Helsinki University of Technology
Department of Engineering Physics and Mathematics

Master’s thesis

Electronic Transport in Superconducting Nanostructures: Scattering Approach

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Läheisilmio vaikutuksea voidaan tarkastella ns. Andreevin interferometreissä (AI), joissa ilmiön voimakkuutta voidaan säädetä muuttamalla kahden normaaliaineeseen yhteydessä olevan suprajohteen järjestysparametriä vältää vaihe-eroa. Tuloksena on ominaisjohtavuuden vähättely vaihe-eron funktiona. Värähtelyyn voimakkuus riippuu energiasta ja se mittaa eroa vahvan ja heikon läheisilmön välillä.

Tässä työssä kuvaamme kvanttikuljetusteoriaa mesoskooppisissa normaalisuojrahtavissa (NS) heterorakenteissa käyttäen sirotaamattiaan perustuvaa numerista menetelmää. Erityisesti tarkastelemme Andreevin interferometrinen kuljetusoiminaisuuksia: johtavuusvärähtelyjen geometriariippuvuutta, tunneliliitosten vaikutusta ja universaaleja konduktanssisfluktuatioiden (UCF).

Simulaatioiden tuloksena havaitsemme, että värähtelyjen maksimiampitued vähenee potenssilain mukaan suprajohtojen välimatkana kasvaessa. Kun AI-rakenteessa on yksi tai useampia tunneliliitoksia, osoitettuaan, että vahva läheisilmio pienentää konduktanssia matalilla energioilla. Lisäksi havaitsemme, että suprajohtoilla on merkittävä vaikutus universaalisten konduktanssisfluktuatioiden suuruuteen.
When a metallic or semiconducting normal material is in close proximity to a superconductor, the nonvanishing pairing amplitude characteristic for superconductivity “leaks” from the superconductor into the normal side. This proximity effect increases the phase coherence of the normal structure, resulting in an enhanced local conductivity and a significantly modified local density of states. An alternative way to describe the effect of superconductivity on the transport properties of the normal material is the concept of Andreev reflection, where an electron-like quasiparticle excitation is converted into a hole-like excitation.

The consequences of the proximity effect can be studied in so-called Andreev interferometers, where the strength of the effect can be varied by the phase difference between the order parameters of two superconductors in contact with a normal conductor. Changing the phase difference induces oscillations in the conductance through the normal material and the energy-dependent amplitude of these oscillations measures the difference between strong and weak proximity effects.

The objective of the present work is to describe the quantum transport in the mesoscopic normal-superconducting (NS) heterostructures by applying a numerical technique based on the scattering theory. Especially, we consider the transport properties of Andreev interferometers: the dependence of the oscillations on the geometry of the system, the effect of tunnel barriers and the universal conductance fluctuations (UCF).

As a result of our simulations, we find a power-law decay of the maximum amplitude as the separation between the superconductors is increased. Furthermore, we observe that in the presence of a tunnel barrier at one or both ends of the mesoscopic normal conductor, the low-energy conductance is suppressed due to the strong proximity effect. Finally, the magnitude of UCF is found to distinctly decrease due to the presence of superconductivity.
Alkusanat

Tämä diplomityö on tehty osittain Teknillisen korkeakoulun Materiaalifysiikan laboratoriossa ja osittain Lancasterin yliopistossa (School of Physics and Chemistry). Työn ohjaajia ovat professori Colin Lambert Lancasterista sekä professori Gerd Schön Karlsruhen yliopistosta. On ollut suuri kunnia työskennellä heidänlaistensa kansainvälisen huippututkijoiden kanssa.


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<td>$v_F$</td>
<td>Fermi velocity</td>
</tr>
<tr>
<td>$\lambda_F$</td>
<td>Fermi wavelength</td>
</tr>
<tr>
<td>$\tau_{el}$</td>
<td>elastic scattering time</td>
</tr>
<tr>
<td>$l_{el} = v_F \tau_{el}$</td>
<td>elastic mean free path</td>
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<tr>
<td>$\tau_\phi$</td>
<td>inelastic scattering time</td>
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<tr>
<td>$l_\phi = \sqrt{D \tau_\phi}$</td>
<td>phase coherence length</td>
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<tr>
<td>$D$</td>
<td>diffusion constant</td>
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<tr>
<td>$G$</td>
<td>conductance</td>
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<tr>
<td>$E$</td>
<td>energy</td>
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<td>$E_F$</td>
<td>Fermi energy</td>
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<td>$E_T$</td>
<td>Thouless energy</td>
</tr>
<tr>
<td>$a$</td>
<td>tight-binding lattice constant</td>
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<tr>
<td>$i$, $j$</td>
<td>site indices</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>spin index</td>
</tr>
<tr>
<td>$\epsilon_{i,\sigma}$</td>
<td>tight-binding site energy for an electron with spin $\sigma$ at site $i$ (in this work, this is chosen independent of spin)</td>
</tr>
<tr>
<td>$\gamma_{ij}^{\sigma\sigma'}$</td>
<td>tight-binding hopping element between electrons at sites $i$ and $j$ and with spins $\sigma$ and $\sigma'$ (in this work this is chosen to be a constant $\gamma$)</td>
</tr>
<tr>
<td>$W$</td>
<td>width of the “disorder distribution” in the tight-binding Anderson model (site energies $\epsilon_i$ are chosen randomly within the interval $[-W/2, W/2]$)</td>
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LIST OF SYMBOLS

\( \psi_{i,\sigma}^{(1)} \)  
electron annihilation (creation) operator for spin \( \sigma \) at the tight-binding site \( i \)

\( \gamma_{n,\sigma}^{(1)} \)  
\( \textit{bogoliubon} \) annihilation (creation) operator for eigenstate \( n \), spin \( \sigma \)

\( V_{ji} \)  
pairing interaction between sites \( i \) and \( j \)

\( f_{ji} \equiv \langle \psi_{j,\downarrow} \psi_{i,\uparrow} \rangle \)  
pairing amplitude between sites \( i \) and \( j \), spins \( \uparrow, \downarrow \)

\( \Delta_{ji} \equiv V_{ji} f_{ji} \)  
pairing potential (order parameter) between sites \( i \) and \( j \)

\( \mu_i \)  
chemical potential for reservoir \( i \)

\( T_i \)  
temperature for reservoir \( i \)

\( f(E;\mu,T) \)  
Fermi distribution function \( \{ \exp \left[ \frac{(E - \mu)}{kT} \right] + 1 \}^{-1} \)

\( f_i^\alpha(E) \)  
Fermi distribution function \( \{ \exp \left[ \frac{(E - \alpha(\mu_i - \mu))}{kT} \right] + 1 \}^{-1} \)
of \( \alpha \)-type quasiparticles in reservoir \( i \) at the temperature \( T_i \) and chemical potential \( \mu_i \)

\( \nu_i(E) \)  
density of states in lead \( i \)

\( I \)  
unit matrix

\( s^\alpha_{i,a,j,b} \)  
\( s \)-matrix element between \( \beta \)-type channel \( b \) of lead \( j \) and \( \alpha \)-type channel \( a \) of lead \( i \)

\( T_0 \) \( (T_A) \)  
normal (Andreev) transmission probability

\( R_0 \) \( (R_A) \)  
normal (Andreev) reflection probability

\( \Gamma \)  
transmittivity of a tunnel barrier, defined by the ratio of conductances of a ballistic structure in the presence of the barrier and the corresponding conductance in the absence of the barrier

For notation used in Chapter 5, “Results”, see Fig. 5.1, pp. 45.

Transverse wavefunctions

In the leads, the quasiparticles get into transverse modes of type Eq. (2.29).

Here the transverse wavefunctions \( \chi_i^\alpha(\rho) \) depend on the dimensionality of
the system and transverse boundary conditions. Two boundary conditions are commonly applied in the numerical method: fixed end and periodic. These will be introduced separately.

**Fixed-end boundary conditions**

Fixed-end boundary conditions correspond to the case where the leads contain “hard walls”, i.e. infinite potential restricting the quasiparticles inside a certain area. Assume that the leads contain $M$ sites in the transverse ($y$-) direction in the 2D case or $M_y$ and $M_z$ sites in the $y$- and $z$-directions, respectively, in the 3D case. These boundary conditions read (from now on, we will set the lattice constant $a = 1$ and omit here the lead and quasiparticle indices; the transverse wavefunctions look similar for both types of quasiparticles, only the corresponding eigenenergies have a different sign)

$$
\chi_a(0) = \chi_a(M + 1) = 0, \quad (2D),
$$

$$
\chi_a(0, z) = \chi_a(y, 0) = \chi_a(M_y + 1, z) = \chi_a(y, M_z + 1) = 0, \quad (3D). \quad (2)
$$

Applying these boundary conditions for the tight-binding Hamiltonian, Eq. (2.1), we obtain the wavefunctions

$$
\chi_a(y) = \sqrt{\frac{2}{M + 1}} \sin \left( \frac{a 2\pi}{M + 1} y \right), \quad (2D),
$$

$$
\chi_a(y, z) = \sqrt{\frac{4}{(M_y + 1)(M_z + 1)}} \sin \left( \frac{2\pi a_y}{M_y + 1} y \right) \sin \left( \frac{2\pi a_z}{M_z + 1} z \right), \quad (3D). \quad (3)
$$

Here $a, a_y$ and $a_z \in \mathbb{N}$.

**Periodic boundary conditions**

Periodic boundary conditions correspond to a two-dimensional system formed in the surface of a cylinder. (In general, periodic boundary conditions could also be used to describe a system of infinite width, but with a periodic pat-
tern of length \((M_i + 1)\) to direction \(i\). Now the boundary conditions are

\[
\begin{align*}
\chi_a(y) &= \chi_a(y + m(M_y)), \quad \text{(2D),} \\
\chi_a(y, z) &= \chi_a(y + m_y(M_y), z + m_z(M_z)), \quad \text{(3D),}
\end{align*}
\]

where \(m, m_y\) and \(m_z \in \mathbb{Z}\). The eigenfunctions corresponding to these boundary conditions are

\[
\begin{align*}
\chi_a(y) &= \sqrt{\frac{1}{M}} \exp \left(i \frac{2\pi a}{M} y\right), \quad \text{(2D),} \\
\chi_a(y, z) &= \sqrt{\frac{1}{(M_y)(M_z)}} \exp \left(i \frac{2\pi a_y}{M_y} y\right) \exp \left(i \frac{2\pi a_z}{M_z} z\right), \quad \text{(3D).}
\end{align*}
\]

In this case \(a, a_y\) and \(a_z \in \mathbb{Z}\).

**Dispersion relations and group velocities**

**Nearly free electron approximation**

In the absence of a magnetic field, the Hamiltonian written in the nearly free electron approximation for an electronlike quasiparticle in lead \(i\) is

\[
\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m} \nabla^2 - E_{F}^{\text{nelectron}} + U_i(\mathbf{r}),
\]

where \(U(\mathbf{r})\) describes the boundaries of the lead.

