm{A}}(X, p)\right\}\tanh\left(\frac{\beta E}{2}\right),} \tag{C.15}$$

and the same relation applies also to the quasiclassical Green's functions.

Using this result we will prove a relation which is needed in connection with the normalization of the full 8×8 quasiclassical Green's function matrix, $\check{g}$,

$$\begin{aligned}\hat{g}^{\mathrm{R}}\hat{g}^{\mathrm{K}} + \hat{g}^{\mathrm{K}}\hat{g}^{\mathrm{A}} &= \left\{\left(\hat{g}^{\mathrm{R}}\right)^2 - \hat{g}^{\mathrm{R}}\hat{g}^{\mathrm{A}} + \hat{g}^{\mathrm{R}}\hat{g}^{\mathrm{A}} - \left(\hat{g}^{\mathrm{A}}\right)^2\right\}\tanh\left(\frac{\beta E}{2}\right) \\ &= \left\{\hat{1} - \hat{1}\right\}\tanh\left(\frac{\beta E}{2}\right) = 0.\end{aligned} \tag{C.16}$$

We will conclude this section by demonstrating how the gap may be calculated from the quasiclassical Green's functions using Equation (4.54)

$$\Delta = -\frac{1}{8}N_0\lambda\mathrm{Tr}\left\{\frac{\hat{\rho}_1 - \mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3 \int \mathrm{d}E\hat{g}^{\mathrm{K}}(X, \boldsymbol{p}_{\mathrm{F}}, E)\right\}\Bigg|_{X=(\boldsymbol{r_1},t_1)}.$$

To this end (C.15) will once again be used since we can now find $\hat{g}^{\mathrm{K}}$ from the known retarded and advanced solutions. We find that

$$\hat{g}^{\mathrm{R}} - \hat{g}^{\mathrm{A}} = 2\hat{\rho}_3\frac{|E|}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2) - 2\hat{\Delta}\frac{\mathrm{sgn}(E)}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2), \tag{C.17}$$

but since $\mathrm{Tr}\left\{\frac{\hat{\rho}_1-\mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\hat{\rho}_3\right\} = 0$, $\mathrm{Tr}\left\{\frac{\hat{\rho}_1-\mathrm{i}\hat{\rho}_2}{2}\hat{\tau}_3\hat{\Delta}\right\} = 2\Delta$, only one term survives. Inserted into the gap equation we get

$$\Delta = \frac{1}{2}N_0\lambda\int_{-\infty}^{\infty}\mathrm{d}E\Delta\frac{\mathrm{sgn}(E)}{\sqrt{E^2-|\Delta|^2}}\Theta(E^2-|\Delta|^2)\tanh\left(\frac{\beta E}{2}\right).$$

The Δ can be canceled from the equation since we are considering a BCS reservoir in equilibrium where this quantity is a constant. Since both $\tanh\left(\frac{\beta E}{2}\right)$ and $\mathrm{sgn}(E)$ are odd functions of E the integrand is even and we may simplify the integral taking the step function into account

$$1 = N_0\lambda\int_{|\Delta|}^{\infty}\mathrm{d}E\frac{\tanh\left(\frac{\beta E}{2}\right)}{\sqrt{E^2-|\Delta|^2}}.$$

To make the analogy with standard BCS theory more evident let us change integration variable to ξ. Since $\xi = \sqrt{E^2-|\Delta|^2}$ we have $\frac{\mathrm{d}\xi}{\mathrm{d}E} = \frac{E}{\sqrt{E^2-|\Delta|^2}}$. This brings our gap equation into

$$\begin{aligned}\frac{1}{N_0\lambda} &= \int_0^{\infty}\mathrm{d}\xi\left(\frac{\mathrm{d}\xi}{\mathrm{d}E}\right)^{-1}\frac{\tanh\left(\frac{\beta E}{2}\right)}{\sqrt{E^2-|\Delta|^2}} \\ &= \int_0^{\infty}\mathrm{d}\xi\frac{\tanh\left(\frac{\beta E}{2}\right)}{E},\end{aligned} \tag{C.18}$$

which with the introduction of a Debye cut-off for the integral corresponds to Equation (2-53) in the textbook by Tinkham [6].

