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Chapter 2

Theoretical concepts

2.1 Fundamentals of superconductivity

2.1.1 Foundation of the microscopical description

The work of Cooper [11] (1956) shows that if the interaction between electrons leads to a net attraction between two electrons close to the Fermi surface, then bound states can be formed located below the Fermi surface. The density of these bound states strongly depends on the total momentum K of the pair, being at a maximum where K = 0 and rapidly going to zero for non-zero K. It was therefore suggested that the elementary excitations of the pair were most likely to correspond to the splitting of the pair rather than to increasing the kinetic energy of the pair (since its density falls of so quickly with increasing K). Such net attractive interaction between electrons can occur when the attractive phonon interaction dominates the Coulomb repulsion. Where the latter mechanism is just the direct repulsion between two particles of the same charge, the first mechanism is an indirect interaction. The negatively charged electron slightly deforms the surrounding lattice by pulling on the positively charged atoms and while the electron moves around, it leaves a trail (or wave) of such deformations (or phonons). As this is an area with slightly increased positive charge, it attracts new electrons. Effectively, by this mechanism electrons attract each other mediated by phonons. In the works of Bardeen, Cooper and Schrieffer [12, 13] (BCS theory, 1957) and of Bogoliubov [14] (1958) a systematic theory of superconductivity has been erected on this principle of attraction. It was shown that the ground state of such a system of interacting Fermi particles is located below the normal state with a filled Fermi sphere and, in consequence, it is separated from the excited states by an energy gap with a magnitude of the order of the coupling energy of an individual pair. Furthermore, the net attraction between electrons takes place inside an energy shell of order k_BT_c around the Fermi surface, with T_c the superconducting transition temperature. For the elemental superconductors, like Aluminum (Al), Mercury (Hg), Niobium (Nb), Tin (Sn) and Lead (Pb), this coupling ranges up to about 1 meV, with a corresponding T_c up to about 10 K. An essential feature of the BCS theory is that all the Cooper pairs must behave in exactly the same way, which makes that they can be described by a single wave function. According to BCS theory: "The pairs should be chosen so that transitions between them are possible, i.e. they all have the same total momentum". As a best choice for the ground state pairing they took pairs with zero total momentum and opposite spin. The latter because exchange terms enhance the repulsive interaction for parallel spins. The Cooper pairs are located at the Fermi energy which is separated by an energy gap Δ from the quasiparticle states. The total gap between the (occupied) quasiparticle

spectrum below E_F and the (unoccupied) quasiparticle spectrum above E_F is $2\Delta \approx 3.5 k_B T_c$. This approximation is valid in the weak coupling limit, which means superconductors for which $N_0 V < 0.3$ where N_0 is the normal density of states at the Fermi energy and V the attractive interaction. Most classical superconductors belong to this limit (Al has a bulk T_c of 1.2 K with $\Delta \sim 180 \ \mu eV$) but for example Pb with a bulk T_c of 7.2 K and $\Delta \sim 1.3 \ meV$ does not. The left panel of Fig. 2.1 shows the pairing of states in k-space, for both a filled pair state $(|\mathbf{k}| > k_F)$ and an empty pair state $|\mathbf{k}| < k_F$. The elementary excitations are broken paired states, which means that one of the two states of the paired state is occupied and one is empty. If $|\mathbf{k}| < k_F$ the excitation is hole-like in its behavior, while for $|\mathbf{k}| > k_F$ it is electron-like. The k-space represents only kinetic energy and thus the (potential) energy lowering of the paired states due to condensation is not "included". The paired states assemble in the condensate which is at the Fermi energy E_F while the excitations (broken states) occupy single electron states in the quasiparticle spectrum (right panel of Fig. 2.1, with $E_F = 0$). Electron-like excitation have $E > E_F$ and hole-like excitations have $E < E_F$. The Cooper pairs can be bro-



Figure 2.1: Pairing of states in k-space (left panel) and quasiparticle spectrum (right panel) for a BCS superconductor. The light/dark shaded areas represent empty/occupied states, the black/white dots represent electron/hole excitations and the wiggled lines represents the paired states. Left panel: The Fermi wave vector k_F is much larger than the shell δk around k_F where the pairing takes place (for clarity k_z is taken zero). Right panel: The density of states N_S is normalized to the normal state density of states N_0 , the energy E is normalized to the gap energy Δ , and the Fermi energy E_F is set to zero.

ken into excited states by temperature, but also by mechanisms that change the pairing itself. The Cooper pairs in a conventional bulk superconductor (s-wave, spin-singlet = BCS superconductor) consist of two electrons with opposite spin and momentum close to Fermi momentum. The Fermi spheres to which the two particles (\mathbf{k},\uparrow) and $(-\mathbf{k},\downarrow)$ belong are identical, say symmetrical. Whenever this symmetry is lifted the Cooper pair starts to experience a pair breaking force, weakening the superconducting state. Two types of symmetry breaking effects are recognized. The orbital effect is related to a shift between the Fermi spheres, which happens if the one acquires a net momentum with respect to the other. The paramagnetic effect is related to a change in the *size* between the Fermi spheres, which translates to an exchange energy between the two spin states. The orbital effect is responsible for the limitation of the supercurrent density and magnetic flux expulsion. In terms of momentum **p** the two electrons of the Cooper pair are (\mathbf{p},\uparrow) and $(-\mathbf{p},\downarrow)$, but in the presence of an electromagnetic field described by the vector potential A, the potential (or field) momentum eA/c needs to be added to the kinetic momentum $m\mathbf{v}$, with c the velocity of light. For the Cooper pair this results in $(\mathbf{p} + e\mathbf{A}/c, \uparrow)$ and $(-\mathbf{p} + e\mathbf{A}/c, \downarrow)$, which gives a total momentum of $2e\mathbf{A}/c$. The exerted Lorentz force is directed in opposite directions for the two electrons, trying to break the Cooper pair. Whenever the associated energy of the pair momentum exceeds the condensation energy, the Cooper pair is no longer a stable ground state. A transition from the superconducting state to the normal state by the orbital effect is essentially due to the kinetic energy of the pairs becoming larger than the condensation energy, while by the paramagnetic effect it is if the exchange energy becomes larger then the condensation energy.

The BCS Hamiltonian that describes superconductivity is valid for a superconductor in equilibrium at zero temperature in the absence of any interactions other than the attractive interaction that causes the formation of Cooper pairs. Using the creation and annihilation operators $(c_{k\sigma}^{\dagger} \text{ and } c_{k\sigma})$ for Bloch states specified by wave vector **k** and spin σ , it can be expressed as:

$$\mathcal{H}_{BCS} = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \sum_{kk'} V_{kk'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$
(2.1)

where $n_{k\sigma} = c_{k\sigma}^{\dagger} c_{k\sigma}$ is the single-particle number operator (which counts the number of particles in a specific state), $\epsilon_k = \hbar^2 k^2 / (2m)$ is the corresponding (kinetic) energy with *m* the electron mass, measured with respect to the

momentum **p**, velocity **v** and wave vector **k** are related by $\mathbf{p} = m\mathbf{v} = \hbar \mathbf{k}$

Fermi energy, and $V_{kk'}$ is the attractive interaction. The first term appearing in the Hamiltonian is the standard kinetic energy term, while the second term describes the scattering of a Cooper pair from state $(k'\uparrow, -k'\downarrow)$ to state $(k\uparrow, -k\downarrow)$ under the influence of the attractive interaction. In the BCS model, the attractive interaction is taken constant, $V_{kk'} = V$, for energies up to a certain cut-off energy (the Debye energy), otherwise it is zero. The Hamiltonian is accompanied by a self-consistency relation for the energy gap:

$$\frac{1}{V} = \frac{1}{2} \sum_{k} \frac{1}{\sqrt{\Delta^2 + \epsilon_k^2}} \tag{2.2}$$

Solving the Hamiltonian for a certain potential V gives the eigenstates and eigenenergies of the superconductor. By inserting these into the self-consistency equation, the chosen potential V should be regained if the chosen value was correct. These two equations (Eq. 2.1, 2.2) form the basis for the modern description of superconductivity, which is written in the language of Green functions.