The dispersion relation corresponding to this Hamiltonian is

\[
\epsilon_{a,\kappa}^{+1} = \frac{\hbar^2 \kappa^2}{2m} + \epsilon_{a,0}^{+1} - E_{F}^{\text{nelectron}},
\]

where \(\kappa\) is the longitudinal wave number, \(m\) is the effective mass of the quasiparticle and \(\epsilon_{a,0}\) is the eigenenergy corresponding to the transverse mode \(a\):

\[
\epsilon_{a,0}^{+1} = \frac{\hbar^2}{2m} \sum_i \left(\frac{2\pi a}{(M_i + 1)}\right)^2.
\]

Here the sum goes over all the transverse dimensions (in the case of periodic boundary conditions, use \(M_i\) instead of \(M_i + 1\)).

The eigenenergies for quasiholes are obtained by \(\epsilon_{a,\kappa}^{-1} = -\epsilon_{a,\kappa}^{+1}\).
LIST OF SYMBOLS

Longitudinal group velocity corresponding to the electronlike quasiparticle mode $a$ is given by the $\kappa$-derivative of the mode energy:

$$v_{a,\kappa} = \frac{1}{\hbar} \frac{\partial \epsilon_{a,\kappa}}{\partial \kappa} = \frac{\hbar \kappa}{m}. \quad (12)$$

The nearly free electron approximation will be used as a continuum version of the tight-binding model in Appendices 6 and 6.

Tight-binding approximation

The tight-binding Hamiltonian is given in Eq. (2.1). In the absence of a magnetic field in the leads, its eigenenergies are of the form

$$\epsilon_{a,\kappa} = -E_F^{\text{lb}} - 2\gamma \cos(\kappa) + \epsilon_{a,0}. \quad (13)$$

The transverse-mode eigenenergies $\epsilon_{a,0}$ are given by

$$\epsilon_{a,0} = -2\gamma \sum_i \cos \left( \frac{2\pi a}{M_i + 1} \right) \quad (14)$$

and the group velocities by

$$v_{a,\kappa} = \frac{2\gamma}{\hbar} \sin(\kappa). \quad (15)$$

In Eq. (14), the sum goes over all the transverse dimensions. Also here, if one considers periodic boundary conditions, $M_i + 1$ should be replaced by $M$.

Note that if we set $E_F^{\text{lb}} = E_F^{\text{nm}} - 4\gamma$ and $\gamma = \hbar^2/2ma^2$, the limit $a \to 0$ yields the corresponding nearly free electron quantities.
Chapter 1

Introduction

In recent years, the pace of miniaturization of electronic devices has exceeded even the boldest predictions. Since the development of the world’s first transistor in 1947, roughly of one centimeter across, the size of new electronic devices has steadily shrunk. In the 1980s, the characteristic length scale was already micrometers, but the boost given by computer technology within the past decade is making rapid advance towards the age of nanoelectronics. Within the next 10-20 years, the lateral dimensions of the features in integrated circuits are expected to decrease down to a few tens of nanometers and their thickness will be even smaller. Nanoscience and nanotechnology will revolutionize future technologies.

In the minuscule length scales where the smallest details in the electronic devices are only tens of atoms wide, one starts to observe novel phenomena which can be explained only by considering the quantum-mechanical wave nature of electrons. Phenomena such as the universal conductance fluctuations (UCF) due to the specific realization of impurities, the quantization of conductance, low dimensionality of certain nanoscale structures and the discreteness of the charge of an electron strongly affect the transport properties of these devices. While these phenomena may create difficulties in the conventional design, they simultaneously also provide opportunities to fabricate entirely new types of devices, such as the single-electron transistor. One may start to talk about quantum engineering [1].

Transport phenomena in these mesoscopic structures have attracted a lot
of attention in recent years [2–5]. One of the most important findings in this field has been the recognition that elastic scattering is not phase-breaking. Even if the elastic scattering time $\tau_{el}$ and the corresponding elastic mean free path $l_{el} = v_F \tau_{el}$ are generally quite small, usually of the order of tens of nanometers, the electrons may retain their phase memory at much larger length scales. For low temperatures, inelastic processes such as collisions with phonons are rare events and, consequently, diffusive electronic motion may be phase-coherent over distances $l_\phi = \sqrt{D \tau_\phi} \gg l_{el}$. At $T \sim 1$ K, typical values for the phase coherence length in disordered conductors range from hundreds of nanometers to even micrometers [4, 5].

Due to progress in the fabrication technologies, it has become possible to grow pure ultrathin perfect crystals in layers between different materials with different conductance and valence band energies (c.f., Fig. 1.1). Typically, the thickness of these layers is only a few nanometers. Consequently, a practically two-dimensional electron gas (2DEG) is formed.\(^1\) Usually, these layers are constructed either in metal-oxide-semiconductor (MOS) structures, involving Si, or between GaAs and Al\(_x\)Ga\(_{1-x}\)As. The electron density (and thus the Fermi energy) in these 2DEGs can be controlled by depositing metallic gates on top of the uppermost material. Furthermore, the electrons of the 2DEG can be confined by using appropriately shaped gates. Hence, structures of almost arbitrary shape can be constructed, including in particular one-dimensional channels.

Novel alternatives for mesoscopic nanoscale structures are the carbon nanotubes [6] (c.f., Fig. 1.2). By laser-vapouring carbon with an admixture of Ni/Co and imaging by an atomic force microscope, one has obtained tubular structures with lengths of the order of micrometers and heights down to one nanometer. In these nanotubes, electric conduction seems to occur through well separated, discrete electron states that are quantum-mechanically coherent over relatively long distances, at least over 100 nm.

In mesoscopic conductors, electronic transport is described in terms of

\(^1\)The energy of the “first excited” state in this ($z$) direction is much higher than the ground-state energy, such that transport is essentially two-dimensional at low bias energies and/or temperatures.
travelling electron waves interfering with each other. In contrast, superconductors feature a slightly different quantum-mechanical transport mechanism: below the critical temperature, the current is carried without dissipation by the Cooper pairs. The superconducting condensate may be described through a single wavefunction with macroscopic phase coherence extending throughout the structure. The presence of the macroscopic condensate wavefunction is manifested experimentally, for example, through the quantization of magnetic flux in superconducting rings, or via the Josephson effects between two superconductors with different phases. In addition to the “supercurrent” due to the Cooper pairs, a dissipative “normal” current can also be carried by single electrons (quasiparticle excitations) with energy exceeding the energy gap $\Delta$ of the superconductor.

It has been known for long [7] that when a superconductor is in close proximity to a normal (nonsuperconducting) material, the macroscopic wavefunction “leaks” from the superconductor into the normal side. At low temperatures, the penetration depth of this proximity effect is of the order of
hundreds of nanometers and its influence on the properties of the normal material has been difficult to probe until the present decade. However, the recent advances in nanofabrication techniques have served to renew the interest in this phenomenon. The proximity effect is now known to drastically change the local density of states of the normal material near the normal-superconducting (NS) interface [8]; moreover, the transport properties are also modified [9]. For example, one may expect the local conductivity to display a dependence on the macroscopic phase of the superconducting condensate.

A NS heterostructure may be described by the Bogoliubov–de Gennes (BdG) equations, which introduce the coupled quasiparticle picture of electrons (quasiparticles above the Fermi energy) and holes (quasiparticles below $E_F$). An electronlike quasiparticle just above the Fermi energy injected from the normal side enters the superconductor as an evanescent wave. One would expect to observe another electronlike quasiparticle to be reflected back to the normal metal. But if the NS interface is clean, it is much more probable that another kind of a reflection process occurs. Andreev [10] showed that the electron is retroreflected as a hole to the normal metal and the net result is an additional Cooper pair in the superconductor. This is a result of the
coupling between electron- and holelike quasiparticle states in the superconductor. The existence of this Andreev reflection may actually be considered as an equivalent picture with the proximity effect; the amplitude of the Andreev reflection is proportional to the pairing amplitude at the interface.

In the Andreev reflection, the retroreflected hole contains three interesting properties related to the incident electron. First of all, it has opposite spin and charge. Therefore, Andreev reflection enhances the current and reduces the resistance. Secondly, at $E_F$, the dynamical phase of the hole is conjugated and thirdly, the hole acquires an additional phase shift due to the macroscopic phase of the superconducting wavefunction. This latter property causes an observable effect on transport if the hole may further reflect from an interface with another superconductor having another macroscopic phase. Namely, if the phase difference between these two superconductors is varied, one finds oscillations in the conductance through the normal sample [11]. This is why these kinds of devices are called the Andreev interferometers (AIs).

Another interesting phenomenon in the field of mesoscopic superconductivity is provided by finite-size effects on the superconductivity itself. Anderson [12] proposed in 1959 that superconductivity may exist only if the energy gap $\Delta$ is much larger than the energy-level spacing $d$ in the superconductor. The typical size of the energy gap is one thousandth of the Fermi energy. Hence, if one assumes that the energy levels are uniformly spaced, the finite energy-level spacing would be seen in a crystal lattice with a few thousand unit cells. This corresponds to particle sizes on the order of 10 nm. The experiments by Ralph, Black and Tinkham [13, 14] in the past few years have confirmed this prediction: the pairing potential decreases when particle size is lowered and in small enough particles, superconductivity can no longer be observed.

There are two commonly applied theoretical approaches to the description of transport in NS heterostructures. One approach starts from the Dyson equation for the Keldysh Green’s functions at thermal equilibrium. This is further simplified by introducing quasiclassical Green’s functions to describe transport in either clean (Eilenberger equation) or dirty systems.
This quasiclassical formalism is suitable for evaluating analytical formulae for ensemble-averaged quantities. However, these equations do not allow for effects due to weak localization.

The present work utilizes mainly the other approach: the scattering formalism \[9, 16\]. This simplifies the calculation of the conductance to the determination of the transmission and reflection amplitudes between the different quantum channels in the ends of the mesoscopic structure. These quantities can be evaluated from the Green’s function for the Bogoliubov - de Gennes equation in a tight-binding lattice describing the system and the description may also include Andreev reflection and/or transmission. This formalism is especially suited for evaluating sample-specific vs. ensemble-averaged quantities for systems with different geometries.

This thesis considers the transport properties of Andreev interferometers. It has been found \[17, 18\] that the ensemble-averaged conductance oscillations display a reentrant behaviour in the quasiparticles energy: the amplitude of the oscillations is maximal at a finite energy proportional to the Thouless energy of the normal structure between the superconductors. Employing a numerical technique based on the scattering formalism, we investigate the geometry dependence of the maximum amplitude. Also the sample-specific vs. ensemble-averaged properties are compared by calculating the rms amplitude of the universal conductance fluctuations (UCF). Finally, calculations of these quantities in systems involving d-wave superconductors are reported.

Even if the proximity effect is attenuated exponentially into the normal material, we find that the conductance oscillation amplitude decreases only as a power law as the separation between the superconductors is increased (provided that the energy \(E/E_T\) is varied accordingly). This is an interesting property since one suggested application for Andreev interferometers is SQUID-like detection of magnetic field. The Josephson effect utilized in SQUIDs decreases exponentially as the width of the insulator between the superconductors is increased. Because of the power-law dependence, the Andreev Interferometers would perhaps be more stable to variations in the fabrication techniques.