C.3 Normal Metal

In the limiting case of a normal metal the gap disappears, $\Delta = 0$. Taking this limit in the results above we find

$$\hat{g}^{\mathrm{R}} = \hat{\rho}_3 = -\hat{g}^{\mathrm{A}}. \tag{C.19}$$

The Keldysh component of the propagator is determined by the upper right block of Equation (C.2),

$$\left(E\hat{\rho}_3 - \hat{\xi}_{\boldsymbol{p}} - \hat{\Delta}\right)\hat{G}^{\mathrm{K}}(\boldsymbol{p}, E) = 0, \tag{C.20}$$

which seems to suggest that $\hat{G}^{\mathrm{K}} = 0$. However, the situation is not as simple as that. Consider the definition of the 2×2 Keldysh Green's function in the absence of a superconducting gap,

$$\mathrm{i}\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(1,2) = \left\langle \psi_\sigma(1)\psi^\dagger_\sigma(2) - \psi^\dagger_\sigma(2)\psi_\sigma(1) \right\rangle. \tag{C.21}$$

We will now substitute the following plane-wave representation of the field operators

$$\psi_\sigma(1) = \sum_{\boldsymbol{p}_1} \frac{1}{\sqrt{V}} \mathrm{e}^{\mathrm{i}\boldsymbol{p}_1\cdot\boldsymbol{r}_1 - \mathrm{i}E_{\boldsymbol{p}_1}t_1} c_{\boldsymbol{p}_1\sigma}, \tag{C.22}$$

$$\psi^\dagger_{\sigma'}(2) = \sum_{\boldsymbol{p}_2} \frac{1}{\sqrt{V}} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}_2\cdot\boldsymbol{r}_2 + \mathrm{i}E_{\boldsymbol{p}_2}t_2} c^\dagger_{\boldsymbol{p}_2\sigma'}, \tag{C.23}$$

into the definition of $\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(1,2)$. This gives

$$\begin{aligned}
\mathrm{i}\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(1,2) =& \frac{1}{V}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} \left(\left\langle c_{\boldsymbol{p}_1\sigma} c^\dagger_{\boldsymbol{p}_2\sigma'} \right\rangle - \left\langle c^\dagger_{\boldsymbol{p}_2\sigma'} c_{\boldsymbol{p}_1\sigma} \right\rangle \right) \mathrm{e}^{\mathrm{i}(\boldsymbol{p}_1\cdot\boldsymbol{r}_1 - \boldsymbol{p}_2\cdot\boldsymbol{r}_2) - \mathrm{i}\left(E_{\boldsymbol{p}_1}t_1 - E_{\boldsymbol{p}_2}t_2\right)} && \text{(C.24)}\\
=& \frac{1}{V}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} \left(\delta_{\boldsymbol{p}_1,\boldsymbol{p}_2}\delta_{\sigma,\sigma'} - 2\left\langle c^\dagger_{\boldsymbol{p}_2\sigma'} c_{\boldsymbol{p}_1\sigma} \right\rangle \right) \mathrm{e}^{\mathrm{i}(\boldsymbol{p}_1\cdot\boldsymbol{r}_1 - \boldsymbol{p}_2\cdot\boldsymbol{r}_2) - \mathrm{i}\left(E_{\boldsymbol{p}_1}t_1 - E_{\boldsymbol{p}_2}t_2\right)} && \text{(C.25)}\\
=& \frac{1}{V}\delta_{\sigma\sigma'} \sum_{\boldsymbol{p}} \left(1 - 2n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right)\right) \mathrm{e}^{\mathrm{i}\boldsymbol{p}(\boldsymbol{r}_1 - \boldsymbol{r}_2) - \mathrm{i}E_{\boldsymbol{p}}(t_1 - t_2)}. && \text{(C.26)}
\end{aligned}$$

