Full Proximity Effect in Spin-Textured Superconductor|Ferromagnet Bilayers

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Abstract

The quasiclassical transport equation for superconductor/ferromagnet hybrid structures with electromagnetic fields, spin-orbit coupling, impurity scattering, and spin-flip scattering is derived from a microscopic Hamiltonian. We then derive the Usadel equation describing a superconductor/ferromagnet bilayer in diffusive equilibrium, and perform a Riccati parametrization of this equation. The result is a set of second-order differential equations, which can form the basis for future numerical investigations into the behaviour of such structures.

Contents

Preface

This thesis was submitted as a specialization project in theoretical condensed matter physics at the Norwegian University of Science and Technology, under supervision of professor Jacob Linder. It was produced as part of a 10 semester integrated Master's programme in Applied Physics and Mathematics, and amounts to 15 ECTS credits in the 9th semester of the programme.

I would especially like to thank my supervisor Jacob Linder for introducing me to the fascinating topic of superconductivity in proximity-coupled hybrid structures, and for his insightful guidance and discussions throughout the semester. I would also like to thank doctor Sol Jacobsen for some useful discussions about the technical details of the calculations. I look forward to continue the collaboration with both of you during the spring. Finally, I also want to thank my parents for always encouraging me to keep going and study hard.

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1 Introduction

1.1 Superconductivity

The first observations of superconductivity were made in 1911, when H. K. Onnes used liquid helium to cool mercury down to a temperature of 4.2 K, and observed that its electrical resistance suddenly vanished. The next major discovery was made in 1933, when W. Meissner and R. Ochsenfeld noted that superconductors expel magnetic fields. After these empirical discoveries, an early milestone in the quest for a theoretical description was the work of the F. and H. London in 1935, which related supercurrents to electromagnetic fields. Another major advancement was the subsequent work of V. L. Ginzburg and L. Landau in 1950, which described superconductivity in terms of a complex wavefunction that serves as an order parameter during the phase transition to a superconductor.[1,2] However, the exact microscopic origin of this wavefunction was still a mystery.

It was soon realized that the metals with a high resistivity at room temperature (e.g. niobium, lead, mercury, tin) became superconductive at higher temperatures than the ones with a low resistivity at room temperature (e.g. gold, silver, copper). Since the resistivity of a material was attributed to electron–phonon scattering, this suggested that phonons had to be involved in the mechanism behind superconductivity. This suggestion was further supported by observations that heavier isotopes of mercury became superconductive at lower temperatures, since the mass of an isotope is directly related to the phonon energy spectrum. Finally, J. Bardeen, L. N. Cooper, and J. R. Schrieffer managed to derive the first microscopic theory of superconductivity in 1957.[3] According to the BCS theory, attractive interactions between electrons can result in the formation of bosonic *Cooper pairs*, and these pairs can then condense to an electronic superfluid. It is precisely this electronic superfluid that the wavefunction in the earlier Ginzburg–Landau theory had described, and which was behind all of the peculiar features associated with superconductors. In all the superconductors that were known by the end of the 1950s, this attractive force was mediated by phonons. While the BCS theory has been very successful for low-temperature superconductors, the exact mechanism behind high-temperature superconductivity is still an open problem in condensed matter physics.

While the predictive power of the BCS theory lies in the full quantum mechanical formulation, the essential physics can be understood from a classical model of metals. Consider a positively charged ionic lattice permeated by a swarm of negatively

[1] An *order parameter* is a physical quantity that vanishes in some thermodynamic phases but not in others. For example, the magnetization of a ferromagnet is finite below the Curie temperature, but zero above this temperature; it is therefore an order parameter that characterizes this phase transition.

[2] For a history of superconductivity, see e.g. the first two chapters of Fossheim and Sudbø (2004) or the first chapter of Tinkham (1996).

[3] Bardeen, Cooper, and Schrieffer 1957.

charged electrons. As an electron moves through this structure, it will attract the ions in the surrounding lattice, which are then pulled out of their equilibrium positions and towards the electron. But since the electron is tens of thousands of times lighter than the ions, it can also move around hundreds of times faster, and so the ions will stay in this distorted state for a relatively long time after the electron has moved on. So the electron leaves an increased ion concentration in its wake, and the resulting positively charged tunnel may then attract a new electron. When the new electron travels through the tunnel, there is a finite energy barrier that must be overcome before it can be knocked out of the tunnel, and so the electron is protected against resistive scattering at low temperatures. This presents a simplified answer to how a supercurrent can flow through the superconductor.

The most significant attraction is actually between two electrons moving in opposite directions, since each electron can then move through the positive tunnel left by the other one. Furthermore, assuming that both electrons have roughly the Fermi velocity v_F, moving in opposite directions will maximize the relative velocity. This in turn minimizes the time spent in each others vicinity and the associated electrostatic repulsions. This kind of pairing between two electrons moving in opposite directions is what we call a Cooper pair. Since the two electrons in the Cooper pair are moving apart, individual Cooper pairs are not stable entities, but rather something that continuously form and break. In the quantum mechanical description of the phenomenon, the ionic lattice distortion discussed above is what we would call a phonon, and the Cooper pairs are unstable bosons with charge $2e$, no momentum, and no spin. For a visualization of the mechanism, see Figure 1.1.

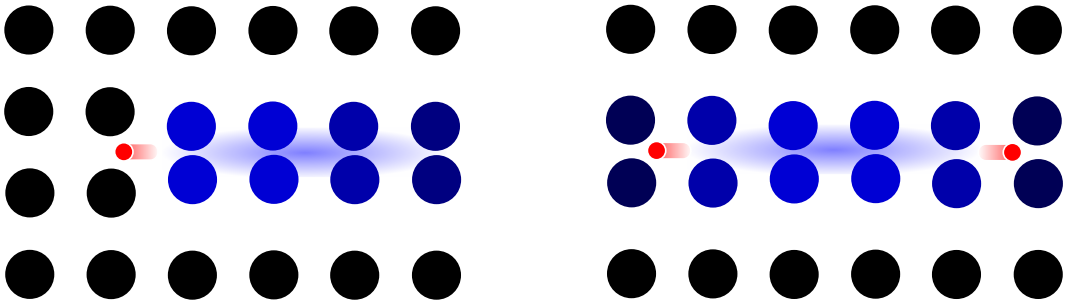

Figure 1.1: In the left figure, a single electron moves through the ionic lattice and leaves behind a positively charged lattice distortion. In the right figure, each electron in a Cooper pair moves through the lattice distortion left by the other electron.

1.2 Proximity effect

Particularly interesting physics can arise in mesoscopic hybrid structures that involve superconducting components in conjunction with other materials. One such phenomenon that has been known for a long time is the *proximity effect*, in which Cooper pairs leak across an interface from a superconductor into a normal metal. This means that the special properties of the superconductor can be induced in materials that originally did not possess them. Conversely, the normal metal drains the superconductor of Cooper pairs, and this has an adverse effect on the special properties of the superconductor, including a reduction of the critical temperature. This is known as the *inverse proximity effect*. When both effects are significant, the phenomenon is called the *full proximity effect*, and the Cooper pair wavefunction of such a system is illustrated in Figure 1.2.

The proximity effect in structures with ferromagnetic components has garnered a lot of interest in later years. At first, this might seem a bit odd, since it is well-known that superconductivity and ferromagnetism are competing forces. On one hand, superconductors expel magnetic fields through the Meissner effect; on the other hand, conventional Cooper pairs consist of a spin-up and a spin-down electron, and these would be pulled apart by a ferromagnetic exchange field. Thus the proximity effect in a superconductor/ferromagnet system is quite weak, and this has made many experiments on such systems prohibitively difficult until recently.

The theoretical consideration of the interplay between superconductivity and ferromagnetic exchange fields goes back to 1964, with the independent work of P. Fulde and R. A. Ferrell in the United States, and A. Larkin and Y. Ovchinnikov in the Soviet Union. They realized that the energy splitting between the spin-up and spin-down electron in a Cooper pair leads to a finite pair momentum, which in turn causes a spatial modulation of the wavefunction.[4] The difference between the wavefunction in a normal metal and a ferromagnet is shown in Figure 1.2.

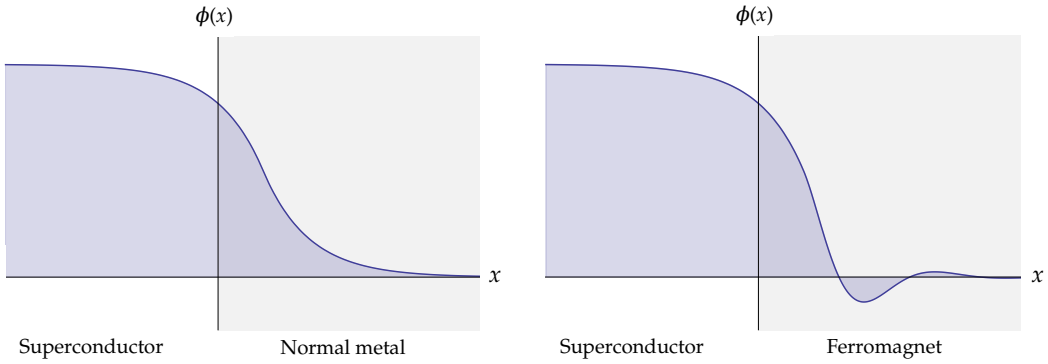

Figure 1.2: Sketch of the superconducting wavefunction $\phi(x)$ near the interface to a normal metal and homogeneous ferromagnet, assuming negligible interface resistance.

[4] For a quick summary of the existing research on superconductor/ferromagnet hybrid structures, see Eschrig (2011). A mathematical introduction to the subject is given by Buzdin (2005).

These oscillations led to several surprising predictions for the behaviour of superconductor/ferromagnet hybrid structures. Usually, when two superconductors are separated by some other material, they interact through the proximity effect in such a way that their complex phases align in the ground state. This structure is known as a Josephson junction, and one of its characteristics is that a supercurrent can flow between the superconductors, even though they are separated by a normal metal or even insulator. However, if the separating material is replaced by a ferromagnet, then the oscillations in the ferromagnetic region can lead to a ground state that is either symmetric (0-junction) or antisymmetric (π-junction). Furthermore, whether the structure is a 0-junction or a π-junction depends on parameters such as the temperature, the size of the ferromagnet, and the strength of the exchange field. The difference between sandwiching a normal metal and a ferromagnet between two superconductors is shown in Figure 1.3.

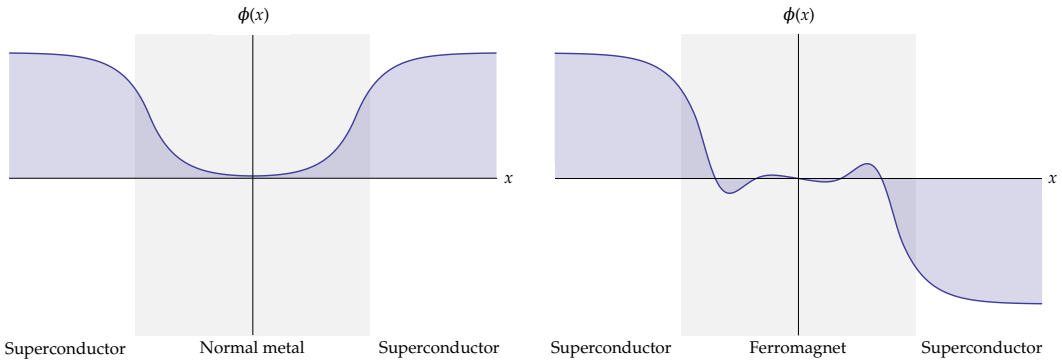

Figure 1.3: The left figure shows the behaviour of the superconducting wavefunction $\phi(x)$ in a socalled SNS structure, and the right figure shows the same situation for an SFS structure. While the wavefunction in a symmetric SNS structure has a symmetric ground state, it can also become antisymmetric in an SFS structure.

A series of experimental breakthroughs were then made in the early 2000s. Ryazanov et al. connected superconducting niobium electrodes to a ferromagnetic copper/nickel alloy, and measured the critical current across this Josephson junction as a function of temperature and applied magnetic field. They observed regions where the critical current dropped rapidly to zero and bounced back up, which was the first empirical evidence of transitions between a 0-junction and π-junction.[5] These findings were published almost simultaneously as the results by Kontos et al., who had had used tunneling spectroscopy to measure the density of states of a bilayer consisting of superconducting niobium and a ferromagnetic palladium/nickel alloy, which also clearly indicated the existence of both a 0-state and a π-state.[6]

The Cooper pairs in conventional superconductors have zero spin, which means that they are in the singlet state $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$.[7] However, it was realized that the spin-splitting of the energy bands in a ferromagnet introduces an oscillating phase

[5] Ryazanov et al. 2001.
[6] Kontos et al. 2001.
[7] We suppress overall normalization factors of $1/\sqrt{2}$ and $i/\sqrt{2}$ in this qualitative discussion.

difference between $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, which permits the singlet state to oscillate into a triplet state $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ and back, in a process known as *singlet–triplet mixing*. In other words, the ferromagnetic exchange field can actually generate new kinds of Cooper pairs, which are not present in sizeable quantities in conventional superconductors. F. S. Bergeret, A. F. Volkov, and K. B. Efetov published two papers in 2001 and 2005 demonstrating that an inhomogeneous magnetic field can lead to a *triplet–triplet mixing*, which further rotates $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ into the other triplet states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$.[8] Note that these new kinds of triplet pairs consist of electrons with the same spin, and they are therefore immune to usual pair-breaking effect of ferromagnets. This means that they can penetrate very deep into ferromagnets compared to other kinds of Cooper pairs, and they are therefore known as *long-range triplet components*. In half-metals, which are conductive for spin-up electrons and insulating for spin-down electrons, $|\uparrow\uparrow\rangle$ is the only contribution that survives deep inside the ferromagnet, leading to 100% spin-polarized supercurrents.

The first empirical observations of this effect were published in 2006, when Keizer et al. passed a supercurrent through up to 1 µm thick layers of half-metallic chromium dioxide, using superconducting niobium titanium nitride electrodes. This is much larger than the typical coherence length of around 1 nm for singlet components in ferromagnets.[9] Further evidence for the existence of long-range triplet superconductivity was found by Khaire et al. when studying a sophisticated multilayer Josephson junction in 2009.[10] A recent development on the theoretical side, was that F. S. Bergeret and I. V. Tokatly published two papers in 2013 and 2014 which showed that instead of using magnetic inhomogeneities, the long-range triplet components can also be generated by a spin-orbit coupling in the material.[11]

The mesoscopic superconductor/ferromagnet structures are interesting from a fundamental physics point of view because they produce entirely new physical phenomena, such as triplet pairing and spin-polarized supercurrents. It has also been shown that the dominant contributions to the long-range triplet component has even parity. Since the Pauli principle only allows the formation of Cooper pairs with an antisymmetric two-particle wavefunction, the only way for the pair to be symmetric in spin and spatial coordinates would be that it is antisymmetric in time, which leads to a peculiar phenomenon known as *odd-frequency superconductivity*. These hybrid structures also have great potential with respect to future applications. For instance, controlled creation and manipulation of spin-polarized supercurrents would revolutionize the emerging field of spintronics,[12] and the recent realization of Josephson π-junctions has already led to suggestions for novel circuit designs in both digital and quantum computing.[13]

[8] Bergeret, Volkov, and Efetov 2001; Bergeret, Volkov, and Efetov 2005.
[9] Keizer et al. 2006.
[10] Khaire et al. 2010.
[11] Bergeret and Tokatly 2013; Bergeret and Tokatly 2014.
[12] Eschrig 2011.
[13] Feofanov et al. 2010.

1.3 Structure

In this thesis, we rederive the celebrated Usadel equation under general conditions, so that all kinds of singlet and triplet superconductivity can be studied in the full proximity regime. The endeavour starts with a quick review of the preliminaries in chapter 2, including a brief discussion of nonequilibrium Green's functions and the quasiclassical approximation. Chapter 3 contains a derivation of the Hamiltonian for superconductor/ferromagnet hybrid structures with inhomogeneous exchange fields and spin-orbit coupling, which in the first half of chapter 4 is used to derive the exact transport equation for such a system. This is then followed by a series of approximations which culminates in the Usadel equation in the end of chapter 4. The original work presented in this thesis is the Riccati parametrization of these equations and their appropriate boundary conditions in chapter 5, which leads to a numerically tractable boundary value problem for the system.

2 Preliminaries

2.1 Mathematical conventions

Most of of the mathematical notation will follow the usual conventions in physics; real and complex numbers are written with a slightly slanted typeface as in a, b, c, while vectors and matrices are usually written with a boldfaced font as in $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The Cartesian unit vectors are $\hat{\mathbf{e}}_x$, $\hat{\mathbf{e}}_y$ and $\hat{\mathbf{e}}_z$. We write complex conjugation as $(a+ib)^* = a - ib$, matrix transposition as $\mathbf{M}^{\mathrm{T}}$, and Hermitian conjugation as $\psi^\dagger$. The symbols $\mathbf{0}$ and $\mathbf{1}$ represent the zero matrix and identity matrix, respectively. The commutator of two operators or matrices is defined as $[\mathbf{A}, \mathbf{B}]_- \equiv \mathbf{AB} - \mathbf{BA}$, and the anticommutator is $[\mathbf{A}, \mathbf{B}]_+ \equiv \mathbf{AB} + \mathbf{BA}$. Partial differentiation is written in the short-hand notation $\partial_t f(\mathbf{r}, t) \equiv \partial f(\mathbf{r}, t)/\partial t$, and the gradient is $\nabla \equiv \partial_x \hat{\mathbf{e}}_x + \partial_y \hat{\mathbf{e}}_y + \partial_z \hat{\mathbf{e}}_z$. Integration limits and summation ranges may be left implicit, at least when they should either be clear from context (like a sum over the possible spin configurations of an electron), or if they are yet unknown (such as an integral over the extent of a not yet defined system). The function $\theta(t)$ is the Heaviside step function, $\delta(t)$ is the Dirac delta function, and δ_{ij} is the Kronecker delta. Unless otherwise stated, $\mathbf{r}$ will usually mean a spatial coordinate, $\mathbf{p}$ a momentum value, σ a spin, ϵ an energy, and t a point in time. The Pauli matrices that span spin space are defined as:

$$\sigma^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.1}$$

The last three Pauli matrices are often collected in a mathematical object called the Pauli vector, which is defined as $\boldsymbol{\sigma} \equiv \sigma^1 \hat{\mathbf{e}}_x + \sigma^2 \hat{\mathbf{e}}_y + \sigma^3 \hat{\mathbf{e}}_z$. We will also be using the corresponding ladder matrices $\sigma^\pm \equiv \sigma^1 \pm i\sigma^2$:

$$\sigma^+ = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \qquad \sigma^- = \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix} \tag{2.2}$$

The Pauli matrices in Nambu space are defined in exactly the same way, but will be denoted by $\boldsymbol{\tau}$ instead of $\boldsymbol{\sigma}$. We will also use the convention that sums and products of incompatible matrices are evaluated by promoting the smaller matrix $\mathbf{M}$ to its Kronecker product $\mathbf{1} \otimes \mathbf{M}$ with the appropriate identity matrix. For example, if A is a scalar, $\mathbf{B}$ is a 2×2 matrix, and $\mathbf{C}$ is a 4×4 matrix, then we would interpret $A + \mathbf{BC}$ as follows:

$$A + \mathbf{BC} = \begin{bmatrix} A & 0 & 0 & 0 \\ 0 & A & 0 & 0 \\ 0 & 0 & A & 0 \\ 0 & 0 & 0 & A \end{bmatrix} + \begin{bmatrix} B_{11} & B_{12} & 0 & 0 \\ B_{21} & B_{22} & 0 & 0 \\ 0 & 0 & B_{11} & B_{12} \\ 0 & 0 & B_{21} & B_{22} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix} \tag{2.3}$$

2.2 Natural units

The laws of physics can be made simpler and more elegant by an appropriate choice of physical units. It is therefore common practice in theoretical physics to choose a unit system where the most common constants get numerical values of one, such that these constants can be removed from our equations. For example, Poisson's equations for gravity $\nabla^2\phi_{\mathrm{m}}(\mathbf{r},t) = -4\pi G\rho_{\mathrm{m}}(\mathbf{r})$ and electrostatics $\nabla^2\phi_{\mathrm{e}}(\mathbf{r}) = -\rho_{\mathrm{e}}(\mathbf{r})/\epsilon_0$ encourage us to pick a unit system where $4\pi G = \epsilon_0 = 1$. Similarly, Einstein's equation for a relativistic free particle $E^2 = p^2c^2 + m^2c^4$ would simplify to just $E^2 = p^2 + m^2$ if we could set the speed of light $c = 1$. In this thesis, we will use *rationalized natural units*, which means that the following constants are normalized to unity: Planck's reduced constant $\hbar$, Boltzmann's constant k, Newton's gravitational constant $4\pi G$, and the speed of light c. Since $c = 1/\sqrt{\epsilon_0\mu_0}$, we can also set the vacuum permittivity ϵ_0 and permeability μ_0 to unity. In other words:

$$\hbar = k = 4\pi G = c = \epsilon_0 = \mu_0 = 1 \tag{2.4}$$

This equation uniquely defines a system of physical units, which can be related to any other unit system by plugging in the experimental values of the constants in the equation. So we can say that the philosophy of natural units is the exact opposite of conventional units: instead of *defining* the base units and *measuring* the physical constants, we define the physical constants and then determine the basic measures by experiment. A short list of common natural units, as well as conversion factors for equivalent SI units, is provided in Table 2.1.

Table 2.1: Conversion table between rationalized natural units and some common SI units.

Quantity	Natural unit	Conversion factor
Length	$\sqrt{4\pi G\hbar/c^3}$	5.73×10^{-35} m
Time	$\sqrt{4\pi G\hbar/c^5}$	1.91×10^{-43} s
Mass	$\sqrt{\hbar c/4\pi G}$	6.14×10^{-9} kg
Energy	$\sqrt{\hbar c^5/4\pi G}$	5.52×10^{8} J
Temperature	$\sqrt{\hbar c^5/4\pi G k^2}$	4.00×10^{31} K
Charge	$\sqrt{\hbar c\epsilon_0}$	5.29×10^{-19} C

2.3 Quantum mechanics

From elementary quantum mechanics, we know that the state of a physical system can be represented as a *ket vector* $|\phi\rangle$ in Hilbert space. Each of these ket vectors is accompanied by a unique *bra vector* $\langle\phi|$, which is defined as the Hermitian conjugate of $|\phi\rangle$. All physically observable properties of the system are then represented as Hermitian operators A that act on such state vectors. The arguably most important role of these operators, is that they can be used to calculate the expectation values of physical observables. Specifically, if a system is prepared in the state $|\phi\rangle$ at time zero, and the observable corresponding to operator A is measured at some later time t, then the expectation value $\langle A\rangle$ for this measurement is:

$$\langle A\rangle = \langle\phi|e^{iHt}Ae^{-iHt}|\phi\rangle \tag{2.5}$$

Note the *time evolution operator* $e^{\pm iHt}$, which connects states and measurements defined at different times. The symbol H is the Hamiltonian operator of the system. In practice, we usually choose to absorb this time evolution into either the states, the observables, or both.

(i) **Schrödinger picture.** If we define time-dependent states $|\phi(t)\rangle \equiv e^{-iHt}|\phi\rangle$, then the expectation value of the observation becomes $\langle A\rangle = \langle\phi(t)|A|\phi(t)\rangle$. These states have to satisfy what is known as the *Schrödinger equation*:

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\phi(t)\rangle = H|\phi(t)\rangle \tag{2.6}$$

(ii) **Heisenberg picture.** If we define time-dependent operators $A(t) \equiv e^{iHt}Ae^{-iHt}$, then the expectation value $\langle A\rangle = \langle\phi|A(t)|\phi\rangle$. These operators satisfy the *Heisenberg equation*:[1]

$$i\frac{\mathrm{d}}{\mathrm{d}t}A(t) = [A(t), H]_- \tag{2.7}$$

(iii) **Interaction picture.** It is also possible to do both, meaning that $\langle A\rangle = \langle\phi(t)|A(t)|\phi(t)\rangle$. If we split the Hamiltonian into two parts H_0 and H_i, and define the time-dependent states $|\phi(t)\rangle \equiv e^{iH_0t}e^{-iHt}|\phi\rangle$ and operators $A(t) \equiv e^{iH_0t}Ae^{-iH_0t}$, then the states follow a Schrödinger equation while the operators follow a Heisenberg equation:[2]

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\phi(t)\rangle = H_i|\phi(t)\rangle \qquad\qquad i\frac{\mathrm{d}}{\mathrm{d}t}A(t) = [A(t), H_0]_- \tag{2.8}$$

If we use a position space representation of quantum mechanics, then the ket vector is often called a *wave function*, and denoted $\phi(\mathbf{r}, t) \equiv \langle\mathbf{r}|\phi(t)\rangle$. In this basis, the Hamiltonian operator is just like the Hamiltonian function from classical mechanics, except for the substitution $\mathbf{p} \to -i\nabla$ of the momentum variable. This goes for all the other operators as well: if an observable can be expressed as a function $A(\mathbf{r}, \mathbf{p})$ in classical mechanics, then the transformation $\mathbf{p} \to -i\nabla$ generates the corresponding quantum mechanical operator in position space.