This thesis is organized as follows. The next chapter describes the
theory underlying the scattering formalism for NS heterostructures. The Bogoliubov-de Gennes equations are motivated and their consequences, the proximity effect and Andreev reflection, are discussed. Also the Landauer-Büttiker formalism is introduced with the formulae relating the conductance and the scattering amplitudes. The numerical scheme is outlined in the third chapter. Some alternative methods are mentioned, but the main focus is on the decimation method applied in this work. The fourth chapter reviews recent experiments on the AIs and their theoretical interpretations and the fifth chapter presents results of the numerical calculations. The final chapter includes a discussion of the results and a glance at the future. This is followed by appendices detailing derivations of formulae essential for this research.
Chapter 2

Formalism

This chapter presents a theoretical framework for calculating the conductance of a hybrid normal/superconducting (NS) heterostructure. The mathematical description is basically an extended Landauer - Büttiker formalism [19–21], where the presence of superconductivity is introduced by applying the Bogoliubov - de Gennes Hamiltonian in the tight-binding picture. In addition to this basic phenomena and central quantities considered in this work are defined and derived.

There are two approaches to the description of the physics of the NS heterostructures: The first alternative is the language of the proximity effect, where the nonzero pairing potential “leaks” from the superconductor to the normal structure and modifies its physical properties. On the other hand, one may describe the electronic properties of the structure by the picture of the Andreev reflection, where a quasiparticle (quasihole) is converted to a quasihole (quasiparticle). These two approaches are nothing more than different pictures of the same phenomenon, and usually to obtain a fair understanding of the observed effect in question, both approaches should be applied. An example of this is especially provided by the case of the Andreev interferometers in Chapter 4.
CHAPTER 2. FORMALISM

2.1 Tight-binding Bogoliubov - de Gennes equation

A non-superconducting cubic\(^{1}\) crystal lattice is here characterized by the tight-binding Hamiltonian [22]

\[
H_0 = \sum_{i,\sigma} \psi_{i,\sigma}^\dagger (\epsilon_{i,\sigma} - E_F) \psi_{i,\sigma} - \sum_{\langle i,j \rangle_{\sigma,\sigma'}} \gamma_{ji}^{\sigma\sigma'} \left( \psi_{j,\sigma'}^\dagger \psi_{i,\sigma} + \text{h.c.} \right),
\]

(2.1)

where \(i\) and \(j\) represent the crystal lattice sites and \(\langle i, j \rangle\) denotes the nearest neighbours \(i\) and \(j\). The Hamiltonian is written in terms of the real-space field operators \(\psi_{i,\sigma}^\dagger\) and \(\psi_{i,\sigma}\), which create or destroy an electron of spin \(\sigma\) at site \(i\). These operators satisfy the anticommutation relations

\[
\{\psi_{i,\sigma}^\dagger, \psi_{j,\sigma'}\} = 0, \quad \{\psi_{i,\sigma}^\dagger, \psi_{j,\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}. \quad (2.2)
\]

When the crystal is nonferromagnetic and there are no magnetic impurities, we have \(\gamma_{ji}^{\sigma\sigma'} = \gamma_{ji}\) and \(\epsilon_{i,\sigma} = \epsilon_i\). In the so called Anderson model considered in this work, the site energies \(\epsilon_i\) are chosen randomly from an interval\(^{2}\) \([-W/2, W/2]\) where the parameter \(W\) describes the amount of disorder in the system. Moreover, in the absence of an external magnetic field\(^{3}\), \(\gamma_{ji} = \gamma\) is a constant.

The derivation of the Bogoliubov-de Gennes equation is usually performed in the continuum \([7]\). However, the numerical calculations employ the tight-binding picture for discrete lattice sites (unit cells of the crystal lattice). Therefore, we will consider the BCS interaction connecting pairs of electrons in different tight-binding sites already at the outset. In the

---

\(^{1}\)Phenomena dependent on the symmetry of the lattice can be studied by a suitable choice of couplings between the lattice sites.

\(^{2}\)In this work the site energies are assumed uniformly distributed. Another commonly considered distribution is Gaussian. Usually this choice does not have a significant effect on the calculated observables.

\(^{3}\)The effect of a magnetic field can be included into the model by the Peierls substitution \(\gamma_{ji} = \gamma \exp[i \frac{e}{\hbar} \int \frac{\mathbf{A}}{2} \cdot d\mathbf{l}]\).
tight-binding picture this corresponds to overlap integrals of the form

$$\int dr dr' \phi^*_n(r-r_1)\phi^*_m(r'-r_0) V(r-r_1, r'-r_0) \phi_m(r-r_j) \phi_{m'}(r'-r_{j'}) ,$$

(2.3)

where $\phi_n(r-r_1)$ is the atomic wavefunction for the state $n$ at site $i$.

The only interaction Eq. (2.1) governs between the electrons is the “Fermi interaction”, i.e. that induced by the Pauli exclusion principle (actually, the quantities $\epsilon_i$ and $\gamma$ may also be slightly dependent on the Coulomb interaction between the electrons). This interaction is included into the definition of the field operators. However, the theory of superconductivity assumes an attractive nonvanishing interaction between pairs in time-reversed electronic states (Cooper pairs). It is customary to assume this interaction extremely local, i.e. acting only on a single site, but the actual BCS interaction with the cutoff energy at some finite value extends over multiple sites (c.f., Sect. 3.5). Thus we arrive at a Hamiltonian of the form

$$H_{\text{eff}} = H_0 + \sum_{ij} \frac{1}{2} V_{ij} \sum_{\sigma, \sigma'} \psi_{i,\sigma}^{\dagger} \psi_{j,\sigma'}^{\dagger} \psi_{j,\sigma'} \psi_{i,\sigma} .$$

(2.4)

Superconductivity can be characterized by the so called pairing potential

$$\Delta_{ji}^{\sigma \sigma'} \equiv V_{ji}^{\sigma \sigma'} f_{ji}^{\sigma \sigma'}$$

(2.5)

where the pairing amplitude $f_{ji}^{\sigma \sigma'}$ is defined as

$$f_{ji}^{\sigma \sigma'} \equiv \langle \psi_{j,\sigma'} \psi_{i,\sigma} \rangle$$

(2.6)

and the angular brackets denote an average over the state of the system. The anticommutation relations, Eq. (2.2), force the terms $f_{ii}^{\sigma \sigma'}$ to vanish. In what follows, we assume spin singlet superconductivity,\(^4\) and therefore take into account only terms with $f_{ji}^{\sigma -\sigma}$, defining $f_{ji}^{\uparrow \downarrow} \equiv f_{ji}$. In general, the terms $\Delta_{ji}^{\sigma -\sigma}$ are nonzero, at least for $i = j$, for superconductors below their critical temperature (and critical magnetic field) but zero otherwise.

\(^4\)“Total spin of a Cooper pair” is zero, i.e. $\sigma + \sigma' = 0$.  

The interaction term in the Hamiltonian Eq. (2.4) may now be written in terms of pairing amplitudes, the operators $\delta \sigma_{ij}^\sigma$ describing fluctuations around the mean field, and their complex conjugates:

$$
\psi_{j,\sigma}^\dagger \psi_{i,\sigma} = f_{ji}^{\sigma} + \delta_{ji}^{\sigma} \\
\psi_{i,\sigma}^\dagger \psi_{j,\sigma}^\dagger = (f_{ji}^{\sigma})^\dagger + (\delta_{ji}^{\sigma})^\dagger.
$$

(2.7)

Since $\delta_{ji}^{\sigma}$ describe quantum fluctuations, they are chosen to satisfy $\langle \delta_{ji}^{\sigma} \rangle = 0$. We may now make the assumption that the fluctuations are small and expand the interaction term to the first order in $\delta_{ji}^{\sigma}$. By defining $E_0 \equiv -\sum_{ji} V_{ji} |f_{ji}|^2$, we obtain

$$
H_{\text{eff}} = H_0 + E_0 + \\
\frac{1}{2} \sum_{ij} \left[ (\Delta_{ji}^{\dagger})^\dagger \psi_{j,i} \psi_{i,i}^\dagger + (\Delta_{ji}^{\dagger})^\dagger \psi_{j,i} \psi_{i,i}^\dagger + \Delta_{ji}^{\dagger} \psi_{i,i}^\dagger \psi_{j,i}^\dagger + \Delta_{ji}^{\dagger} \psi_{i,i}^\dagger \psi_{j,i}^\dagger \right].
$$

(2.8)

In the absence of a magnetic field neither spin direction is preferred, and hence the sum of the first terms on the second line of Eq. (2.8) is equal to the sum of the second terms. Analogously, the sums of the third and fourth terms are equal and one may reorder them to find

$$
H_{\text{eff}} = E_0 + \sum_{ij} \left( \psi_{i,i}^\dagger \psi_{i,i}^\dagger \right) H \left( \psi_{j,j}^\dagger \psi_{j,j}^\dagger \right)
$$

(2.9)

where

$$
H = \begin{pmatrix} H_0 & \Delta \\ \Delta^\dagger & -H_0^\dagger \end{pmatrix}.
$$

(2.10)

The operator (2.10) is known as the Bogoliubov - de Gennes (BdG) Hamiltonian after its originators [7] and the corresponding eigenvalue equation

$$
H \Psi_{n,j} = H \begin{pmatrix} u_{n,j} \\ v_{n,j} \end{pmatrix} = E_n \begin{pmatrix} u_{n,i} \\ v_{n,i} \end{pmatrix}
$$

(2.11)

is the Bogoliubov - de Gennes equation. For each positive eigenvalue $E_n$ of $H$ with the eigenvector $\Psi_{n,i}$, there exists a corresponding negative eigenvalue $-E_n$ with the eigenvector

$$
\Psi_{-n,i} = \begin{pmatrix} -v_{n,i}^* \\ u_{n,i}^* \end{pmatrix}.
$$

(2.12)
Consequently, $\mathcal{H}_{\text{eff}}$ can be diagonalized by the transformation

$$
\begin{pmatrix}
\psi_{i\uparrow} \\
\psi_{i\downarrow}
\end{pmatrix} = \sum_{n>0} \begin{pmatrix}
u_{n,i} & -\gamma_{n,i}^* \\
v_{n,i} & u_{n,i}
\end{pmatrix} \begin{pmatrix}
\gamma_{n\uparrow} \\
\gamma_{n\downarrow}
\end{pmatrix}.
$$

(2.13)

Indeed, substituting (2.13) into Eq. (2.9) and noting that for a closed system, eigenstates can be chosen to be orthonormal, yields

$$
\mathcal{H}_{\text{eff}} = E_0 - \sum_{n>0} E_n + \sum_{\sigma} E_n \gamma_{n,\sigma}^\dagger \gamma_{n,\sigma}.
$$

(2.14)

Furthermore, one may invert Eq. (2.13) to find the Bogoliubov quasiparticle ($bogoliubon$) field operators $\gamma_{n\sigma}^\dagger$,

$$
\begin{pmatrix}
\gamma_{n\uparrow} \\
\gamma_{n\downarrow}
\end{pmatrix} = \sum_{i} \begin{pmatrix}
u_{n,i}^* & \gamma_{i,i}^* \\
v_{n,i}^* & u_{n,i}
\end{pmatrix} \begin{pmatrix}
\psi_{i\uparrow} \\
\psi_{i\downarrow}
\end{pmatrix}.
$$