2.1.2 Bogoliubov-de Gennes equation

The BCS theory is written in (standard) single particle creation and annihilation operators for Bloch states specified by wave vector **k** and spin σ . However, the elementary excitations of the superconductor are no longer the single particle states which we have for a normal metal, instead they are broken Cooper pair states. This makes the usage of the standard single particle creation and annihilation operators very cumbersome (for finite temperatures). A mathematical formulation based on the BCS theory was developed by Bogoliubov where he introduced the concept of coherent mixtures of particles and holes to describe a superconductor at finite temperatures. These mixed particle-hole excited states are known as Bogoliubons. The introduction of operators for these Bogoliubons has been generalized and evolved into what is now known as the Bogoliubov-deGennes (BdG) equation [15]. In this description, the standard momentum operators (k-space) have been replaced by field operators (real-space), which have the advantage that they are able to describe systems in which k is no longer a good quantum number and thus the eigenfunctions are no longer plane waves (dirty systems for example). The solutions (eigenfunctions) are given by an electron-like part, $\psi_e(r)$, and a hole-like part, $\psi_h(r)$, which have to be solved in a self-consistent manner fulfilling the gap equation. The Bogoliubov-deGennes equation can be expressed as:

$$\begin{pmatrix} H_0 & \Delta(r) \\ \Delta(r)^* & -H_0^* \end{pmatrix} \begin{pmatrix} \psi_e(r) \\ \psi_h(r) \end{pmatrix} = E \begin{pmatrix} \psi_e(r) \\ \psi_h(r) \end{pmatrix}$$
(2.3)

The Hamiltonian H_0 contains the kinetic energy term plus all interactions other than Δ (like the crystal potential and impurity potential). The * symbol denoted the complex conjugate. Clearly, the coupling between electron and hole states exists for nonzero Δ only. One of the many applications of the BdG equations is the model of Blonder-Tinkham-Klapwijk [16] (BTK, 1982), which solves the BdG equations for an N/S interface with arbitrary interface barrier potential. They consider all possible reflection/transmission processes at the interface (normal reflection, Andreev reflection, normal transmission, branch-crossing transmission) and calculate the energy dependent transport probabilities, which allows for the calculation of current (I) - voltage (V) characteristics. While the BTK model seems the "end of the story" for N/S interfaces, in 1991 it was shown [17] that it breaks down when transport is dominated by impurity scattering. Strictly speaking, BTK remains correct but its validity becomes limited to the interface itself (which remains ballistic) and so looses is functionality for determining transport properties. So, although potentially the BdG model can deal with impurities, in real systems it is often still of not much use. This is because the positions (and therefore the potential) of the impurities are generally unknown, making it a serious difficulty to add the effects of scattering processes near the interface. This shifted the attention towards the usage of quasiclassical Green functions, which by then was already solidly formulated for about 20 years. The theoretical framework exhibits a higher complexity of mathematical concepts, but its functionality is more powerful. Currently, this framework is the modern way to describe superconductivity.

2.1.3 Green functions and the Gor'kov equation

A large amount of theoretical work has been done in describing superconductivity using quantum field theory, which had proved to be a very powerful and effective tool for microscopic theories of solid state systems (for a thorough description see for example [18, 19]). Green functions contain the information of the transport probabilities of single particles. They describe how particles propagate through the system influenced by all kind of interactions. Once the Green functions of a system are known, all single-particle properties of the system are known (for example, the density of states and electrical current) The single-particle normal Green function is defined by:

$$G_{\alpha\beta}(x,x') = -i\left\langle T_t\left(\psi_\alpha(x)\,\psi_\beta^\dagger(x')\right)\right\rangle_{\rm st} \tag{2.4}$$

with $x = (\mathbf{r}, t)$ and $\psi_{\alpha}^{\dagger}(x)$ and $\psi_{\alpha}(x)$ are the time dependent electron creation and annihilation (Heisenberg) operators respectively, satisfying the usual

commutation rules for Fermi statistics. The Green function is a statistical average over all possible paths from x' to x, denoted by $\langle ... \rangle_{st}$ and T_t is the time-ordering operator which orders the operators logically in time, giving a minus sign for each permutation. Effectively, the normal Green function $G_{\alpha\beta}(x,x')$ describes the movement of a particle from x' to x, or more precise, the probability amplitude for a particle to move coherently from x' to x, where β and α are the initial and final spin direction of the particle (the particle being an electron if t > t' and a hole if t < t'). Note that the normal Green function depends on the standard electron operators and not on the quasiparticle operators introduced by Bogoliubov (to describe single-particle motion). The normal Green function is complemented by a Green function that describes the opposite movement:

$$\overline{G}_{\alpha\beta}\left(x,x'\right) = -i\left\langle T_t\left(\psi_{\alpha}^{\dagger}\left(x\right)\psi_{\beta}\left(x'\right)\right)\right\rangle_{\rm st}$$
(2.5)

and they are related through $G_{\alpha\beta}(x, x')^* = -\overline{G}_{\alpha\beta}(x, x')$, where * denotes the complex conjugate. In addition to the normal Green functions which describes coherent motion of single-particles (using single-particle electron states), a second type of Green function is needed to deal with the Cooper pairs, which occupy the paired states. These so-called anomalous Green functions are defined by:

$$F_{\alpha\beta}(x,x') = -i \left\langle T_t \left(\psi_\alpha(x) \psi_\beta(x') \right) \right\rangle_{\text{st}}$$

$$\overline{F}_{\alpha\beta}(x,x') = -i \left\langle T_t \left(\psi_\alpha^{\dagger}(x) \psi_\beta^{\dagger}(x') \right) \right\rangle_{\text{st}}$$