[1] If the operator A that we started with has an explicit time-dependence, then we need to add a term $i\partial_t A$ to the right-hand side of the Heisenberg equation.

[2] The reason for not writing $|\phi(t)\rangle = e^{iH_0t}e^{-iHt}|\phi\rangle$ as just $|\phi(t)\rangle = e^{-iH_it}|\phi\rangle$, is that these two expressions are only equivalent in the special case where $[H_0, H_i]_- = 0$. But it can still be shown that the resulting Heisenberg equation only depends on H_i.

2.4 Quantum field theory

When we wish to treat systems with large numbers of particles, it is convenient to use the language of quantum field theory. We introduce a *creation operator* $\psi_\sigma^\dagger(\mathbf{r},t)$ that makes an electron with spin σ pop into existence at position $\mathbf{r}$ and time t, and an *annihilation operator* $\psi_\sigma(\mathbf{r},t)$ that make the same electron pop out of existence again. These *field operators* act on superpositions of the many-particle states $|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_n\sigma_n\rangle = |\mathbf{r}_1\sigma_1\rangle \oplus \cdots \oplus |\mathbf{r}_n\sigma_n\rangle$ in Fock space. These many-particle basis vectors can be constructed by simply adding particles to a special *vacuum state* $|0\rangle$, which represents a system with no electrons at all:

$$|\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_n\sigma_n\rangle = \psi_{\sigma_1}^\dagger(\mathbf{r}_1,t)|\mathbf{r}_2\sigma_2,\ldots,\mathbf{r}_n\sigma_n\rangle = \cdots = \psi_{\sigma_1}^\dagger(\mathbf{r}_1,t)\cdots\psi_{\sigma_n}^\dagger(\mathbf{r}_n,t)|0\rangle \quad (2.9)$$

The electron field operators satisfy the *fermionic anticommutation relations*:

$$[\psi_\sigma^\dagger(\mathbf{r},t),\, \psi_{\sigma'}^\dagger(\mathbf{r}',t)]_+ = 0 \quad (2.10)$$

$$[\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma'}^\dagger(\mathbf{r}',t)]_+ = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'} \quad (2.11)$$

$$[\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)]_+ = 0 \quad (2.12)$$

If we have a system that can be described by a non-interacting Hamiltonian H_0 in quantum mechanics, then the equivalent operator $\mathcal{H}_0$ in quantum field theory is:

$$\mathcal{H}_0 = \int \mathrm{d}^3\mathbf{r} \sum_\sigma \psi_\sigma^\dagger(\mathbf{r},t) H_0 \psi_\sigma(\mathbf{r},t) \quad (2.13)$$

To describe the interacting part of the Hamiltonian, we need to consider the propagation of at least two particles. If the interaction is described by a spin-independent potential $V(\mathbf{r},\mathbf{r}')$, then there are two possibilities that preserve angular momentum:

(i) **Direct interaction.** This means that two particles at $\mathbf{r}$ and $\mathbf{r}'$ interact through the potential $V(\mathbf{r},\mathbf{r}')$, and stay in the same spin states after the interaction. The integrand is in this case just a product $n_\sigma(\mathbf{r},t)n_{\sigma'}(\mathbf{r}',t)$ of two number operators.

$$\mathcal{H}_\mathrm{d} = +\frac{1}{2}\int \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}') \sum_{\sigma\sigma'} \psi_\sigma^\dagger(\mathbf{r},t)\psi_\sigma(\mathbf{r},t)\psi_{\sigma'}^\dagger(\mathbf{r}',t)\psi_{\sigma'}(\mathbf{r}',t) \quad (2.14)$$

(ii) **Exchange interaction.** This means that two particles at $\mathbf{r}$ and $\mathbf{r}'$ interact through the potential $V(\mathbf{r},\mathbf{r}')$, and somehow swap spin states during the interaction.

$$\mathcal{H}_\mathrm{e} = -\frac{1}{2}\int \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'\, V(\mathbf{r},\mathbf{r}') \sum_{\sigma\sigma'} \psi_\sigma^\dagger(\mathbf{r},t)\psi_{\sigma'}(\mathbf{r},t)\psi_{\sigma'}^\dagger(\mathbf{r}',t)\psi_\sigma(\mathbf{r}',t) \quad (2.15)$$

We will also introduce a field that describes the spin orientation of the electron cloud, namely the *spin field operator* $\boldsymbol{\sigma}(\mathbf{r},t)$. The spin field operator is basically just the second-quantized operator that corresponds to the Pauli vector $\boldsymbol{\sigma}$:

$$\boldsymbol{\sigma}(\mathbf{r},t) \equiv \sum_{\sigma\sigma'} \psi^\dagger_\sigma(\mathbf{r},t)\boldsymbol{\sigma}_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r},t) \tag{2.16}$$

If we perform the summation over the elements of the Pauli matrices, we see that the components of the spin field are:

$$\sigma^1(\mathbf{r},t) = \psi^\dagger_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t) + \psi^\dagger_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t) \tag{2.17}$$

$$i\sigma^2(\mathbf{r},t) = \psi^\dagger_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t) - \psi^\dagger_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t) \tag{2.18}$$

$$\sigma^3(\mathbf{r},t) = \psi^\dagger_\uparrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t) - \psi^\dagger_\downarrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t) \tag{2.19}$$

We will also define the corresponding ladder operators $\sigma^\pm(\mathbf{r},t) \equiv \sigma^1(\mathbf{r},t) \pm i\sigma^2(\mathbf{r},t)$:

$$\sigma^+(\mathbf{r},t) = 2\psi^\dagger_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t) \qquad \sigma^-(\mathbf{r},t) = 2\psi^\dagger_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t) \tag{2.20}$$

2.5 Green's functions

In the context of many-particle physics, *Green's functions* refer to certain correlation functions between quantum fields evaluated at different positions and times.[3] There are several ways to define these functions, but we will use the Keldysh definitions:[4]

$$G^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv -i\langle[\psi_\sigma(\mathbf{r},t),\,\psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+\rangle\,\theta(t-t') \tag{2.21}$$

$$G^{\mathrm{A}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv +i\langle[\psi_\sigma(\mathbf{r},t),\,\psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+\rangle\,\theta(t'-t) \tag{2.22}$$

$$G^{\mathrm{K}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv -i\langle[\psi_\sigma(\mathbf{r},t),\,\psi^\dagger_{\sigma'}(\mathbf{r}',t')]_-\rangle \tag{2.23}$$

The Green's functions contain useful information about the transport properties of a physical system. Straight from the definition, we see that the *retarded function* G^{R} vanishes unless we let $t > t'$, which means that the electron creation $\psi^\dagger_\sigma(\mathbf{r}',t')$ has to happen before the annihilation $\psi_\sigma(\mathbf{r},t)$. Conversely, the *advanced function* G^{A} vanishes unless $t < t'$, which means that the annihilation happens first. Thus we may conclude that G^{R} describes the flow of electrons, while G^{A} describes the flow of holes. The *Keldysh function* G^{K} is the only one of the Green's functions that contains information about the non-equilibrium properties of the system. Note that the retarded and advanced functions are defined as anticommutators, while the Keldysh function is instead a commutator.

[3] Note that this definition differs from the usual one in mathematics, where a Green's function is defined as the inverse of a differential operator.

[4] For an introduction to the Keldysh formalism, see Rammer (1986) or Belzig et al. (1998).

We will also be using the *anomalous Green's functions*, which describe correlations between the states of electrons at different points in space and time:

$$F^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv -i\langle[\psi_\sigma(\mathbf{r},t),\,\psi_{\sigma'}(\mathbf{r}',t')]_+\rangle\,\theta(t-t') \tag{2.24}$$

$$F^{\mathrm{A}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv +i\langle[\psi_\sigma(\mathbf{r},t),\,\psi_{\sigma'}(\mathbf{r}',t')]_+\rangle\,\theta(t'-t) \tag{2.25}$$

$$F^{\mathrm{K}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') \equiv -i\langle[\psi_\sigma(\mathbf{r},t),\,\psi_{\sigma'}(\mathbf{r}',t')]_-\rangle \tag{2.26}$$

In most physical systems, these correlations will just vanish. However, in superconductors below the critical temperature, an electronic condensate will form which establishes anomalous electron correlations in the system. It is precisely these correlations that we can quantify with the anomalous Green's functions. A similar description of anomalous correlations between holes is obtained by taking the complex conjugates of the functions defined above.

The different spin-dependent Green's functions defined on the previous page are usually combined to form 2×2 matrices in spin space:

$$\mathbf{G}^{\mathrm{R}} \equiv \begin{bmatrix} G^{\mathrm{R}}_{\uparrow\uparrow} & G^{\mathrm{R}}_{\uparrow\downarrow} \\ G^{\mathrm{R}}_{\downarrow\uparrow} & G^{\mathrm{R}}_{\downarrow\downarrow} \end{bmatrix} \qquad \mathbf{G}^{\mathrm{A}} \equiv \begin{bmatrix} G^{\mathrm{A}}_{\uparrow\uparrow} & G^{\mathrm{A}}_{\uparrow\downarrow} \\ G^{\mathrm{A}}_{\downarrow\uparrow} & G^{\mathrm{A}}_{\downarrow\downarrow} \end{bmatrix} \qquad \mathbf{G}^{\mathrm{K}} \equiv \begin{bmatrix} G^{\mathrm{K}}_{\uparrow\uparrow} & G^{\mathrm{K}}_{\uparrow\downarrow} \\ G^{\mathrm{K}}_{\downarrow\uparrow} & G^{\mathrm{K}}_{\downarrow\downarrow} \end{bmatrix} \tag{2.27}$$

$$\mathbf{F}^{\mathrm{R}} \equiv \begin{bmatrix} F^{\mathrm{R}}_{\uparrow\uparrow} & F^{\mathrm{R}}_{\uparrow\downarrow} \\ F^{\mathrm{R}}_{\downarrow\uparrow} & F^{\mathrm{R}}_{\downarrow\downarrow} \end{bmatrix} \qquad \mathbf{F}^{\mathrm{A}} \equiv \begin{bmatrix} F^{\mathrm{A}}_{\uparrow\uparrow} & F^{\mathrm{A}}_{\uparrow\downarrow} \\ F^{\mathrm{A}}_{\downarrow\uparrow} & F^{\mathrm{A}}_{\downarrow\downarrow} \end{bmatrix} \qquad \mathbf{F}^{\mathrm{K}} \equiv \begin{bmatrix} F^{\mathrm{K}}_{\uparrow\uparrow} & F^{\mathrm{K}}_{\uparrow\downarrow} \\ F^{\mathrm{K}}_{\downarrow\uparrow} & F^{\mathrm{K}}_{\downarrow\downarrow} \end{bmatrix} \tag{2.28}$$

In the absence of magnetic fields and spin-flip scattering processes, the $\mathbf{G}$ matrices become diagonal and the $\mathbf{F}$ matrices antidiagonal. The regular and anomalous Green's functions can be further collected as 4×4 matrices in Nambu space:

$$\hat{\mathbf{G}}^{\mathrm{R}} \equiv \begin{bmatrix} \mathbf{G}^{\mathrm{R}} & \mathbf{F}^{\mathrm{R}} \\ \mathbf{F}^{\mathrm{R}*} & \mathbf{G}^{\mathrm{R}*} \end{bmatrix} \qquad \hat{\mathbf{G}}^{\mathrm{A}} \equiv \begin{bmatrix} \mathbf{G}^{\mathrm{A}} & \mathbf{F}^{\mathrm{A}} \\ \mathbf{F}^{\mathrm{A}*} & \mathbf{G}^{\mathrm{A}*} \end{bmatrix} \qquad \hat{\mathbf{G}}^{\mathrm{K}} \equiv \begin{bmatrix} \mathbf{G}^{\mathrm{K}} & \mathbf{F}^{\mathrm{K}} \\ -\mathbf{F}^{\mathrm{K}*} & -\mathbf{G}^{\mathrm{K}*} \end{bmatrix} \tag{2.29}$$

Note the sign discrepancy between the definitions of $\hat{\mathbf{G}}^{\mathrm{K}}$ and the other Green's functions, which stems from the fact that $\hat{\mathbf{G}}^{\mathrm{K}}$ is defined as a commutator instead of an anticommutator. Finally, all the Green's functions can be expressed as a single 8×8 matrix in Keldysh space:

$$\check{\mathbf{G}} \equiv \begin{bmatrix} \hat{\mathbf{G}}^{\mathrm{R}} & \hat{\mathbf{G}}^{\mathrm{K}} \\ 0 & \hat{\mathbf{G}}^{\mathrm{A}} \end{bmatrix} \tag{2.30}$$

The most interesting physical observables in superconductor/ferromagnet systems, such as the density of states and electrical currents, can all be expressed as functions of the Green's function matrix $\check{\mathbf{G}}$. The majority of this thesis is therefore dedicated to finding numerically tractable equations of motion for this matrix.

2.6 Quasiclassical approximation

The Green's function $\check{\mathbf{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2)$ varies with respect to its coordinates in two different ways. The main contributions come from nearly free electrons at the Fermi surface $|\mathbf{p}| = p_\mathrm{F}$.[5] Since the wave function of an electron with momentum $\mathbf{p}$ and energy ϵ has the form $e^{i\mathbf{p}\cdot\mathbf{r}-i\epsilon t}$, we should expect a phase contribution of roughly $e^{ip_\mathrm{F}|\mathbf{r}_1-\mathbf{r}_2|-i\epsilon|t_1-t_2|}$ in the Green's function, which oscillates over the characteristic length scale $\lambda_\mathrm{F} = 2\pi/p_\mathrm{F}$. The other source of variation is the material that the electrons move through, which varies over the length scales $\xi_0 = p_\mathrm{F}/m\Delta$ and $\xi_T = p_\mathrm{F}/mT$ in the case of superconductors. Since both $\xi_0 \gg \lambda_\mathrm{F}$ and $\xi_T \gg \lambda_\mathrm{F}$ in most systems of interest, we may approximate the full Green's function as a monochromatic electron wave modulated by an envelope $\check{\mathbf{g}}$, where the envelope is primarily a function of the center of mass coordinates $(\mathbf{r}_1 + \mathbf{r}_2)/2$ and $(t_1 + t_2)/2$:

$$\check{\mathbf{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) \cong e^{ip_\mathrm{F}|\mathbf{r}_1-\mathbf{r}_2|-i\epsilon|t_1-t_2|}\,\check{\mathbf{g}}\left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}, \frac{t_1+t_2}{2}\right) \tag{2.31}$$

Since we are usually interested in the overall properties of the material, and not the phases of the constituent electrons, we can discard the wave function $e^{ip_\mathrm{F}|\mathbf{r}_1-\mathbf{r}_2|-i\epsilon|t_1-t_2|}$ and study the envelope $\check{\mathbf{g}}$ by itself.

We will now attempt to give a more rigorous definition of $\check{\mathbf{g}}$. First we switch to the *mixed representation* $\check{\mathbf{G}}(\mathbf{r}, \mathbf{s}, t, u)$ of the Green's function, where the mixed variables are defined as:

$$\mathbf{r} \equiv (\mathbf{r}_1 + \mathbf{r}_2)/2 \qquad \mathbf{s} \equiv \mathbf{r}_1 - \mathbf{r}_2 \tag{2.32}$$

$$t \equiv (t_1 + t_2)/2 \qquad u \equiv t_1 - t_2 \tag{2.33}$$

We then proceed to Fourier transform the relative variables $\mathbf{s}$ and u, such that we obtain a function $\check{\mathbf{G}}(\mathbf{r}, \mathbf{p}, \epsilon, t)$ that depends on the momentum $\mathbf{p}$ and energy ϵ instead:

$$\check{\mathbf{G}}(\mathbf{r}, \mathbf{p}, \epsilon, t) = \int \mathrm{d}u\; e^{i\epsilon u} \int \mathrm{d}^3\mathbf{s}\; e^{-i\mathbf{p}\cdot\mathbf{s}}\,\check{\mathbf{G}}(\mathbf{r}, \mathbf{s}, t, u) \tag{2.34}$$

We may then restrain the momentum $\mathbf{p}$ to the Fermi surface. This is done by defining the variable $\xi_\mathbf{p} \equiv \mathbf{p}^2/2m - \mu$, which is the kinetic energy measured relative to the Fermi level μ, and then setting $\xi_\mathbf{p} = 0$ with a delta function:

$$\check{\mathbf{G}}(\mathbf{r}, \mathbf{p}, \epsilon, t) \cong -i\pi\delta(\xi_\mathbf{p})\,\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_\mathrm{F}, \epsilon, t) \tag{2.35}$$

[5] This claim can be motivated from the Pauli exclusion principle. At low temperatures, most of the states inside the Fermi sphere are already occupied. Since the Pauli principle prevents double occupancy of the states, this implies that there are few available states with $|\mathbf{p}| \ll p_\mathrm{F}$ that particles may be scattered *into*. On the other hand, most states outside the Fermi sphere are unoccupied, so there are also few states with $|\mathbf{p}| \gg p_\mathrm{F}$ that particles may be scattered *from*. Conservation of momentum then dictates that most of the allowed scatterings have to be between different states with $|\mathbf{p}| \cong p_\mathrm{F}$. These are the interactions that have to drive the transport processes in the system.

This is just a different way of saying that $|\mathbf{p}| \cong p_\mathrm{F} \equiv \sqrt{2m\mu}$, which is known as the *quasiclassical approximation* in the literature. The prefactor $-i\pi$ normalizes the quasiclassical Green's function such that $\check{\mathbf{g}} \circ \check{\mathbf{g}} = \mathbf{1}$, where the ring product is defined in the next section. The symbol $\hat{\mathbf{p}}_\mathrm{F}$ refers to the direction of the momentum vector at the Fermi surface, which determines the transport direction. This equation may then be integrated over all values of $\xi_\mathbf{p}$ to obtain the *quasiclassical Green's function* $\check{\mathbf{g}}$:

$$\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_\mathrm{F}, \epsilon, t) = \frac{i}{\pi} \int \mathrm{d}\xi_\mathbf{p} \check{\mathbf{G}}(\mathbf{r}, \mathbf{p}, \epsilon, t) \tag{2.36}$$

Putting all the steps above together, we get the following equation for the quasiclassical Green's function $\check{\mathbf{g}}(\mathbf{r}, \mathbf{p}_\mathrm{F}, \epsilon, t)$ in terms of the Green's function $\check{\mathbf{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2)$:

$$\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_\mathrm{F}, \epsilon, t) = \frac{i}{\pi} \int \mathrm{d}\xi_\mathbf{p} \int \mathrm{d}u \int \mathrm{d}^3\mathbf{s}\, e^{i\epsilon u - i\mathbf{p}\cdot\mathbf{s}} \check{\mathbf{G}}(\mathbf{r} + \mathbf{s}/2, t + u/2; \mathbf{r} - \mathbf{s}/2, t - u/2) \tag{2.37}$$

The result is a function of the coordinates $\mathbf{r}$ and t, the transport direction $\hat{\mathbf{p}}_\mathrm{F}$, and the energy ϵ. Note the presence of an imaginary unit in the prefactor, which implies that the quasiclassical Green's function changes sign under complex conjugation. This ends up altering the sign structure of (2.29) after the quasiclassical approximation:

$$\hat{\mathbf{g}}^\mathrm{R} = \begin{bmatrix} \mathbf{g}^\mathrm{R} & \mathbf{f}^\mathrm{R} \\ -\mathbf{f}^{\mathrm{R}*} & -\mathbf{g}^{\mathrm{R}*} \end{bmatrix} \qquad \hat{\mathbf{g}}^\mathrm{A} = \begin{bmatrix} \mathbf{g}^\mathrm{A} & \mathbf{f}^\mathrm{A} \\ -\mathbf{f}^{\mathrm{A}*} & -\mathbf{g}^{\mathrm{A}*} \end{bmatrix} \qquad \hat{\mathbf{g}}^\mathrm{K} = \begin{bmatrix} \mathbf{g}^\mathrm{K} & \mathbf{f}^\mathrm{K} \\ \mathbf{f}^{\mathrm{K}*} & \mathbf{g}^{\mathrm{K}*} \end{bmatrix} \tag{2.38}$$

2.7 Product notation for integrals

To simplify notation in the chapters ahead, we will introduce a product that takes two functions $\mathbf{A}$ and $\mathbf{B}$, that depend on two spacetime coordinates each, and creates a new function $\mathbf{A} \bullet \mathbf{B}$ of the same kind. We define this *bullet product* by connecting the second coordinate of the first function to the first coordinate of the second function, and integrating over the possible choices for these intermediate coordinates:[6]

$$(\mathbf{A} \bullet \mathbf{B})(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) \equiv \int \mathrm{d}t' \int \mathrm{d}^3\mathbf{r}'\, \mathbf{A}(\mathbf{r}_1, t_1; \mathbf{r}', t')\mathbf{B}(\mathbf{r}', t'; \mathbf{r}_2, t_2) \tag{2.39}$$

In the special case that $\mathbf{A}$ or $\mathbf{B}$ is a function of only one or zero spacetime points, we should interpret $\mathbf{A} \bullet \mathbf{B}$ as an ordinary matrix product $\mathbf{AB}$. If we switch to the mixed representation, and Fourier transform the relative variables, it can be shown that the bullet product becomes:

$$\mathbf{A} \bullet \mathbf{B} = \exp\left\{\frac{i}{2}(\partial_t^\mathbf{A}\partial_\epsilon^\mathbf{B} - \partial_\epsilon^\mathbf{A}\partial_t^\mathbf{B})\right\} \exp\left\{\frac{i}{2}(\nabla_\mathbf{r}^\mathbf{A}\nabla_\mathbf{p}^\mathbf{B} - \nabla_\mathbf{p}^\mathbf{A}\nabla_\mathbf{r}^\mathbf{B})\right\} \mathbf{A}(\mathbf{r}, \mathbf{p}, \epsilon, t)\mathbf{B}(\mathbf{r}, \mathbf{p}, \epsilon, t) \tag{2.40}$$

[6] The bullet product is sometimes called a *convolution* in the literature, although it is a somewhat different procedure from the more common product $f \star g = \int \mathrm{d}x'\, f(x)g(x - x')$ with the same name.