(2.15)

When solved for the positive energy eigenvalues, the Bogoliubov - de Gennes equation yields all the system observables in terms of the amplitudes $u_n, v_n$ and the operators $\gamma_{n\sigma}^\dagger$. For example, the current density is given by

$$
\mathbf{j}_i \equiv (e/m) \text{Re} \sum_{\sigma} \langle \psi_{i\sigma}^\dagger (\mathbf{p}_i - e\mathbf{A}_i/c) \psi_{i\sigma} \rangle
$$

$$
= (e/m) \text{Re} \left[ 2 \sum_{n>0} \langle v_{n,i} (\mathbf{p}_i - e\mathbf{A}_i/c) \psi_{n,i}^* \rangle \right]
$$

$$
+ (e/m) \text{Re} \left[ \sum_{n>0} \langle u_{n,i}^* (\mathbf{p}_i - e\mathbf{A}_i/c) u_{n,i} \rangle \langle \gamma_{n,\sigma}^\dagger \gamma_{n,\sigma} \rangle \right]
$$

$$
- (e/m) \text{Re} \left[ \sum_{n>0} \langle v_{n,i} (\mathbf{p}_i - e\mathbf{A}_i/c) v_{n,i}^* \rangle \langle \gamma_{n,-\sigma}^\dagger \gamma_{n,-\sigma} \rangle \right].
$$

(2.16)

Note that the quantity $\langle \gamma_{n,\sigma}^\dagger \gamma_{n,\sigma} \rangle$ is nothing else but the average number of the bogoliubon quasiparticles at the energy $E_n$ and hence, in the equilibrium, it may be replaced by the Fermi distribution function $f(E_n)$. 
2.1.1 Proximity effect

The Bogoliubov - de Gennes Hamiltonian Eq. (2.10) itself depends on the amplitudes $u_n$ and $v_n$ via

$$\Delta^{\downarrow \uparrow}_{ij} = V_{ij} f_{ij} = V_{ij} \sum_n \left[-u_n i^* v_{n,j} + u_{n,j} v_{n,i} \langle \gamma_{n,i} \gamma_{n,j} \rangle + v_{n,i} v_{n,j} \langle \gamma_{n,i} \gamma_{n,j} \rangle\right].$$

(2.17)

Consequently, Eq. (2.11) must be solved self-consistently: choosing an initial ansatz for the $\Delta$-matrix, solving $u_n$ and $v_n$, substituting these into Eq. (2.17) and solving again until convergence. As a result, the pairing amplitude is found to "leak" (it becomes nonzero) into the normal side$^5$, decaying exponentially with the distance from the interface (c.f., Fig. 2.1). The characteristic penetration depth is given by

$$\xi_T = \frac{\hbar v_F}{2\pi E}$$

(2.18)

for clean normal materials (ballistic transport), and by

$$\xi_T = \sqrt{\frac{\hbar D}{2\pi E}},$$

(2.19)

in the diffusive (dirty) case. Here $v_F$ is the Fermi velocity, $D$ is the diffusion constant for the normal material and $E$ is the energy of an electron experiencing the proximity effect.

In the present work, only the first step of the self-consistent solution is taken such that $\Delta_{ij}$ only depends on $|i - j|$. With this choice, solving Eq. (2.11) once yields approximately the correct penetration of the pairing amplitude and further corrections from the self-consistent procedure do not have a significant effect on the conductance.

$^5$"Normally conducting" in this work refers to a material where the pairing interaction $V$ is zero.
Figure 2.1: When in contact with a normal material, the nonzero pair amplitude "leaks" from the superconductor into the normal side.

2.1.2 Andreev reflection

In the absence of superconductivity, $\Delta = 0$, and the amplitudes $u_n$ and $v_n$ are decoupled, satisfying

\begin{align}
\mathcal{H}_0 u_n &= E_n u_n \\
-\mathcal{H}_0^t v_n &= E_n v_n.
\end{align}

In the nearly free electron approximation [22], the eigenfunctions for a clean normal lattice are

\begin{align}
u_n(r) &= u_n e^{ik_n^e r} \\
v_n(r) &= v_n e^{ik_n^h r},
\end{align}

where the wavevectors satisfy

\begin{align}
|k_n^e| &= \frac{2m}{\hbar} \sqrt{E_F + E_n} \\
|k_n^h| &= \frac{2m}{\hbar} \sqrt{E_F - E_n}
\end{align}

and normalization implies $|u_n|^2 + |v_n|^2 = 1$. Since the $u_n(r)$ describe excitations above the Fermi energy, they are called electron-like quasiparticle (or simply quasiparticle) wavefunctions. Similarly, $v_n(r)$ are the hole-like quasiparticle (quasihole) wavefunctions.
Then consider an incident electron-like quasiparticle propagating towards a normal-superconducting interface from the normal side. Assume that the superconductor is characterized by a local order parameter $\Delta e^{i\varphi_S}$. Since the order parameter couples the electron-like and hole-like quasiparticles, there are four possible final states propagating away from the interface:

Normal conductor: 
\[
\begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(i k^e x) \rightarrow
\]

Superconductor ($\Delta e^{i\varphi_S}$): 
\[
\begin{pmatrix} t^{ee} (u \exp(i \varphi_S) & \exp(i q^+ x) \\ v & \exp(i q^- x) \end{pmatrix} \rightarrow
\]

\[
\begin{pmatrix} t^{he} (v \exp(i \varphi_S) & \exp(i q^- x) \\ u & \exp(i q^+ x) \end{pmatrix} \rightarrow
\]

In the superconductor, a gap $\Delta$ appears in the dispersion relation:
\[
E^2 = \left(\hbar q^2 / 2m - E_F\right)^2 + \Delta^2.
\]
Solving this for $q$ yields $q^\pm = 2m/\hbar^2 \left(E_F \pm \sqrt{E^2 - \Delta^2}\right)$, which shows that whenever the excitation energy is lower than $\Delta$, an imaginary component develops in the wavenumber and the solution is decaying.

The amplitudes for different processes can be obtained by matching the wavefunctions at the boundary. In the absence of a tunnel barrier and a mismatch in the Fermi wavevectors ($k_F = q_F$), the amplitude for normal reflection as well as for the hole-like wave in the superconductor vanishes ($r^{ee} = 0$ and $t^{he} = 0$). Hence the Andreev reflection [10,23], where the quasiparticle reflects from the interface as a quasihole or vice versa, is the dominant process. The amplitudes for these processes, $r^{he}$ and $r^{eh}$, respectively, are

\[
r^{he}(E) = \exp(-i \varphi_S) \exp(-i \arccos(E/\Delta))
\]

\[
r^{eh}(E) = \exp(+i \varphi_S) \exp(-i \arccos(E/\Delta)).
\]

The reflected quasihole has opposite charge and spin with respect to the incident quasiparticle. To ensure the conservation of charge and spin, the net result has to be a removal of an additional electron from the normal side and an addition of a Cooper pair in the superconducting condensate. Moreover, the conservation of particle momentum requires that the reflected quasihole
propagates along the same path (but in the opposite direction) as the incoming particle. Therefore, the process is conventionally called retroreflection. At the Fermi energy, the dynamical phase of the incoming electron, \(k^eL\), is exactly cancelled by the dynamical phase of the Andreev-reflectected quasihole, \(k^hL\). At finite quasiparticle energies, this phase conjugation is destroyed at lengths of the order of the penetration depth of the proximity effect, \(\xi_T\).

In the continuum and in the case of local pairing potential independent of spin, the pairing amplitude is given by 

\[
f(r) = \sum_{n>0} u_n(r) v_n(r)^*(2f(E_n) - 1),
\]

where \(f(E_n)\) is the Fermi distribution. Substituting the incident and reflected wavefunctions, one finds for the pairing amplitude on the normal side:

\[
f(r) = \sum_{n>0} (r^{he})^n \exp(-i k^h x) \left[ \exp(ik^e x) + r^{ee} \exp(-ik^e x) \right] (2f(E_n) - 1).
\]

(2.28)

In the absence of Andreev reflection, \(r^{he} = 0\), the pairing amplitude is zero. Thus the Andreev reflection generates the proximity effect.

### 2.2 Extended Landauer - Büttiker formalism

The Landauer - Büttiker formalism [4, 19, 20] has been widely used for describing transport properties of normal mesoscopic systems but it was only in the beginning of 90s that this formalism was extended to partly superconducting structures involving Andreev scattering processes [21].

The formalism considers \(L\) normal and \(L_S\) \((i = L + 1 \ldots L + L_S)\) superconducting quasiparticle reservoirs connected to the scattering area by perfectly clean, crystalline leads (c.f., Fig. 2.2). The reservoirs are characterized by their chemical potentials \(\mu_i\) and temperatures \(T_i\). It is assumed that the quasiparticles undergo inelastic scatterings inside the reservoirs such that the outgoing particles are uncorrelated and their distribution may be described by the Fermi function \(f(E; \mu, T)\). Furthermore, it is assumed that the number of quasiparticles in the reservoirs is infinite, such that they can act as constant sources of particles and the chemical potential is not affected by a removal of one particle. The leads serve to transfer the quasiparticles between the reservoirs and the scattering area. The basic assumption is that
the leads contain no backscattering. Therefore, they have to be considered semi-infinite and clean.

\[ \psi_{i,a}^\alpha(x) e^{i k_n^\alpha x} = \left( \frac{\delta_{\alpha,+1}}{\delta_{\alpha,-1}} \right) [v_{i,a}^+ - \frac{1}{2}] \chi_{i,a}^\alpha(\rho) e^{i k_n^\alpha x}, \quad (2.29) \]

where \( \chi_{i,n}^\alpha(\rho) \) is the wavefunction of the \( \alpha \)-type (\( \alpha = +1 \) for a quasiparticle and \( \alpha = -1 \) for a quasihole) transverse quasiparticle mode (channel) \( n \) with an eigenenergy \( E_n \) at the transverse coordinate \( \rho \). The normalization by the inverse square-root of the group velocity is chosen to obtain a wave carrying a unit flux of particles. If the quasiparticles injected from a reservoir have an energy \( E \) (relative to the Fermi energy \( E_F \)), all the modes with \( E_n < E_F + E \) are filled (open for transmission) and all the others empty (closed).