(2.6)

and satisfy $F_{\alpha\beta}(x,x')^* = -\overline{F}_{\alpha\beta}(x,x')$. Clearly, $F_{\alpha\beta}(x,x')$ annihilates a Cooper pair (empties a Cooper pair state) and $\overline{F}_{\alpha\beta}(x,x')$ creating one (fills a Cooper pair state). Just as for the normal Green function, the transport nature is visible again as the highest probability to create(annihilate) a Cooper pair is at, or very near the position where the first(remaining) electron has coherently travelled to during the time interval from t' to t. Fig. 2.2 shows a graphical representation of the normal and anomalous Green function. Next to these real time Green functions, the imaginary time Matsubara Green function is often encountered in literature within the field of superconductivity. The Matsubara Green function is valid for systems in equilibrium (i.e. no potential differences) and has the advantage that at finite temperatures the ordering of the electron operators is still unambiguously defined. For the real-time Green functions special time ordering rules (Keldysh technique) are necessary (adding

$$\left\{\psi_{\alpha}\left(x\right),\psi_{\beta}^{\dagger}\left(x'\right)\right\}=\delta\left(x-x'\right)\delta_{\alpha\beta}\text{ and }\left\{\psi_{\alpha}\left(x\right),\psi_{\beta}\left(x'\right)\right\}=\left\{\psi_{\alpha}^{\dagger}\left(x\right),\psi_{\beta}^{\dagger}\left(x'\right)\right\}=0.$$



superconductor

Figure 2.2: (Left) A spin up electron is added to the superconductor (location r', time t') and at time t > t' the probability to find that electron at location r is probed (where the electron could have taken any possible path from r' to r). This represents the normal Green function $G_{\uparrow\uparrow}(x, x')$. (Right) The spin up electron of a Cooper pair is taken out of the superconductor (location r', time t') and at time t > t' the probability to find the remaining electron of the Cooper pair is probed. This represents the anomalous Green function $F_{\downarrow\uparrow}(x, x')$.

to the mathematical complexity), but it is applicable to non-equilibrium systems as well. The anomalous Green functions describe the superconducting correlations and are related to the order parameter Δ of the superconductor. This order parameter is a measure for the strength of the superconducting energy gap and uses the same symbol. For an s-wave superconductor we have:

$$\Delta_{\alpha\beta}(x) = -\lambda F_{\alpha\beta}(x, x)$$

$$\overline{\Delta}_{\alpha\beta}(x) = -\lambda \overline{F}_{\alpha\beta}(x, x)$$
(2.7)

where λ is the attractive interaction ($\lambda < 0$). Using the anti-commutation rules one can obtain: $\Delta_{\alpha\alpha}(x) = -\Delta_{\alpha\alpha}(x)$ and $\overline{\Delta}_{\alpha\alpha}(x) = -\overline{\Delta}_{\alpha\alpha}(x)$. As a consequence, the order parameter (for an s-wave superconductor) has to be zero for equal spin directions. Only the pairing of electrons/states with opposite spin directions contribute to the superconducting order parameter, which is a fundamental assumption within the BCS theory.

The Green functions can be conveniently written/ordered into 2×2 matrices in spin space, where the elements contain all possible spin combinations. The set of matrices that span the spin space are the Pauli spin matrices given by:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(2.8)

where σ_0 is the unity matrix in spin space and $\sigma_i \sigma_i = \sigma_0$. For the normal Green function and the order parameter we write:

$$\hat{G}(x,x') = \begin{pmatrix} G_{\uparrow\uparrow}(x,x') & G_{\uparrow\downarrow}(x,x') \\ G_{\downarrow\uparrow}(x,x') & G_{\downarrow\downarrow}(x,x') \end{pmatrix}, \quad \hat{\Delta}(x) = \begin{pmatrix} 0 & \Delta_{\uparrow\downarrow}(x) \\ \Delta_{\downarrow\uparrow}(x) & 0 \end{pmatrix}$$
(2.9)

Similar definitions hold for $\hat{\overline{G}}(x, x')$, $\hat{F}(x, x')$, $\hat{\overline{F}}(x, x')$ and $\hat{\overline{\Delta}}(x)$. These (2×2) matrix Green functions can be further collected/ordered into a single (4×4) matrix Green function in the Nambu \otimes spin space, with \otimes the tensor product. In the Nambu space (particle-hole space) the Green functions are ordered based on the different combinations of electron/hole operators (ψ^{\dagger} creates an electron, ψ creates a hole). The elementary matrices of the Nambu space are identical to the ones that span the spin space, but now are denoted by τ_0 , τ_1 , τ_2 and τ_3 . The matrix Green functions \hat{G} , $\hat{\overline{G}}$, \hat{F} and $\hat{\overline{F}}$ each consist of a different combination of the two types of electron operators. The matrix Green function and matrix order parameter in Nambu \otimes spin space are written as:

$$\check{G}(x,x') = \begin{pmatrix} \hat{G}(x,x') & \hat{F}(x,x') \\ \hat{\overline{F}}(x,x') & \hat{\overline{G}}(x,x') \end{pmatrix}, \\ \check{\Delta}(x) = \begin{pmatrix} 0 & \hat{\Delta}(x) \\ \hat{\overline{\Delta}}(x) & 0 \end{pmatrix}$$
(2.10)

For stationary systems the Green functions no longer depend on the explicit time coordinates, but rather on the time difference between the two operations: $\check{G}(x, x') \rightarrow \check{G}(\mathbf{r}, \mathbf{r}', t - t')$. By making a Fourier transform over the time difference the energy dependent Green functions are obtained:

$$\check{G}\left(\mathbf{r},\mathbf{r}',\epsilon\right) = \int e^{-i\epsilon(t-t')/\hbar} \check{G}\left(\mathbf{r},\mathbf{r}',t,t'\right) d(t-t')$$
(2.11)

with ϵ the energy of the single-particle (state). When using the imaginary time Matsubara Green functions this works out a bit different. The Matsubara Green functions are defined at the finite time interval: $-\frac{\hbar}{k_BT} < \tau - \tau' < \frac{\hbar}{k_BT}$, and as a result, the Fourier transformed Green functions are non-zero only for a discrete set of frequencies: $\hbar\omega_n = (2n+1)\pi k_BT$, where ω_n are the Matsubara frequencies. This series of frequencies continues up to the cut-off frequency ω_D , which is the Debye frequency. Just as within the BCS model where the Debye energy limits the range over which the attractive interaction is non-zero.

Gor'kov rewrote the original BCS Hamiltonian (Eq. 2.1) into an equation for the Green functions of the system [20]. In matrix form this equation takes a similar form as the BdG equations (Eq. 2.3) with the main difference that the eigenstate functions of BdG are replaced by the Green functions of the system. Using the τ_i and σ_i matrices, the stationary Gor'kov equation can be expressed as:

$$\left(-\epsilon \left(\sigma_{0} \otimes \tau_{3}\right) + H\left(\mathbf{r}\right) \left(\sigma_{0} \otimes \tau_{0}\right) - \check{\Delta}\left(\mathbf{r}\right)\right) \check{G}\left(\mathbf{r}, \mathbf{r}', \epsilon\right) = \hbar \delta\left(\mathbf{r} - \mathbf{r}'\right) \left(\sigma_{0} \otimes \tau_{0}\right) \quad (2.12)$$

with $\delta(x)$ the Dirac delta function and $H(\mathbf{r}) = -\frac{\hbar^2}{2m} \left(\partial_{\mathbf{r}} + \frac{q}{i\hbar} \mathbf{A}\right)^2 + q\varphi$ is the Hamiltonian of a particle (of mass m and charge q) in an electromagnetic field (with vector potential \mathbf{A} and scalar potential φ). Furthermore, $q\varphi = E_F - \mu$ is the energy difference between the Fermi energy and the chemical potential, and $\partial_{\mathbf{r}} \equiv \partial/\partial \mathbf{r}$. With this new set of equations, Gor'kov showed [21] that the famous phenomenological Ginzburg-Landau theory [22] can be microscopically derived from the BCS theory for temperatures close to the transition temperature. This is a solid proof for the "correctness" of the phenomenological Ginzburg-Landau model.