The exponential of a differential operator should be interpreted in terms of the Taylor series $\exp(i\mathbf{D}) = 1 + i\mathbf{D} + \cdots$. The notations $\nabla_{\mathbf{r}}^{\mathbf{A}}$ and $\partial_t^{\mathbf{A}}$ are defined as differentiations with respect to $\mathbf{r}$ and t that only affect the function $\mathbf{A}$, and so on.[7] It is also convenient to introduce a *ring product*, which consists of only the energy/time differentiations from the full bullet product:

$$\mathbf{A} \bullet \mathbf{B} = \exp\left\{\frac{i}{2}(\nabla_{\mathbf{r}}^{\mathbf{A}}\nabla_{\mathbf{p}}^{\mathbf{B}} - \nabla_{\mathbf{p}}^{\mathbf{A}}\nabla_{\mathbf{r}}^{\mathbf{B}})\right\} \mathbf{A}(\mathbf{r},\mathbf{p},\epsilon,t) \circ \mathbf{B}(\mathbf{r},\mathbf{p},\epsilon,t) \tag{2.41}$$

$$\mathbf{A} \circ \mathbf{B} = \exp\left\{\frac{i}{2}(\partial_t^{\mathbf{A}}\partial_\epsilon^{\mathbf{B}} - \partial_\epsilon^{\mathbf{A}}\partial_t^{\mathbf{B}})\right\} \mathbf{A}(\mathbf{r},\mathbf{p},\epsilon,t)\, \mathbf{B}(\mathbf{r},\mathbf{p},\epsilon,t) \tag{2.42}$$

Note that in the stationary limit $\partial_t = 0$, the ring product reduces to just ordinary matrix multiplication. Under the quasiclassical approximation, we assume that the spatial variation of $\mathbf{A}$ and $\mathbf{B}$ is slow on the scale of the Fermi length λ_{F}, which means that we may linearize the gradient expansion of the bullet product:

$$\mathbf{A} \bullet \mathbf{B} \cong \mathbf{A} \circ \mathbf{B} + \frac{i}{2}\Big\{(\nabla_{\mathbf{r}}\mathbf{A}) \circ (\nabla_{\mathbf{p}}\mathbf{B}) - (\nabla_{\mathbf{p}}\mathbf{A}) \circ (\nabla_{\mathbf{r}}\mathbf{B})\Big\} \tag{2.43}$$

This is also called the *gradient approximation* in the literature. We will also define some commutators and anticommutators for the bullet and ring products:

$$[\mathbf{A},\mathbf{B}]_-^\bullet \equiv \mathbf{A}\bullet\mathbf{B} - \mathbf{B}\bullet\mathbf{A} \qquad [\mathbf{A},\mathbf{B}]_+^\bullet \equiv \mathbf{A}\bullet\mathbf{B} + \mathbf{B}\bullet\mathbf{A} \tag{2.44}$$

$$[\mathbf{A},\mathbf{B}]_-^\circ \equiv \mathbf{A}\circ\mathbf{B} - \mathbf{B}\circ\mathbf{A} \qquad [\mathbf{A},\mathbf{B}]_+^\circ \equiv \mathbf{A}\circ\mathbf{B} + \mathbf{B}\circ\mathbf{A} \tag{2.45}$$

Using equation (2.43) together with the definitions above, the commutator becomes:

$$[\mathbf{A},\mathbf{B}]_-^\bullet \cong [\mathbf{A},\mathbf{B}]_-^\circ + \frac{i}{2}\Big\{[\nabla_{\mathbf{r}}\mathbf{A},\nabla_{\mathbf{p}}\mathbf{B}]_+^\circ - [\nabla_{\mathbf{p}}\mathbf{A},\nabla_{\mathbf{r}}\mathbf{B}]_+^\circ\Big\} \tag{2.46}$$

Since the transport equations we derive in chapter 4 will involve bullet commutators, and it is a lot easier to evaluate ring products than bullet products, this could be a useful approximation.

[7] It might be instructive to interpret these operators as just a short-hand notation for the following:

$$(\nabla_{\mathbf{r}}^{\mathbf{A}}\nabla_{\mathbf{p}}^{\mathbf{B}} - \nabla_{\mathbf{p}}^{\mathbf{A}}\nabla_{\mathbf{r}}^{\mathbf{B}})\,\mathbf{A}(\mathbf{r},\mathbf{p})\mathbf{B}(\mathbf{r},\mathbf{p}) = \Big[(\nabla_{\mathbf{r}_1}\nabla_{\mathbf{p}_2} - \nabla_{\mathbf{p}_1}\nabla_{\mathbf{r}_2})\,\mathbf{A}(\mathbf{r}_1,\mathbf{p}_1)\mathbf{B}(\mathbf{r}_2,\mathbf{p}_2)\Big]_{\mathbf{r}_1=\mathbf{r}_2=\mathbf{r};\,\mathbf{p}_1=\mathbf{p}_2=\mathbf{p}}$$

3 Hamiltonian

3.1 Non-interacting electrons

When we wish to describe a complicated physical system, a natural first step is to isolate and describe the non-interacting parts of the system.[1] In our case, an appropriate choice would be to consider non-interacting electrons moving in an electromagnetic background field, which we describe using a scalar field $\varphi(\mathbf{r},t)$ and vector field $\mathbf{A}(\mathbf{r},t)$. From classical mechanics, we know the Hamiltonian for a particle with charge e moving in such fields:[2]

$$H_0 = \frac{(\mathbf{p} - e\mathbf{A}(\mathbf{r},t))^2}{2m} + e\varphi(\mathbf{r},t) - \mu \tag{3.1}$$

Note that we use the convention where the quantity $e < 0$ refers to the *electron charge*, not the elementary charge. We have also subtracted the chemical potential μ above, which just means that all energies are measured with respect to the Fermi level. The first-quantized Hamiltonian is obtained by the usual prescription $\mathbf{p} \to -i\nabla$:

$$H_0 = -\frac{(\nabla - ie\mathbf{A}(\mathbf{r},t))^2}{2m} + e\varphi(\mathbf{r},t) - \mu \tag{3.2}$$

The notation can be simplified by introducing the usual *gauge covariant derivative*, which is defined as $\tilde{\nabla} \equiv \nabla - ie\mathbf{A}(\mathbf{r},t)$. To then find the second-quantized Hamiltonian, we just have to plug (3.2) into (2.13):

$$\mathcal{H}_0 = \int \mathrm{d}^3\mathbf{r} \sum_\sigma \psi_\sigma^\dagger(\mathbf{r},t)\left\{-\frac{1}{2m}\tilde{\nabla}^2 + e\varphi(\mathbf{r},t) - \mu\right\}\psi_\sigma(\mathbf{r},t) \tag{3.3}$$

[1] Note that in this context, *non-interacting electrons* just means that the electrons *don't interact with each other*. They can still interact with externally applied fields like $\varphi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$.

[2] Goldstein, Poole, and Safko 2001, pp. 341–342.

3.2 Ferromagnetism

We will now derive how exchange interactions can lead to ferromagnetism, and then simplify the model with a mean field approximation.[3] From classical electromagnetism, we know that the electrostatic interaction between two electrons at positions $\mathbf{r}$ and $\mathbf{r}'$ is given by the Coulomb potential:

$$V(\mathbf{r},\mathbf{r}') = \frac{e^2}{4\pi|\mathbf{r}-\mathbf{r}'|} \tag{3.4}$$

This potential $V(\mathbf{r},\mathbf{r}')$ leads to two kinds of two-particle interaction terms in the second-quantized Hamiltonian: direct interactions $\mathcal{H}_\mathrm{d}$ and exchange interactions $\mathcal{H}_\mathrm{e}$. We will now consider the exchange interactions. Substituting (3.4) into (2.15), and moving constant factors out of the integral, we obtain:

$$\mathcal{H}_\mathrm{e} = -\frac{e^2}{8\pi}\int \frac{\mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\sum_{\sigma\sigma'}\psi^\dagger_\sigma(\mathbf{r},t)\psi_{\sigma'}(\mathbf{r},t)\psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi_\sigma(\mathbf{r}',t) \tag{3.5}$$

In the following, we will use the shorthand notation $\psi_{1\sigma} \equiv \psi_\sigma(\mathbf{r},t)$ and $\psi_{2\sigma} \equiv \psi_\sigma(\mathbf{r}',t)$ to keep the derivations somewhat tidy. The sum over spins in the integrand can then be expanded as follows:

$$\begin{aligned}\sum_{\sigma\sigma'}\psi^\dagger_{1\sigma}\psi_{1\sigma'}\psi^\dagger_{2\sigma'}\psi_{2\sigma} = {}& \psi^\dagger_{1\uparrow}\psi_{1\uparrow}\psi^\dagger_{2\uparrow}\psi_{2\uparrow} + \psi^\dagger_{1\downarrow}\psi_{1\downarrow}\psi^\dagger_{2\downarrow}\psi_{2\downarrow} \\ & + \psi^\dagger_{1\uparrow}\psi_{1\downarrow}\psi^\dagger_{2\downarrow}\psi_{2\uparrow} + \psi^\dagger_{1\downarrow}\psi_{1\uparrow}\psi^\dagger_{2\uparrow}\psi_{2\downarrow}\end{aligned} \tag{3.6}$$

Using the relation $(a+b)(c+d)+(a-b)(c-d) = 2ac+2bd$, the first line on the right-hand side of the equation can be factorized:

$$\begin{aligned}\sum_{\sigma\sigma'}\psi^\dagger_{1\sigma}\psi_{1\sigma'}\psi^\dagger_{2\sigma'}\psi_{2\sigma} = {}& \frac{1}{2}\left(\psi^\dagger_{1\uparrow}\psi_{1\uparrow} + \psi^\dagger_{1\downarrow}\psi_{1\downarrow}\right)\left(\psi^\dagger_{2\uparrow}\psi_{2\uparrow} + \psi^\dagger_{2\downarrow}\psi_{2\downarrow}\right) \\ & + \frac{1}{2}\left(\psi^\dagger_{1\uparrow}\psi_{1\uparrow} - \psi^\dagger_{1\downarrow}\psi_{1\downarrow}\right)\left(\psi^\dagger_{2\uparrow}\psi_{2\uparrow} - \psi^\dagger_{2\downarrow}\psi_{2\downarrow}\right) \\ & + \psi^\dagger_{1\uparrow}\psi_{1\downarrow}\psi^\dagger_{2\downarrow}\psi_{2\uparrow} + \psi^\dagger_{1\downarrow}\psi_{1\uparrow}\psi^\dagger_{2\uparrow}\psi_{2\downarrow}\end{aligned} \tag{3.7}$$

The factors $\psi^\dagger_{i\uparrow}\psi_{i\uparrow}+\psi^\dagger_{i\downarrow}\psi_{i\downarrow}$ are just the spin-independent number operators $n_i = \psi^\dagger_i\psi_i$. Furthermore, comparison with (2.19) and (2.20) reveal that the rest of the terms can be identified as the spin field components σ^3_i and their ladder operators $\sigma^\pm_i$. So (3.7) can be rewritten in the form:

$$\sum_{\sigma\sigma'}\psi^\dagger_{1\sigma}\psi_{1\sigma'}\psi^\dagger_{2\sigma'}\psi_{2\sigma} = \frac{1}{2}n_1n_2 + \frac{1}{2}\sigma^3_1\sigma^3_2 + \frac{1}{4}\sigma^+_1\sigma^-_2 + \frac{1}{4}\sigma^-_1\sigma^+_2 \tag{3.8}$$

[3] This derivation is partly based on Keeling 2008, pp. 3–5, 37–38.

This becomes more compact if we use the identity $\sigma_1 \cdot \sigma_2 = \sigma_1^3\sigma_2^3 + \frac{1}{2}\sigma_1^+\sigma_2^- + \frac{1}{2}\sigma_1^-\sigma_2^+$:

$$\sum_{\sigma\sigma'} \psi_{1\sigma}^\dagger \psi_{1\sigma'} \psi_{2\sigma'}^\dagger \psi_{2\sigma} = \frac{1}{2} n_1 n_2 + \frac{1}{2} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \tag{3.9}$$

In this section, we will focus on the behaviour of electron spins, and will therefore ignore the number density term. Switching back to the explicit notation $\boldsymbol{\sigma}_1 = \boldsymbol{\sigma}(\mathbf{r}, t)$, $\boldsymbol{\sigma}_2 = \boldsymbol{\sigma}(\mathbf{r}', t)$, and substituting the result back into integral (3.5), we obtain:

$$\mathcal{H}_\mathrm{e} = -\frac{e^2}{16\pi} \int \frac{\mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \boldsymbol{\sigma}(\mathbf{r}, t) \cdot \boldsymbol{\sigma}(\mathbf{r}', t) \tag{3.10}$$

So in systems where this term is important, the ground state clearly has to be some state which maximizes the spin field autocorrelation function $\langle \boldsymbol{\sigma}(\mathbf{r}, t) \cdot \boldsymbol{\sigma}(\mathbf{r}', t) \rangle$ with a Coulomb weight $1/|\mathbf{r} - \mathbf{r}'|$. This process is commonly known as *spontaneous magnetization*, since each electron spin is associated with a magnetic moment, so a self-alignment of the spin field also results in a macroscopic magnetic field.

Now that we have a Hamiltonian that can describe ferromagnetic behaviour, we wish to simplify it using a mean field approximation. The first step is to define a mean field $\boldsymbol{\sigma}_\mu(\mathbf{r}, t)$ and fluctuation field $\boldsymbol{\sigma}_\delta(\mathbf{r}, t)$:

$$\boldsymbol{\sigma}_\mu(\mathbf{r}, t) \equiv \langle \boldsymbol{\sigma}(\mathbf{r}, t) \rangle \qquad\qquad \boldsymbol{\sigma}_\delta(\mathbf{r}, t) \equiv \boldsymbol{\sigma}(\mathbf{r}, t) - \langle \boldsymbol{\sigma}(\mathbf{r}, t) \rangle \tag{3.11}$$

We then substitute the identity $\boldsymbol{\sigma}(\mathbf{r}, t) = \boldsymbol{\sigma}_\mu(\mathbf{r}, t) + \boldsymbol{\sigma}_\delta(\mathbf{r}, t)$ into (3.10), and obtain:

$$\begin{aligned} \mathcal{H}_\mathrm{e} = -\frac{e^2}{16\pi} \int \frac{\mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \Big\{ & \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) + \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\delta(\mathbf{r}', t) \\ & + \boldsymbol{\sigma}_\delta(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) + \boldsymbol{\sigma}_\delta(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\delta(\mathbf{r}', t) \Big\} \end{aligned} \tag{3.12}$$

We assume that the spin field fluctuations are relatively weak, i.e. that $|\boldsymbol{\sigma}_\delta| \ll |\boldsymbol{\sigma}_\mu|$, so that we may discard the term that is quadratic in $\boldsymbol{\sigma}_\delta(\mathbf{r}, t)$:

$$\mathcal{H}_\mathrm{e} \cong -\frac{e^2}{16\pi} \int \frac{\mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \Big\{ \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) + \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\delta(\mathbf{r}', t) + \boldsymbol{\sigma}_\delta(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) \Big\} \tag{3.13}$$

Substituting $\boldsymbol{\sigma}_\delta(\mathbf{r}, t) = \boldsymbol{\sigma}(\mathbf{r}, t) - \boldsymbol{\sigma}_\mu(\mathbf{r}, t)$ back into the equation, we get:

$$\begin{aligned} \mathcal{H}_\mathrm{e} = & -\frac{e^2}{16\pi} \int \frac{\mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \Big\{ \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}(\mathbf{r}', t) + \boldsymbol{\sigma}(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) \Big\} \\ & + \frac{e^2}{16\pi} \int \frac{\mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \Big\{ \boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t) \Big\} \end{aligned} \tag{3.14}$$

Since we integrate over the same range for $\mathbf{r}$ and $\mathbf{r}'$, the terms $\boldsymbol{\sigma}_\mu(\mathbf{r}, t) \cdot \boldsymbol{\sigma}(\mathbf{r}', t)$ and $\boldsymbol{\sigma}(\mathbf{r}, t) \cdot \boldsymbol{\sigma}_\mu(\mathbf{r}', t)$ are equivalent, and can be written as a single term $2\boldsymbol{\sigma}(\mathbf{r}, t) \cdot \langle \boldsymbol{\sigma}(\mathbf{r}', t) \rangle$.

As for the integral of $\sigma_\mu(\mathbf{r},t)\cdot\sigma_\mu(\mathbf{r}',t)$, this is a constant with no direct dependence on the operator $\sigma(\mathbf{r},t)$, and will therefore be ignored below. So the interaction part of the Hamiltonian has now been reduced to:

$$\mathcal{H}_{\mathrm{e}} = -\frac{e^2}{8\pi}\int \frac{\mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\sigma(\mathbf{r},t)\cdot\langle\sigma(\mathbf{r}',t)\rangle \tag{3.15}$$

Let us define the *magnetic order parameter* or *exchange field* $\mathbf{h}(\mathbf{r},t)$ as follows:

$$\mathbf{h}(\mathbf{r},t) \equiv \frac{e^2}{8\pi}\int \mathrm{d}^3\mathbf{r}'\,\frac{\langle\sigma(\mathbf{r}',t)\rangle}{|\mathbf{r}-\mathbf{r}'|} \tag{3.16}$$

Equation (3.15) then simplifies to:

$$\mathcal{H}_{\mathrm{e}} = -\int \mathrm{d}^3\mathbf{r}\;\sigma(\mathbf{r},t)\cdot\mathbf{h}(\mathbf{r},t) \tag{3.17}$$

Reexpressing the spin field $\sigma(\mathbf{r},t)$ in terms of the electron field $\psi_\sigma(\mathbf{r},t)$, we arrive at the following description of ferromagnetism in the mean field approximation:

$$\mathcal{H}_{\mathbf{h}} = -\int \mathrm{d}^3\mathbf{r}\sum_{\sigma\sigma'}\psi^\dagger_\sigma(\mathbf{r},t)\left[\sigma\cdot\mathbf{h}(\mathbf{r},t)\right]_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r},t) \tag{3.18}$$

Note that the symbol σ that appears in the equation above is the Pauli vector, not the spin field $\sigma(\mathbf{r},t)$ that we treated earlier.

3.3 Superconductivity

In this section, we will first derive how the electronic condensate which is associated with superconductivity can arise, and then simplify the model using a mean field approximation followed by a gauge transformation.[4] Let us begin by considering the effects of electron–electron scattering by some attractive potential $V(\mathbf{r},\mathbf{r}')$. In the context of low-temperature superconductors, it is usually phonons that mediate this interaction, but in principle it could also represent any other attractive interaction. The Hamiltonian describing direct interactions is then given by (2.14):

$$\mathcal{H}_{\mathrm{d}} = \frac{1}{2}\int \mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{r}'\; V(\mathbf{r},\mathbf{r}')\sum_{\sigma\sigma'}\psi^\dagger_\sigma(\mathbf{r},t)\psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi_{\sigma'}(\mathbf{r}',t)\psi_\sigma(\mathbf{r},t) \tag{3.19}$$

If the particles that mediate this electron–electron interaction have a short range, we can approximate the potential by $V(\mathbf{r},\mathbf{r}') \cong \lambda(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$. But remember that the Pauli principle prevents electrons from entering the same quantum state. This means that if $\sigma = \sigma'$, then the factors $\psi^\dagger_\sigma(\mathbf{r},t)\psi^\dagger_{\sigma'}(\mathbf{r}',t)$ and $\psi_{\sigma'}(\mathbf{r}',t)\psi_\sigma(\mathbf{r},t)$ both have to vanish in the limit $\mathbf{r}\to\mathbf{r}'$. Thus the only terms that survive in the limit of local interactions are those where $\sigma = -\sigma'$, leaving the Hamiltonian in the form:

$$\mathcal{H}_{\mathrm{d}} = \frac{1}{2}\int \mathrm{d}^3\mathbf{r}\;\lambda(\mathbf{r})\sum_{\sigma}\psi^\dagger_\sigma(\mathbf{r},t)\psi^\dagger_{-\sigma}(\mathbf{r},t)\psi_{-\sigma}(\mathbf{r},t)\psi_\sigma(\mathbf{r},t) \tag{3.20}$$

If we write out the sum above, we see that the resulting terms are actually equivalent because of the fermionic anticommutation relations:

$$\psi^\dagger_\uparrow(\mathbf{r},t)\psi^\dagger_\downarrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t) = \psi^\dagger_\downarrow(\mathbf{r},t)\psi^\dagger_\uparrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t) \tag{3.21}$$

So the sum is just $2\psi^\dagger_\downarrow(\mathbf{r},t)\psi^\dagger_\uparrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)$, and the Hamiltonian can be written:

$$\boxed{\mathcal{H}_{\mathrm{d}} = \int \mathrm{d}^3\mathbf{r}\;\lambda(\mathbf{r})\,\psi^\dagger_\downarrow(\mathbf{r},t)\psi^\dagger_\uparrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)} \tag{3.22}$$

This is the interaction term which leads to superconductivity. At this point, it is convenient to introduce a bosonic field $\phi(\mathbf{r},t) \equiv \psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)$ that describes pairs of electrons with opposite spin states, also known as *Cooper pairs*. The Hamiltonian above then takes the form of a number operator for such electron pairs:

$$\mathcal{H}_{\mathrm{d}} = \int \mathrm{d}^3\mathbf{r}\;\lambda(\mathbf{r})\,\phi^\dagger(\mathbf{r},t)\,\phi(\mathbf{r},t) \tag{3.23}$$

Since we assumed that the interaction was attractive, i.e. that $\lambda(\mathbf{r}) < 0$, we see that increasing the number density of electron pairs decreases the energy of the system. So at low temperatures we expect a large number of electrons to form such pairs, and this phenomenon is referred to as the *formation of an electronic condensate*.

[4] This section is inspired by Fossheim and Sudbø 2004, pp. 66–83; Morten 2005, pp. 15, 26–30.

We will now proceed to treat this Hamiltonian in the mean field approximation. The first step is to define the mean field $\phi_\mu(\mathbf{r},t)$ and the fluctuation field $\phi_\delta(\mathbf{r},t)$:

$$\phi_\mu(\mathbf{r},t) \equiv \langle\phi(\mathbf{r},t)\rangle \qquad\qquad \phi_\delta(\mathbf{r},t) \equiv \phi(\mathbf{r},t) - \langle\phi(\mathbf{r},t)\rangle \tag{3.24}$$

Substituting the relation $\phi(\mathbf{r},t) = \phi_\mu(\mathbf{r},t) + \phi_\delta(\mathbf{r},t)$ into (3.23), we get:

$$\mathcal{H}_\mathrm{d} = \int \mathrm{d}^3\mathbf{r}\ \ \lambda(\mathbf{r})\Big\{\phi_\mu^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t) + \phi_\mu^\dagger(\mathbf{r},t)\phi_\delta(\mathbf{r},t) + \phi_\delta^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t) + \phi_\delta^\dagger(\mathbf{r},t)\phi_\delta(\mathbf{r},t)\Big\}$$

In the mean field approximation, we then assume that the fluctuations are weak, so in other words $|\phi_\delta| \ll |\phi_\mu|$. We will therefore keep only leading order terms in ϕ_δ, and discard the quadratic term $\phi_\delta^\dagger(\mathbf{r},t)\phi_\delta(\mathbf{r},t)$:

$$\mathcal{H}_\mathrm{d} \cong \int \mathrm{d}^3\mathbf{r}\ \ \lambda(\mathbf{r})\Big\{\phi_\mu^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t) + \phi_\mu^\dagger(\mathbf{r},t)\phi_\delta(\mathbf{r},t) + \phi_\delta^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t)\Big\} \tag{3.25}$$

We then substitute $\phi_\delta(\mathbf{r},t) = \phi(\mathbf{r},t) - \phi_\mu(\mathbf{r},t)$ into this result and obtain:

$$\mathcal{H}_\mathrm{d} = \int \mathrm{d}^3\mathbf{r}\ \ \lambda(\mathbf{r})\Big\{\phi_\mu^\dagger(\mathbf{r},t)\phi(\mathbf{r},t) + \phi^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t)\Big\} - \int \mathrm{d}^3\mathbf{r}\ \ \lambda(\mathbf{r})\,\phi_\mu^\dagger(\mathbf{r},t)\phi_\mu(\mathbf{r},t) \tag{3.26}$$

The second integral is a constant with no direct dependence on the operator $\phi(\mathbf{r},t)$, and will therefore be ignored. We then define the *superconducting order parameter* as $\zeta(\mathbf{r},t) \equiv \lambda(\mathbf{r})\langle\phi(\mathbf{r},t)\rangle$, and get:

$$\mathcal{H}_\mathrm{d} = \int \mathrm{d}^3\mathbf{r}\ \ \Big\{\zeta(\mathbf{r},t)\phi^\dagger(\mathbf{r},t) + \zeta^*(\mathbf{r},t)\phi(\mathbf{r},t)\Big\} \tag{3.27}$$

After rewriting the Cooper pair field $\phi(\mathbf{r},t)$ in terms of the electron field $\psi(\mathbf{r},t)$, the following mean field description of superconductivity is obtained:

$$\boxed{\mathcal{H}_\mathrm{d} = \int \mathrm{d}^3\mathbf{r}\ \ \Big\{\zeta(\mathbf{r},t)\psi_\uparrow^\dagger(\mathbf{r},t)\psi_\downarrow^\dagger(\mathbf{r},t) + \zeta^*(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)\Big\}} \tag{3.28}$$

We will now attempt to simplify the above result by exploiting the gauge freedom of the fields. The superconducting order parameter $\zeta(\mathbf{r},t)$ is in general a complex number, which can be written on the form $\zeta(\mathbf{r},t) = \Delta(\mathbf{r},t)e^{i\nu(\mathbf{r},t)}$ for two real-valued functions $\Delta(\mathbf{r},t)$ and $\nu(\mathbf{r},t)$, which we refer to as the *superconducting band gap* and the *superconducting phase*. Equation (3.28) can then be written on the form:

$$\mathcal{H}_\mathrm{d} = \int \mathrm{d}^3\mathbf{r}\ \ \Big\{\Delta(\mathbf{r},t)\psi_\uparrow^\dagger(\mathbf{r},t)\psi_\downarrow^\dagger(\mathbf{r},t)e^{i\nu(\mathbf{r},t)} + \Delta(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)e^{-i\nu(\mathbf{r},t)}\Big\} \tag{3.29}$$

Note that the factor $e^{i\nu(\mathbf{r},t)}$ is placed next to two creation operators, while $e^{-i\nu(\mathbf{r},t)}$ is next to two annihilation operators. This means that we can exactly cancel both phase factors by performing the following U(1) gauge transformation of the fields:[5]

$$\psi_\sigma(\mathbf{r},t) \to e^{i\nu(\mathbf{r},t)/2}\psi_\sigma(\mathbf{r},t) \tag{3.30}$$

$$\mathbf{A}(\mathbf{r},t) \to \mathbf{A}(\mathbf{r},t) + \nabla\nu(\mathbf{r},t)/2e \tag{3.31}$$

$$\varphi(\mathbf{r},t) \to \varphi(\mathbf{r},t) - \partial_t\nu(\mathbf{r},t)/2e \tag{3.32}$$

In other words, we simply pick a gauge where the superconducting phase vanishes:

$$\mathcal{H}_\Delta = \int \mathrm{d}^3\mathbf{r}\ \ \Delta(\mathbf{r},t)\left\{\psi^\dagger_\uparrow(\mathbf{r},t)\psi^\dagger_\downarrow(\mathbf{r},t) + \psi_\downarrow(\mathbf{r},t)\psi_\uparrow(\mathbf{r},t)\right\} \tag{3.33}$$

In this particular gauge, any potentially interesting behaviour related to the superconducting phase will appear as spatiotemporal fluctuations in the electromagnetic background fields.