In the absence of inelastic scattering, all the dc transport properties of the system can be determined from the quantum-mechanical scattering matrix \( s(E; \mathcal{H}) \), composed of the transmission (reflection) coefficients \( s_{i,j,a,b}^\alpha \) between the \( \beta \)-type modes \( m \) of lead \( j \) and the \( \alpha \)-type modes \( n \) of lead \( i \) connected to the scattering area described by the Hamiltonian \( \mathcal{H} \). In order for the current to be conserved, this \( s \)-matrix has to be unitary:

\[ \sum_{j:b,\beta} \left| s_{i,a,b}^{\alpha\beta} \right|^2 = \sum_{i:a,\alpha} \left| s_{i,a,b}^{\alpha\beta} \right|^2 = 1. \quad (2.30) \]
In the quasiparticle picture, it is customary to define the so-called $P$-matrix, consisting of the probabilities for transmission from $\beta$-type modes in lead $j$ to $\alpha$-type modes in lead $i$:

$$ P_{ij}^{\alpha\beta}(E; \mathcal{H}) = \sum_{a \in i} \left| \tilde{\rho}_{(i,a),(j,b)}^{\alpha\beta}(E; \mathcal{H}) \right|^2. \quad (2.31) $$

From the current conservation property of the $s$-matrix, Eq. (2.30), one obtains the following conditions for the $P$-matrix:

$$ \sum_{j,\beta} P_{ij}^{\alpha\beta}(E, \mathcal{H}) = N_i^{\alpha}(E) \quad (2.32) $$

$$ \sum_{i,\alpha} P_{ij}^{\alpha\beta}(E, \mathcal{H}) = N_j^{\beta}(E), \quad (2.33) $$

where $N_i^{\alpha}(E)$ is the number of open channels at the energy $E$ in lead $i$. Furthermore, time-reversal symmetry of the $s$-matrix implies that

$$ P_{ij}^{\alpha\beta}(E, \mathcal{H}) = P_{ji}^{\beta\alpha}(E, \mathcal{H}) \quad (2.34) $$

and finally, in the presence of particle-hole symmetry,

$$ P_{ij}^{\alpha\beta}(E, \mathcal{H}) = P_{ij}^{-\alpha-\beta}(-E, \mathcal{H}). \quad (2.35) $$

In what follows, the main focus will be on the case of two normal reservoirs. Now it is convenient to define the normal and Andreev transmission and reflection probabilities from lead 1 as $T_0(E) \equiv P_{21}^{++}(E, \mathcal{H})$, $T_a(E) \equiv P_{21}^{-+}(E, \mathcal{H})$, $R_0(E) \equiv P_{11}^{++}(E, \mathcal{H})$ and $R_a(E) \equiv P_{11}^{-+}(E, \mathcal{H})$ and the corresponding quantities from lead 2 with a prime ($T'_0(E)$ etc.).

In the presence of Andreev reflection the conductance between reservoirs 1 and 2 at $T = 0$ is given by (see Appendix 6)

$$ G = \frac{\hbar}{2e^2 (v_1 - v_2)} = (T_0 + T_a) + 2 \left[ \frac{R_a R'_a - T_a T'_a}{R_a + R'_a + T_a + T'_a} \right]. \quad (A.10) $$

To simplify the treatment, the conductance has been normalized by twice the Klitzing resistance $e^2/h$.

Since Eq. (A.10) is rather complicated, it is instructive to consider simple limits. Firstly, if the system is totally left-right symmetric, i.e. the primed
probabilities equal the corresponding unprimed ones, the conductance simplifies into the form

\[ G = T_0 + R_a, \]  

(2.36)

showing how the Andreev reflection increases the current. Secondly, in the absence of Andreev scattering with \( R_a = T_a = 0 \), the conductance is given by the well-known Landauer formula

\[ G = T_0. \]  

(2.37)

### 2.3 Quasiclassical theory

An alternative formalism for describing electronic transport in NS heterostructures is the quasiclassical theory [15]. It is based on Gor'kov's Green's function theory involving equations for the particle-particle and particle-hole correlators. Since the Gor'kov equations are almost impossible to solve even in the homogenous case, one has to consider some simplifications. The quasiclassical Green's functions are introduced by integrating out all the oscillations whose wavelengths are smaller than \( \lambda_F \). In a ballistic (clean) conductor, this leads to a closed-form equation, which was first derived by Eilenberger [24]. In the dirty limit, further simplifications can be made by expanding the quasiclassical Green's function in spherical harmonics and keeping only the s- and p-wave terms. As a result, one arrives at a diffusion-like equation proposed by Usadel [25].

Since the quasiclassical approach does not consider single scatterings, the viewpoint is merely that of the proximity effect and the local increase in conductivity resulting from it. One remarkable result of the theory is the finding that due to the proximity effect, the local density of states in the normal material near the superconducting interface contains a pseudogap with magnitude of the order of the Thouless energy [8].

The advantage of the quasiclassical theory as compared to the scattering approach is twofold. First of all, it is capable of producing analytical formulae for the physical quantities at different limits and hence sometimes a better physical insight on the problem is obtained. Secondly, it does not rely on
the microscopic description of the structure\(^6\) and hence it can be applied to much larger structures than the calculations based on the scattering theory.

However, the quasiclassical theory contains a few handicaps not present in the scattering approach. Since the quasi-classical theory averages out the different disorder realisations, it cannot describe conductance fluctuations. Furthermore, the so-called weak-localisation (WL) effects are ignored.\(^7\) And finally, the quasiclassical theory is less versatile in describing different geometries of the scattering area as compared to the scattering theory. Thus, a fair description of the transport properties of NS heterostructures can only be obtained by combining these two approaches.

### 2.4 Thouless energy

In general, mesoscopic structures are characterized by the small system size and low electron energies (low bias and/or low temperature). In these kinds of systems, changes in the boundary conditions have a significant effect on such system properties as conductance. A characteristic energy displaying this sensitivity to boundary conditions is the Thouless energy \(E_T\), usually defined in diffusive materials as the inverse diffusion time through the structure,

\[
E_T = \frac{\hbar D}{L^2}.
\]  

(2.38)

Here \(D\) is the diffusion constant and \(L\) the linear size of the system. (See Ref. [26] for alternate definitions of this quantity and extensions to ballistic structures.)

One example of the appearance of the Thouless energy is the proximity effect. When the penetration depth of the pairing amplitude, \(\sqrt{\frac{\hbar D}{E}}\) is of the size of the normal structure \(L_N\), the corresponding energy scale is exactly the Thouless energy. This can be seen, for example, in Andreev

\(^6\)Remember that at least in disordered structures, the scattering theory is based on the microscopic Hamiltonian, for example the tight-binding Hamiltonian.

\(^7\)WL arises in phase-coherent structures from an increase in the probability for a particle to backscatter into its time-reversed trajectory.
interferometers, where the conductance oscillations obtain a maximum for energies of the order of the Thouless energy.
Chapter 3

Numerical scattering method

In this chapter the numerical method for calculating the $s$-matrix elements is presented. The method is based on evaluating the Green’s function of the scattering area and relating it through the Dyson equation to the Green’s function of the total structure. When the total Green’s function is obtained, it is straightforward to calculate the $s$-matrix by the Fisher-Lee relation [27] generalised to structures involving Andreev scattering.

The chapter introduces the so-called decimation method for the computation of the Green’s function. It is basically an efficient Gaussian elimination algorithm, which also has a nice physical interpretation in terms of the quasiparticle paths. The second part of the chapter includes a brief introduction to the transfer matrix technique, which is an alternative numerical method for solving the $s$-matrix, and a few comments on the validity of the model for numerical calculations.

3.1 Scattering matrix and surface Green’s functions

The relation between the $s$-matrix elements and the Green’s function describing the structure is given by the generalised Fisher-Lee relation (c.f., Appendix 6)

\[
s_{(j,b),(i,a)}^{\beta\alpha} = -\delta_{(j,b),(i,a)}^{\beta\alpha} + i\hbar \sqrt{v_b^\alpha v_a^\beta} \langle b,\beta, j | \mathcal{G}_j^+ | a,\alpha, i \rangle ,
\]

(B.21)
where $G^+_{ji}$ is the retarded Green’s function describing coupling between the leads $i$ and $j$ and $|a, \alpha, i\rangle$ is the $a$-type transverse quasiparticle mode $a$ in the lead $i$. From hereon we consider only the retarded Green’s function and thus drop the superscript $+$. Typically $G_{ji}$ is chosen to couple the sites nearest to the scattering region (see Fig. 3.1). This is why it is frequently called the “surface Green’s function”. Choosing some other site further inside the leads would yield only an unimportant phase factor.

![Figure 3.1: Surface Green’s function $G_{ji}(y_j, y_i)$ in two-dimensional tight-binding lattice coupling surface slices of leads $j$ and $i$.](image)

Numerical solution of the Green’s function involves typically an inversion of the matrix $EI - \mathcal{H}$. Since the leads are assumed semi-infinite, this matrix is infinite dimensional and hence has to be truncated in some way. To do this, let us first partition the Hamiltonian into parts describing the leads and the scattering region. From now on we concentrate on the case of two normal leads of an equal cross section, but the generalisation to multi-probe systems is rather obvious. The Hamiltonian is of the form

$$
\mathcal{H} = \begin{pmatrix}
\mathcal{H}_{LL} & \tau^\dagger_{SL} & 0 \\
\tau_{SL} & \mathcal{H}_S & \tau_{SR} \\
0 & \tau^\dagger_{SR} & \mathcal{H}_{RL}
\end{pmatrix},
$$

where $\tau_{CD}$ ($D \in \{R, L\}$) describes coupling between the scattering region and the leads and no coupling between the leads is assumed. In the tight-binding model, the matrix $\tau_{CD}$ contains only the coupling terms between the sites of the surfaces of the scattering area and the lead $D$. Let us now
define a lead Hamiltonian $H_L$ to consist of the parts $H_{LL}$ and $H_{RL}$ and the Hamiltonian of the scattering region, $H_S \equiv H - H_L$. Between these it is straightforward to find the Dyson equation relating the total Green’s function $G$ to the lead Green’s function $G_L$

$$G_L \equiv (EI - H_L)^{-1} = \begin{pmatrix} (EI - H_{LL})^{-1} & 0 \\ 0 & (EI - H_{RL})^{-1} \end{pmatrix}$$

(3.2)

and the scattering Hamiltonian $H_S$:

$$G = (I - GLH_S)^{-1} G_L.$$  

(3.3)

### 3.2 Decimation method

The Green’s function $G_L$ for the leads can be calculated analytically (see Appendix 6) to yield

$$G_L = \begin{pmatrix} G_{LL}^{+1} & 0 & 0 & 0 \\ 0 & G_{RL}^{+1} & 0 & 0 \\ 0 & 0 & G_{LL}^{-1} & 0 \\ 0 & 0 & 0 & G_{RL}^{-1} \end{pmatrix},$$

(C.26)

with

$$G_{DL}^{\alpha} = \frac{1}{\gamma} \sum_{a} \chi_{D,a}^{\alpha}(\rho) e^{i\kappa_{D,a}^{\alpha}} \chi_{D,a}^{\alpha}(\rho').$$

(C.27)

but in the presence of disorder or a complicated geometry of the scattering region, the inversion of the matrix $EI - G_LH_S$ must be carried out numerically. The order of the matrix $H_S$ is $2(M^{d-1}L) \times 2(M^{d-1}L)$, where $M$ and $L$ are the numbers of sites in transverse and longitudinal direction, respectively, and $d - 1$ is the transverse dimension of the structure. This is, in general, quite large and the matrix inversion as such would take too much CPU time. Therefore, we have to remove some information irrelevant to us from the Hamiltonian $H_S$. One way to do this is to use the so called decimation method. It starts from the $N \times N$ matrix Schrödinger eigenvalue equation

$$\sum_{j=1}^{N} H_{ij}\phi_j = E\phi_i, \ i = 1, \ldots, N.$$  

(3.4)
If $\phi_1$ does not belong to the boundary sites of the scattering area, the
information in it is not relevant to the transport properties between the
leads. Therefore, let us separate it from the Eq. (3.4):

$$\sum_{j=1}^{N} \mathcal{H}_{ij} \phi_j = \sum_{j=2}^{N} \mathcal{H}_{ij} + \mathcal{H}_{11} \phi_1 = E \phi_i.$$  \hfill (3.5)