2.1.4 Quasiclassical approximation: Usadel equation

Cooper pairs are non-local objects and much larger (size is of order ξ_s) than the Fermi wavelength λ_F . Therefore, their transport properties (or Green functions) do not vary strongly on the scale of λ_F . This is the key to the quasiclassical approximation which greatly reduces the complexity of the Gor'kov equations. The approximation is based on the observation that the Green functions entering the Gor'kov equations contain (in most cases) fast oscillations on the scale of λ_F due to self-interference effects (like weak localization). These fast oscillations are all redundant information when interested in superconductivity, which only feels the average of such oscillations. The main idea of the quasiclassical approximation is that the relative coordinate of the Green functions $\rho = \mathbf{r} - \mathbf{r}'$ is responsible for the fast oscillations, while the center-of-mass coordinate $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$, is responsible for the slow oscillations. Therefore, to lose the redundant information, one could average out the relative coordinate. A convenient way to do this is by first applying a Wigner transformation: $\mathbf{r} \to \mathbf{R} + \rho/2$ and $\mathbf{r}' \to \mathbf{R} - \rho/2$, which is an exact transformation to go from coordinates $(\mathbf{r}, \mathbf{r}')$ to (\mathbf{R}, ρ') . Next to make a Fourier transform over the relative coordinate (to separate the fast and slow oscillations in the obtained spectrum) resulting in the relative momentum \mathbf{p} , and finally to integrate over the magnitude of the momentum. The precise definition of the quasiclassical Green functions, defined through the Gor'kov Green functions, reads:

$$\check{g}\left(\mathbf{R},\hat{\mathbf{p}},\epsilon\right) = \frac{i}{\pi} \int d\xi_p \int d(\mathbf{r}-\mathbf{r}')\check{G}\left(\mathbf{r},\mathbf{r}',\epsilon\right) e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')/\hbar}$$
(2.13)

where $\hat{\mathbf{p}} = \mathbf{p}/p$ is the unit vector in the direction of momentum (*p* is the momentum magnitude) and ξ_p is the kinetic energy variable which is connected to the momentum: $\xi_p = v_F (p - p_F)$, where $p_F = mv_F$ is the Fermi momentum and v_F the Fermi velocity. Application of this quasiclassical approximation on the Gor'kov equation (Eq. 2.12) leads to the Eilenberger equation [23], which in the absence of electromagnetic fields is written as:

$$-i\hbar \mathbf{v}_{\mathbf{F}}\partial_{\mathbf{R}}\check{g} - \left[\epsilon\left(\sigma_{0}\otimes\tau_{3}\right) + \check{\Delta},\check{g}\right] = \left[\check{\Sigma},\check{g}\right]$$
(2.14)

where the commutator of two elements [a, b] = ab - ba, and we used that $v_F \hat{\mathbf{p}} = \mathbf{v}_F$. Furthermore, $\check{g}(\mathbf{R}, \hat{\mathbf{p}}, \epsilon)$ and $\check{\Delta}(\mathbf{R})$ are the quasiclassical variants of Eq. 2.10 and the right-hand-side of the Eilenberger equation adds the effect of self-energies (see below). The Eilenberger equation is called quasiclassical since it describes the system using a mixture of classical and quantum mechanics. It uses the quantum mechanical field operators to find the probability amplitudes (the Green functions) of the motion of classical particles with velocity v_F and direction $\hat{\mathbf{p}}$.

The presented form of the Gor'kov equation (Eq. 2.12) does not contain any interaction term other than the attractive interaction responsible for superconductivity. Taking $\Delta = 0$ (or $T > T_c$) makes it a normal metal and one could say the Green functions are now all of "non-interacting" types. In general, the Green functions are complemented by something called self-energy, usually denoted by Σ . Loosely speaking, the self-energy dresses up the non-interacting Green function by adding the effects of other interactions, such as electronelectron interactions, electron-phonon interactions and impurity scattering. The resulting Green function is then the "real" Green function of the system. In general, the self-energy is a complex function with the real part describing the change in energy (which is a renormalization of mass) and the imaginary part describing the lifetime of the energy state. Since Σ describes the changes of electron states, it depends on Green functions having equal coordinates i.e. $\Sigma_{\alpha\beta}(x) \propto G_{\alpha\beta}(x,x)$. Comparing Σ to Δ (see Eq. 2.7) we can say that Δ is the anomalous equivalent of the self-energies, but now associated with a twoparticle state. The interactions of importance are the interactions between or with quasiparticles (the elementary excitations). These interactions are responsible for the relaxation of the system to an equilibrium state, where it is assumed that the crystal lattice (phonons + impurities) itself is already in

equilibrium and forms a heat bath. The main contributions to the relaxation (in descending order of importance) are scattering with impurities (both nonmagnetic and magnetic), electron-phonon interactions and electron-electron interactions. A powerful method to incorporate the interaction between electrons and random impurities has been developed by Abrikosov and Gor'kov [24]. It is assumed that physical properties of superconductors containing a large amount of random impurities can be obtained by averaging over realizations of the disordered impurity potentials. A second assumption is the Born approximation, which implies that the scattering potential is small compared to the characteristic atomic potential (which is of the order of the Fermi energy). For isotropic scattering (there is no preferred direction to scatter into, and the dependence on $\hat{\mathbf{p}}$ is lost) the self-energy becomes:

$$\check{\Sigma}\left(\mathbf{R},\epsilon\right) = \frac{i\hbar}{2\tau_{\rm imp}} \left\langle \check{g}\left(\mathbf{R},\hat{\mathbf{p}}_{1},\epsilon\right) \right\rangle_{\mathbf{p}_{1}} + \frac{i\hbar}{2\tau_{\rm sf}} \left(\sigma_{3}\otimes\tau_{0}\right) \left\langle \check{g}\left(\mathbf{R},\hat{\mathbf{p}}_{1},\epsilon\right) \right\rangle_{\mathbf{p}_{1}} \left(\sigma_{3}\otimes\tau_{0}\right) \ (2.15)$$

where the momentum average $\langle A(\hat{\mathbf{p}}) \rangle_{\mathbf{p}} = \int A(\hat{\mathbf{p}}) \frac{d\Omega_{\mathbf{p}}}{4\pi}$. Furthermore, τ_{imp} and τ_{sf} are the scattering times for scattering at non-magnetic impurities and magnetic impurities respectively. The first term thus describes non-magnetic impurity scattering while the second describes the magnetic impurity scattering.