[5] Berche and Medina 2013, p. 170.

3.4 Spin-orbit coupling

If the scalar field $\varphi(\mathbf{r},t)$ is spatially inhomogeneous, then there is an electric field $\mathbf{E}(\mathbf{r},t) = -\nabla\varphi(\mathbf{r},t)$ in the system. To accurately determine how this affects an electron, we should perform a Lorentz transformation from the lab frame to the momentary rest frame of the electron. The leading order terms of this transformation are:[6]

$$\mathbf{E} \to \mathbf{E}' = \mathbf{E} + \mathbf{v}\times\mathbf{B} \qquad\qquad \mathbf{B} \to \mathbf{B}' = \mathbf{B} - \mathbf{v}\times\mathbf{E} \tag{3.34}$$

So even when $\mathbf{B} = 0$ in the lab frame, the electron will still experience a magnetic field $\mathbf{B}'(\mathbf{r},t) = \mathbf{v}\times\nabla\varphi(\mathbf{r},t)$ in its own reference frame. For an electron with momentum $\mathbf{p} = m\mathbf{v}$ and magnetic moment $\boldsymbol{\mu} = ge\boldsymbol{\sigma}/4m$, which couples to the magnetic field through the Zeeman interaction $H_i = -\boldsymbol{\mu}\cdot\mathbf{B}'$, we get:[7]

$$H_i = -\frac{ge}{4m^2}\boldsymbol{\sigma}\cdot(\mathbf{p}\times\nabla\varphi(\mathbf{r},t)) \tag{3.35}$$

Note that the interaction above is linear in both momentum and spin. An interaction like this, where the spin $\boldsymbol{\sigma}$ couples to the momentum $\mathbf{p}$, is called a *spin-orbit coupling*.

In practice, it is not straight-forward to calculate the spin-orbit coupling from first principles. First of all, $\varphi(\mathbf{r},t)$ should not only include the externally applied field, but also the internal field of the crystal structure. Furthermore, a rigorous treatment of the subject would have to include the detailed electron band structure of the material, which in general results in a non-linear coupling. Nonetheless, a linearized interaction is sufficient to describe the mesoscopic behaviour of most materials of interest.[8] Such a linearized interaction can in general be parametrized by some 3×3 matrix $\mathbf{w}(\mathbf{r},t)$:

$$H_i = -\frac{\mathbf{p}}{m}\cdot\mathbf{w}(\mathbf{r},t)\,\boldsymbol{\sigma} \tag{3.36}$$

The interaction matrix above is defined such that the component w_{nm} quantifies the coupling between momentum component p_n and spin component σ^m.

For a concrete example of such an interaction, consider a thin crystal layer placed in the yz-plane such that the growth direction of the crystal is $\hat{\mathbf{e}}_x$. One way to produce a spin-orbit coupling in this material, would be to introduce a *structure inversion asymmetry*, where we break the inversion symmetry of the system perpendicular to the yz-plane by e.g. applying an electric field along the x-axis.

[6] Set $\gamma \cong 1$ in the transformations found in e.g. Jackson 1998, p. 558; Griffiths 1999, pp. 528–532.

[7] Another way to derive the spin-orbit coupling, is to expand the positive-energy components of the Dirac equation to order $1/c^2$, which leads to the following Hamiltonian:

$$H = \underbrace{\frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2 + e\varphi}_{H_0} \quad \underbrace{-\frac{e}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}}_{\text{Zeeman interaction}} \quad \underbrace{-\frac{e}{4m^2}\boldsymbol{\sigma}\cdot(\mathbf{E}\times(\mathbf{p}-e\mathbf{A})) - \frac{ie}{8m^2}\boldsymbol{\sigma}\cdot(\nabla\times\mathbf{E})}_{\text{Spin-orbit interaction}} \quad \underbrace{+\frac{e}{8m^2}\nabla^2\varphi}_{\text{Darwin correction}}$$

See e.g. Sinova and MacDonald (2009, pp. 48–51) for the details.

[8] Bergeret and Tokatly 2014, pp. 2–3.

This leads to the *Rashba coupling* $H_{\mathrm{R}} = \alpha(p_z\sigma^2 - p_y\sigma^3)$. Another possibility would be to use a material with a noncentrosymmetric crystal structure, which leads to a *bulk inversion asymmetry*, and causes the *Dresselhaus coupling* $H_{\mathrm{D}} = \beta(p_z\sigma^3 - p_y\sigma^2)$. The interaction matrix $\mathbf{w}$ for a system where both of these effects are present can be expressed in terms of the *Rashba constant* α and *Dresselhaus constant* β:[9]

$$\mathbf{w} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & m\beta & m\alpha \\ 0 & -m\alpha & -m\beta \end{bmatrix} \qquad \mathbf{w}\boldsymbol{\sigma} = m(\beta\sigma^2 + \alpha\sigma^3)\hat{\mathbf{e}}_y - m(\alpha\sigma^2 + \beta\sigma^3)\hat{\mathbf{e}}_z \tag{3.37}$$

There are several other ways to produce spin-orbit couplings that may be more convenient experimentally, such as e.g. subjecting the system to a biaxial strain. These alternatives usually result in spin-orbit couplings with the same symmetry as the Rashba–Dresselhaus interactions discussed above.[10]

We will now return to the case of a general interaction matrix $\mathbf{w}$. Let us first write out the Hamiltonian $H = H_0 + H_i$ for a particle subject to such an interaction:

$$H = \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}}{m} \cdot \mathbf{w}(\mathbf{r}, t)\,\boldsymbol{\sigma} \tag{3.38}$$

Assuming that any spatiotemporal variations in the spin-orbit coupling are relatively weak, we can add a $\mathcal{O}(\mathbf{w}^2)$ term to the Hamiltonian without affecting the dynamics of the system, and then complete the square:

$$H \cong \frac{1}{2m}\left(\mathbf{p} - \mathbf{w}(\mathbf{r}, t)\,\boldsymbol{\sigma}\right)^2 \tag{3.39}$$

By comparison to (3.1), we see that the spin-orbit coupling enters the equation as an effective background field. It is therefore convenient to define a spin-dependent vector field $\boldsymbol{\mathcal{A}}(\mathbf{r}, t)$, and redefine the covariant derivative in terms of this quantity:[11]

$$\tilde{\nabla} \equiv \nabla - i\boldsymbol{\mathcal{A}}(\mathbf{r}, t) \qquad \boldsymbol{\mathcal{A}}(\mathbf{r}, t) \equiv e\mathbf{A}(\mathbf{r}, t) + \mathbf{w}(\mathbf{r}, t)\,\boldsymbol{\sigma} \tag{3.40}$$

The spin-orbit interactions may then be incorporated into our equations by using the spin-dependent covariant derivative in the non-interacting Hamiltonian (3.3):[12]

$$\mathcal{H}_0 = \int \mathrm{d}^3\mathbf{r} \sum_{\sigma\sigma'} \psi^\dagger_\sigma(\mathbf{r}, t)\left\{-\frac{1}{2m}\tilde{\nabla}^2_{\sigma\sigma'} + e\varphi(\mathbf{r}, t)\delta_{\sigma\sigma'} - \mu\delta_{\sigma\sigma'}\right\}\psi_{\sigma'}(\mathbf{r}, t) \tag{3.41}$$

[9] Bergeret and Tokatly 2014, p. 11.

[10] For a discussion of different kinds of spin-orbit coupling, see e.g. Studer (2010, pp. 4–8).

[11] Note that the background field $\boldsymbol{\mathcal{A}}$ is similar to the Pauli vector $\boldsymbol{\sigma}$ in the sense that it has $3 \times 2 \times 2$ dimensions, which we interpret as a vector structure in real space and a matrix structure in spin space. This is perhaps more transparent if we rewrite the definition of $\boldsymbol{\mathcal{A}}$ in index notation:

$$\mathcal{A}_{n\sigma\sigma'} = eA_n\sigma^0_{\sigma\sigma'} + \sum_m w_{nm}\sigma^m_{\sigma\sigma'}$$

[12] Technically, we have now promoted the U(1) gauge field $\mathbf{A}(\mathbf{r}, t)$ to a U(2) gauge field $\boldsymbol{\mathcal{A}}(\mathbf{r}, t)$, and this introduces SU(2) degrees of freedom related to the spin-orbit interactions. For a discussion of how SU(2) gauge transformations can be used to relate the effects of inhomogeneous magnetic fields and spin-orbit couplings, see Bergeret and Tokatly (2014).

3.5 Impurity scattering

Any real material is likely to contain at least *some* impurities, which interact with and scatter the electrons in the system. These impurities can be divided into two groups: non-magnetic impurities and magnetic impurities. The non-magnetic impurities can be thought of as an effective background potential $V_{\text{imp}}(\mathbf{r})$ for the electrons, which inserted into (2.13) yields:

$$\mathcal{H}_{\text{imp}} = \int \mathrm{d}^3\mathbf{r}\; V_{\text{imp}}(\mathbf{r}) \sum_{\sigma} \psi_\sigma^\dagger(\mathbf{r},t)\psi_\sigma(\mathbf{r},t) \tag{3.42}$$

The magnetic impurities have a spin field $\mathbf{s}(\mathbf{r},t)$ that couple to the electron spin field $\boldsymbol{\sigma}(\mathbf{r},t)$ through a scattering potential $V_{\text{sf}}(\mathbf{r})$, in a process known as *spin-flip scattering*:

$$\mathcal{H}_{\text{sf}} = \int \mathrm{d}^3\mathbf{r}\; V_{\text{sf}}(\mathbf{r})\, \boldsymbol{\sigma}(\mathbf{r},t) \cdot \mathbf{s}(\mathbf{r},t) \tag{3.43}$$

If we rewrite $\boldsymbol{\sigma}(\mathbf{r},t)$ in terms of the electron field $\psi_\sigma(\mathbf{r},t)$, this becomes:

$$\mathcal{H}_{\text{sf}} = \int \mathrm{d}^3\mathbf{r}\; V_{\text{sf}}(\mathbf{r}) \sum_{\sigma\sigma'} \psi_\sigma^\dagger(\mathbf{r},t) \left[\boldsymbol{\sigma} \cdot \mathbf{s}(\mathbf{r},t)\right]_{\sigma\sigma'} \psi_{\sigma'}(\mathbf{r},t) \tag{3.44}$$

This interaction looks very similar to (3.18), except that the magnetization $\mathbf{h}(\mathbf{r},t)$ has been replaced by the impurity spin field $\mathbf{s}(\mathbf{r},t)$.

3.6 Complete system

We now have everything we need to construct an effective field theory for materials with electromagnetic fields, superconducting properties, ferromagnetic properties, spin-orbit coupling, and impurity scattering. The appropriate Hamiltonian for such a system is a synthesis of equations (3.18), (3.33), (3.41), (3.42) and (3.44):

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_\Delta + \mathcal{H}_{\mathbf{h}} + \mathcal{H}_{\text{sf}} + \mathcal{H}_{\text{imp}} \tag{3.45}$$

4 Equations of motion

4.1 Time evolution of the electron field

In the previous chapter, we derived a Hamiltonian for impure materials with ferromagnetic and superconducting properties. We will now use this Hamiltonian to derive the equations of motion for the electron field in such a material. The time evolution of the field operators is governed by the Heisenberg equation (2.7):

$$i\partial_t \psi_\sigma(\mathbf{r},t) = [\psi_\sigma(\mathbf{r},t), \mathcal{H}]_- \qquad i\partial_t \psi^\dagger_\sigma(\mathbf{r},t) = [\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}]_- \tag{4.1}$$

Since commutators are linear in both arguments, we can pull the sums and integrals out of the commutators above, and expand the integrand term by term using the commutation relations derived in appendix A.

Let us first consider the non-interacting Hamiltonian (3.41). If we evaluate $[\psi_\sigma(\mathbf{r},t), \mathcal{H}_0]_-$ using (A.8) and (A.18), and then $[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_0]_-$ with (A.11) and (A.19), then we obtain:

$$[\psi_\sigma(\mathbf{r},t), \mathcal{H}_0]_- = -\frac{1}{2m}\sum_{\sigma'} \tilde{\nabla}^2_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r},t) + e\varphi(\mathbf{r},t)\psi_\sigma(\mathbf{r},t) - \mu\psi_\sigma(\mathbf{r},t) \tag{4.2}$$

$$[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_0]_- = \frac{1}{2m}\sum_{\sigma'} \tilde{\nabla}^{2*}_{\sigma\sigma'}\psi^\dagger_{\sigma'}(\mathbf{r},t) - e\varphi(\mathbf{r},t)\psi^\dagger_\sigma(\mathbf{r},t) + \mu\psi^\dagger_\sigma(\mathbf{r},t) \tag{4.3}$$

The commutators with impurity scattering terms from (3.42) can also be simplified using (A.8) and (A.11), followed by a summation over the Kronecker delta symbols:

$$[\psi_\sigma(\mathbf{r},t), \mathcal{H}_{\text{imp}}]_- = V_{\text{imp}}(\mathbf{r})\psi_\sigma(\mathbf{r},t) \tag{4.4}$$

$$[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_{\text{imp}}]_- = -\psi^\dagger_\sigma(\mathbf{r},t)V_{\text{imp}}(\mathbf{r}) \tag{4.5}$$

We then turn to the terms that describe superconductivity (3.33). Applying (A.7) and (A.9) to $[\psi_\sigma(\mathbf{r},t), \mathcal{H}_\Delta]_-$, and then (A.10) and (A.12) to $[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_\Delta]_-$, we get:

$$[\psi_\sigma(\mathbf{r},t), \mathcal{H}_\Delta]_- = \Delta(\mathbf{r},t)\left\{\delta_{\sigma\uparrow}\psi^\dagger_\downarrow(\mathbf{r},t) - \delta_{\sigma\downarrow}\psi^\dagger_\uparrow(\mathbf{r},t)\right\} \tag{4.6}$$

$$[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_\Delta]_- = \Delta(\mathbf{r},t)\left\{\delta_{\sigma\downarrow}\psi_\uparrow(\mathbf{r},t) - \delta_{\sigma\uparrow}\psi_\downarrow(\mathbf{r},t)\right\} \tag{4.7}$$

To expand the commutators with the ferromagnetic terms (3.18), we apply (A.8) to $[\psi_\sigma(\mathbf{r},t), \mathcal{H}_\mathbf{h}]_-$ and (A.11) to $[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_\mathbf{h}]_-$. Summation over the resulting Kronecker delta symbols yields:

$$[\psi_\sigma(\mathbf{r},t), \mathcal{H}_\mathbf{h}]_- = -\sum_{\sigma'} [\mathbf{h}(\mathbf{r},t)\cdot\boldsymbol{\sigma}]_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r},t) \tag{4.8}$$

$$[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_\mathbf{h}]_- = \sum_{\sigma'} [\mathbf{h}(\mathbf{r},t)\cdot\boldsymbol{\sigma}]_{\sigma'\sigma}\psi^\dagger_{\sigma'}(\mathbf{r},t) \tag{4.9}$$

The spin-flip terms from (3.44) have the same form as the ferromagnetic terms, so:

$$[\psi_\sigma(\mathbf{r},t), \mathcal{H}_{\text{sf}}]_- = \quad V_{\text{sf}}(\mathbf{r}) \sum_{\sigma'} [\mathbf{s}(\mathbf{r},t)\cdot\boldsymbol{\sigma}]_{\sigma\sigma'}\, \psi_{\sigma'}(\mathbf{r},t) \tag{4.10}$$

$$[\psi^\dagger_\sigma(\mathbf{r},t), \mathcal{H}_{\text{sf}}]_- = -V_{\text{sf}}(\mathbf{r}) \sum_{\sigma'} [\mathbf{s}(\mathbf{r},t)\cdot\boldsymbol{\sigma}]_{\sigma'\sigma}\, \psi^\dagger_{\sigma'}(\mathbf{r},t) \tag{4.11}$$

If we finally collect all of the results above, we can express the equations of motion for the electron field as follows:

$$i\partial_t \psi_\sigma(\mathbf{r},t) = P(\mathbf{r},t)\psi_\sigma(\mathbf{r},t) + \sum_{\sigma'} Q_{\sigma\sigma'}(\mathbf{r},t)\psi_{\sigma'}(\mathbf{r},t) + \sum_{\sigma'} R_{\sigma\sigma'}(\mathbf{r},t)\psi^\dagger_{\sigma'}(\mathbf{r},t) \tag{4.12}$$

$$-i\partial_t \psi^\dagger_\sigma(\mathbf{r},t) = \psi^\dagger_\sigma(\mathbf{r},t)P(\mathbf{r},t) + \sum_{\sigma'} \psi^\dagger_{\sigma'}(\mathbf{r},t)Q^\dagger_{\sigma'\sigma}(\mathbf{r},t) - \sum_{\sigma'} \psi_{\sigma'}(\mathbf{r},t)R_{\sigma'\sigma}(\mathbf{r},t) \tag{4.13}$$

For the sake of brevity, the results are written in terms of the following operators:

$$P(\mathbf{r},t) \equiv e\varphi(\mathbf{r},t) - \mu + V_{\text{imp}}(\mathbf{r},t) \tag{4.14}$$

$$\mathbf{Q}(\mathbf{r},t) \equiv -\frac{1}{2m}\tilde{\nabla}^2 - \mathbf{h}(\mathbf{r},t)\cdot\boldsymbol{\sigma} + V_{\text{sf}}(\mathbf{r})\mathbf{s}(\mathbf{r},t)\cdot\boldsymbol{\sigma} \tag{4.15}$$

$$\mathbf{R}(\mathbf{r},t) \equiv \Delta(\mathbf{r},t) i\sigma^2 \tag{4.16}$$

Note that the differential operators hidden in $\mathbf{Q}^\dagger$ should be interpreted as acting on $\psi^\dagger_{\sigma'}(\mathbf{r},t)$ from the right. Other than that, the only difference between $\mathbf{Q}$ and $\mathbf{Q}^\dagger$ is that the former contains $\tilde{\nabla}^2 = (\nabla - i\boldsymbol{\mathcal{A}})^2$ and the latter $\tilde{\nabla}^{2\dagger} = (\nabla + i\boldsymbol{\mathcal{A}})^2$. Finally, note that the matrix $\mathbf{R}$ is real and antisymmetric, which means that $\mathbf{R}^\dagger = \mathbf{R}^{\text{T}} = -\mathbf{R}$. These observations are all consistent with the fact that Hermitian conjugation of (4.12) should also produce (4.13).

4.2 Time evolution of the Green's functions

We will now use the results from the previous section to calculate the time evolution of the Green's functions. Let us commence by differentiating the definition (2.21) of the retarded Green's function with respect to t and t':

$$i\partial_t G^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') = -i\langle[i\partial_t\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+\rangle\theta(t-t') + \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.17}$$

$$i\partial_{t'} G^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') = -i\langle[\psi_\sigma(\mathbf{r},t),\ i\partial_{t'}\psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+\rangle\theta(t-t') - \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.18}$$

The anticommutators above can be expanded using (4.12) and (4.13):

$$\begin{aligned}[i\partial_t\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ &= P(\mathbf{r},t)[\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ \\ &+ \sum_{\sigma''} Q_{\sigma\sigma''}(\mathbf{r},t)[\psi_{\sigma''}(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ \\ &+ \sum_{\sigma''} R_{\sigma\sigma''}(\mathbf{r},t)[\psi^\dagger_{\sigma''}(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ \end{aligned} \tag{4.19}$$

$$\begin{aligned}[\psi_\sigma(\mathbf{r},t),\ i\partial_{t'}\psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ &= -[\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma'}(\mathbf{r}',t')]_+ P(\mathbf{r}',t') \\ &- \sum_{\sigma''}[\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma''}(\mathbf{r}',t')]_+ Q^\dagger_{\sigma''\sigma'}(\mathbf{r}',t') \\ &+ \sum_{\sigma''}[\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma''}(\mathbf{r}',t')]_+ R_{\sigma''\sigma'}(\mathbf{r}',t') \end{aligned} \tag{4.20}$$

We then substitute these identities into (4.17) and (4.18), and use (2.21) and (2.24) to express the expectation values of the remaining anticommutators in terms of Green's functions again, and obtain:

$$i\partial_t G^{\mathrm{R}}_{\sigma\sigma'} = P\,G^{\mathrm{R}}_{\sigma\sigma'} + \sum_{\sigma''} Q_{\sigma\sigma''}\,G^{\mathrm{R}}_{\sigma''\sigma'} - \sum_{\sigma''} R_{\sigma\sigma''}\,F^{\mathrm{R}^*}_{\sigma''\sigma'} + \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.21}$$

$$-i\partial_{t'} G^{\mathrm{R}}_{\sigma\sigma'} = G^{\mathrm{R}}_{\sigma\sigma'}P' + \sum_{\sigma''} G^{\mathrm{R}}_{\sigma\sigma''}\,Q'^\dagger_{\sigma''\sigma'} - \sum_{\sigma''} F^{\mathrm{R}}_{\sigma\sigma''}\,R'_{\sigma''\sigma'} + \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.22}$$

One subtlety one should be aware of when deriving the above, is that since the definition of F^{R} contains an imaginary unit, the term F^{R^*} introduces an extra minus sign. For the sake of brevity, the spacetime arguments of the functions above have been suppressed; all the Green's functions should be interpreted as functions of both primed and unprimed coordinates, while $P, \mathbf{Q}, \mathbf{R}$ only depend on unprimed coordinates, and $P', \mathbf{Q}'^\dagger, \mathbf{R}'$ only depend on primed coordinates. We can identify the sums above as matrix products, and recast the equations of motion in matrix form:

$$i\partial_t \mathbf{G}^{\mathrm{R}} = [\,P\ +\ \mathbf{Q}\,]\mathbf{G}^{\mathrm{R}} - \mathbf{R}\,\mathbf{F}^{\mathrm{R}^*} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.23}$$

$$-i\partial_{t'}\mathbf{G}^{\mathrm{R}} = \mathbf{G}^{\mathrm{R}}[P' + \mathbf{Q}'^\dagger] - \mathbf{F}^{\mathrm{R}}\mathbf{R}' + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.24}$$

If we take the complex conjugates of these results, we also get equations for $\mathbf{G}^{\mathrm{R}^*}$:

$$-i\partial_t \mathbf{G}^{\mathrm{R}^*} = [\,P\ +\ \mathbf{Q}^*\,]\mathbf{G}^{\mathrm{R}^*} - \mathbf{R}\,\mathbf{F}^{\mathrm{R}} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.25}$$

$$i\partial_{t'}\mathbf{G}^{\mathrm{R}^*} = \mathbf{G}^{\mathrm{R}^*}[P' + \mathbf{Q}'^{\mathrm{T}}] - \mathbf{F}^{\mathrm{R}^*}\mathbf{R}' + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.26}$$

We will now turn to the corresponding anomalous Green's functions $\mathbf{F}^{\mathrm{R}}$ and $\mathbf{F}^{\mathrm{R}^*}$. After differentiating definition (2.24) with respect to t and t', we get:

$$i\partial_t F^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') = -i\langle[i\partial_t\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+\rangle\theta(t-t') \tag{4.27}$$

$$i\partial_{t'} F^{\mathrm{R}}_{\sigma\sigma'}(\mathbf{r},t;\mathbf{r}',t') = -i\langle[\psi_\sigma(\mathbf{r},t),\ i\partial_{t'}\psi_{\sigma'}(\mathbf{r}',t')]_+\rangle\theta(t-t') \tag{4.28}$$