From this equation with $i = 1$ we can calculate $\phi_1$:

$$\phi_1 = \sum_{j=2}^{N} \frac{\mathcal{H}_{1j}}{E - \mathcal{H}_{11}}.$$  \hfill (3.6)

Substituting this to Eq. (3.4) and “forgetting” the equation with $i = 1$ we
get

$$\sum_{j=2}^{N} \mathcal{H}_{ij}^{[1]} \phi_j = E \phi_i, \ i = 2, \ldots, N.$$  \hfill (3.7)

with

$$\mathcal{H}_{ij}^{[1]} = \mathcal{H}_{ij} + \frac{\mathcal{H}_{11} \mathcal{H}_{1j}}{E - \mathcal{H}_{11}}.$$  \hfill (3.8)

Repeating this procedure $k$ times for the site wavefunctions (“decimating
the sites”) in the scattering area excluding the boundary sites, we get reduced
equations of the form (3.7) with

$$\mathcal{H}_{ij}^{(k)} = \mathcal{H}_{ij}^{k-1} + \frac{\mathcal{H}_{kj}^{(k-1)} \mathcal{H}_{kj}^{(k-1)}}{D^{(k-1)}(E)},$$  \hfill (3.9)

where the denominator $D^{(k-1)}(E) = E - \mathcal{H}_{kk}^{(k-1)}$. The above procedure
 corresponds to substituting the information from all the paths via $k$th site
(with weight $\frac{1}{D^{(k-1)}(E)}$) to the reduced Hamiltonian (c.f., Fig. 3.2). In the
end we are left with a Hamiltonian $\mathcal{H}^{(l)}$ connecting the boundary sites of the
leads only and now by applying Eq. (3.3) with $\mathcal{H}_S = \mathcal{H}^{(l)}$, we get the desired
Green’s function.

With the decimation method it is also possible to calculate energy eigen-
values by decimating all but one site and requiring $D^{(N)}(E) = 0$. The ener-
gies satisfying this are eigenvalues of Eq. (3.4) and vice versa. Alternatively
for large systems, one can calculate the density of these eigenvalues. According to the so called “negative eigenvalue theorem”, the number of eigenvalues of $\mathcal{H}$ less than $E$ is the number of positive denominators in the sequence $D^{[1]}(E), D^{[2]}(E), \ldots, D^{[N]}(E)$. Dividing this by the number of sites $N$, one gets the density of states in the system.

When the decimation method reduces the dimension of the eigenequation (3.4), it necessarily removes some information from it. But since all the paths between different sites in the leads are “saved” into the couplings between the leads, the removed information is irrelevant for the transport properties between the leads. What is removed is rather the information about different paths between the sites inside the scattering area.

### 3.3 Form of pairing interaction

Typically the form of the pairing potential (Eq. (2.5)) is chosen extremely local: $\Delta = \Delta \delta_{ij}$ such that the interaction between the pairs in time-reversed electronic states is a nonzero constant for electrons within the same site and zero elsewhere. In a two-dimensional clean superconductor (i.e. with a constant site energy $\epsilon_i = \mu$ and a constant $\Delta_i = \Delta$) this form of $V$ yields the dispersion relation

$$E^2 = \epsilon_k^2 + |\Delta_k|^2,$$

(3.10)
where \(\epsilon_k = -2\gamma (\cos(k_x a) + \cos(k_y a)) - \mu\) is the usual tight-binding dispersion relation and

\[
\Delta_k = \Delta. \quad (3.11)
\]

Since the gap \(\Delta\) in the energy spectrum Eq. (3.10) is not \(k\)-dependent, the symmetry of this choice for \(V_{ij}\) is called the s-wave symmetry. The above described way is the easiest implementation of the s-wave pairing\(^1\). Another often considered symmetry is the d-wave symmetry, where (in 2D) \(\Delta\) depends on \(k\) in the following way:

\[
\Delta_k = \Delta(\cos(k_x a) - \cos(k_y a)), \quad (3.12)
\]

i.e. with \(k_x = \pm k_y + n2\pi, \Delta = 0\). It is assumed that this kind of a pairing could be found in such novel phenomena as high-temperature and heavy-fermion superconductivity. Simplest way to get the dispersion relation (3.12) in a two-dimensional lattice is to choose

\[
V_{ij} = \begin{cases} 
  V_i/2, & \text{when } j \text{ is the nearest neighbour of } i \text{ in x-direction} \\
  -V_i/2, & \text{when } j \text{ is the nearest neighbour of } j \text{ in y-direction} \\
  0, & \text{otherwise.}
\end{cases} \quad (3.13)
\]

Figure 3.3 illustrates the forms of \(V_{ij}\) for different pairings.

### 3.4 Transfer matrix method

An alternative method for calculating the s-matrix is given by the transfer matrix method. This method yields a transfer matrix \(T\) satisfying

\[
\begin{pmatrix} O_L \\ I_L \end{pmatrix} = T \begin{pmatrix} I_R \\ O_R \end{pmatrix}, \quad (3.14)
\]

where \(O_i\) (\(I_i\)) refer to vectors of outgoing (incoming) plane-wave amplitudes of lead \(i\), normalized to a unit flux at each mode. The s-matrix couples the

\(^1\)In general, s-wave symmetry is obtained if and only if particle-hole coupling has a spherical symmetry in the real space.
outgoing amplitudes to the incoming amplitudes and hence the corresponding representation for the \( s \)-matrix is given by

\[
\begin{pmatrix}
O_L \\
O_R
\end{pmatrix} = \begin{pmatrix}
I_L \\
I_R
\end{pmatrix}.
\] (3.15)

Once the \( T \)-matrix has been evaluated, the calculation of the corresponding \( s \)-matrix is straightforward. Namely, if one defines

\[
s = \begin{pmatrix}
r_{LL} & t_{LR} \\
t_{RL} & r_{RR}
\end{pmatrix},
\] (3.16)

then \( T \) has the form

\[
T = \begin{pmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{pmatrix} = \begin{pmatrix}
(t_{RL})^{-1} & r_{RR}(t_{LR})^{-1} \\
-(t_{LR})^{-1}r_{LL} & (t_{LR})^{-1}
\end{pmatrix}.
\] (3.17)

from which one obtains the following inverse relation:

\[
s = \begin{pmatrix}
-T_{22}^{-1}T_{21} & T_{22}^{-1} \\
(T_{11})^{-1} & T_{12}T_{22}^{-1}
\end{pmatrix}.
\] (3.18)
The $T$-matrix can be determined for example as follows. For simplicity, we consider a two-dimensional lead and local $s$-wave superconductivity. Denote the amplitude of an $\alpha$-type quasiparticle wavefunction at site $(n,i)$ of the scattering region by $a^\alpha_{n,i}$. Here $n$ $(i)$ is the index for the transverse (longitudinal) direction. Combine the amplitudes of each transverse slice $n$ into a vector $A^\alpha_n$, yielding the Schrödinger equations for the electron- and hole-like quasiparticle vectors

\[
EA^+_n = \mathcal{H}_n A^+_n - \gamma (A^+_n - A^+_n - A^+_n + A^+_n + A_{n+1}^-) + \Delta_n A^-_n \tag{3.19}
\]

\[
EA^-_n = -\mathcal{H}_n A^+_n + \gamma (A^-_n - A^-_n + A^-_n + A^-_n + A_{n+1}^-) + \Delta_n A^+_n, \tag{3.20}
\]

where $\Delta_n$ is a diagonal matrix consisting of the particle-hole couplings in slice $n$ and $\mathcal{H}_n$ is the transverse quasiparticle Hamiltonian describing couplings within the slice $n$. Rearranging one obtains the relation between the $n$'th and $(n+1)$'th vectors:

\[
\begin{pmatrix}
A^+_{n+1} \\
A^-_{n+1} \\
A^+_n \\
A^-_n
\end{pmatrix} = \begin{pmatrix}
-\frac{1}{\gamma}(E - \mathcal{H}_n) & \frac{1}{\gamma}\Delta_n & -\mathcal{I} & 0 \\
\frac{1}{\gamma}\Delta_n & \frac{1}{\gamma}(E + \mathcal{H}_n) & 0 & -\mathcal{I} \\
\mathcal{I} & 0 & 0 & 0 \\
0 & \mathcal{I} & 0 & 0
\end{pmatrix} \begin{pmatrix}
A^+_{n+1} \\
A^-_{n+1} \\
A^+_n \\
A^-_n
\end{pmatrix}
\]

\[
= \prod_{m=1}^{n} \begin{pmatrix}
-\frac{1}{\gamma}(E - \mathcal{H}_m) & \frac{1}{\gamma}\Delta_m & -\mathcal{I} & 0 \\
\frac{1}{\gamma}\Delta_m & \frac{1}{\gamma}(E + \mathcal{H}_m) & 0 & -\mathcal{I} \\
\mathcal{I} & 0 & 0 & 0 \\
0 & \mathcal{I} & 0 & 0
\end{pmatrix} \begin{pmatrix}
A^+_{n+1} \\
A^-_{n+1} \\
A^+_n \\
A^-_n
\end{pmatrix} \equiv \bar{T}_n \begin{pmatrix}
A^+_{n+1} \\
A^-_{n+1} \\
A^+_n \\
A^-_n
\end{pmatrix}.
\]

This equation describes site-to-site couplings and hence the $T$-matrix can be found by $T_n = \sum_\alpha \langle \alpha | \bar{T}_n | \alpha \rangle$.

In the $T$-matrix technique, there is no need for matrix inversions taking huge amounts of CPU time. However, the matrix to be handled is four times as large as in the corresponding decimation method. Therefore, the decimation method is usually faster than the corresponding transfer matrix method. It is also more versatile to more complicated forms of pairing potential than the local $s$-wave case.
3.5 Comments on the validity of the model

The model described above has been successfully used for analysing a variety of phenomena involved with the electronic transport in NS heterostructures. However, there are a couple of rather weakly reasoned points in the formalism. These are at least the form of the particle-hole pairing potential and the possible effects of the small structure size. These issues will here be discussed briefly.