When a material is in the dirty limit, a particle scatters a lot of times before losing its phase coherence and this results in the loss of the initial momentum direction. The Green functions, which describe the electron and hole motion, become nearly isotropic in this limit. In a first approximation, they no longer depend on momentum directions and the first-order correction is linear in $\hat{\mathbf{p}}$, which is the unit vector in the direction of momentum (and is equal to $\hat{\mathbf{v}}_F$). For the quasiclassical Green functions in the dirty limit we write:

$$\check{g}\left(\mathbf{R}, \hat{\mathbf{p}}, \epsilon\right) = \check{g}_0\left(\mathbf{R}, \epsilon\right) + \hat{\mathbf{p}}\check{\mathbf{g}}$$
(2.16)

where both the isotropic part \check{g}_0 and the correction $\check{\mathbf{g}}$ do not depend on the direction of momentum. Furthermore $|\check{\mathbf{g}}| \ll \check{g}_0$ and the normalization condition $\check{g}^2 = \check{1}$ applies. Inserting this expansion into the Eilenberger equation and averaging over momentum directions results in the Usadel equation [25], which is fully isotropic. For the stationary system, in the absence of electromagnetic fields, it reads:

$$i\hbar D\partial_{\mathbf{R}} \left(\check{g}_0 \partial_{\mathbf{R}} \check{g}_0 \right) - \left[\check{\Delta} + \epsilon \left(\sigma_0 \otimes \tau_3 \right), \check{g}_0 \right] = \left[\check{\Sigma}_{sf}, \check{g}_0 \right]$$
(2.17)

Where $\dot{\Sigma}_{sf}(\mathbf{R},\epsilon) = \frac{i\hbar}{2\tau_{sf}}(\sigma_3 \otimes \tau_0) \check{g}_0(\mathbf{R},\epsilon) (\sigma_3 \otimes \tau_0)$ and we used that the diffusion constant D is coupled to the Fermi velocity and the elastic mean free path by $D = \frac{1}{3} v_F \ell_e$ where the elastic mean free path $\ell_e = v_F \tau_{imp}$. From the scattering at impurities, only the magnetic impurity term remains, which acts as pair breaker. The matrix Green function $\check{g}_0(\mathbf{R}, \epsilon)$ and $\check{\Delta}(\mathbf{R})$ have the usual form in Nambu \otimes spin space.

An important limitation of the quasiclassical approximation is the inability to account for different (non-identical) spin bands with different Fermi velocities, as it poses problems to make the integration over $d\xi_p$. As a result, identical spin bands are used, which in general is correct for normal metals and superconductors. However, for a ferromagnet such a model can only be correct if the spin polarization is about zero. This, in combination with the general limitation of correlations between particles separated by energies of the order E_F , is the weak ferromagnetic limit. It has $E_{\rm ex} \ll E_F$ and a polarization of 0%. A weak ferromagnet is treated as a normal metal with the inclusion of a small exchange field. The strong ferromagnetic limit is when $E_{\rm ex} \sim E_F$, and usually the polarization is no longer close to zero. The incapability of dealing with non-identical spin bands does not mean that the model cannot treat spin dependent interactions. In fact, the attractive interaction itself depends on spin directions, and also spin-flip processes were already included. As long as the spin dependent interactions are not caused by non-identical spin bands, they can be included in the Hamiltonian.

For spin independent systems a simplification is possible, which comes down to dropping the spin space ordering. Such systems do not contain any coherent spin dependent interactions at all (i.e. changing the spin direction of a particle without disturbing its energy), however, they do include for example spin scattering which randomizes spin. In this case, several components of the Green functions will vanish. For the normal Green functions, components with opposite spin directions vanish while for the anomalous Green functions the components having equal spin directions vanish. The reason for this is that there are no interactions to coherently flip the spin of a particle. For a single particle (normal Green function) this means that a non-zero probability amplitude is only possible if the particle stays in a single spin band. It also means that for a Cooper pair the correlation exists only between opposite spin directions (pairing only occurs between opposite spin directions, and an electron of the Cooper pair cannot flip its spin coherently to create a correlation between equal spin directions). For the non-zero Green functions we get: $G_{\uparrow\uparrow} = G_{\downarrow\downarrow} = G$ and $\overline{G}_{\uparrow\uparrow} = \overline{G}_{\downarrow\downarrow} = \overline{G}$ (the two spin bands are identical). For the anomalous Green functions we get: $F_{\uparrow\downarrow} = -F_{\downarrow\uparrow} = F$ and $\overline{F}_{\uparrow\downarrow} = -\overline{F}_{\downarrow\uparrow} = \overline{F}$. The matrix Green function and order parameter in Nambu⊗spin space now

reduce to:

$$\check{g}_0 = \begin{pmatrix} G\sigma_0 & iF\sigma_2 \\ i\overline{F}\sigma_2 & \overline{G}\sigma_0 \end{pmatrix} , \, \check{\Delta} = \begin{pmatrix} 0 & i\Delta\sigma_2 \\ i\overline{\Delta}\sigma_2 & 0 \end{pmatrix} , \qquad (2.18)$$

while for the spin-flip self-energy matrix we find:

$$\check{\Sigma}_{\rm sf} = \frac{i\hbar}{2\tau_{\rm sf}} \begin{pmatrix} G\sigma_0 & -iF\sigma_2 \\ -i\overline{F}\sigma_2 & G\sigma_0 \end{pmatrix}$$
(2.19)

We see that the Nambu space matrices all have a σ_0 spin symmetry on the diagonal and a σ_2 spin symmetry on the off-diagonal. Multiplication of two such matrices results in a matrix having the same spin symmetry, therefore the spin space effectively drops out of the equations. We then find for the spin independent Usadel equation, using now the $\hat{}$ notation for the 2×2 matrix in Nambu space:

$$i\hbar D\partial_{\mathbf{R}} \left(\hat{g}_0 \partial_{\mathbf{R}} \hat{g}_0 \right) - \left[\hat{\Delta} \left(\mathbf{R} \right) + \epsilon \tau_3, \hat{g}_0 \right] = \left[\hat{\Sigma}_{sf}, \hat{g}_0 \right]$$
(2.20)

with:

$$\hat{g}_0 = \begin{pmatrix} G & iF \\ i\overline{F} & \overline{G} \end{pmatrix} , \hat{\Delta} = \begin{pmatrix} 0 & i\Delta \\ i\overline{\Delta} & 0 \end{pmatrix} , \hat{\Sigma}_{\rm sf} = \frac{i\hbar}{2\tau_{\rm sf}}\tau_3\hat{g}_0\tau_3$$
(2.21)

The self-consistency relation for Δ as well as the special boundary condition necessary to describe interfaces between materials are given in Chapter 7.

2.1.5 Unconventional Cooper pairs

Stimulated by the observation or idea that the 3-Helium superfluid state should have a p-wave orbital state (below 0.07 K) the BCS theory has been generalized for non-zero orbital angular momentum. First in the works of Anderson and Morel [26] and improved by Balian and Werthamer [27] (see Leggett's nobel lecture for a review [28]). A condensation of pairs into $\ell = 1$ or higher states can become favorable when for example there is a strong short-range repulsion preventing condensation into the s-wave configuration, which is the case for the 3-Helium superfluid. Because a Cooper pair consists of two Fermi particles and obeys Fermi statistics, an anti-symmetric wave function is required under the exchange of the two particles (the Pauli principle). This puts restraints on the possible types of pairing (i.e. the possible combinations of orbital and spin states). The orbital state is symmetric if the orbital quantum number

in this thesis we use , `and `to respectively denote a 2×2, 4×4 and 8×8 matrix

 $\ell = 0, 2, ...$ (even) and anti-symmetric if $\ell = 1, 3, ...$ (odd). The $\ell = 0, 1, 2$ are the s-, p- and d-wave respectively. The spin state of a pair is either in the symmetrical spin singlet state (S=0) or in the anti-symmetrical spin triplet state (S=1). The implication of this is that pairs in s- or d-wave orbital states should be in spin singlet states, while pairs in p-wave orbital state should be in spin triplet states.