Both the anticommutators above can be expanded using (4.12):

$$\begin{aligned}[i\partial_t\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+ &= P(\mathbf{r},t)[\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+ \\ &\quad+\sum_{\sigma''} Q_{\sigma\sigma''}(\mathbf{r},t)[\psi_{\sigma''}(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+ \\ &\quad+\sum_{\sigma''} R_{\sigma\sigma''}(\mathbf{r},t)[\psi^\dagger_{\sigma''}(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+ \end{aligned} \tag{4.29}$$

$$\begin{aligned}[\psi_\sigma(\mathbf{r},t),\ i\partial_{t'}\psi_{\sigma'}(\mathbf{r}',t')]_+ &= P(\mathbf{r}',t')[\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma'}(\mathbf{r}',t')]_+ \\ &\quad+\sum_{\sigma''} Q_{\sigma'\sigma''}(\mathbf{r}',t')[\psi_\sigma(\mathbf{r},t),\ \psi_{\sigma''}(\mathbf{r}',t')]_+ \\ &\quad+\sum_{\sigma''} R_{\sigma'\sigma''}(\mathbf{r}',t')[\psi_\sigma(\mathbf{r},t),\ \psi^\dagger_{\sigma''}(\mathbf{r}',t')]_+ \end{aligned} \tag{4.30}$$

We then insert these identities into (4.27) and (4.28), and use definitions (2.21) and (2.24) to rewrite the results in terms of Green's functions:

$$i\partial_t F^{\mathrm{R}}_{\sigma\sigma'} = PF^{\mathrm{R}}_{\sigma\sigma'} + \sum_{\sigma''} Q_{\sigma\sigma''}F^{\mathrm{R}}_{\sigma''\sigma'} - \sum_{\sigma''} R_{\sigma\sigma''}G^{\mathrm{R}^*}_{\sigma''\sigma'} \tag{4.31}$$

$$i\partial_{t'} F^{\mathrm{R}}_{\sigma\sigma'} = P'F^{\mathrm{R}}_{\sigma\sigma'} + \sum_{\sigma''} Q'_{\sigma'\sigma''}F^{\mathrm{R}}_{\sigma\sigma''} + \sum_{\sigma''} R'_{\sigma'\sigma''}G^{\mathrm{R}}_{\sigma\sigma''} \tag{4.32}$$

These results can also be recast as matrix equations by interpreting the sums as matrix multiplication, and using the antisymmetry $\mathbf{R}^{\mathrm{T}} = -\mathbf{R}$ to simplify one term:

$$i\partial_t\mathbf{F}^{\mathrm{R}} = [\ P\ +\ \mathbf{Q}\ ]\mathbf{F}^{\mathrm{R}} - \mathbf{R}\,\mathbf{G}^{\mathrm{R}^*} \tag{4.33}$$

$$i\partial_{t'}\mathbf{F}^{\mathrm{R}} = \mathbf{F}^{\mathrm{R}}[P' + \mathbf{Q}'^{\mathrm{T}}] - \mathbf{G}^{\mathrm{R}}\mathbf{R}' \tag{4.34}$$

By taking the complex conjugate of these results, we also obtain equations for $\mathbf{F}^{\mathrm{R}^*}$:

$$-i\partial_t\mathbf{F}^{\mathrm{R}^*} = [\ P\ +\ \mathbf{Q}^*\ ]\mathbf{F}^{\mathrm{R}^*} - \mathbf{R}\,\mathbf{G}^{\mathrm{R}} \tag{4.35}$$

$$-i\partial_{t'}\mathbf{F}^{\mathrm{R}^*} = \mathbf{F}^{\mathrm{R}^*}[P' + \mathbf{Q}'^{\dagger}] - \mathbf{G}^{\mathrm{R}^*}\mathbf{R}' \tag{4.36}$$

Now that we have differential equations that describe the retarded Green's functions in spin space, the next item on the agenda is to merge these into an equation for the retarded Green's function in Nambu space. All the 2×2 matrix equations that we have derived so far can be collected as two 4×4 matrix equations:

$$i\partial_t \begin{bmatrix} \mathbf{G}^{\mathrm{R}} & \mathbf{F}^{\mathrm{R}} \\ -\mathbf{F}^{\mathrm{R}*} & -\mathbf{G}^{\mathrm{R}*} \end{bmatrix} = \begin{bmatrix} P+\mathbf{Q} & -\mathbf{R} \\ -\mathbf{R} & P+\mathbf{Q}^* \end{bmatrix} \begin{bmatrix} \mathbf{G}^{\mathrm{R}} & \mathbf{F}^{\mathrm{R}} \\ \mathbf{F}^{\mathrm{R}*} & \mathbf{G}^{\mathrm{R}*} \end{bmatrix} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.37}$$

$$-i\partial_{t'} \begin{bmatrix} \mathbf{G}^{\mathrm{R}} & -\mathbf{F}^{\mathrm{R}} \\ \mathbf{F}^{\mathrm{R}*} & -\mathbf{G}^{\mathrm{R}*} \end{bmatrix} = \begin{bmatrix} \mathbf{G}^{\mathrm{R}} & \mathbf{F}^{\mathrm{R}} \\ \mathbf{F}^{\mathrm{R}*} & \mathbf{G}^{\mathrm{R}*} \end{bmatrix} \begin{bmatrix} P'+\mathbf{Q}'^{\dagger} & -\mathbf{R}' \\ -\mathbf{R}' & P'+\mathbf{Q}'^{\mathrm{T}} \end{bmatrix} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.38}$$

Comparing this to definition (2.29), we note that both the equations above have $\hat{\mathbf{G}}^{\mathrm{R}}$ on the right-hand side. However, the left-hand side matrices differ from $\hat{\mathbf{G}}^{\mathrm{R}}$ by some signs; this can be resolved by factoring out $\tau^3\otimes\sigma^0 = \mathrm{diag}(\mathbf{1},-\mathbf{1})$ to the left in the first equation, and to the right in the second equation. We then arrive at the following equations of motion for $\hat{\mathbf{G}}^{\mathrm{R}}$:

$$i(\tau^3\otimes\sigma^0)(\partial_t\hat{\mathbf{G}}^{\mathrm{R}}) = \mathbf{H}\hat{\mathbf{G}}^{\mathrm{R}} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.39}$$

$$-i(\partial_{t'}\hat{\mathbf{G}}^{\mathrm{R}})(\tau^3\otimes\sigma^0) = \hat{\mathbf{G}}^{\mathrm{R}}\overline{\mathbf{H}}' + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.40}$$

To keep the notation succinct, we have implicitly defined the following matrices:

$$\mathbf{H} \equiv \begin{bmatrix} P+\mathbf{Q} & -\mathbf{R} \\ -\mathbf{R} & P+\mathbf{Q}^* \end{bmatrix} \qquad \overline{\mathbf{H}}' \equiv \begin{bmatrix} P'+\mathbf{Q}'^{\dagger} & -\mathbf{R}' \\ -\mathbf{R}' & P'+\mathbf{Q}'^{\mathrm{T}} \end{bmatrix} \tag{4.41}$$

The derivation of equations of motion for $\hat{\mathbf{G}}^{\mathrm{A}}$ and $\hat{\mathbf{G}}^{\mathrm{K}}$ proceeds in the same way as for $\hat{\mathbf{G}}^{\mathrm{R}}$, and is therefore omitted here. The results are:[1]

$$i(\tau^3\otimes\sigma^0)(\partial_t\hat{\mathbf{G}}^{\mathrm{A}}) = \mathbf{H}\hat{\mathbf{G}}^{\mathrm{A}} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.42}$$

$$-i(\partial_{t'}\hat{\mathbf{G}}^{\mathrm{A}})(\tau^3\otimes\sigma^0) = \hat{\mathbf{G}}^{\mathrm{A}}\overline{\mathbf{H}}' + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.43}$$

$$i(\tau^3\otimes\sigma^0)(\partial_t\hat{\mathbf{G}}^{\mathrm{K}}) = \mathbf{H}\hat{\mathbf{G}}^{\mathrm{K}} \tag{4.44}$$

$$-i(\partial_{t'}\hat{\mathbf{G}}^{\mathrm{K}})(\tau^3\otimes\sigma^0) = \hat{\mathbf{G}}^{\mathrm{K}}\overline{\mathbf{H}}' \tag{4.45}$$

If we finally combine the equations for $\hat{\mathbf{G}}^{\mathrm{R}}$, $\hat{\mathbf{G}}^{\mathrm{A}}$ and $\hat{\mathbf{G}}^{\mathrm{K}}$ using definition (2.30), we obtain two 8×8 matrix equations of motion that cover all of the Green's functions:

$$i(\tau^3\otimes\sigma^0)(\partial_t\check{\mathbf{G}}) = \mathbf{H}\check{\mathbf{G}} + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.46}$$

$$-i(\partial_{t'}\check{\mathbf{G}})(\tau^3\otimes\sigma^0) = \check{\mathbf{G}}\overline{\mathbf{H}}' + \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{4.47}$$

[1] Note that the equations of motion for $\hat{\mathbf{G}}^{\mathrm{K}}$ are the only ones without delta functions. The reason is just that definitions (2.21) and (2.22) contains step functions, while (2.23) does not.

4.3 Quantum transport equation

In the preceding section, two equations of motion for the $\check{\mathbf{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2)$ were derived: one that describes variation with respect to t_1, and another that describes variation with respect to t_2. The purpose of the following section is to fuse these equations of motion into a single transport equation. We start by subtracting (4.47) from (4.46):[2]

$$i(\tau^3 \otimes \sigma^0)(\partial_{t_1} \check{\mathbf{G}}) + i(\partial_{t_2} \check{\mathbf{G}})(\tau^3 \otimes \sigma^0) = \mathbf{H}_1 \check{\mathbf{G}} - \check{\mathbf{G}} \overline{\mathbf{H}}_2 \tag{4.48}$$

Let us start by considering the left-hand side. If we switch to the mixed variables $t \equiv (t_1 + t_2)/2$ and $u \equiv t_1 - t_2$, the time derivatives can be rewritten as $\partial_{t_1} = \frac{1}{2}\partial_t + \partial_u$ and $\partial_{t_2} = \frac{1}{2}\partial_t - \partial_u$. Furthermore, when we then Fourier transform with respect to the relative variable u as shown in (2.34), the transformation replaces time derivatives with energy factors according to $\partial_u \to -i\epsilon$. So in other words, we can substitute $\partial_{t_1} = \frac{1}{2}\partial_t - i\epsilon$ and $\partial_{t_2} = \frac{1}{2}\partial_t + i\epsilon$ into (4.48), which yields the following equation:

$$[\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]_- + \frac{i}{2}[\tau^3 \otimes \sigma^0, \partial_t \check{\mathbf{G}}]_+ = \mathbf{H}_1 \check{\mathbf{G}} - \check{\mathbf{G}} \overline{\mathbf{H}}_2 \tag{4.49}$$

Note that $\epsilon\tau^3 \otimes \sigma^0$ is linear in ϵ and independent of t, which means that an infinite series of differentiations would truncate at first order in ϵ and zeroth order in t. Consequently, the ring products (2.42) between $\epsilon\tau^3 \otimes \sigma^0$ and $\check{\mathbf{G}}$ become:

$$(\epsilon\tau^3 \otimes \sigma^0) \circ \check{\mathbf{G}} = \sum_{n=0}^{\infty} \frac{i^n}{2^n n!} \Big\{ (\partial_\epsilon^n \epsilon\tau^3 \otimes \sigma^0)(\partial_t^n \check{\mathbf{G}}) - (\partial_t^n \epsilon\tau^3 \otimes \sigma^0)(\partial_\epsilon^n \check{\mathbf{G}}) \Big\} \tag{4.50}$$

$$= (\epsilon\tau^3 \otimes \sigma^0)\check{\mathbf{G}} + \frac{i}{2}(\tau^3 \otimes \sigma^0)(\partial_t \check{\mathbf{G}}) \tag{4.51}$$

$$\check{\mathbf{G}} \circ (\epsilon\tau^3 \otimes \sigma^0) = \sum_{n=0}^{\infty} \frac{i^n}{2^n n!} \Big\{ (\partial_\epsilon^n \check{\mathbf{G}})(\partial_t^n \epsilon\tau^3 \otimes \sigma^0) - (\partial_t^n \check{\mathbf{G}})(\partial_\epsilon^n \epsilon\tau^3 \otimes \sigma^0) \Big\} \tag{4.52}$$

$$= \check{\mathbf{G}}(\epsilon\tau^3 \otimes \sigma^0) - \frac{i}{2}(\partial_t \check{\mathbf{G}})(\tau^3 \otimes \sigma^0) \tag{4.53}$$

We subtract these two equations and use definition (2.45) of the ring commutator:

$$[\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]_-^\circ = [\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]_- + \frac{i}{2}[\tau^3 \otimes \sigma^0, \partial_t \check{\mathbf{G}}]_+ \tag{4.54}$$

Since $\epsilon\tau^3 \otimes \sigma^0$ is independent of momentum and spatial variables, definition (2.41) implies that the bullet product and ring product are equivalent in this case, so we may also write the above as:

$$[\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]_-^\bullet = [\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]_- + \frac{i}{2}[\tau^3 \otimes \sigma^0, \partial_t \check{\mathbf{G}}]_+ \tag{4.55}$$

[2] Note that in this section, we will use numbered coordinates $(\mathbf{r}_1, t_1)$, $(\mathbf{r}_2, t_2)$ instead of primed coordinates $(\mathbf{r}, t)$, $(\mathbf{r}', t')$ to prevent the notation from clashing with the mixed variables $(\mathbf{r}, t)$, $(\mathbf{s}, u)$.

By comparing (4.49) to (4.55), we conclude that the transport equation becomes:

$$[\epsilon\tau^3 \otimes \sigma^0, \check{\mathbf{G}}]^\bullet_- = \mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2 \tag{4.56}$$

We will now consider the right-hand side of the equation. Substituting definition (4.41) of $\mathbf{H}$ and $\bar{\mathbf{H}}$ into the equation, we may rewrite the right-hand side as:

$$\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2 = \begin{bmatrix} P_1 + \mathbf{Q}_1 & -\mathbf{R}_1 \\ -\mathbf{R}_1 & P_1 + \mathbf{Q}_1^* \end{bmatrix}\check{\mathbf{G}} - \check{\mathbf{G}}\begin{bmatrix} P_2 + \mathbf{Q}_2^\dagger & -\mathbf{R}_2 \\ -\mathbf{R}_2 & P_2 + \mathbf{Q}_2^{\mathrm{T}} \end{bmatrix} \tag{4.57}$$

The contribution from the P components is clearly:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_P = P_1\check{\mathbf{G}} - \check{\mathbf{G}}P_2 \tag{4.58}$$

Since the bullet product was defined as just an ordinary matrix product when one of the arguments is a function of only one spacetime point, which is true for both P_1 and P_2, we may rewrite the result using $P_1\check{\mathbf{G}} = P \bullet \check{\mathbf{G}}$ and $\check{\mathbf{G}}P_2 = \check{\mathbf{G}} \bullet P$. So in other words, the P contribution can be expressed as:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_P = [P, \check{\mathbf{G}}]^\bullet_- \tag{4.59}$$

Using (4.14), this can also be written in terms of the physical quantities that we started with:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_P = [e\varphi + V_{\mathrm{imp}}, \check{\mathbf{G}}]^\bullet_- \tag{4.60}$$

Note the absence of the chemical potential μ from the equation above, since the bullet commutator with a constant vanishes.

We will then turn to the contributions from the $\mathbf{R}$ components. Consulting (4.57) again, we see that this contribution can be written:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_{\mathbf{R}} = (-\tau^1 \otimes \mathbf{R}_1)\check{\mathbf{G}} - \check{\mathbf{G}}(-\tau^1 \otimes \mathbf{R}_2) \tag{4.61}$$

Just like the P contributions, this can be rewritten as a bullet commutator:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_{\mathbf{R}} = [-\tau^1 \otimes \mathbf{R}, \check{\mathbf{G}}]^\bullet_- \tag{4.62}$$

If we then restore definition (4.16) of $\mathbf{R}$, this becomes:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_{\mathbf{R}} = [-\Delta(\tau^1 \otimes i\sigma^2), \check{\mathbf{G}}]^\bullet_- \tag{4.63}$$

Note that $-\Delta(\tau^1 \otimes i\sigma^2)$ is just another way of writing the $\mathbf{R}$ dependent parts of (4.41).

Finally, we have to compute the contributions from the $\mathbf{Q}$ components as well, which is a bit more challenging since it is a complex matrix containing differential operators. We begin by computing the complex conjugate, matrix transpose, and transpose conjugate of $\mathbf{Q}$, and then use the facts that σ and $\mathcal{A}$ are Hermitian to simplify the results:

$$\mathbf{Q}_1 = -\frac{1}{2m}(\nabla_1 - i\mathcal{A}_1)^2 - \mathbf{h}_1 \cdot \boldsymbol{\sigma} + V_{\mathrm{sf}}\mathbf{s}_1 \cdot \boldsymbol{\sigma} \tag{4.64}$$

$$\mathbf{Q}_1^* = -\frac{1}{2m}(\nabla_1 + i\mathcal{A}_1^*)^2 - \mathbf{h}_1 \cdot \boldsymbol{\sigma}^* + V_{\mathrm{sf}}\mathbf{s}_1 \cdot \boldsymbol{\sigma}^* \tag{4.65}$$

$$\mathbf{Q}_2^{\mathrm{T}} = -\frac{1}{2m}(\nabla_2 - i\mathcal{A}_2^*)^2 - \mathbf{h}_2 \cdot \boldsymbol{\sigma}^* + V_{\mathrm{sf}}\mathbf{s}_2 \cdot \boldsymbol{\sigma}^* \tag{4.66}$$

$$\mathbf{Q}_2^{\dagger} = -\frac{1}{2m}(\nabla_2 + i\mathcal{A}_2)^2 - \mathbf{h}_2 \cdot \boldsymbol{\sigma} + V_{\mathrm{sf}}\mathbf{s}_2 \cdot \boldsymbol{\sigma} \tag{4.67}$$

Switching to the mixed coordinates $\mathbf{r} \equiv (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{s} \equiv \mathbf{r}_1 - \mathbf{r}_2$, the derivatives with respect to $\mathbf{r}_1$ and $\mathbf{r}_2$ can be written $\nabla_1 = \frac{1}{2}\nabla_{\mathbf{r}} + \nabla_{\mathbf{s}}$ and $\nabla_2 = \frac{1}{2}\nabla_{\mathbf{r}} - \nabla_{\mathbf{s}}$. Furthermore, if we perform a Fourier transformation of the separation $\mathbf{s}$ as shown in (2.34), differentiation with respect to $\mathbf{s}$ transforms into multiplication by the momentum $\mathbf{p}$ according to $\nabla_{\mathbf{s}} \to i\mathbf{p}$. So we substitute $\nabla_1 = \frac{1}{2}\nabla_{\mathbf{r}} + i\mathbf{p}$ into (4.68) and (4.69), and $\nabla_2 = \frac{1}{2}\nabla_{\mathbf{r}} - i\mathbf{p}$ into (4.70) and (4.71):

$$\mathbf{Q}_1 = -\frac{1}{2m}(\nabla_{\mathbf{r}} + i\mathbf{p} - i\mathcal{A}_1)^2 - \mathbf{h}_1 \cdot \boldsymbol{\sigma} + V_{\mathrm{sf}}\mathbf{s}_1 \cdot \boldsymbol{\sigma} \tag{4.68}$$

$$\mathbf{Q}_1^* = -\frac{1}{2m}(\nabla_{\mathbf{r}} + i\mathbf{p} + i\mathcal{A}_1^*)^2 - \mathbf{h}_1 \cdot \boldsymbol{\sigma}^* + V_{\mathrm{sf}}\mathbf{s}_1 \cdot \boldsymbol{\sigma}^* \tag{4.69}$$

$$\mathbf{Q}_2^{\mathrm{T}} = -\frac{1}{2m}(\nabla_{\mathbf{r}} - i\mathbf{p} - i\mathcal{A}_2^*)^2 - \mathbf{h}_2 \cdot \boldsymbol{\sigma}^* + V_{\mathrm{sf}}\mathbf{s}_2 \cdot \boldsymbol{\sigma}^* \tag{4.70}$$

$$\mathbf{Q}_2^{\dagger} = -\frac{1}{2m}(\nabla_{\mathbf{r}} - i\mathbf{p} + i\mathcal{A}_2)^2 - \mathbf{h}_2 \cdot \boldsymbol{\sigma} + V_{\mathrm{sf}}\mathbf{s}_2 \cdot \boldsymbol{\sigma} \tag{4.71}$$

Since (4.57) contains the matrix structures $\mathrm{diag}(\mathbf{Q}, \mathbf{Q}^*)$ and $\mathrm{diag}(\mathbf{Q}^{\dagger}, \mathbf{Q}^{\mathrm{T}})$, the above equations suggest that we define the following matrices to simplify the notation:

$$\hat{\mathcal{A}} \equiv \begin{bmatrix} \mathcal{A} & 0 \\ 0 & -\mathcal{A}^* \end{bmatrix} \qquad \hat{\boldsymbol{\sigma}} \equiv \begin{bmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma}^* \end{bmatrix} \tag{4.72}$$

These definitions are not entirely unrelated. If we substitute in the original definition (3.40) of the background field $\mathcal{A}$, we see that $\hat{\mathcal{A}}$ can be expressed in terms of $\hat{\boldsymbol{\sigma}}$ by decomposing it into magnetic and spin-orbit contributions:

$$\hat{\mathcal{A}} = (e\mathbf{A} + \mathbf{w}\hat{\boldsymbol{\sigma}})(\tau^3 \otimes \sigma^0) \tag{4.73}$$

If we substitute the above results into (4.57), we see that the $\mathbf{Q}$ contributions are:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_{\mathrm{Q}} = \left[-\frac{1}{2m}(\nabla_{\mathbf{r}} + i\mathbf{p} - i\hat{\mathcal{A}})^2 - \mathbf{h}\cdot\hat{\sigma} + V_{\mathrm{sf}}\,\mathbf{s}\cdot\hat{\sigma}\right]\bullet\check{\mathbf{G}} - \check{\mathbf{G}}\bullet\left[-\frac{1}{2m}(\nabla_{\mathbf{r}} - i\mathbf{p} + i\hat{\mathcal{A}})^2 - \mathbf{h}\cdot\hat{\sigma} + V_{\mathrm{sf}}\,\mathbf{s}\cdot\hat{\sigma}\right] \tag{4.74}$$

Let us then expand the differential operators in the equation above:

$$(\nabla_{\mathbf{r}} + i\mathbf{p} - i\hat{\mathcal{A}})^2 = \nabla_{\mathbf{r}}^2 + i\mathbf{p}\cdot\nabla_{\mathbf{r}} + i\nabla_{\mathbf{r}}\cdot\mathbf{p} - \mathbf{p}^2 - i\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}} - i\hat{\mathcal{A}}\cdot\nabla_{\mathbf{r}} + \mathbf{p}\cdot\hat{\mathcal{A}} + \hat{\mathcal{A}}\cdot\mathbf{p} - \hat{\mathcal{A}}^2 \tag{4.75}$$

$$(\nabla_{\mathbf{r}} - i\mathbf{p} + i\hat{\mathcal{A}})^2 = \nabla_{\mathbf{r}}^2 - i\mathbf{p}\cdot\nabla_{\mathbf{r}} - i\nabla_{\mathbf{r}}\cdot\mathbf{p} - \mathbf{p}^2 + i\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}} + i\hat{\mathcal{A}}\cdot\nabla_{\mathbf{r}} + \mathbf{p}\cdot\hat{\mathcal{A}} + \hat{\mathcal{A}}\cdot\mathbf{p} - \hat{\mathcal{A}}^2 \tag{4.76}$$