In the traditional BCS theory the electron-electron pairing interaction is usually written in the $k$-space as follows:

$$ V_{\bar{k} \bar{k}'} = \begin{cases} V \delta(\bar{k} + \bar{k}'), & \text{for } E_F < \epsilon_{\bar{k}} < E_F + \hbar \omega_D \\ 0, & \text{otherwise.} \end{cases} (3.22) $$

Here $V$ is a constant, $\epsilon_{\bar{k}}$ is the energy of an electron whose wave vector is $\bar{k}$ and $\hbar \omega_D$ is the Debye energy. This cutoff energy for the pairing interaction has only been argued and not strictly proven. If this pairing interaction is Fourier-transformed to $\mathbf{r}$-space, one obtains the form

$$ V(\mathbf{r}, \mathbf{r}') = \frac{V k_D^2 j_0(k_D R)}{\pi^2 R}, \quad (3.23) $$

where $R = |\mathbf{r} - \mathbf{r}'|$, $j_0(x)$ is the spherical Bessel function of the zeroth order and the Debye wave number $k_D$ satisfies $\epsilon_{k_D} = E_F + \hbar \omega_D$ (for simplicity it is assumed that this energy does not depend on the direction of $k_D$). Function (3.23) resembles the sinc-function rather closely, i.e. it is peaked around $r = 0$ and its half-width is $\frac{2.5}{k_D}$. Thus, one could argue that the pairing interaction should couple all the sites within some $1/k_D$ instead of coupling only the electrons inside single sites (local s-wave pairing) or the nearest neighbour sites (nonlocal s-wave or d-wave pairing). Apparently including higher-order couplings would make the results more accurate, but here it is assumed that the corrections would be rather quantitative than qualitative (as long as the proper symmetries for the energy gap are satisfied) and the most important factor arising from superconductivity is coupling between quasiparticles and quasiholes.

Another weak point of the formalism becomes apparent when one starts to make numerical calculations. To be able to calculate disorder-averaged
quantities even with the present supercomputers, the width of the structures cannot be more than few tens of lattice sites. According to the Anderson criterion [12, 28], superconductivity disappears when the level spacing \( d \) exceeds the superconducting energy gap \( \Delta \) (see Chapter 1). Thus, a rather large \( \Delta \) must be chosen (even \( E_F/10 \)) for the calculated structures. On the other hand, in the conventional superconductors the energy gap is few thousandths of \( E_F \). In the present calculations we try to choose a compromising value between these two requirements. It is assumed that even if superconductivity does not persist as such when \( d \approx \Delta \), the pairing potential is still present and has a similar effect on the transport properties as in the slightly larger structures.

Claughton et al. [29] compared the predictions obtained by scattering approach and the quasiclassical theory. The conclusion was that even for the simplified assumptions of the scattering theory, it yields ensemble-averaged results which are in good correspondence with the quasiclassical theory.
Chapter 4

Andreev interferometers

The proximity effect has a couple of consequences on the transport properties of the normal structure in contact with a superconductor. First of all, the local conductivity near the superconducting interface is typically increased at finite energies [30]. Secondly, if the size of the normal layer is comparable to the superconducting coherence length, the proximity effect provides a significant modification in the local density of states of the normal structure, including the appearance of a pseudogap of the order of the Thouless energy $E_T$ [8].

In order to be able to study the proximity effect on the physical observables of the normal structure, one has to be able to somehow vary its strength. One tool for this is provided by the Andreev interferometers (AI), where a normal structure is coupled to two superconductors with order-parameter phases $\phi_1$ and $\phi_2$. Since in the Andreev reflection the reflected wave acquires the phase of the superconducting order parameter (c.f., Sect. 2.1), transport quantities in AIs display an oscillatory dependence on the phase difference $\Delta \phi \equiv \phi_1 - \phi_2$. It turns out that for $\Delta \phi = 0$, the proximity effect is at its strongest and for $\Delta \phi = \pi$ at weakest (for an explanation, see Fig. 4.1).\footnote{The quasiclassical theory predicts an equal conductance for the case $\Delta \phi = \pi$ as for the normal structure. This does not exactly hold, as demonstrated by the scattering approach [31], and is probably due to the one-dimensional nature of the currently available quasiclassical theory.}

Figure 4.2 shows an example of an Andreev interferometer consisting of a two-dimensional electron gas in contact with a superconducting loop.
The phase difference between the two contacts can be varied either by a supercurrent between the ends of the superconductor or by a magnetic flux through the loop.

The observed AI effects do not depend strongly on the dimensionality of the normal structure; the same qualitative behaviour of the conductance oscillations can be found in a two-dimensional electron gas [32] as well as in a three-dimensional metallic normal structures [33] having two contacts with a superconductor.
CHAPTER 4. ANDREEV INTERFEROMETERS

Figure 4.2: Layout of Andreev interferometer formed by T-shaped 2DEG in contact with interrupted superconducting Nb loop. The contacts (0) are connected to the Nb loop and (1) and (2) are connected to the T-shaped 2DEG. It is found that the conductance between the electrodes (1) and (2) oscillates as a function of the magnetic flux $\Phi$ through the loop. The right-hand panel shows a scanning electron micrograph of the device. From Ref. [18].

4.1 Experimental results

The sensitivity of the conductance $G_N$ through the normal structure on the phase difference between two superconducting contacts was theoretically predicted already in the beginning of 80s [34]. The progress in lithographic techniques, which made possible the fabrication of highly transparent NS interfaces, recreated the interest in the subject and further predictions and suggestions for the experimental devices were made in the early 90s [35-37]. First experiments were made in 1994 and today several experimental realisations of the Andreev Interferometers have been carried out. Examples of these are a superconducting fork coupled to a normal metal [38, 39], a 2DEG or a normal metal coupled to the different sides of a Josephson junction [40, 41] and a Cu loop coupled to two superconducting Al islands [42].

In many of the experiments the superconducting pieces connecting to the normal structure are separate. This property brings in a Josephson coupling
between the superconductors and to find the AI oscillations, the Josephson-effect oscillations have to be first resolved from the data [11, 42]. At low energies and for small separation of superconductors, the Josephson effect is the dominant effect and all the AI-oscillations are smeared out. But since the Josephson effect decays exponentially both with the distance and the energy, and AI oscillations only as a power law (see below and the next chapter), they can be disentangled by varying the geometry of the experiments or the bias voltage.

4.1.1 Reentrant effect

Artemenko [43] predicted that at zero energy, the conductance is not changed due to the proximity effect. However, Petrashev et al. [33] observed strong oscillations in conductance as a function of the modulating supercurrent in a sample consisting of silver in contact with superconducting aluminium. Furthermore, it was found that these oscillations were at strongest at low $T$ and decreased with increasing temperatures as an inverse power law [42].

Later experiments [11, 18, 44, 45] indicated that indeed the low-energy effect is small, but at a finite energy of the order of the Thouless energy of the normal structure, the oscillation amplitude $\delta G$ is huge, even multiple conductance quanta $e^2/h$. This reentrant behaviour (see Fig. 4.3) is typical for the proximity effect and can be observed also in systems involving only a single superconductor [46].

4.1.2 Zero-bias amplitude

On the contrary to the Artemenko’s prediction of the vanishing of the zero-energy oscillation amplitude, several experiments indicate a nonzero amplitude even at $E = 0$. However, the results seem to be contradictory: while some groups show a positive oscillation amplitude at low energies (i.e. the zero-phase conductance is larger than the $\pi$-phase conductance, see e.g. Fig. 4.3) [18], other experiments show a crossover between positive and negative amplitudes at a finite energy [11] (c.f., Fig. 4.4). The question is not yet totally settled and it is discussed more in the next chapter.
Figure 4.3: Energy dependence of resistance oscillation amplitude $\Delta R = R(\Delta \phi = \pi) - R(\Delta \phi = 0)$ for three different implementations of the device depicted in Fig. 4.2. The reentrant effect is clearly observable. The first two samples involve cryogenic filtering and, consequently, the zero-energy amplitude for them is slightly lower than for the third sample. The temperatures in the measurements were 250 mK, 170 mK and 50 mK for structures a), b) and c), respectively. From Ref. [18].

Another kind of an observation of finite low-energy oscillations has been recently made by Antonov et al. [47]. This experiment included tunnel barriers between the conductance measuring electrodes and a T-shaped normal structure in contact with two superconductors (see Fig. 4.5). The low-temperature conductance oscillations were found to be shifted by $\pi$ with respect to the oscillations in a structure without barriers, corresponding to a conductance minimum at $\Delta \phi = 0$. At larger temperatures corresponding to the Thouless energy of the T-shaped structure, the zero-phase conductance again exceeded the $\pi$-phase conductance.
Figure 4.4: Amplitude of the conductance oscillations $\Delta G \equiv G(\Delta \phi = 0) - G(\Delta \phi = \pi)$ as function of dc voltage bias, for three different temperatures. From Ref. [11].

4.1.3 Conductance fluctuations

Every mesoscopic sample with dimensions smaller than the phase-coherence length contain universal conductance fluctuations (UCF) due to their specific realization of impurities. Typically the magnitude of these fluctuations is of the order of $e^2/h$. Experimentally these fluctuations can be studied by applying a magnetic field through the disordered sample and thus effectively varying the set of impurities faced by the individual particle trajectories. The magnitude of these fluctuations - for example the rms amplitude of the conductance modulation due to the applied magnetic field - is universal for the symmetry obeyed by the structure. Since the phase difference of the superconductors is varied by an applied magnetic field, universal conductance fluctuations have an effect on the measured conductance [48], which has to be taken into account by some kind of ensemble averaging.

Moreover, the presence of superconductivity introduces new universality classes for mesoscopic systems [54] and as a result, the magnitude of
the universal conductance fluctuations of the normal structure may change depending on the presence or absence of the proximity effect (see Chapter 5).

4.2 Theoretical analysis

The theoretical explanations for the abovementioned effects utilize the languages of the two main phenomena of the NS heterostructures: namely, the proximity effect and the Andreev scattering. Some of the following explanations are oversimplified, their main object is to provide an intuitive physical picture about the situation underlying all of the phenomena. But all of the effects can be described at least qualitatively with the exact scattering approach (see Chapter 5) without further assumptions such as a nonzero pairing potential in the normal area [49] or the Coulomb interaction between the electrons.
Let us first make a closer look at the phase dependence of the conductance. Figure 4.6 shows one example of a quasiparticle trajectory (Feynman path) between the reservoirs $R_1$ and $R_2$. Consider a quasiparticle incoming from $R_1$ (solid line), diffusing through the normal structure to the superconductor $S_1$, and Andreev reflecting from it as a quasihole (dashed line). Now this quasihole follows the path of the initial quasielectron until at the impurity $I$, where it has a finite probability to scatter away from this path. This scattered hole may now diffuse to the other superconductor $S_2$, Andreev reflect as a quasiparticle and diffuse to the reservoir $R_2$. Since at the first Andreev reflection, the hole wavefunction is shifted by $-\phi_1$ (particle-to-hole) and at the second by $\phi_2$ (hole-to-particle), the final quasiparticle carries information about the phase difference $\phi_2 - \phi_1$.

### 4.2.1 Reentrant effect

The reentrant effect can be theoretically explained by both the quasiclassical theory and the scattering approach [17, 49]. The main argument for the “thermal effect” increasing the oscillations at a finite energy is the breaking of the particle-hole symmetry at finite energies. There does not yet exist a clear intuitive way of understanding the effect, but a couple of explanations based on the multiple scattering picture of Andreev reflected holes or the
proximity-effect induced pseudogap in the density of states [50] have been suggested. The approach followed here is based on the explanation by den Hartog [32].

Consider a quasiparticle Andreev reflected as a quasihole from the superconducting interface (see Fig. 4.7). In a disordered structure it is possible for the quasihole to collide with an impurity such that it reflects away from the trajectory of the incoming quasiparticle\(^2\). Now assume that this quasihole goes on to the same NS interface and Andreev reflects again to a quasielectron state. The most probable trajectory of this quasielectron is the one followed by the quasihole, i.e. back to the first Andreev reflection point. Here the particle undergoes a third Andreev reflection and returns back to the reservoir as a quasihole following the path of the first quasiparticle.