An important difference between s-, p- and d-wave is that only in case of pairing into s-wave orbital states, the superconducting energy gap is isotropic. It does not depend on momentum \mathbf{k} and no single particle states exist for energies within the gap region. This makes the s-wave superconductor robust against impurity scattering because there are no available normal electron states which can "absorb" a pair after scattering at an impurity. However, when we consider a p- or d-wave orbital state, the energy gap is no longer isotropic. This means that for a certain absolute value of k (with energy ε_k), some directions have a full or reduced gap, while other direction don't have a gap at all. As a result, the density of single particle states becomes non-zero (and non-constant) for energies inside the gap region. These superconductors are not robust against impurity scattering and only survive in clean systems, where the superconducting coherence length is (much) smaller than the elastic mean free path. The Cooper pairs as suggested by BCS theory are in a spin singlet state with s-wave orbital state, which is called conventional superconductivity. Triplet superconductivity in conventional thin film superconductors thus seems a non-existing phenomena, and yet it was recently measured in experiments of Keizer et al. [29] en Sosnin et al. [30]. In the first, triplet pairing was induced in the half-metallic ferromagnet CrO_2 (100 % spin polarized material), while in the latter is was induced in Holmium (Ho) which is a conical ferromagnet. Somehow the above discussion about the possible combinations between orbital and spin states is circumvented. The answer to this lies in the time coordinate/symmetry which thus far was not really taken into account. If the time dependent part of the Cooper pair wave function is anti-symmetric under the exchange of the two particles, a s-wave spin-triplet pairing becomes possible [31]. This mechanism should also allow for p-wave singlets, but they have not been observed (yet).

Another type of unconventional superconductivity is what is now known as the LOFF state, named after Fulde and Ferrell (1964) [32] and Larkin and Ovchinnikov (1964) [33] whom considered this situation for the first time. The LOFF state is an inhomogeneous superconducting state, where the two single electron states forming the paired-state belong to different Fermi surfaces. This difference between the Fermi surfaces for the two spin bands is (in the model systems) created by a homogeneous exchange field generated by polarized magnetic impurities, making the LOFF state a display for the coexistence of ferromagnetism and superconductivity. The parameter which determines if the LOFF state is viable is the strength of the exchange field compared to the condensation energy (the paramagnetic effect). Unlike the conventional BCS state, the Cooper pairs in the LOFF state have acquired a non-zero total momentum. This gives rise to a spatially varying Cooper pair density (and gap potential). Electronegativity is maintained by the normal electrons created from the breaking of pairs (which is the cause for the density changes). The description of the LOFF state is very similar to the induced superconductivity (or proximity effect) in S/F junctions.

2.2 Fundamentals of ferromagnetism

In our experimental works the ferromagnets are "used" for their exchange field to investigate their interaction with superconductivity. In this section a brief description of magnetism is given, focussed on the type and appearance it takes in our devices (see ref [34] for a more detailed description).

Magnetism is a phenomenon encountered in nature, for example it is found in the magnetic mineral Fe₃O₄ (known as Magnetite). Magnetism is well integrated in nowadays technology, especially in the area of digital data storage. The strength of magnetism, or actually, the magnetic induction or magnetic flux density, is expressed in Tesla. The earth's field is around 30-50 μ T at the surface, which is very weak compared to magnetic materials which can have surface strengths up to 1 or 2 Tesla. A magnetic field can be connected to electrical currents. These can be macroscopic, as e.g. utilized in electromagnetic coils. In superconductors, macroscopic screening currents are able to expel magnetic flux from its interior. They can also be microscopic, and it are the atomic electrical currents together with the magnetic moments connected to the electron spin, which lead to the magnetization of matter.

Whenever a piece of material is put into a magnetic field, the electron spin and its associated magnetic moments will start to align with the field, which behavior is know as paramagnetism (it typically only involves a small fraction of the electrons and the induced field is rather weak). However, only few materials show a spontaneous alignment of the spins in the absence of external magnetic fields. This phenomenon is another display of a condensed state of the electrons, just as superconductivity is. Again, the ordering appears *below* a certain critical temperature, while *above* this temperature the directions of the magnetic moments randomize resulting in a zero net magnetization. Different types of magnetic alignment exist. In a ferromagnetic material, the alignment is parallel and the critical temperature is called the Curie temperature $T_{\rm C}$. In an antiferromagnetic material the alignment is perfectly antiparallel and the critical temperature is called the Néel temperature $T_{\rm N}$. All the alignments in between are the ferrimagnetic materials.

All materials are built up from atoms, which consist of a positively charged core of protons and neutrons with negatively charged electrons orbiting around it. Both the electron cloud and the nucleus carry an intrinsic magnetic moment, but in general the magnetic moment of the nucleus is much smaller than that of the electrons, and therefore we narrow down the discussion to the electron part. In isolated atoms, incompletely filled electronic shells carry both an orbital angular momentum and a spin angular momentum, and therefore a magnetic moment. As long as the orbits do not overlap, these "local moments" also occur in solids matter, but we shall not be concerned with such magnetism either. Instead, we focus on so-called band ferromagnets, which are found in particular in alloys of 3d-transition metals (Ti, V, Cr, Mn, Fe, Co, Ni and Cu). In a band ferromagnet, the two spin bands are asymmetrically as depicted in Fig. 2.3. Where in the normal metal (in the ground state) both spin bands are filled up to the Fermi energy E_F and contain an equally number of electrons. In case of a ferromagnet one spin band (majority band) contains more electrons n_{\uparrow} and is filled up to a higher energy level compared to the other spin band (minority band), which contains n_{\perp} electrons. The energy of the electron states are now given by $\epsilon_{\uparrow,\downarrow}(k) = \epsilon_0(k) - I \frac{n_{\uparrow,\downarrow}}{n}$ with I a measure for the exchange correlation and $n = n_{\uparrow} + n_{\downarrow}$. In this new state, the kinetic



Figure 2.3: Filling of the density of states N(E) of the two spin bands for a normal metal and a ferromagnet, with E_F the Fermi energy and E_{ex} the exchange energy

energy has increased (electrons originally occupying states with $k < k_F$ now occupy states with $k > k_F$, increasing the kinetic energy $\propto k^2$). However, the potential energy has decreased (with less degenerate states doubly occupied, the total spatially overlap of electron states has reduced, which reduces the Coulomb repulsion energy). This new state is stable if the potential energy decrease is larger than the kinetic energy increase. This leads to the Stoner criterium for ferromagnetism to occur: $N(E_F) I > 1$, with $N(E_F)$ the density of states at the Fermi energy.