When inserted into (4.74), the Laplacian terms become $\nabla_{\mathbf{r}}^2\check{\mathbf{G}} - \nabla_{\mathbf{r}}^2\check{\mathbf{G}} = 0$ and therefore cancel. Furthermore, the momentum variable $\mathbf{p}$ is independent of any spacetime point, so $\nabla_{\mathbf{r}}\cdot\mathbf{p} = 0$. For the same reason, the term $-\mathbf{p}^2$ will also disappear from the bullet commutator. So the nonvanishing terms in the equations above are:

$$(\nabla_{\mathbf{r}} + i\mathbf{p} - i\hat{\mathcal{A}})^2 = \quad i\mathbf{p}\cdot\nabla_{\mathbf{r}} - i(\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}} + \hat{\mathcal{A}}\cdot\nabla_{\mathbf{r}}) + (2\mathbf{p}\cdot\hat{\mathcal{A}} - \hat{\mathcal{A}}^2) \tag{4.77}$$

$$(\nabla_{\mathbf{r}} - i\mathbf{p} + i\hat{\mathcal{A}})^2 = -i\mathbf{p}\cdot\nabla_{\mathbf{r}} + i(\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}} + \hat{\mathcal{A}}\cdot\nabla_{\mathbf{r}}) + (2\mathbf{p}\cdot\hat{\mathcal{A}} - \hat{\mathcal{A}}^2) \tag{4.78}$$

We then substitute these relations into (4.74), and rewrite the results in terms of commutators and anticommutators:

$$[\mathbf{H}_1\check{\mathbf{G}} - \check{\mathbf{G}}\bar{\mathbf{H}}_2]_{\mathrm{Q}} = -\frac{i\mathbf{p}}{m}\cdot\left\{\nabla_{\mathbf{r}}\check{\mathbf{G}} - i[\hat{\mathcal{A}}, \check{\mathbf{G}}]_-^\bullet\right\} - [\mathbf{h}\cdot\hat{\sigma} - V_{\mathrm{sf}}\,\mathbf{s}\cdot\hat{\sigma}, \check{\mathbf{G}}]_-^\bullet + \frac{i}{2m}\left\{[\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}}, \check{\mathbf{G}}]_+^\bullet + [\hat{\mathcal{A}}, \nabla_{\mathbf{r}}\check{\mathbf{G}}]_+^\bullet - i[\mathcal{A}^2, \check{\mathbf{G}}]_-^\bullet\right\} \tag{4.79}$$

We have now calculated everything we need to write out the transport equation of the system. Note that no approximations were performed during this procedure, which means that any inaccuracies in the transport equation will be solely due to the assumptions and approximations related to the Hamiltonian itself. So when we finally combine (4.56), (4.60), (4.63) and (4.79), we arrive at the exact transport equation for a system described by (3.45):

$$\frac{\mathbf{p}}{m}\cdot\left\{\nabla_{\mathbf{r}}\check{\mathbf{G}} - i[\hat{\mathcal{A}}, \check{\mathbf{G}}]_-^\bullet\right\} = i[\epsilon(\tau^3\otimes\sigma^0) + \Delta(\tau^1\otimes i\sigma^2) + \mathbf{h}\cdot\hat{\sigma} - e\varphi - V_{\mathrm{imp}} - V_{\mathrm{sf}}\,\mathbf{s}\cdot\hat{\sigma}, \check{\mathbf{G}}]_-^\bullet + \frac{1}{2m}\left\{[\nabla_{\mathbf{r}}\cdot\hat{\mathcal{A}}, \check{\mathbf{G}}]_+^\bullet + [\hat{\mathcal{A}}, \nabla_{\mathbf{r}}\check{\mathbf{G}}]_+^\bullet - i[\hat{\mathcal{A}}^2, \check{\mathbf{G}}]_-^\bullet\right\} \tag{4.80}$$

4.4 Quasiclassical transport equation

Although the transport equation (4.80) is exact, a direct solution can easily become unwieldy in practical systems of interest, especially because each of the bullet products involves infinite series of differentiations with respect to position, time, energy, *and* momentum. The rest of the chapter is therefore dedicated to analytical approximations that will yield a more amenable transport equation. In most systems of interest, any characteristic length scale L of the system will be much larger than the Fermi wavelength λ_{F} of the constituent electrons. This means that the leading order contributions to the transport equation are given by the terms of lowest order in the expansion parameter $\eta \equiv \lambda_{\mathrm{F}}/L$, which was the basis for the quasiclassical approximation discussed in section 2.6.

Let us commence by performing some order of magnitude estimates of the terms in the exact transport equation (4.80). We will assume that the covariant derivative $\tilde{\nabla} = \nabla - i\boldsymbol{\mathcal{A}}$ varies over the characteristic scale $1/L$, while the momentum $\mathbf{p}$ is roughly equal to the Fermi momentum, and therefore inversely proportional to λ_{F}. All the terms on the left-hand side of (4.80) are then of order $1/mL\lambda_{\mathrm{F}}$, which can also be written as $\eta/m\lambda_{\mathrm{F}}^2$. If we however consider the terms on the second line of the right-hand side, these are all of order $1/mL^2$, or equivalently $\eta^2/m\lambda_{\mathrm{F}}^2$. So to leading order in η, we can simply discard the second line of the exact transport equation (4.80).[3]

It would also be tremendously useful if we could somehow reduce the bullet products in the transport equation to simpler ring products. One way to accomplish this task, would be to perform a leading order gradient expansion as shown in (2.46). However, we can go even further: since $\nabla_{\mathbf{r}} \sim 1/L$ and $\nabla_{\mathbf{p}} \sim \lambda_{\mathrm{F}}$, we see that the gradient expansion of the bullet product is equivalent to an expansion in η. This means that to leading order in η, we can throw away everything but the zeroth order term of the expansion, which permits us to replace bullet products with ring products.

Henceforth, we will also assume that the background field $\boldsymbol{\mathcal{A}}$ is time-independent. This implies that the left-hand side of (4.80) further reduces to a covariant derivative of the Green's function, where the covariant derivative in this context is defined as:

$$\tilde{\nabla}\check{\mathbf{G}} \equiv \nabla_{\mathbf{r}}\check{\mathbf{G}} - i[\hat{\boldsymbol{\mathcal{A}}}, \check{\mathbf{G}}]_{-} \tag{4.81}$$

[3] Physically, the $[\hat{\boldsymbol{\mathcal{A}}}, \nabla_{\mathbf{r}} G]_{+}$ term corresponds to a U(2) Lorentz force, so one consequence of this approximation is the suppression of Hall effects. See also Bergeret and Tokatly (2014, pp. 7–8).

The covariant derivative of a Green's function is intimately related to the previously defined covariant derivative of a field operator. Let us first go back to the definition $\tilde{\nabla}\psi \equiv \nabla\psi - i\boldsymbol{\mathcal{A}}\psi$ and its Hermitian conjugate $(\tilde{\nabla}\psi)^\dagger = \nabla\psi^\dagger + i\psi^\dagger\boldsymbol{\mathcal{A}}$. If we were to *define* the covariant derivative of a string of field operators with a product rule that reduces to factors of $(\tilde{\nabla}\psi)$ and $(\tilde{\nabla}\psi)^\dagger$, then applying it to a Green's function proportional to $\psi\psi^\dagger$ would produce the expansion:

$$\begin{aligned}\tilde{\nabla}(\psi\psi^\dagger) &\equiv (\tilde{\nabla}\psi)\psi^\dagger + \psi(\tilde{\nabla}\psi)^\dagger \\ &= (\nabla\psi - i\boldsymbol{\mathcal{A}}\psi)\psi^\dagger + \psi(\nabla\psi^\dagger + i\psi^\dagger\boldsymbol{\mathcal{A}}) \\ &= (\nabla\psi)\psi^\dagger + \psi(\nabla\psi^\dagger) - i\boldsymbol{\mathcal{A}}(\psi\psi^\dagger) + i(\psi\psi^\dagger)\boldsymbol{\mathcal{A}} \\ &= \nabla(\psi\psi^\dagger) - i[\boldsymbol{\mathcal{A}}, \psi\psi^\dagger]_- \end{aligned} \tag{4.82}$$

This result has the same mathematical structure as definition (4.81). In light of this result, we can think of the commutator in (4.81) as a manifestation of the fact that electrons and holes interact oppositely with the background field.

If we perform the approximations discussed above, replace $\mathbf{p}/m$ with the Fermi velocity $\mathbf{v}_\mathrm{F}$, and replace $\check{\mathbf{G}}(\mathbf{r}, \mathbf{p}, \epsilon, t)$ by the quasiclassical Green's function $\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_\mathrm{F}, \epsilon, t)$, then we obtain the quasiclassical transport equation for the system:

$$\mathbf{v}_\mathrm{F} \cdot \tilde{\nabla}\check{\mathbf{g}} = i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h}\cdot\hat{\boldsymbol{\sigma}} - e\varphi - V_\mathrm{imp} - V_\mathrm{sf}\,\mathbf{s}\cdot\hat{\boldsymbol{\sigma}}, \check{\mathbf{g}}]_-^\circ \tag{4.83}$$

This is also known as the *Eilenberger equation* in the literature. The result is clearly a lot simpler than the exact transport equation (4.80); not only could we discard three nontrivial terms, but the remaining terms are no longer subject to an infinite series of differentiations with respect to position and momentum. Furthermore, since the quasiclassical Green's function $\check{\mathbf{g}}$ is independent of the magnitude of $\mathbf{p}$, there is one degree of freedom less to worry about when solving the equation. We also note that the right-hand side of the simplified equation reduces to just a regular commutator in the stationary limit $\partial_t = 0$, which makes it easier to work with in equilibrium.

4.5 Diffusive limit

We will now consider *dirty materials*, i.e. systems with a relatively high concentration of non-magnetic impurities, which means that V_{imp} will be the dominant term in the Eilenberger equation.[4] In systems of this kind, the high frequency of random scattering events results in a nearly isotropic Green's function. This suggests that we approximate the Green's function by a first-order expansion in spherical harmonics:

$$\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_{\text{F}}, \epsilon, t) \cong \check{\mathbf{g}}_s(\mathbf{r}, \epsilon, t) + \hat{\mathbf{p}}_{\text{F}} \cdot \check{\mathbf{g}}_p(\mathbf{r}, \epsilon, t) \tag{4.84}$$

The s-wave component $\check{\mathbf{g}}_s$ is the isotropic part of the Green's function, while $\check{\mathbf{g}}_p$ is the p-wave component that describes the linearized anisotropy with respect to the transport direction $\hat{\mathbf{p}}_{\text{F}}$. Furthermore, the impurity and spin-flip potentials may in dirty materials be expressed as:[5]

$$V_{\text{imp}} \cong -\frac{i}{2\tau_0}\langle \check{\mathbf{g}} \rangle \qquad\qquad V_{\text{sf}}\, \mathbf{s} \cdot \hat{\boldsymbol{\sigma}} \cong -\frac{i}{2\tau_s}(\tau^3 \otimes \sigma^0)\langle \check{\mathbf{g}} \rangle (\tau^3 \otimes \sigma^0) \tag{4.85}$$

Here, τ_0 is the momentum relaxation time, τ_s is the spin relaxation time, and the angle brackets denote an average over the Fermi surface. We will for notational convenience also define $\nu_0 \equiv 1/2\tau_0$ and $\nu_s \equiv 1/2\tau_s$. Since $\langle \check{\mathbf{g}} \rangle \cong \langle \check{\mathbf{g}}_s \rangle + \langle \hat{\mathbf{p}}_{\text{F}} \cdot \check{\mathbf{g}}_p \rangle = \check{\mathbf{g}}_s$ if we use expansion (4.84), we see that:

$$V_{\text{imp}} \cong -i\nu_0 \check{\mathbf{g}}_s \qquad\qquad V_{\text{sf}}\, \mathbf{s} \cdot \hat{\boldsymbol{\sigma}} \cong -i\nu_s (\tau^3 \otimes \sigma^0) \check{\mathbf{g}}_s (\tau^3 \otimes \sigma^0) \tag{4.86}$$

We substitute (4.84) and (4.86) into (4.83), and rewrite the Fermi velocity as $v_{\text{F}}\hat{\mathbf{p}}_{\text{F}}$:

$$\begin{aligned} & v_{\text{F}}\hat{\mathbf{p}}_{\text{F}} \cdot \tilde{\nabla}\check{\mathbf{g}}_s + v_{\text{F}}\hat{\mathbf{p}}_{\text{F}}^2 \tilde{\nabla} \cdot \check{\mathbf{g}}_p \\ &= i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\boldsymbol{\sigma}} - e\varphi + i\nu_0 \check{\mathbf{g}}_s + i\nu_s (\tau^3 \otimes \sigma^0)\check{\mathbf{g}}_s(\tau^3 \otimes \sigma^0), \check{\mathbf{g}}_s]_-^\circ \\ &+ i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\boldsymbol{\sigma}} - e\varphi + i\nu_0 \check{\mathbf{g}}_s + i\nu_s (\tau^3 \otimes \sigma^0)\check{\mathbf{g}}_s(\tau^3 \otimes \sigma^0), \check{\mathbf{g}}_p]_-^\circ \cdot \hat{\mathbf{p}}_{\text{F}} \end{aligned} \tag{4.87}$$

If we average this over the Fermi surface, then all the odd powers of $\hat{\mathbf{p}}_{\text{F}}$ vanish:[6]

$$\frac{1}{3} v_{\text{F}} \tilde{\nabla} \cdot \check{\mathbf{g}}_p = i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\boldsymbol{\sigma}} - e\varphi + i\nu_s (\tau^3 \otimes \sigma^0)\check{\mathbf{g}}_s(\tau^3 \otimes \sigma^0), \check{\mathbf{g}}_s]_-^\circ \tag{4.88}$$

Note that the impurity scattering has also vanished in the equation above, since $[\check{\mathbf{g}}_s, \check{\mathbf{g}}_s]_-^\circ = 0$. On the other hand, if we multiply by $\hat{\mathbf{p}}_{\text{F}}$ before averaging, then only the terms with even powers of $\hat{\mathbf{p}}_{\text{F}}$ disappear from the equation:

$$v_{\text{F}} \tilde{\nabla} \check{\mathbf{g}}_s = i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\boldsymbol{\sigma}} - e\varphi + i\nu_0 \check{\mathbf{g}}_s + i\nu_s (\tau^3 \otimes \sigma^0)\check{\mathbf{g}}_s(\tau^3 \otimes \sigma^0), \check{\mathbf{g}}_p]_-^\circ \tag{4.89}$$

[4] This derivation is based on Chandrasekhar (2004), Morten (2005), and Rammer (1986).

[5] This result is derived by making a continuum approximation of the sum over impurity locations, and then replacing the interactions by the self-energies in the first-order Born approximation. See for example Morten (2005, pp. 39–40,45–46) and Rammer (1986, pp. 351–352).

[6] The reason for the factor 1/3 is that the derivative term was quadratic in $\hat{\mathbf{p}}_{\text{F}}$, and $\langle \hat{\mathbf{p}}_{\text{F}}^2 \rangle = 1/3$.

We assumed that the equation is dominated by the impurity scattering, which means that we can discard everything but the ν_0 term in the commutator above:

$$v_{\mathrm{F}}\tilde{\nabla}\check{\mathbf{g}}_s \cong -\nu_0[\check{\mathbf{g}}_s, \check{\mathbf{g}}_p]^\circ_- \tag{4.90}$$

To further simplify this result, we turn to the normalization condition $\check{\mathbf{g}} \circ \check{\mathbf{g}} = \mathbf{1}$ of the quasiclassical Green's function. If we insert (4.84) into this, we get:

$$\check{\mathbf{g}}_s \circ \check{\mathbf{g}}_s + \hat{\mathbf{p}}_{\mathrm{F}} \cdot \check{\mathbf{g}}_p \circ \check{\mathbf{g}}_s + \hat{\mathbf{p}}_{\mathrm{F}} \cdot \check{\mathbf{g}}_s \circ \check{\mathbf{g}}_p + \hat{\mathbf{p}}_{\mathrm{F}}^2 \check{\mathbf{g}}_p \circ \check{\mathbf{g}}_p = \mathbf{1} \tag{4.91}$$

For a nearly isotropic Green's function, $\check{\mathbf{g}}_p \circ \check{\mathbf{g}}_p$ should be negligible compared to $\check{\mathbf{g}}_s \circ \check{\mathbf{g}}_s$. So if we average the above equation over the Fermi surface, we obtain:

$$\check{\mathbf{g}}_s \circ \check{\mathbf{g}}_s \cong \mathbf{1} \tag{4.92}$$

If we instead multiply (4.91) by $\hat{\mathbf{p}}_{\mathrm{F}}$ before averaging, we obtain another identity:

$$\check{\mathbf{g}}_p \circ \check{\mathbf{g}}_s + \check{\mathbf{g}}_s \circ \check{\mathbf{g}}_p = \mathbf{0} \tag{4.93}$$

Applying (4.93) to (4.90), we get:

$$v_{\mathrm{F}}\tilde{\nabla}\check{\mathbf{g}}_s \cong -2\nu_0 \check{\mathbf{g}}_s \circ \check{\mathbf{g}}_p \tag{4.94}$$

We then ring multiply this equation with $\check{\mathbf{g}}_s$ from the left, use (4.92) to get rid of the $\check{\mathbf{g}}_s \circ \check{\mathbf{g}}_s$ factor, reinstate $\tau_0 = 1/2\nu_0$, and solve for $\check{\mathbf{g}}_p$:

$$\check{\mathbf{g}}_p = -\tau_0 v_{\mathrm{F}} \check{\mathbf{g}}_s \circ \tilde{\nabla}\check{\mathbf{g}}_s \tag{4.95}$$

This equation shows that if we manage to solve the transport equation for the isotropic component $\check{\mathbf{g}}_s$, then we may directly compute the anisotropic component $\check{\mathbf{g}}_p$ from the result. In other words, the isotropic component $\check{\mathbf{g}}_s$ appears to capture the most essential physics of the system. We may therefore with a clear conscience eliminate $\check{\mathbf{g}}_p$ from our equations, and from now on focus on determining $\check{\mathbf{g}}_s$. If we substitute (4.95) into (4.88), then we finally obtain a diffusion equation for the isotropic Green's function $\check{\mathbf{g}}_s$:

$$iD\tilde{\nabla} \cdot (\check{\mathbf{g}}_s \circ \tilde{\nabla}\check{\mathbf{g}}_s) = [\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\sigma} - e\varphi + i\nu_s(\tau^3 \otimes \sigma^0)\check{\mathbf{g}}_s(\tau^3 \otimes \sigma^0), \check{\mathbf{g}}_s]^\circ_- \tag{4.96}$$

This result is also known as the *Usadel equation* in the literature. Note that we introduced the *diffusion coefficient* $D \equiv \frac{1}{3}\tau_0 v_{\mathrm{F}}^2$ above. At first, this result might look more complicated than the Eilenberger equation (4.83), since we went from a first-order to a second-order differential equation. However, the crucial point is that we have reduced an equation for $\check{\mathbf{g}}(\mathbf{r}, \hat{\mathbf{p}}_{\mathrm{F}}, \epsilon, t)$ to an equation for only the isotropic part $\check{\mathbf{g}}_s(\mathbf{r}, \epsilon, t)$. This means that we have eliminated two degrees of freedom from our equations, which drastically simplifies practical calculations.

4.6 Equilibrium

After the system reaches equilibrium, the state of the system will cease to evolve in time. In this limit, the Green's function above becomes a time-independent quantity $\check{\mathbf{g}}_s(\mathbf{r}, \epsilon)$, and all the ring products in the Usadel equation (4.96) reduce to ordinary matrix products. Furthermore, $e\varphi$ is just a scalar and therefore commutes with the Green's function, which means that it will drop out of (4.96) in this limit. So the Usadel equation will then reduce to:

$$iD\tilde{\nabla}\cdot(\check{\mathbf{g}}_s\tilde{\nabla}\check{\mathbf{g}}_s) = [\epsilon(\tau^3\otimes\sigma^0) + \Delta(\tau^1\otimes i\sigma^2) + \mathbf{h}\cdot\hat{\boldsymbol{\sigma}} + i\nu_s(\tau^3\otimes\sigma^0)\check{\mathbf{g}}_s(\tau^3\otimes\sigma^0), \check{\mathbf{g}}_s]_- \tag{4.97}$$

Notably, not all the components of $\check{\mathbf{g}}$ are independent, which means that the equation above contains some redundant degrees of freedom. First of all, it is straightforward to show that the retarded and advanced components are related by $\hat{\mathbf{g}}^{\mathrm{A}} = -(\tau^3\otimes\sigma^0)\hat{\mathbf{g}}^{\mathrm{R}\dagger}(\tau^3\otimes\sigma^0)$ from their definitions in terms of field operators. Moreover, these can also be related to the Keldysh component by $\hat{\mathbf{g}}^{\mathrm{K}} = (\hat{\mathbf{g}}^{\mathrm{R}} - \hat{\mathbf{g}}^{\mathrm{A}})\tanh(\epsilon/2T)$ at equilibrium at temperature T.[7] In other words, at equilibrium it is sufficient to solve the Usadel equation for the retarded component $\hat{\mathbf{g}}^{\mathrm{R}}$:

$$iD\tilde{\nabla}\cdot(\hat{\mathbf{g}}_s^{\mathrm{R}}\tilde{\nabla}\hat{\mathbf{g}}_s^{\mathrm{R}}) = [\epsilon(\tau^3\otimes\sigma^0) + \Delta(\tau^1\otimes i\sigma^2) + \mathbf{h}\cdot\hat{\boldsymbol{\sigma}} + i\nu_s(\tau^3\otimes\sigma^0)\hat{\mathbf{g}}_s^{\mathrm{R}}(\tau^3\otimes\sigma^0), \hat{\mathbf{g}}_s^{\mathrm{R}}]_- \tag{4.98}$$

[7] Morten 2005, pp. 57,61.

5 Physical system

5.1 Description

Up until this point, we have considered a somewhat general class of physical systems: three-dimensional materials with electromagnetic background fields, superconductivity, ferromagnetism, spin-orbit coupling, impurity scattering, and spin-flip scattering. We started by creating an effective Hamiltonian for this class of systems in chapter 3, and then derived the corresponding diffusion equation in chapter 4. In this chapter, we will restrict our attention to one particular instance, namely the superconductor/ferromagnet bilayer shown in Figure 5.1. The bilayer consists of a superconductor of thickness L_1 and a ferromagnet of thickness L_2 with a common interface at $x = 0$, and this structure is bounded by a region of practically infinite electrical resistance. We will assume that the dynamics are effectively one-dimensional, so that we only have to consider variations along the x-axis. There are two different ways to construct such a system. One way would be to make the material so large along the y- and z-axes that the system may be considered translation invariant in the yz-plane. Note that this translation invariance would also imply that the x-component of the background field $\mathcal{A}_x \to 0$. Alternatively, one could make the system infinitesimal along either the y- or z-axis, which would again result in a one-dimensional diffusion equation, but allow for a finite value of $\mathcal{A}_x$, which may lead to other kinds of interesting behaviour. In the derivations below, we will not pick an explicit form for the background field $\mathcal{A}$, but merely assume that all of its elements are real constants throughout the ferromagnet and zero elsewhere.[1]

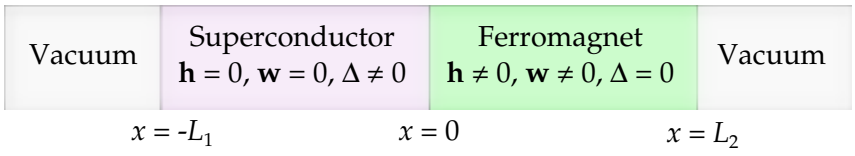

Figure 5.1: Conceptual sketch of a superconductor/ferromagnet bilayer.

We will treat the problem in diffusive equilibrium, and neglige spin-flip scattering processes. The system can then be described by a simplified version of the Usadel equation (4.98):

$$\tilde{\nabla} \cdot (\hat{\mathbf{g}} \tilde{\nabla} \hat{\mathbf{g}}) = -i[\epsilon(\tau^3 \otimes \sigma^0) + \Delta(\tau^1 \otimes i\sigma^2) + \mathbf{h} \cdot \hat{\boldsymbol{\sigma}}, \hat{\mathbf{g}}]_- \tag{5.1}$$

[1] The assumption that $\mathcal{A} = e\mathbf{A} + \mathbf{w}\boldsymbol{\sigma}$ is real-valued means that the σ^2 component has to vanish, and also implies that $\hat{\mathcal{A}} = \mathrm{diag}(\mathcal{A}, -\mathcal{A})$. In effectively two-dimensional materials, the spin-orbit coupling will usually involve only two spin components (Studer 2010, pp. 4–8), which means that we can satisfy this assumption by rotating the coordinate system such that the σ^2 contribution to $\mathcal{A}$ vanishes.