Here we have used the anticommutation relation for the momentum fermion creation/ annihilation-operators, orthogonality of states and taken the Fermi distribution at equilibrium to be defined by $n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right) = \left\langle c^\dagger_{\boldsymbol{p}\sigma} c_{\boldsymbol{p}\sigma} \right\rangle$. In the continuum limit we let $\frac{1}{V}\sum_{\boldsymbol{p}} \to \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}$, which gives

$$\mathrm{i}\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(\boldsymbol{r}_1 - \boldsymbol{r}_2, t_1 - t_2) = \delta_{\sigma\sigma'} \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \left(1 - 2n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right)\right) \mathrm{e}^{\mathrm{i}\boldsymbol{p}(\boldsymbol{r}_1 - \boldsymbol{r}_2) - \mathrm{i}E_{\boldsymbol{p}}(t_1 - t_2)}. \tag{C.27}$$

We will now perform the Fourier transform with respect to the relative coordinate $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. But we can recognize the inverse of this transformation already present in the expression, so that we get simply

$$\mathrm{i}\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(\boldsymbol{p}, t_1 - t_2) = \delta_{\sigma\sigma'} \left(1 - 2n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right)\right) \mathrm{e}^{-\mathrm{i}E_{\boldsymbol{p}}(t_1 - t_2)}. \tag{C.28}$$

The next step is to Fourier transform the relative-time coordinate, $t = t_1 - t_2$. Remembering that the Dirac delta function can be written as $2\pi\delta(\omega) = \int \mathrm{d}t\mathrm{e}^{\mathrm{i}\omega t}$ we get

$$\begin{aligned}
\mathrm{i}\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(\boldsymbol{p}, E) =& \delta_{\sigma\sigma'} \left(1 - 2n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right)\right) \int \mathrm{d}t\mathrm{e}^{\mathrm{i}(E - E_{\boldsymbol{p}})t} && \text{(C.29)}\\
=& 2\pi\delta_{\sigma\sigma'} \left(1 - 2n_{\mathrm{F}}\left(E_{\boldsymbol{p}}\right)\right) \delta(E - E_{\boldsymbol{p}}). && \text{(C.30)}
\end{aligned}$$

Using the identity

$$1 - 2n_{\mathrm{F}}(E) = 1 - 2\frac{1}{1 + \mathrm{e}^{-\beta E}} = \tanh\left(\frac{\beta E}{2}\right), \tag{C.31}$$

we find that

$$\bar{G}^{\mathrm{K}}_{\sigma\sigma'}(E, \boldsymbol{p}) = -2\pi\mathrm{i}\delta_{\sigma\sigma'} \tanh\left(\frac{\beta E_{\boldsymbol{p}}}{2}\right) \delta(E - E_{\boldsymbol{p}}). \tag{C.32}$$

The off-diagonal elements of $\hat{G}^{\mathrm{K}}$ are given by anomalous propagators. In the absence of a superconducting gap all these are zero. These arguments show that instead of simply being equal to zero, the Keldysh component should in the homogeneous, equilibrium case be diagonal and proportional to a delta function, i.e.

$$\hat{G}^{\mathrm{K}}(E,\boldsymbol{p}) = -\,2\pi\mathrm{i}\hat{\rho}_3 \tanh\left(\frac{\beta E}{2}\right)\delta(E-\xi_{\boldsymbol{p}}-|\Delta|). \tag{C.33}$$

The quasiclassical Keldysh Green's function is obtained by integrating with respect to $\xi_{\boldsymbol{p}}$, which gives

$$\hat{g}^{\mathrm{K}}(E,\boldsymbol{p}) = \frac{\mathrm{i}}{\pi}\int \xi_{\boldsymbol{p}}\hat{G}^{\mathrm{K}}(E,\boldsymbol{p}) = 2\hat{\rho}_3 \tanh\left(\frac{\beta E}{2}\right). \tag{C.34}$$

The above formulas also show that in this case

$$\hat{g}^{\mathrm{K}} = \left(\hat{g}^{\mathrm{R}} - \hat{g}^{\mathrm{A}}\right)\tanh\left(\frac{\beta E}{2}\right), \tag{C.35}$$

corresponding nicely with the result (C.15).

Appendix D

Star Product

In this appendix we will derive some relations concerning the "star-product" involving an infinite series of differentiations. This is a form of convolution which is a convenient starting point for the quasiclassical approximations.