2.2.1 Magnetic domains and switching

A ferromagnet at a temperature below its Curie temperature thus shows spontaneous magnetization. However, the magnetization is not necessarily homogeneous. Moreover, the net magnetization of a ferromagnet (in absence of any field) is usually close to zero! Energetically there is a strong preference



Figure 2.4: Different possible domain configurations in a ferromagnet, with from left to right a decrease of the induced field outside the ferromagnet.

to keep the magnetization inside the material, and this typically leads to the formation of domains (see Fig. 2.4). Each domain has a single orientation of the magnetization vector and the domains are separated by domain walls, which have typically a much smaller lateral dimension. In the domain wall, the the magnetization vector rotates from the direction of the domain on the one side to the direction of the domain on the other side. Two main classes of domain walls are distinguished (see Fig. 2.5). In Bloch walls the rotation goes out-of-plane, while in Néel walls it goes in-plane (where the plane is spanned by the two magnetization vectors). Other more complex rotations exists, but are always a combination of the Bloch and Néel type.



Figure 2.5: Rotation of the magnetization vector \mathbf{M} in an out-of-plane Bloch domain wall (top) and an in-plane Néel domain wall (bottom)

The appearance of the domain configuration is the result of minimizing the total energy of the system. For a ferromagnet, the following terms are to be considered. The exchange energy (E_{ex}) relates to the interaction between electron spins and is minimized for parallel alignment of the spins. The Zeeman energy ($E_{\rm H}$) relates to the direction of the magnetization with respect to the external field. It minimizes for parallel alignment. The crystalline anisotropy energy (E_{ca}) relates to the direction of the magnetization with respect to the lattice orientation (it is minimized for alignment with the so-called lattice easy-axes). The magnetostatic (or demagnetization) energy $(E_{\rm D})$ is an effect of the dipole fields and therefore connected to the shape of the ferromagnet. It is minimized by keeping flux inside the ferromagnet (or inducing a lowest field outside the ferromagnet). The demagnetization energy is responsible for the presence of domains, while the competition between the exchange energy and crystalline anisotropy energy determines the width of the domain walls. The first favors a (infinitely) broad wall, while the latter favors a thin as possible wall. When the sample dimension becomes of the order of the typical domain sizes, which are usually in the μm range, the shape anisotropy becomes the dominant energy term (because it cannot become lower anymore by making domains), especially in elongated shapes. For a long and thin wire, this often leads to a magnetization aligned with the wire direction. The actual magnetic configuration in the ferromagnet is coupled to an external magnetic field (\mathbf{H}) through the Zeeman term. Whenever this field **H** increases or decreases, the magnetic configuration in the ferromagnet usually changes as well, leading to a change in the (average) magnetization vector **M**. Fig. 2.6 illustrates this

behavior, where the origin gives the initial state of the ferromagnet (practically zero net magnetization). The curve then passes the points a to f in alphabetic order and ends up again in point a. The foremost characteristic of this curve is that it shows hysteresis (i.e. there is a difference in the path for going up and down in field), and it is generally known as the hysteresis curve. For high enough (absolute) field, the ferromagnet saturates. It has become a single domain, with its magnetization vector pointing along the applied field. Points b and e are the remanent (or residual) magnetization points. After being (partly) saturated once, the ferromagnet now shows a significant magnetization in zero applied field. Points c and f are the coercive field points. They indicate the field required to return to a net magnetization of zero, or, to change the direction of magnetization. The hysteresis curve shows, for the chosen direction of applied field, what field strengths are required to fully magnetize the ferromagnet. It also shows over which field range there is a presence of magnetic domains, and it shows how "easy" or "hard" it is to magnetize along the chosen direction. An easy direction result in a squarish hysteresis curve, with the remanent field values close to the saturation values. For a hard direction the remanent field values are much reduced (points b and e close to 0) and the hysteresis curve starts to close.

Being two very different phenomena, antagonistic even, because the superconductor tries to expel any magnetic field from its interior. The two states are very similar at the same time. Both superconductivity and ferromagnetism are mean field orders of electron spins, parameterized by Δ and $E_{\rm ex}$ respectively. Both orders appear below a certain critical temperature and change the normal metal density of states near the Fermi energy. However, the ferromagnetic density of states is (usually) just an energy shifted version of the normal density of states and the charge, energy and spin transport are governed by normal electrons. The superconductor is much more special in this aspect, as now a gap region has appeared near the Fermi energy. Charge transport is now governed by Cooper pair, which don't transport any heat (the energy is always the Fermi energy, no extra energy can be carried by the Cooper pair), and only the non conventional types can carry spin. Ferromagnetism is an ordering/allignment of electron spin such that one spin band contains more filled states (the majority band) and one contains less filled states (the minority band). As a result, there is a polarization of the electron spin and a potential (and kinetic) energy difference between the two spin bands. In the conventional superconductor, the spin ordering goes in k-space, and in real space no differences exists between the two spin populations.



Figure 2.6: Hysteresis curve showing saturation magnetization (points a and d) remanent magnetization (points b and e) and coercive fields (points c and f).

2.3 Proximity effect

2.3.1 Proximity effect in S/N

Although Cooper pairs are only generated inside a superconductor (for $T < T_c$), they are not confined to the interior of the superconductor itself. In a junction between a superconductor (S) and a normal metal (N) Cooper pairs can move from S to N, inducing superconducting properties into the normal metal. This is called the (superconducting) proximity effect. At first sight, this proximity effect does not seem possible as the Cooper pairs are not eigenfunctions of any non-superconducting material. Besides that, normal electron transport is blocked by the energy gap for all energies close to the Fermi energy. However, a unique mechanism exists that allows for the transfer of a Cooper pair from S to N (and visa versa). This process is the Andreev reflection [35] and is depicted in Fig. 2.7 (right panel). An incoming (excited) electron at energy $\epsilon < \Delta$ reaches the S/N interface. But, instead of being reflected it drags along a second electron at energy $-\epsilon$, with opposite direction of momentum and spin, to enter the superconductor as a Cooper pair. This

second electron is taken from the valence band and consequently leaves a hole behind. This hole then travels back along the path of the original incoming electron because it has opposite direction of momentum. The reverse mech-



Figure 2.7: The right panel shows the Andreev reflection at a normal metal - superconductor interface. Upon reaching the interface, the incoming electron at energy ϵ causes a hole reflection at energy $-\epsilon$ (together they form the correlated electron-hole pair). The incoming electron itself and the missing electron in the valence band have entered the superconductor where they are converted into a Cooper pair. The left panel shows the correlated electron-hole in k-space.

anism takes place as well. In that case the incoming particle is a hole in the valence band (energy $-\epsilon$), which upon arriving at the interface pulls a Cooper pair out of the condensate. One of the electrons occupies the hole, while the other electron occupies an excited state in de conduction band (energy ϵ , with opposite direction of momentum and spin compared to the incoming hole) and travels back along the path of the original incoming hole. The net result of an Andreev reflection is thus a charge transfer of -2e from N to S. No excessive energy is transferred as in N the electron excitation is swapped for an energy-equivalent hole excitation, while in S the Cooper pair is simply added to the condensate (the ground state). The Andreev reflection is thus purely a transfer of charge.