The symbol $\hat{\mathbf{g}}$ represents the retarded isotropic Green's function $\hat{\mathbf{g}}_s^{\mathrm{R}}$, where we drop the superscripts and subscripts from now on. Furthermore, note that the energy ϵ, band gap Δ, and exchange field $\mathbf{h}$ have all been rescaled to absorb the diffusion coefficient D in (4.98). The Green's function $\hat{\mathbf{g}}$ is a function of both position x and energy ϵ, while the band gap Δ and exchange field $\mathbf{h}$ are only functions of x. Since we assume that the system is governed by one-dimensional dynamics, the covariant derivative takes the form $\tilde{\nabla}\hat{\mathbf{g}} = \partial_x\hat{\mathbf{g}} - i[\hat{\mathcal{A}}, \hat{\mathbf{g}}]_-$.

Before we can attempt to solve the Usadel equation for the system shown in FIGURE 5.1, we need some boundary conditions for the problem. We will use the Kuprianov–Lukichev boundary conditions, which can be written as follows:[2][3]

$$\hat{\mathbf{g}}_n\tilde{\nabla}_x\hat{\mathbf{g}}_n\big|_{x=0} = \frac{1}{2}\Omega_n[\mathbf{g}_1, \mathbf{g}_2]_- \tag{5.2}$$

The notation $\hat{\mathbf{g}}_n$ refers to the Green's function in region n, where $n = 1$ for the superconductor and $n = 2$ for the ferromagnet. The interface parameter is defined as $\Omega_n \equiv R_n/L_nR_{\mathrm{B}}$, where R_n is the bulk resistance of material n, L_n is the length of region n, and R_{B} is the barrier resistance of the interface. The boundaries to the vacuum regions obey a similar condition, but assuming that the vacuum barrier has an infinite resistance, the corresponding interface parameter drops to zero. This simplifies the boundary conditions at those two boundaries:

$$\tilde{\nabla}_x\hat{\mathbf{g}}_1\big|_{x=-L_1} = 0 \qquad\qquad \tilde{\nabla}_x\hat{\mathbf{g}}_2\big|_{x=L_2} = 0 \tag{5.3}$$

In order to fully determine the behaviour of the system, we also need a way to determine the superconducting band gap Δ. In the case of a weak proximity effect, we can use the conventional self-consistency equation:[4]

$$-N_0\lambda\int_{-\infty}^{\infty}\mathrm{d}\xi\,\frac{\tanh[\sqrt{\xi^2+\Delta^2}/2T]}{\sqrt{\xi^2+\Delta^2}} = 1 \tag{5.4}$$

T is the temperature of the system and N_0 is the density of states at the Fermi level. However, in general the band gap $\Delta(x)$ would have to be calculated from the Green's functions. This can be done by noting that definition (2.26) can be written as $F^{\mathrm{K}}_{\uparrow\downarrow}(x,t;x,t) = -2i\langle\psi_\uparrow(x,t)\psi_\downarrow(x,t)\rangle$ when the two arguments are evaluated at the same spacetime coordinate. The band gap was defined as the absolute value of the order parameter $\lambda\langle\psi_\uparrow(x,t)\psi_\downarrow(x,t)\rangle$, and the interaction strength $\lambda < 0$, so we see that:

$$\Delta(x,t) = -\frac{1}{2}\lambda|F^{\mathrm{K}}_{\uparrow\downarrow}(x,t;x,t)| \tag{5.5}$$

In the limit of quasiclassical equilibrium, the above can be expressed as a function of the retarded isotropic Green's function in (5.1). However, due to time limitations, these calculations have not been performed.

[2] Kuprianov and Lukichev 1988.

[3] The Kuprianov–Lukichev boundary condition is conventionally written as $2\gamma_n\hat{\mathbf{g}}_n\partial_x\hat{\mathbf{g}}_n = [\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2]_-$, where γ_n is the ratio between the interface resistance per unit area and the resistivity of material n (Bergeret, Volkov, and Efetov 2005, pp. 1327,1367). However, in the presence of a background field $\mathcal{A}$, the partial derivative is replaced by a covariant derivative (Bergeret and Tokatly 2014, p. 5).

[4] Tinkham 1996, p. 63; Morten 2005, p. 62.

5.2 Parametrization

The 4×4 components of the matrix $\hat{\mathbf{g}}$ are not independent, but can be expressed as:

$$\hat{\mathbf{g}}(x,\epsilon) = \begin{bmatrix} \mathbf{g}(x,+\epsilon) & \mathbf{f}(x,+\epsilon) \\ -\mathbf{f}^*(x,-\epsilon) & -\mathbf{g}^*(x,-\epsilon) \end{bmatrix} \tag{5.6}$$

The above suggests that we introduce the *tilde conjugation* $\tilde{\mathbf{g}}(x,+\epsilon) \equiv \mathbf{g}^*(x,-\epsilon)$ to simplify the notation from now on. Moreover, the normalization condition $\hat{\mathbf{g}}^2 = \mathbf{1}$ further constrains the form of $\hat{\mathbf{g}}$ by relating the $\mathbf{g}$ components to the $\mathbf{f}$ components:

$$\mathbf{g}\mathbf{g} - \mathbf{f}\tilde{\mathbf{f}} = \mathbf{1} \qquad\qquad \mathbf{g}\mathbf{f} - \mathbf{f}\tilde{\mathbf{g}} = \mathbf{0} \tag{5.7}$$

Remarkably, if we pick a suitable parametrization of $\hat{\mathbf{g}}$ which automatically satisfies the symmetry and normalization requirements discussed above, then the 4×4 matrix equations (5.1), (5.2) and (5.3) can be reduced to three equivalent 2×2 equations. In this thesis, we will employ the socalled *Riccati parametrization* of $\hat{\mathbf{g}}$ for this purpose:

$$\hat{\mathbf{g}} = \begin{bmatrix} \mathbf{N} & 0 \\ 0 & -\tilde{\mathbf{N}} \end{bmatrix} \begin{bmatrix} 1+\gamma\tilde{\gamma} & 2\gamma \\ 2\tilde{\gamma} & 1+\tilde{\gamma}\gamma \end{bmatrix} \tag{5.8}$$

The normalization matrices are defined as $\mathbf{N} \equiv (1-\gamma\tilde{\gamma})^{-1}$ and $\tilde{\mathbf{N}} \equiv (1-\tilde{\gamma}\gamma)^{-1}$. Using the parametrization above, solving the equations for the 2×2 matrix function $\gamma(x,\epsilon)$ is sufficient to uniquely construct the whole Green's function $\hat{\mathbf{g}}(x,\epsilon)$. It is also noteworthy that $\hat{\mathbf{g}} \to \mathbf{1}$ when $\gamma \to \mathbf{0}$, while all the elements of $\hat{\mathbf{g}}$ diverge to infinity when $\gamma \to \mathbf{1}$; so we see that a finite range of variation in γ parametrizes an infinite range of variation in the elements of $\hat{\mathbf{g}}$.

Before we perform any calculations using the Riccati parametrization, it is convenient to derive some basic identities that relate the different matrices. Let us start by calculating the inverses of the two matrix products $\mathbf{N}\gamma$ and $\gamma\tilde{\mathbf{N}}$:

$$(\mathbf{N}\gamma)^{-1} = \gamma^{-1}\mathbf{N}^{-1} = \gamma^{-1}(\mathbf{1}-\gamma\tilde{\gamma}) = \gamma^{-1} - \tilde{\gamma} \tag{5.9}$$

$$(\gamma\tilde{\mathbf{N}})^{-1} = \tilde{\mathbf{N}}^{-1}\gamma^{-1} = (\mathbf{1}-\tilde{\gamma}\gamma)\gamma^{-1} = \gamma^{-1} - \tilde{\gamma} \tag{5.10}$$

By comparison of the results above, we see that $\mathbf{N}\gamma = \gamma\tilde{\mathbf{N}}$. Similar calculations for other combinations of the Riccati matrices reveal that we can move normalization matrices past gamma matrices if we also perform a tilde conjugation in the process:

$$\mathbf{N}\gamma = \gamma\tilde{\mathbf{N}} \qquad \tilde{\mathbf{N}}\gamma = \gamma\mathbf{N} \qquad \mathbf{N}\tilde{\gamma} = \tilde{\gamma}\tilde{\mathbf{N}} \qquad \tilde{\mathbf{N}}\tilde{\gamma} = \tilde{\gamma}\mathbf{N} \tag{5.11}$$

Since we intend to parametrize a differential equation, we should also try to relate the derivatives of the Riccati matrices. This can be done by differentiating the definition of $\mathbf{N}$ using the matrix version of the chain rule:

$$\begin{aligned} \partial_x\mathbf{N} &= \partial_x(\mathbf{1}-\gamma\tilde{\gamma})^{-1} \\ &= -(\mathbf{1}-\gamma\tilde{\gamma})^{-1}\left[\partial_x(\mathbf{1}-\gamma\tilde{\gamma})\right](\mathbf{1}-\gamma\tilde{\gamma})^{-1} \\ &= (\mathbf{1}-\gamma\tilde{\gamma})^{-1}\left[(\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma})\right](\mathbf{1}-\gamma\tilde{\gamma})^{-1} \\ &= \mathbf{N}\left[(\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma})\right]\mathbf{N} \end{aligned} \tag{5.12}$$

Performing a tilde conjugation of the equation above, we get a similar result for $\partial_x\tilde{\mathbf{N}}$. So the derivatives of the normalization matrices satisfy the following identities:

$$\partial_x\mathbf{N} = \mathbf{N}[(\partial_x\gamma)\tilde{\gamma} + \gamma(\partial_x\tilde{\gamma})]\mathbf{N} \qquad \partial_x\tilde{\mathbf{N}} = \tilde{\mathbf{N}}[(\partial_x\tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x\gamma)]\tilde{\mathbf{N}} \tag{5.13}$$

In addition to the identities derived above, one should note that the definition of the normalization matrix $\mathbf{N} = (\mathbf{1} - \gamma\tilde{\gamma})^{-1}$ can be rewritten in many forms which may be of use when simplifying Riccati parametrized expressions, such as $\gamma\tilde{\gamma} = \mathbf{1} - \mathbf{N}^{-1}$ and $\mathbf{1} = \mathbf{N} - \mathbf{N}\gamma\tilde{\gamma}$.

Now that the basic identities are in place, we can commence the parametrization of the Usadel equation. Let us expand the covariant derivatives in (5.1), and then simplify the result using the normalization $\hat{\mathbf{g}}^2 = \mathbf{1}$ and its derivative $[\hat{\mathbf{g}}, \partial_x\hat{\mathbf{g}}]_+ = \mathbf{0}$:

$$\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}}) = \partial_x(\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}) - i\partial_x(\hat{\mathbf{g}}\hat{\mathcal{A}}_x\hat{\mathbf{g}}) - i[\hat{\mathcal{A}}_x, \hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]_- - [\hat{\mathcal{A}}, \hat{\mathbf{g}}\hat{\mathcal{A}}\hat{\mathbf{g}}]_- \tag{5.14}$$

We then write $\hat{\mathbf{g}}$ on component form using (5.6), and write $\hat{\mathcal{A}}$ on the same form using (4.73). Since we made the assumption that the elements of $\mathcal{A}$ are real constants, the latter equation reduces to $\hat{\mathcal{A}} = \mathrm{diag}(\mathcal{A}, -\mathcal{A})$. The terms that appear in (5.14) may then be written as follows:

$$\partial_x(\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}) = \begin{bmatrix} \partial_x(\mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}) & \partial_x(\mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}) \\ \partial_x(\tilde{\mathbf{g}}\partial_x\tilde{\mathbf{f}} - \tilde{\mathbf{f}}\partial_x\mathbf{g}) & \partial_x(\tilde{\mathbf{g}}\partial_x\tilde{\mathbf{g}} - \tilde{\mathbf{f}}\partial_x\mathbf{f}) \end{bmatrix} \tag{5.15}$$

$$\partial_x(\hat{\mathbf{g}}\hat{\mathcal{A}}\hat{\mathbf{g}}) = \begin{bmatrix} \partial_x(\mathbf{g}\mathcal{A}\mathbf{g} + \mathbf{f}\mathcal{A}\tilde{\mathbf{f}}) & \partial_x(\mathbf{g}\mathcal{A}\mathbf{f} + \mathbf{f}\mathcal{A}\tilde{\mathbf{g}}) \\ -\partial_x(\tilde{\mathbf{g}}\mathcal{A}\tilde{\mathbf{f}} + \tilde{\mathbf{f}}\mathcal{A}\mathbf{g}) & -\partial_x(\tilde{\mathbf{g}}\mathcal{A}\tilde{\mathbf{g}} + \tilde{\mathbf{f}}\mathcal{A}\mathbf{f}) \end{bmatrix} \tag{5.16}$$

$$[\hat{\mathcal{A}}, \hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]_- = \begin{bmatrix} [\mathcal{A}, \mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}]_- & [\mathcal{A}, \mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}]_+ \\ -[\mathcal{A}, \tilde{\mathbf{g}}\partial_x\tilde{\mathbf{f}} - \tilde{\mathbf{f}}\partial_x\mathbf{g}]_+ & -[\mathcal{A}, \tilde{\mathbf{g}}\partial_x\tilde{\mathbf{g}} - \tilde{\mathbf{f}}\partial_x\mathbf{f}]_- \end{bmatrix} \tag{5.17}$$

$$[\hat{\mathcal{A}}, \hat{\mathbf{g}}\hat{\mathcal{A}}\hat{\mathbf{g}}]_- = \begin{bmatrix} [\mathcal{A}, \mathbf{g}\mathcal{A}\mathbf{g} + \mathbf{f}\mathcal{A}\tilde{\mathbf{f}}]_- & [\mathcal{A}, \mathbf{g}\mathcal{A}\mathbf{f} + \mathbf{f}\mathcal{A}\tilde{\mathbf{g}}]_+ \\ [\mathcal{A}, \tilde{\mathbf{g}}\mathcal{A}\tilde{\mathbf{f}} + \tilde{\mathbf{f}}\mathcal{A}\mathbf{g}]_+ & [\mathcal{A}, \tilde{\mathbf{g}}\mathcal{A}\tilde{\mathbf{g}} + \tilde{\mathbf{f}}\mathcal{A}\mathbf{f}]_- \end{bmatrix} \tag{5.18}$$

Substituting these results back into (5.14), we can find the upper blocks of $\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})$:[5]

$$\begin{aligned}[\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,1)} &= \partial_x(\mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}) - i\partial_x(\mathbf{g}\mathcal{A}_x\mathbf{g} + \mathbf{f}\mathcal{A}_x\tilde{\mathbf{f}}) \\ &\quad - i[\mathcal{A}_x, \mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}]_- - [\mathcal{A}, \mathbf{g}\mathcal{A}\mathbf{g} + \mathbf{f}\mathcal{A}\tilde{\mathbf{f}}]_-\end{aligned} \tag{5.19}$$

$$\begin{aligned}[\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,2)} &= \partial_x(\mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}) - i\partial_x(\mathbf{g}\mathcal{A}_x\mathbf{f} + \mathbf{f}\mathcal{A}_x\tilde{\mathbf{g}}) \\ &\quad - i[\mathcal{A}_x, \mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}]_+ - [\mathcal{A}, \mathbf{g}\mathcal{A}\mathbf{f} + \mathbf{f}\mathcal{A}\tilde{\mathbf{g}}]_+\end{aligned} \tag{5.20}$$

[5] In this context, the notation $\mathbf{M}^{(n,m)}$ refers to the n'th row and m'th column of $\mathbf{M}$ in Nambu space. Since the Green's function $\hat{\mathbf{g}}$ and background field $\hat{\mathcal{A}}$ also have a spin space structure, the $(1,1)$ element in Nambu space is the upper left 2×2 block of the matrix, and the $(1,2)$ element is the upper right one.

There are two kinds of expressions that recur in the equations above, namely the components of $\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}$ and $\hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}$. After we substitute in the Riccati parametrization $\mathbf{g} = 2\mathbf{N} - \mathbf{1}$ and $\mathbf{f} = 2\mathbf{N}\gamma$, these matrix blocks take the form:

$$\begin{aligned}[\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]^{(1,1)} &= \mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}} \\ &= 2\mathbf{N}[(\partial_x\gamma)\tilde{\gamma} - \gamma(\partial_x\tilde{\gamma})]\mathbf{N} \end{aligned} \tag{5.21}$$

$$\begin{aligned}[\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]^{(1,2)} &= \mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}} \\ &= 2\mathbf{N}[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{\mathbf{N}} \end{aligned} \tag{5.22}$$

$$\begin{aligned}[\hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}]^{(1,1)} &= \mathbf{g}.\mathcal{A}\mathbf{g} + \mathbf{f}.\mathcal{A}\tilde{\mathbf{f}} \\ &= 4\mathbf{N}(\mathcal{A} + \gamma\mathcal{A}\tilde{\gamma})\mathbf{N} - 2[\mathcal{A}, \mathbf{N}]_+ + \mathcal{A} \end{aligned} \tag{5.23}$$

$$\begin{aligned}[\hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}]^{(1,2)} &= \mathbf{g}.\mathcal{A}\mathbf{f} + \mathbf{f}.\mathcal{A}\tilde{\mathbf{g}} \\ &= 4\mathbf{N}(\mathcal{A}\gamma + \gamma.\mathcal{A})\tilde{\mathbf{N}} - 2[\mathcal{A}, \mathbf{N}\gamma]_+ \end{aligned} \tag{5.24}$$

If we calculate the commutators of $\hat{\mathcal{A}}$ with the matrices $\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}$ and $\hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}$, then we find:

$$\begin{aligned}[\hat{\mathcal{A}}, \hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]_-^{(1,1)} &= [\mathcal{A}, \mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}]_- \\ &= 2\mathbf{N}(\mathbf{1} - \gamma\tilde{\gamma}).\mathcal{A}\mathbf{N}[(\partial_x\gamma)\tilde{\gamma} - \gamma(\partial_x\tilde{\gamma})]\mathbf{N} \\ &- 2\mathbf{N}[(\partial_x\gamma)\tilde{\gamma} - \gamma(\partial_x\tilde{\gamma})]\mathbf{N}.\mathcal{A}(\mathbf{1} - \gamma\tilde{\gamma})\mathbf{N} \end{aligned} \tag{5.25}$$

$$\begin{aligned}[\hat{\mathcal{A}}, \hat{\mathbf{g}}\partial_x\hat{\mathbf{g}}]_-^{(1,2)} &= [\mathcal{A}, \mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}]_+ \\ &= 2\mathbf{N}(\mathbf{1} - \gamma\tilde{\gamma}).\mathcal{A}\mathbf{N}[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{\mathbf{N}} \\ &+ 2\mathbf{N}[(\partial_x\gamma) - \gamma(\partial_x\tilde{\gamma})\gamma]\tilde{\mathbf{N}}.\mathcal{A}(\mathbf{1} - \tilde{\gamma}\gamma)\tilde{\mathbf{N}} \end{aligned} \tag{5.26}$$

$$\begin{aligned}[\hat{\mathcal{A}}, \hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}]_-^{(1,1)} &= [\mathcal{A}, \mathbf{g}.\mathcal{A}\mathbf{g} + \mathbf{f}.\mathcal{A}\tilde{\mathbf{f}}]_- \\ &= 4\mathcal{A}\mathbf{N}(\mathcal{A} + \gamma\mathcal{A}\tilde{\gamma})\mathbf{N} - 4\mathbf{N}(\mathcal{A} + \gamma\mathcal{A}\tilde{\gamma})\mathbf{N}\mathcal{A} - 2[\mathcal{A}^2, \mathbf{N}]_- \end{aligned} \tag{5.27}$$

$$\begin{aligned}[\hat{\mathcal{A}}, \hat{\mathbf{g}}.\hat{\mathcal{A}}\hat{\mathbf{g}}]_-^{(1,2)} &= [\mathcal{A}, \mathbf{g}.\mathcal{A}\mathbf{f} + \mathbf{f}.\mathcal{A}\tilde{\mathbf{g}}]_+ \\ &= 4\mathcal{A}\mathbf{N}(\mathcal{A}\gamma + \gamma.\mathcal{A})\tilde{\mathbf{N}} + 4\mathbf{N}(\mathcal{A}\gamma + \gamma.\mathcal{A})\tilde{\mathbf{N}}\mathcal{A} - 4\mathcal{A}\mathbf{N}\gamma\mathcal{A} - 2[\mathcal{A}^2, \mathbf{N}\gamma]_+ \end{aligned} \tag{5.28}$$

If we instead differentiate the aforementioned matrices with respect to x, we obtain:

$$\begin{aligned}[\partial_x(\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}})]^{(1,1)} &= \partial_x(\mathbf{g}\partial_x\mathbf{g} - \mathbf{f}\partial_x\tilde{\mathbf{f}}) \\ &= 2\mathbf{N}[(\partial_x^2\boldsymbol{\gamma}) + 2(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}\tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma})]\tilde{\boldsymbol{\gamma}}\mathbf{N} \\ &\quad - 2\mathbf{N}\boldsymbol{\gamma}[(\partial_x^2\tilde{\boldsymbol{\gamma}}) + 2(\partial_x\tilde{\boldsymbol{\gamma}})\mathbf{N}\boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}})]\mathbf{N} \end{aligned} \tag{5.29}$$

$$\begin{aligned}[\partial_x(\hat{\mathbf{g}}\partial_x\hat{\mathbf{g}})]^{(1,2)} &= \partial_x(\mathbf{g}\partial_x\mathbf{f} - \mathbf{f}\partial_x\tilde{\mathbf{g}}) \\ &= 2\mathbf{N}[(\partial_x^2\boldsymbol{\gamma}) + 2(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}\tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma})]\tilde{\mathbf{N}} \\ &\quad - 2\mathbf{N}\boldsymbol{\gamma}[(\partial_x^2\tilde{\boldsymbol{\gamma}}) + 2(\partial_x\tilde{\boldsymbol{\gamma}})\mathbf{N}\boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}})]\boldsymbol{\gamma}\tilde{\mathbf{N}} \end{aligned} \tag{5.30}$$

$$\begin{aligned}[\partial_x(\hat{\mathbf{g}}\mathcal{A}\hat{\mathbf{g}})]^{(1,1)} &= \partial_x(\mathbf{g}\mathcal{A}\mathbf{g} + \mathbf{f}\mathcal{A}\tilde{\mathbf{f}}) \\ &= 2\mathbf{N}(\mathbf{1} + \boldsymbol{\gamma}\tilde{\boldsymbol{\gamma}})\mathcal{A}\mathbf{N}[\boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}}) + (\partial_x\boldsymbol{\gamma})\tilde{\boldsymbol{\gamma}}]\mathbf{N} \\ &\quad + 2\mathbf{N}[\boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}}) + (\partial_x\boldsymbol{\gamma})\tilde{\boldsymbol{\gamma}}]\mathbf{N}\mathcal{A}(\mathbf{1} + \boldsymbol{\gamma}\tilde{\boldsymbol{\gamma}})\mathbf{N} \\ &\quad + 4\mathbf{N}\boldsymbol{\gamma}\mathcal{A}\tilde{\mathbf{N}}[(\partial_x\tilde{\boldsymbol{\gamma}}) + \tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma})\tilde{\boldsymbol{\gamma}}]\mathbf{N} \\ &\quad + 4\mathbf{N}[(\partial_x\boldsymbol{\gamma}) + \boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}})\boldsymbol{\gamma}]\tilde{\mathbf{N}}\mathcal{A}\tilde{\boldsymbol{\gamma}}\mathbf{N} \end{aligned} \tag{5.31}$$

$$\begin{aligned}[\partial_x(\hat{\mathbf{g}}\mathcal{A}\hat{\mathbf{g}})]^{(1,2)} &= \partial_x(\mathbf{g}\mathcal{A}\mathbf{f} + \mathbf{f}\mathcal{A}\tilde{\mathbf{g}}) \\ &= 2\mathbf{N}(\mathbf{1} + \boldsymbol{\gamma}\tilde{\boldsymbol{\gamma}})\mathcal{A}\mathbf{N}[(\partial_x\boldsymbol{\gamma}) + \boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}})\boldsymbol{\gamma}]\tilde{\mathbf{N}} \\ &\quad + 2\mathbf{N}[(\partial_x\boldsymbol{\gamma}) + \boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}})\boldsymbol{\gamma}]\tilde{\mathbf{N}}\mathcal{A}(\mathbf{1} + \tilde{\boldsymbol{\gamma}}\boldsymbol{\gamma})\tilde{\mathbf{N}} \\ &\quad + 4\mathbf{N}\boldsymbol{\gamma}\mathcal{A}\tilde{\mathbf{N}}[\tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma}) + (\partial_x\tilde{\boldsymbol{\gamma}})\boldsymbol{\gamma}]\tilde{\mathbf{N}} \\ &\quad + 4\mathbf{N}[\boldsymbol{\gamma}(\partial_x\tilde{\boldsymbol{\gamma}}) + (\partial_x\boldsymbol{\gamma})\tilde{\boldsymbol{\gamma}}]\mathbf{N}\mathcal{A}\tilde{\boldsymbol{\gamma}}\tilde{\mathbf{N}} \end{aligned} \tag{5.32}$$

Combining all of the equations above, we can express (5.19) and (5.20) using Riccati matrices. In order to isolate the second-order derivative $(\partial_x^2\boldsymbol{\gamma})$ from these, the trick is to multiply (5.19) by $\boldsymbol{\gamma}$ from the right, and subtract the result from (5.20):

$$\begin{aligned}\frac{1}{2}\mathbf{N}^{-1}\Big\{[\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,2)} - [\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,1)}\boldsymbol{\gamma}\Big\} &= (\partial_x^2\boldsymbol{\gamma}) + 2(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}\tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma}) \\ &\quad - 2i(\mathcal{A}_x + \boldsymbol{\gamma}\mathcal{A}_x\tilde{\boldsymbol{\gamma}})\mathbf{N}(\partial_x\boldsymbol{\gamma}) \\ &\quad - 2i(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}(\mathcal{A}_x + \tilde{\boldsymbol{\gamma}}\mathcal{A}_x\boldsymbol{\gamma}) \\ &\quad - 2(\mathcal{A}\boldsymbol{\gamma} + \boldsymbol{\gamma}\mathcal{A})\tilde{\mathbf{N}}(\mathcal{A} + \tilde{\boldsymbol{\gamma}}\mathcal{A}\boldsymbol{\gamma}) \\ &\quad - 2[\mathcal{A}^2, \boldsymbol{\gamma}]_- \end{aligned} \tag{5.33}$$

If we finally rewrite $[\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,1)}$ and $[\tilde{\nabla}\cdot(\hat{\mathbf{g}}\tilde{\nabla}\hat{\mathbf{g}})]^{(1,2)}$ in the equation above by substituting in the Usadel equation (5.1), then we obtain the following equation for the Riccati matrix $\boldsymbol{\gamma}$:

$$\begin{aligned}(\partial_x^2\boldsymbol{\gamma}) + 2(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}\tilde{\boldsymbol{\gamma}}(\partial_x\boldsymbol{\gamma}) &= \Delta(\sigma^2 - \boldsymbol{\gamma}\sigma^2\boldsymbol{\gamma}) - 2i\epsilon\boldsymbol{\gamma} - i\mathbf{h}\cdot(\sigma\boldsymbol{\gamma} - \boldsymbol{\gamma}\sigma^*) \\ &\quad + 2i(\mathcal{A}_x + \boldsymbol{\gamma}\mathcal{A}_x\tilde{\boldsymbol{\gamma}})\mathbf{N}(\partial_x\boldsymbol{\gamma}) + 2i(\partial_x\boldsymbol{\gamma})\tilde{\mathbf{N}}(\mathcal{A}_x + \tilde{\boldsymbol{\gamma}}\mathcal{A}_x\boldsymbol{\gamma}) \\ &\quad + 2(\mathcal{A}\boldsymbol{\gamma} + \boldsymbol{\gamma}\mathcal{A})\tilde{\mathbf{N}}(\mathcal{A} + \tilde{\boldsymbol{\gamma}}\mathcal{A}\boldsymbol{\gamma}) + 2[\mathcal{A}^2, \boldsymbol{\gamma}]_- \end{aligned} \tag{5.34}$$

The corresponding equation for $\tilde{\boldsymbol{\gamma}}$ can be found by tilde conjugation of the above.