D.1 General Formula

In this section we will prove the relation

$$\begin{aligned} A \otimes B(X,p) &= \int \mathrm{d}(x_1 - x_3) \mathrm{e}^{-\mathrm{i}p(x_1 - x_3)} \int \mathrm{d}x_2 A(x_1, x_2) B(x_2, x_3) \\ &= \mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B} - \partial_{p_A}\partial_{X_B}\right)/2} A(X,p) B(X,p). \end{aligned} \tag{D.1}$$

The star product ($\otimes$) is defined as the Fourier transform of the relative coordinate of the convolution of the intermediate variable as seen in the first line. The symbol ∂_{X_A} means the derivative of the function A with respect to the variable X etc. The center and relative coordinates are given by

$$x = x_1 - x_3, \qquad X = \tfrac{x_1 + x_3}{2}. \tag{D.2}$$

These definitions bring our expression for the star product into the form

$$\int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \int \mathrm{d}x_2 A\left(X + \frac{x}{2}, X + x_2\right) B\left(X + x_2, X - \frac{x}{2}\right), \tag{D.3}$$

where we have also shifted the x_2 variable by X, which is possible since the integral is over all of x_2 space. In this integral we will now change the variables of integration from (x, x_2) to the set (u, v) defined by

$$x = u + v, \tag{D.4}$$

$$x_2 = \frac{u - v}{2}. \tag{D.5}$$

The Jacobi determinant is[1]

$$\left| \frac{\partial(x, x_2)}{\partial(u, v)} \right| = \begin{vmatrix} 1 & 1 \\ \frac{1}{2} & -\frac{1}{2} \end{vmatrix} = -1, \tag{D.6}$$

[1]Note that the pipes in this expression denote determinant, not absolute value. However, it is the absolute value of the determinant that enters into the transformed integral.

thus the transformed integral is

$$\int \mathrm{d}u \int \mathrm{d}v \mathrm{e}^{-\mathrm{i}p(u+v)} A\left(X+\frac{u+v}{2}, X+\frac{u-v}{2}\right) B\left(X+\frac{u-v}{2}, X-\frac{u+v}{2}\right). \quad \text{(D.7)}$$

If we now define the related functions $\tilde{A}$ and $\tilde{B}$ by

$$\tilde{A}(x,y) = A\left(x+\frac{y}{2}, x-\frac{y}{2}\right), \quad \text{(D.8a)}$$

$$\tilde{B}(x,y) = B\left(x+\frac{y}{2}, x-\frac{y}{2}\right), \quad \text{(D.8b)}$$

we may write this as

$$\int \mathrm{d}u \int \mathrm{d}v \mathrm{e}^{-\mathrm{i}p(u+v)} \tilde{A}\left(X+\frac{u}{2}, v\right) \tilde{B}\left(X-\frac{v}{2}, u\right). \quad \text{(D.9)}$$

We will now perform a Taylor expansion of $\tilde{A}$ and $\tilde{B}$ in the u and v variables, respectively

$$\tilde{A}\left(X+\frac{u}{2}, v\right) = \sum_{n=0}^{\infty} \frac{u^n}{n!} \left.\frac{\partial^n \tilde{A}\left(X+\frac{u}{2}, v\right)}{\partial u^n}\right|_{u=0} = \sum_{n=0}^{\infty} \frac{u^n}{n!} \left(\frac{1}{2}\right)^n \frac{\partial^n \tilde{A}\left(X, v\right)}{\partial X^n}, \quad \text{(D.10)}$$

$$\tilde{B}\left(X-\frac{v}{2}, u\right) = \sum_{m=0}^{\infty} \frac{v^m}{m!} \left.\frac{\partial^m \tilde{B}\left(X-\frac{v}{2}, u\right)}{\partial v^m}\right|_{v=0} = \sum_{m=0}^{\infty} \frac{v^m}{m!} \left(-\frac{1}{2}\right)^m \frac{\partial^m \tilde{B}\left(X, u\right)}{\partial X^m}. \quad \text{(D.11)}$$