The induced electron-hole pair in N carries superconducting properties along the path of travelling. It is a Cooper pair no longer bound together by the attractive interaction. However, the two electrons that form the Cooper pair through Andreev reflection (and consequently the induced electron-hole pair) do not necessarily have exactly opposite momentum. The electron from the conduction band has $\mathbf{k}_F + \delta \mathbf{k}$, while the electron from the valence band has $-\mathbf{k}_F + \delta \mathbf{k}$ (Fig. 2.7, left panel). This sums up to a net momentum of $2\delta k \sim \frac{\epsilon}{\epsilon_F} k_F \ll k_F$. The result of this k-vector mismatch is that the induced pair dephases, even in the absence of pair breaking mechanisms. Only a correlated pair at the Fermi energy ($\delta \mathbf{k} = 0$) can escape from this dephasing. In case of diffusive systems, the dephasing time corresponds to a travelling distance represented by the (energy averaged) coherence length $\xi_N = \sqrt{(\hbar D_N/(k_B T))} = \int \xi_N(\epsilon) d\epsilon$, with D_N the normal metal diffusion constant and T the temperature, which is taken as the primary source of dephasing. Other sources of dephasing, such as inelastic processes and magnetic fields, will only shorten this coherence length. At the Fermi energy, $\xi_N(\epsilon)$ goes to infinity, while for increasing energy this length becomes shorter. This is why for $T \to 0, \xi_N \to \infty$ as the only possible excitations at zero temperature ar located at the Fermi energy. In reality, the coherence length will still be finite (but pretty long) due to the other forms of dephasing. In S a Cooper pair is being constructed (destructed) from (into) the two electrons from N. This conversion also takes place over a certain distance, which is the superconducting coherence length $\xi_S = \sqrt{(\hbar D_S/(k_B T_c))}$ with D_S the superconductor diffusion constant (also for diffusive systems). Although ξ_S varies per material, it is typically in the range from 10 nm to 1 μ m. This is also the typical range for ξ_N , unless the temperature is close to zero (for conventional superconductors this means at least T < 1 K).

2.3.2 Proximity effect in S/F

When the normal metal is replaced by a ferromagnet (F), the effects of a non-zero spin polarization **P** and exchange energy $E_{\rm ex}$ have to be included. One consequence is a reduction of the Andreev reflections as the mechanism becomes limited by the minority spin band [36]. In case of 100% spin polarization, the Andreev reflection even becomes fully blocked due to absence of a complete spin band. In the presence of an (elastic) spin-rotation/flip mechanism at the interface, this blocking can be partially circumvented as this effectively allows for Andreev reflection using a single spin band. A second consequence is that the induced electron-hole pair experiences the exchange splitting of the spin bands in the ferromagnet. There is a potential energy difference between spin up direction and spin down direction of an electron (which is at a fixed total energy). The minority spin band has an increased potential energy, which means that at a certain energy level (total energy), for example the Fermi energy, the kinetic energy of an electron in the minority spin band is lower compared to the majority spin band. As a result the Cooper pair acquires a net momentum which leads to an oscillation on top of

using $2m(\epsilon_F + \epsilon) = \hbar^2 (k_F + \delta k)^2$ and $\epsilon \ll \epsilon_F$

an exponential decay (see Fig. 1.3), as was shown by Demler and co-workers [37]. The length scales involved are in general much smaller than the "standard decay" (as in S/N) because the exchange energy is usually much higher than the superconductor transition temperature. As an alternative approach to examine the effect of the exchange field on the spin singlet state, we use the Dirac notation and write for the singlet (Ψ^s) and triplet ($\Psi^t_0, \Psi^t_{-1}, \Psi^t_{+1}$) states:

$$\Psi^{s} = \langle \uparrow | \downarrow \rangle - \langle \downarrow | \uparrow \rangle
\Psi^{t}_{0} = \langle \uparrow | \downarrow \rangle + \langle \downarrow | \uparrow \rangle
\Psi^{t}_{-1} = \langle \downarrow | \downarrow \rangle
\Psi^{t}_{+1} = \langle \uparrow | \uparrow \rangle$$
(2.22)

where $|\uparrow\rangle$ and $|\downarrow\rangle$ represent the spin up and spin down state (at fixed energy). In the presence of the exchange energy E_{ex} , the momentum of the electron in the minority (spin down) band is decreased. As a result the spin down state changes into:

$$|\downarrow\rangle \to |\downarrow\rangle \times e^{(-itE_{\rm ex}/h)}$$

$$\langle\downarrow|\to \langle\downarrow|\times e^{(+itE_{\rm ex}/h)}$$
(2.23)

The Cooper pair in the spin singlet state then changes as follows:

$$\Psi^{s} = \langle \uparrow | \downarrow \rangle e^{-itE_{\text{ex}}/h} - \langle \downarrow | \uparrow \rangle e^{+itE_{\text{ex}}/h} = \Psi^{s} \times \cos\left(tE_{\text{ex}}/h\right) - \Psi^{t}_{0} \times i\sin\left(tE_{\text{ex}}/h\right)$$
(2.24)

The amplitude of the singlet state follows indeed an oscillation, and it also shows that the nature of the oscillation is actually a change into the triplet component Ψ_0^t . The period of this oscillation $T = 2\pi h/E_{\rm ex}$, which in a diffusive system (diffusion constant D_F) corresponds to a length of $\sqrt{D_F T}$ = $2\pi\sqrt{\hbar D_F/E_{\rm ex}} = 2\pi\xi_F$. The definition for the ferromagnetic coherence length ξ_F is similar to its normal and superconducting counter parts, except that each coherence length is based on the dominating energy term of the system. When, for example, the temperature is of the same order as the exchange energy, the temperature has to be added to ξ_F . The presence of a homogeneous exchange field thus leads to the appearance of correlated spin triplet pairs. However, only one out of the three spin triplets appears, and since it still consists of both spin directions, the ferromagnet breaks it down just as easy as the conventional singlet pairs. The other two, the spin equal triplets, are generate from the Ψ_0^t triplet once it experiences multiple directions of the exchange field [38, 39]. These "multiple directions" actually means inhomogeneous magnetism, which for example can come from magnetic domains or

magnetic impurities. These are needed to rotate the spins of the Ψ_0^t ($m_z = 0$) component such that it gathers non-zero m_z which are the "spin equal" components. An interface which exhibits inhomogeneous magnetism is called a spin active interface. Fig. 2.8 shows calculations on such spin active interface by Eschrig *et al.* [40]. The amplitudes of all generated components are depicted. In case of a weakly polarized ferromagnet (top curves), the spin-active interface does not generate a significant fraction of long-range triplet components. In case of a strongly polarized ferromagnet (bottom curves) the long-range triplet component which is aligned with the magnetization vector in the ferromagnet arises. The decay of this component in the ferromagnet is much slower than all other induced components in F. In the superconductor, all generated triplet components decay over a characteristic length ξ_S . The singlet component recovers over that distance, being at a lowest amplitude at the interface.



Figure 2.8: Calculation of the triplet components generated at a spin-active S/F interface, as taken from Eschrig *et al.* [40]. Top: weakly polarized ferromagnet, Bottom: strongly polarized ferromagnet