After applying the Riccati parametrization to the Usadel equation, the next step is to do the same to the Kuprianov–Lukichev boundary condition. If we write out the covariant derivative in (5.2), then we get:

$$\hat{\mathbf{g}}_n \partial_x \hat{\mathbf{g}}_n = \frac{1}{2}\Omega_n[\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2]_- + i\hat{\mathbf{g}}_n[\hat{\mathcal{A}}_x, \hat{\mathbf{g}}_n]_- \tag{5.35}$$

We will now restrict our attention to the (1,1) and (1,2) components of the above:

$$\mathbf{g}_n \partial_x \mathbf{g}_n - \mathbf{f}_n \partial_x \tilde{\mathbf{f}}_n = \frac{1}{2}\Omega_n(\mathbf{g}_1\mathbf{g}_2 - \mathbf{g}_2\mathbf{g}_1 - \mathbf{f}_1\tilde{\mathbf{f}}_2 + \mathbf{f}_2\tilde{\mathbf{f}}_1) + i\mathbf{g}_n[\mathcal{A}_x, \mathbf{g}_n]_- + i\mathbf{f}_n[\mathcal{A}_x, \tilde{\mathbf{f}}_n]_+ \tag{5.36}$$

$$\mathbf{g}_n \partial_x \mathbf{f}_n - \mathbf{f}_n \partial_x \tilde{\mathbf{g}}_n = \frac{1}{2}\Omega_n(\mathbf{g}_1\mathbf{f}_2 - \mathbf{g}_2\mathbf{f}_1 - \mathbf{f}_1\tilde{\mathbf{g}}_2 + \mathbf{f}_2\tilde{\mathbf{g}}_1) + i\mathbf{g}_n[\mathcal{A}_x, \mathbf{f}_n]_+ + i\mathbf{f}_n[\mathcal{A}_x, \tilde{\mathbf{g}}_n]_- \tag{5.37}$$

Substituting the Riccati parametrizations $\mathbf{g}_n = 2\mathbf{N}_n - 1$ and $\mathbf{f}_n = 2\mathbf{N}_n\gamma_n$ in the above, we then obtain:

$$\begin{aligned}\mathbf{N}_n[(\partial_x\gamma_n)\tilde{\gamma}_n - \gamma_n(\partial_x\tilde{\gamma}_n)]\mathbf{N}_n = {}& \Omega_n\mathbf{N}_1(\mathbf{1}-\gamma_1\tilde{\gamma}_2)\mathbf{N}_2 \\ & - \Omega_n\mathbf{N}_2(\mathbf{1}-\gamma_2\tilde{\gamma}_1)\mathbf{N}_1 \\ & - i\mathbf{N}_n(\mathbf{1}-\gamma_n\tilde{\gamma}_n)\mathcal{A}\mathbf{N}_n \\ & - i\mathbf{N}_n\mathcal{A}(\mathbf{1}-\gamma_n\tilde{\gamma}_n)\mathbf{N}_n \\ & + 2i\mathbf{N}_n(\mathcal{A}+\gamma_n\mathcal{A}\tilde{\gamma}_n)\mathbf{N}_n\end{aligned} \tag{5.38}$$

$$\begin{aligned}\mathbf{N}_n[(\partial_x\gamma_n) - \gamma_n(\partial_x\tilde{\gamma}_n)\gamma_n]\tilde{\mathbf{N}}_n = {}& \Omega_n\mathbf{N}_1(\mathbf{1}-\gamma_1\tilde{\gamma}_2)\gamma_2\tilde{\mathbf{N}}_2 \\ & - \Omega_n\mathbf{N}_2(\mathbf{1}-\gamma_2\tilde{\gamma}_1)\gamma_1\tilde{\mathbf{N}}_1 \\ & + i\mathbf{N}_n(\mathbf{1}+\gamma_n\tilde{\gamma}_n)\mathcal{A}\gamma_n\tilde{\mathbf{N}}_n \\ & + i\mathbf{N}_n\gamma_n\mathcal{A}(\mathbf{1}+\tilde{\gamma}_n\gamma_n)\tilde{\mathbf{N}}_n\end{aligned} \tag{5.39}$$

If we then multiply (5.38) by γ_n from the right, subtract this from (5.39), and divide by $\mathbf{N}_n$ from the left, then we obtain the following boundary condition for γ_n:

$$\partial_x\gamma_n = \Omega_n[\mathbf{1}-\gamma_1\tilde{\gamma}_2]\mathbf{N}_2[\gamma_2-\gamma_n] + \Omega_n[\mathbf{1}-\gamma_2\tilde{\gamma}_1]\mathbf{N}_1[\gamma_n-\gamma_1] + i[\mathcal{A}_x, \gamma_n]_+ \tag{5.40}$$

When we evaluate the above for $n = 1$ and $n = 2$, then it simplifies to the following:

$$\partial_x\gamma_1 = \Omega_1[\mathbf{1}-\gamma_1\tilde{\gamma}_2]\mathbf{N}_2[\gamma_2-\gamma_1] + i[\mathcal{A}_x, \gamma_1]_+ \tag{5.41}$$

$$\partial_x\gamma_2 = \Omega_2[\mathbf{1}-\gamma_2\tilde{\gamma}_1]\mathbf{N}_1[\gamma_2-\gamma_1] + i[\mathcal{A}_x, \gamma_2]_+ \tag{5.42}$$

The boundary conditions for $\partial_x\tilde{\gamma}_1$ and $\partial_x\tilde{\gamma}_2$ are found by tilde conjugating the above. The boundary conditions at $x = -L_1$ and $x = L_2$ are the same, except that $\Omega_1, \Omega_2 \to 0$.

5.3 Final results

5.3.1 Superconductor

After the Riccati parametrization of the Usadel equation and Kuprianov–Lukichev boundary conditions, we return to the superconductor/ferromagnet bilayer shown in Figure 5.1. Since the superconducting region has no exchange field or spin-orbit coupling, (5.34) and its tilde conjugate become particularly simple in this region:

$$\partial_x^2\gamma_1 = -2(\partial_x\gamma_1)\tilde{\mathbf{N}}_1\tilde{\gamma}_1(\partial_x\gamma_1) - 2i\epsilon\gamma_1 + \Delta(\sigma^2 - \gamma_1\sigma^2\gamma_1) \tag{5.43}$$

$$\partial_x^2\tilde{\gamma}_1 = -2(\partial_x\tilde{\gamma}_1)\mathbf{N}_1\gamma_1(\partial_x\tilde{\gamma}_1) - 2i\epsilon\tilde{\gamma}_1 - \Delta(\sigma^2 - \tilde{\gamma}_1\sigma^2\tilde{\gamma}_1) \tag{5.44}$$

The boundary conditions are given by (5.41) without the spin-orbit term:

$$\partial_x\gamma_1 = \begin{cases} 0 & \text{at } x = -L_1, \\ \Omega_1[\mathbf{1} - \gamma_1\tilde{\gamma}_2]\mathbf{N}_2[\gamma_2 - \gamma_1] & \text{at } x = 0; \end{cases} \tag{5.45}$$

$$\partial_x\tilde{\gamma}_1 = \begin{cases} 0 & \text{at } x = -L_1, \\ \Omega_1[\mathbf{1} - \tilde{\gamma}_1\gamma_2]\tilde{\mathbf{N}}_2[\tilde{\gamma}_2 - \tilde{\gamma}_1] & \text{at } x = 0. \end{cases} \tag{5.46}$$

These equations have to be accompanied by a self-consistency equation for $\Delta(x)$.

5.3.2 Ferromagnet

The ferromagnetic region will in general have both an exchange field and a spin-orbit coupling, while the superconducting band gap Δ vanishes. This means that (5.34) and its tilde conjugate take a more complicated form in this region:

$$\begin{aligned} \partial_x^2\gamma_2 = &-2(\partial_x\gamma_2)\tilde{\mathbf{N}}_2\tilde{\gamma}_2(\partial_x\gamma_2) - 2i\epsilon\gamma_2 - i\mathbf{h}\cdot(\sigma\gamma_2 - \gamma_2\sigma^*) \\ &+ 2i(\mathcal{A}_x + \gamma_2\mathcal{A}_x\tilde{\gamma}_2)\mathbf{N}_2(\partial_x\gamma_2) + 2i(\partial_x\gamma_2)\tilde{\mathbf{N}}_2(\mathcal{A}_x + \tilde{\gamma}_2\mathcal{A}_x\gamma_2) \\ &+ 2(\mathcal{A}\gamma_2 + \gamma_2\mathcal{A})\tilde{\mathbf{N}}_2(\mathcal{A} + \tilde{\gamma}_2\mathcal{A}\gamma_2) + 2[\mathcal{A}^2, \gamma_2]_- \end{aligned} \tag{5.47}$$

$$\begin{aligned} \partial_x^2\tilde{\gamma}_2 = &-2(\partial_x\tilde{\gamma}_2)\mathbf{N}_2\gamma_2(\partial_x\tilde{\gamma}_2) - 2i\epsilon\gamma_2 + i\mathbf{h}\cdot(\sigma^*\tilde{\gamma}_2 - \tilde{\gamma}_2\sigma) \\ &- 2i(\mathcal{A}_x + \tilde{\gamma}_2\mathcal{A}_x\gamma_2)\tilde{\mathbf{N}}_2(\partial_x\tilde{\gamma}_2) - 2i(\partial_x\tilde{\gamma}_2)\mathbf{N}_2(\mathcal{A}_x + \gamma_2\mathcal{A}_x\tilde{\gamma}_2) \\ &+ 2(\mathcal{A}\tilde{\gamma}_2 + \tilde{\gamma}_2\mathcal{A})\mathbf{N}_2(\mathcal{A} + \gamma_2\mathcal{A}\tilde{\gamma}_2) + 2[\mathcal{A}^2, \tilde{\gamma}_2]_- \end{aligned} \tag{5.48}$$

The corresponding boundary conditions are provided by (5.42):

$$\partial_x\gamma_2 = \begin{cases} i[\mathcal{A}_x, \gamma_2]_+ + \Omega_2[\mathbf{1} - \gamma_2\tilde{\gamma}_1]\mathbf{N}_1[\gamma_2 - \gamma_1] & \text{at } x = 0, \\ i[\mathcal{A}_x, \gamma_2]_+ & \text{at } x = L_2; \end{cases} \tag{5.49}$$

$$\partial_x\tilde{\gamma}_2 = \begin{cases} -i[\mathcal{A}_x, \tilde{\gamma}_2]_+ + \Omega_2[\mathbf{1} - \tilde{\gamma}_2\gamma_1]\tilde{\mathbf{N}}_1[\tilde{\gamma}_2 - \tilde{\gamma}_1] & \text{at } x = 0, \\ -i[\mathcal{A}_x, \tilde{\gamma}_2]_+ & \text{at } x = L_2. \end{cases} \tag{5.50}$$

These equations have to be accompanied by an expression for the exchange field $\mathbf{h}(x)$ and spin-orbit coupling $\mathcal{A}$ in the system.

6 Conclusion

In the preceding chapters, we derived a set of equations that describe heterostructures with superconducting and ferromagnetic components under quite general circumstances. After putting together an appropriate Hamiltonian for such a system in chapter 3, we derived the exact transport equations in the first half of chapter 4, followed by a series of analytical approximations that culminated in the Usadel equation. Finally, in chapter 5, we considered the special case of a superconductor/ferromagnet bilayer with spin-orbit coupling in equilibrium, and performed a Riccati parametrization of the Usadel equation and Kuprianov–Lukichev boundary conditions.

The original contribution that has been made in this thesis, is the Riccati parametrized boundary value problem that is presented in section 5.3. In the future, these equations can be used to study how various types of inhomogeneous magnetization textures and spin-orbit coupling affects different physical observables, such as the superconducting band gap, density of states, and critical temperature. Because of the generality of the derivation, these equations can also be used to study the generation and behaviour of long-range triplet components in the full proximity regime. This can ultimately result in predictions that may be tested experimentally.

A Commutation relations for field operators

In this appendix, we will derive some useful commutation identities for products of field operators. The basic strategy is to use $[A, BC]_- = [A, B]_+ C - B[A, C]_+$ to convert commutators into anticommutators, and then use the fermionic anticommutation relations to reduce these to zeros and delta functions.

$$\begin{aligned}
[\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)\psi_{\sigma''}(\mathbf{r}',t)]_- &= [\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)]_+\psi_{\sigma''}(\mathbf{r}',t) - \psi_{\sigma'}(\mathbf{r}',t)[\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma''}(\mathbf{r}',t)]_+ \\
&= 0 && \text{(A.1)} \\
[\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi_{\sigma''}(\mathbf{r}',t)]_- &= [\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)]_+\psi_{\sigma''}(\mathbf{r}',t) - \psi^\dagger_{\sigma'}(\mathbf{r}',t)[\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma''}(\mathbf{r}',t)]_+ \\
&= \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\psi_{\sigma''}(\mathbf{r}',t) && \text{(A.2)} \\
[\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi^\dagger_{\sigma''}(\mathbf{r}',t)]_- &= [\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)]_+\psi^\dagger_{\sigma''}(\mathbf{r}',t) - \psi^\dagger_{\sigma'}(\mathbf{r}',t)[\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma''}(\mathbf{r}',t)]_+ \\
&= \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\psi^\dagger_{\sigma''}(\mathbf{r}',t) - \psi^\dagger_{\sigma'}(\mathbf{r}',t)\delta_{\sigma\sigma''}\delta(\mathbf{r}-\mathbf{r}') && \text{(A.3)} \\
[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)\psi_{\sigma''}(\mathbf{r}',t)]_- &= [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)]_+\psi_{\sigma''}(\mathbf{r}',t) - \psi_{\sigma'}(\mathbf{r}',t)[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi_{\sigma''}(\mathbf{r}',t)]_+ \\
&= \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\psi_{\sigma''}(\mathbf{r}',t) - \psi_{\sigma'}(\mathbf{r}',t)\delta_{\sigma\sigma''}\delta(\mathbf{r}-\mathbf{r}') && \text{(A.4)} \\
[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi_{\sigma''}(\mathbf{r}',t)]_- &= [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)]_+\psi_{\sigma''}(\mathbf{r}',t) - \psi^\dagger_{\sigma'}(\mathbf{r}',t)[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi_{\sigma''}(\mathbf{r}',t)]_+ \\
&= -\psi^\dagger_{\sigma'}(\mathbf{r}',t)\delta_{\sigma\sigma''}\delta(\mathbf{r}-\mathbf{r}') && \text{(A.5)} \\
[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\psi^\dagger_{\sigma''}(\mathbf{r}',t)]_- &= [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)]_+\psi^\dagger_{\sigma''}(\mathbf{r}',t) - \psi^\dagger_{\sigma'}(\mathbf{r}',t)[\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma''}(\mathbf{r}',t)]_+ \\
&= 0 && \text{(A.6)}
\end{aligned}$$

If we multiply the identities above with some operator $\mathbf{F}(\mathbf{r}')$ that commutes with all the field operators, which means that we may move it in and out of commutators at will, and then integrate the results with respect with respect to $\mathbf{r}'$, we get the following identities:

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi_{\sigma''}(\mathbf{r}',t)]_- = 0 \qquad \text{(A.7)}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi_{\sigma''}(\mathbf{r}',t)]_- = \mathbf{F}(\mathbf{r})\,\delta_{\sigma\sigma'}\psi_{\sigma''}(\mathbf{r},t) \qquad \text{(A.8)}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi^\dagger_{\sigma''}(\mathbf{r}',t)]_- = \mathbf{F}(\mathbf{r})\,[\delta_{\sigma\sigma'}\psi^\dagger_{\sigma''}(\mathbf{r},t) - \delta_{\sigma\sigma''}\psi^\dagger_{\sigma'}(\mathbf{r},t)] \qquad \text{(A.9)}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi_{\sigma''}(\mathbf{r}',t)]_- = \mathbf{F}(\mathbf{r})\,[\delta_{\sigma\sigma'}\psi_{\sigma''}(\mathbf{r},t) - \delta_{\sigma\sigma''}\psi_{\sigma'}(\mathbf{r},t)] \qquad \text{(A.10)}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi_{\sigma''}(\mathbf{r}',t)]_- = -\mathbf{F}(\mathbf{r})\,\delta_{\sigma\sigma''}\psi^\dagger_{\sigma'}(\mathbf{r},t) \qquad \text{(A.11)}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi^\dagger_\sigma(\mathbf{r},t),\, \psi^\dagger_{\sigma'}(\mathbf{r}',t)\,\mathbf{F}(\mathbf{r}')\,\psi^\dagger_{\sigma''}(\mathbf{r}',t)]_- = 0 \qquad \text{(A.12)}$$

These commutation relations cover most of the situations that we will encounter. However, there is still one case that requires special care: the covariant derivative $\tilde{\nabla}'^2 = (\nabla' - i\boldsymbol{\mathcal{A}}(\mathbf{r}', t))^2$. Again, we start with the identity $[A, BC]_- = [A, B]_+ C - B[A, C]_+$:

$$\begin{aligned}[\psi_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- &= [\psi_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)]_+ \tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t) \\ &\quad - \psi^\dagger_{\sigma'}(\mathbf{r}', t)[\psi_\sigma(\mathbf{r}, t),\, \tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_+ \end{aligned} \tag{A.13}$$

Since $\tilde{\nabla}'$ only acts on primed coordinates, it commutes with $\psi_\sigma(\mathbf{r}, t)$. We can therefore pull the derivative out of the anticommutator, and then use the fermionic anticommutation relations like before:

$$\begin{aligned}[\psi_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- &= [\psi_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)]_+ \tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t) \\ &\quad - \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}[\psi_\sigma(\mathbf{r}, t),\, \psi_{\sigma''}(\mathbf{r}', t)]_+ \\ &= \delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}')\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t) \end{aligned} \tag{A.14}$$

For the commutator involving $\psi^\dagger_\sigma(\mathbf{r}, t)$, we get something very similar:

$$[\psi^\dagger_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- = -\psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\delta_{\sigma\sigma''}\delta(\mathbf{r} - \mathbf{r}') \tag{A.15}$$

But moving $\delta(\mathbf{r} - \mathbf{r}')$ past the differential operator $\tilde{\nabla}'^2$ requires some special attention. We can accomplish this by expanding $\tilde{\nabla}'^2$, and then using $\nabla'\delta(\mathbf{r} - \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}')\nabla'$:[1]

$$\begin{aligned}\tilde{\nabla}'^2\delta(\mathbf{r} - \mathbf{r}') &= \Big[\nabla'^2 - i\boldsymbol{\mathcal{A}}(\mathbf{r}', t)\cdot\nabla' - i\nabla'\cdot\boldsymbol{\mathcal{A}}(\mathbf{r}', t) + \boldsymbol{\mathcal{A}}^2(\mathbf{r}', t)\Big]\delta(\mathbf{r} - \mathbf{r}') \\ &= \delta(\mathbf{r} - \mathbf{r}')\Big[\nabla'^2 + i\boldsymbol{\mathcal{A}}(\mathbf{r}', t)\cdot\nabla' + i\nabla'\cdot\boldsymbol{\mathcal{A}}(\mathbf{r}', t) + \boldsymbol{\mathcal{A}}^2(\mathbf{r}', t)\Big] \\ &= \delta(\mathbf{r} - \mathbf{r}')(\tilde{\nabla}'^2)^\dagger \end{aligned} \tag{A.16}$$

In the last transition, we used the hermiticity of $\boldsymbol{\mathcal{A}}$. The commutator above becomes:

$$[\psi^\dagger_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- = -\delta_{\sigma\sigma''}\delta(\mathbf{r} - \mathbf{r}')\tilde{\nabla}'^{2*}_{\sigma''\sigma'}\psi^\dagger_{\sigma'}(\mathbf{r}', t) \tag{A.17}$$

Finally, we integrate the above results with respect to $\mathbf{r}'$, and obtain these identities:

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- = \quad \delta_{\sigma\sigma'}\tilde{\nabla}^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}, t) \tag{A.18}$$

$$\int \mathrm{d}^3\mathbf{r}'\, [\psi^\dagger_\sigma(\mathbf{r}, t),\, \psi^\dagger_{\sigma'}(\mathbf{r}', t)\tilde{\nabla}'^2_{\sigma'\sigma''}\psi_{\sigma''}(\mathbf{r}', t)]_- = -\delta_{\sigma\sigma''}\tilde{\nabla}^{2*}_{\sigma''\sigma'}\psi^\dagger_{\sigma'}(\mathbf{r}, t) \tag{A.19}$$

[1] We can motivate this identity by considering the one-dimensional integral of a test function $f(x)$. Using integration by parts, we see that:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta'(x)f(x) = \Big[\delta(x)f(x)\Big]_{-\infty}^{+\infty} - \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x)f'(x)$$

Since $\delta(+\infty) = \delta(-\infty) = 0$, the first term on the right-hand side vanishes. The delta function is *defined* by how it modifies a test function $f(x)$ under integration, so we conclude that $\delta'(x)f(x) = -\delta(x)f'(x)$, or simply $\delta'(x) = -\delta(x)\,\mathrm{d}/\mathrm{d}x$. The three-dimensional generalization is $\nabla\delta(\mathbf{r}) = -\delta(\mathbf{r})\nabla$.

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