Using these expressions in the integral we are considering and collecting terms we get

$$\begin{aligned}
&\sum_{n,m} \frac{1}{n!}\frac{1}{m!} \left(\partial_{X_A}\right)^n \left(\partial_{X_B}\right)^m \int \mathrm{d}v \tilde{A}(X,v) \left(-\frac{v}{2}\right)^m \mathrm{e}^{-\mathrm{i}pv} \int \mathrm{d}u \tilde{B}(X,u) \left(\frac{u}{2}\right)^n \mathrm{e}^{-\mathrm{i}pu} \\
=&\sum_{n,m} \frac{1}{n!}\frac{1}{m!} \left(\partial_{X_A}\right)^n \left(\partial_{X_B}\right)^m \\
&\times \left[\left(-\frac{\mathrm{i}}{2}\right)^m (\partial_p)^m \int \mathrm{d}v \tilde{A}(X,v) \mathrm{e}^{-\mathrm{i}pv}\right] \left[\left(\frac{\mathrm{i}}{2}\right)^n (\partial_p)^n \int \mathrm{d}u \tilde{B}(X,u) \mathrm{e}^{-\mathrm{i}pu}\right] \\
=&\sum_{n,m} \frac{1}{n!}\frac{1}{m!} \left(\partial_{X_A}\right)^n \left(\partial_{p_B}\right)^n \left(\partial_{X_B}\right)^m \left(\partial_{p_A}\right)^m \\
&\times \int \mathrm{d}v \mathrm{e}^{-\mathrm{i}pv} A\left(X+\frac{v}{2}, X-\frac{v}{2}\right) \int \mathrm{d}u \mathrm{e}^{-\mathrm{i}pu} B\left(X+\frac{u}{2}, X-\frac{u}{2}\right) \mathrm{e}^{-\mathrm{i}pu} \\
=&\sum_{n,m} \frac{1}{n!} \left(\partial_{X_A}\right)^n \left(\partial_{p_B}\right)^n \frac{1}{m!} \left(\partial_{X_B}\right)^m \left(\partial_{p_A}\right)^m A(X,p) B(X,p) \\
=&\mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B} - \partial_{p_A}\partial_{X_B}\right)/2} A(X,p) B(X,p),
\end{aligned} \quad \text{(D.12)}$$

which proves relation (D.1). Note that in the 4-vector notation the covariant operator carries an extra negative sign on the time component (because of our definition of the Fourier transformation), so that the expansion of the exponential reads to first order

$$A \otimes B = A \cdot B + \frac{\mathrm{i}}{2}\left[-\frac{\partial A}{\partial T}\frac{\partial B}{\partial E} + \nabla_{\boldsymbol{R}} A \nabla_{\boldsymbol{p}} B + \frac{\partial A}{\partial E}\frac{\partial B}{\partial T} - \nabla_{\boldsymbol{p}} A \nabla_{\boldsymbol{R}} B\right]. \quad \text{(D.13)}$$

In the quasiclassical approximation we only keep these two first terms in the series.

D.2 Special Cases

If one of the functions depends only on one variable, e.g. $A = A(x)$, the star product is understood as simply the Fourier transform of the relative coordinate (no convolution). Formula (D.1) applies to these cases also (with A independent of p in the final expression). These special cases become

$$\begin{aligned}
A \otimes B(X,p) =& \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} A\left(X + \frac{x}{2}\right) B\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{1}{2}\right)^n \frac{\partial^n A(X)}{\partial X^n} x^n B\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \sum_{n=0}^{\infty} \frac{1}{n!}\left(\partial_{X_A}\right)\left(\frac{\mathrm{i}}{2}\right)^n \left(\partial_p\right)^n A(X) \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} B\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B}\right)/2} A(X) B(X,p),
\end{aligned} \tag{D.14}$$

and similarly for $B = B(X)$

$$A \otimes B(X,p) = \mathrm{e}^{-\mathrm{i}\left(\partial_{p_A}\partial_{X_B}\right)/2} A(X,p) B(X). \tag{D.15}$$

The factors A or B might be derivatives, but such cases are also covered by the general formula (D.1). Consider e.g. a divergence

$$(\nabla \cdot \boldsymbol{A}) \otimes B(X,p) = \int \mathrm{d}(x_1 - x_2) \mathrm{e}^{-\mathrm{i}p(x_1 - x_2)} (\nabla_1 \cdot \boldsymbol{A}(x_1)) B(x_1, x_2). \tag{D.16}$$

Define the function $\tilde{A}(x) = \nabla \cdot \boldsymbol{A}(x)$. By the general formula it follows

$$\tilde{A} \otimes B(X,p) = \mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B}\right)/2} \tilde{A}(X) B(X,p), \tag{D.17}$$

where $\tilde{A}(X) = \nabla_{\boldsymbol{R}} \cdot \boldsymbol{A}(X)$ so that

$$(\nabla \cdot \boldsymbol{A}) \otimes B(X,p) = \mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B}\right)/2} \left(\nabla_{\boldsymbol{R}} \cdot \boldsymbol{A}(X)\right) B(X,p), \tag{D.18}$$

and similarly with $\nabla \cdot \boldsymbol{B}(x)$

$$A \otimes (\nabla \cdot B)(X,p) = \mathrm{e}^{-\mathrm{i}\left(\partial_{p_A}\partial_{X_B}\right)/2} A(X,p) \left(\nabla_{\boldsymbol{R}} \cdot \boldsymbol{B}(X)\right). \tag{D.19}$$

The Fourier transform turns derivatives with respect to the relative coordinate into multiplication with the conjugate variable. This can also be incorporated in the formula (D.1). Let us consider two special cases, first with $A = A(x_1)$, $B = B(x_1, x_2)$

$$\begin{aligned}
A \otimes \nabla_1 B(X,p) =& \int \mathrm{d}(x_1 - x_2) \mathrm{e}^{-\mathrm{i}p(x_1 - x_2)} A(x_1) \nabla_1 B(x_1, x_2) \\
=& \sum_n \frac{1}{n!}\left(\frac{1}{2}\right)^n \frac{\partial^n A(X)}{\partial X^n} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} x^n \left(\nabla_{\boldsymbol{r}} + \frac{1}{2}\nabla_{\boldsymbol{R}}\right) B\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \sum_n \frac{1}{n!}\left(\frac{1}{2}\right)^n \frac{\partial^n A(X)}{\partial X^n} \mathrm{i}^n \frac{\partial^n}{\partial p^n} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} \left(\nabla_{\boldsymbol{r}} + \frac{1}{2}\nabla_{\boldsymbol{R}}\right) B\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \sum_n \frac{1}{n!}\left(\frac{1}{2}\right)^n \frac{\partial^n A(X)}{\partial X^n} \mathrm{i}^n \frac{\partial^n}{\partial p^n} \left(\mathrm{i}\boldsymbol{p} B(X,p) + \frac{1}{2}\nabla_{\boldsymbol{R}} B(X,p)\right) \\
=& \mathrm{e}^{\mathrm{i}\left(\partial_{X_A}\partial_{p_B}\right)/2} A(X) \left(\mathrm{i}\boldsymbol{p} B(X,p) + \frac{1}{2}\nabla_{\boldsymbol{R}} B(X,p)\right).
\end{aligned} \tag{D.20}$$

Now we consider $A = A(x_1, x_2)$, $B = B(x_2)$ and obtain in the same way

$$
\begin{aligned}
\nabla_2 A \otimes B(X,p) =& \int \mathrm{d}(x_1 - x_2)\mathrm{e}^{-\mathrm{i}p(x_1-x_2)} \left[\nabla_2 A(x_1,x_2)\right] B(x_2) \\
=& \sum \frac{1}{n!}\left(-\frac{1}{2}\right)^n \frac{\partial^n B(X)}{\partial X^n} \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}px} x^n \left(-\nabla_{\boldsymbol{r}} + \frac{1}{2}\nabla_{\boldsymbol{R}}\right) A\left(X + \frac{x}{2}, X - \frac{x}{2}\right) \\
=& \mathrm{e}^{-\mathrm{i}\left(\partial_{p_A}\partial_{X_B}\right)/2} \left(-\mathrm{i}\boldsymbol{p}A(X,p) + \frac{1}{2}\nabla_{\boldsymbol{R}} A(X,p)\right) B(X).
\end{aligned} \tag{D.21}
$$

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