Now recall the phase change of \(-\pi/2 \pm \phi_S\) in each Andreev reflection (+ corresponding to the reflection from quasihole to quasielectron and - to the opposite case, see Sect. 2.1). Because of the different sign of \(\phi_S\) at each reflection, the “final” quasihole returning to the reservoir carries the

---

\(^2\)This should be interpreted as a beam splitting at each collision; biggest part of the quasihole beam will continue on the time-reversed path of the initial electron, but some of it will take another direction.
same information about the phase of the order parameter, irrespective of the number of reflections. But the phase shift of $-\pi/2$ occurs at each reflection, and thus the final phase of the three times reflected quasihole is $\pi$-shifted with respect to the quasihole reflected once. As a result, constructive interference is obtained for each trajectory with $n + 1$ Andreev reflections and destructive interference for $n + 3$ Andreev reflections ($n \in \mathbb{R}$).

At $E = 0$ all the orders of reflections have to be taken into account. When all the contributions from constructive and destructive interferences are summed up, the result is at most a tiny effect depending on the degree of disorder in the normal structure. But when $E > 0$, the dynamical phase of the quasiparticles and quasiholes differs and the phase information is lost with long enough trajectories. A fair choice for the critical length is the penetration depth $\xi_T$ of the proximity effect. These trajectories can contain only a finite number of Andreev reflections, such that the trajectories leading to destructive interference cancel first out, hence resulting in an increased conductance. The increasing of the conductance continues until $\xi_T$ becomes of the order of the linear size $L$ of the diffusive region, corresponding to the Thouless energy $E_T$. At this length scale only the trajectories including one Andreev reflection give a dominant contribution to the interference and the conductance obtains a maximum. For energies much larger than $E_T$, most of the phase conjugation is lost even for the trajectories containing a single Andreev reflection and conductance is only slightly increased from the corresponding normal value.

Blom et al. [51] have proposed an alternative explanation based on the suppression of oscillations at $E = 0$ because of the retroreflection property of Andreev reflection (they ignore the possible beam splitting because of impurities). However, their approach cannot explain the nonzero oscillations of sample-specific conductances at $E = 0$.

4.2.2 Zero-bias amplitude

The question about the zero-energy oscillation amplitude remains open. The phenomenological multiple scattering picture mentioned above does not provide satisfactory arguments for the total vanishing of $\delta G(0)$ and there seems
to be no symmetry enforcing this result. Furthermore, the experiments mentioned above as also numerical calculations by Leadbeater and Lambert [52] suggest a finite and even a negative $\delta G$ at zero energy.

It is clear that the zero-bias amplitude deviates much from zero in the presence of low-transparency barriers between the leads and the normal structure. Antonov et al. suggest that this is due to the energy gap in the local density of states of the normal material, induced by the proximity effect, suppressing the conductance at $\Delta \phi = 0$ [8, 47]. Note that if the normal material has a direct contact with the reservoirs, no real gap is formed. However, the numerical calculations of the next section show that this suppression of conductance is present also if only either of the contacts between the normal wire and the reservoirs contains a tunnel barrier. Another, oversimplified explanation of the suppression of the conductance can be based on the scattering picture. If the transparency of the barrier is $\Gamma$, the normal transmission probability is proportional to $\Gamma$, but the Andreev reflection, because of its two-particle nature, is proportional to $\Gamma^2$. Thus when $\Gamma \ll 1$, the Andreev reflection is suppressed and along it the conductance at $\Delta \phi = 0$.

The behaviour of the zero-energy amplitude in the absence of barriers is much more difficult to understand. One possible reason for the negative $\delta G$ could be an enhanced weak localisation correction [53] ignored by the quasiclassical theory. Nevertheless, it is possible that all the observed nonzero amplitudes are only a consequence of the universal conductance fluctuations. The next chapter shows how the ensemble-averaged $\delta G(0)$ seems to be always smaller than the rms magnitude of the UCF.

### 4.3 Detectors of magnetic flux?

Since at certain energies, the conductance through an Andreev interferometer can be tuned by a magnetic field applied through a superconducting loop, the AIs could be used as magnetometers with sensitivity comparable with that of a SQUID. However, this contains still a few problems. Firstly, usually the modification of the conductance due to the proximity effect is only a fraction of the total conductance while in the SQUIDs the modulation is typically of
the order of the conductance itself. Furthermore, if one would like to operate on Al's in temperatures close to \( T_C \), the structure size should be quite small (of the order of 100 nm).

The fabrication of conventional SQUIDs and metallic Al's require roughly the same effort. Therefore probably the most interesting difference between them are the noise properties. Since there is no Josephson coupling in the Al's, the noise behaviour is quite different between the two. However, there does not exist a qualitative comparison between the two and this remains an open issue.
Chapter 5

Results

This chapter presents results of the numerical simulations in a two-dimensional Andreev interferometer structure. Simulations probe the geometry dependence of the reentrant effect, the zero-bias amplitude, effect of the tunnel barriers and universal conductance fluctuations in the presence or absence of superconductivity.

If not stated otherwise, all the subsequent energies are expressed in terms of the tight-binding nearest neighbour coupling parameter $\gamma$, which thus can be set to unity. Similarly, all the conductances are scaled by the conductance quantum $2e^2/h$ and lengths by the lattice constant $a$. Most of the simulations consider three different kinds of conductances: the conductance at phase differences of zero and $\pi$ and the conductance of a normal structure in the absence of the superconductors. These three quantities will be denoted by $G_0$, $G_\pi$ and $G_N$, respectively.

5.1 Comments on choosing parameters

The simulated Andreev interferometer structure is depicted in Fig. 5.1. Since the required CPU time restricts the simulations in general to structures smaller than in the experiments, one has to be careful in choosing the parameters in order to find physically observable results. The following list gives a few ideas:

- The Anderson criterion for superconductivity mentioned in the Intro-
CHAPTER 5. RESULTS

Figure 5.1: Simulated Andreev interferometer structure. The superconductors are connected to the center of the diffusive normal region (gray) described by the width $W$ of the disorder distribution. The phase $\phi$ of the order parameter of the upper superconductor is varied keeping the same absolute values of $\Delta$. The transparency of the tunnel barriers is $\Gamma$ and the notation for the different lengths is indicated in the figure.

duction and Sect. 3.5 gives a lower bound for the pairing potential $\Delta$. Namely, the energy-level spacing $d$ in the superconductors has to be smaller than $\Delta$ for the superconductivity to persist. The difference between the lowest-lying states is

$$\epsilon_2 - \epsilon_1 \approx \min\left( \left| (2\pi)^2 \left( \frac{1}{L^2} - \frac{1}{(M')^2} \right) \right|, 3(2\pi)^2 \left/ \left( \max(L, M') \right)^2 \right. \right).$$

(5.1)

However, a typical value for $\Delta$ in conventional superconductors is of the order of $E_F/1000$. Hence it should be chosen as low as possible, but still fulfilling (5.1).

- The penetration depth of the quasiparticle states with $E < \Delta$ vanishing exponentially into a superconductor is proportional to $1/(\Delta - E)$. Hence, to avoid scattering from the boundary of the superconductor by these evanescent states, the dimensions of the superconductors should
not be chosen lower than $1/\Delta$.

- In diffusive conductors, the conductance of the normal structure $G_N$ scales as $G_N \propto M/N$. This property can be used to determine a correct width $W$ of the disorder distribution (see Sect. 2.1). The diffusion constant can then be calculated from $D = G_N/\nu(0)$, where $\nu(0)$ is the density of states at $E = 0$.

- Tunnel barriers can be simulated by locally increasing the site energies $\epsilon_i$. Their transmittivity $\Gamma$ can be defined as the ratio of the conductance of a ballistic structure in the presence of the barrier and the corresponding conductance in the absence of the barrier.

- The Fermi energy $E_F$ of a $d$-dimensional tight-binding model is $E_F \equiv 2d\gamma - \epsilon$, where $\epsilon$ is the average of the site energies. To avoid the van Hove singularity at $E = 0$, we choose $\epsilon = 0.2$.

- For simplicity, we have chosen fixed-end boundary conditions (corresponding to “hard walls”) in the transverse direction.

Table 5.1 summarizes the parameters chosen for the simulations. We have also checked the possible effect of increasing $\Delta$ or $M'$, but the deviations in the results have been only quantitative.

<table>
<thead>
<tr>
<th>$\Delta$</th>
<th>0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W$</td>
<td>2.0</td>
</tr>
<tr>
<td>$D$</td>
<td>$\approx 3.24$</td>
</tr>
<tr>
<td>$E_F$</td>
<td>3.8</td>
</tr>
<tr>
<td>$M'$</td>
<td>10</td>
</tr>
<tr>
<td>$L$</td>
<td>13 ... 25</td>
</tr>
<tr>
<td>$M$</td>
<td>7 ... 35</td>
</tr>
<tr>
<td>$N$</td>
<td>21 ... 75</td>
</tr>
</tbody>
</table>

**Table 5.1:** Parameters of numerical simulations. The length scales $L$, $M$ and $N$ are varied between the indicated extrema.
CHAPTER 5. RESULTS

Figure 5.2: Ensemble-averaged conductances \( G_0 \) (solid line), \( G_\pi \) (solid line with circles) and \( G_N \) (dotted line) as function of energy for structure with \( M = 15 \), \( N = 45 \) and \( L = 15 \). All the quantities are normalized by \( G_N(E = 0) \).

5.2 Reentrant effect and dependence on geometry

Figure 5.2 shows how the different conductances \( G_0 \), \( G_\pi \) and \( G_N \) behave as a function of energy. Near \( E = 0 \), superconductivity does not have a significant effect. As the energy is increased, the proximity effect increases both zero-phased and \( \pi \)-phased quantities, but since the former increases faster, oscillations as a function of \( \phi \) can be observed.

The oscillation amplitude \( \delta G \equiv (G_0 - G_\pi)/G_0 \) was calculated for 21 different geometries \( (M = 7 \ldots 33) \) and the energy dependence for a few of them is shown in Fig. 5.3. Figure 5.3a contains amplitudes for the case \( L = M \) and Fig. 5.3b for a constant \( L = 15 \). The length \( N \) of the diffusive area was chosen three times its width \( M \) to keep the normal-state conductance constant.

Reentrant behaviour can clearly be observed (since we are mainly interested in the amplitude maxima, only the low-energy part is plotted), and the maximum amplitude is obtained with energies within \( (1.5 \ldots 2.5)E_T \). Furthermore, when \( L \) scales with \( M \), the amplitude does not much depend on the geometry and especially no decreasing in the maximum amplitude can
be observed. Thus, it can be argued that the maximum amplitude depends only on the ratio $L/M$, not on the individual lengths.

![Graph a)](image1)

![Graph b)](image2)

**Figure 5.3**: Oscillation amplitude $\delta G = (G_\text{sol} - G_\text{NL})/G_\text{sol}$ for structures with a) $L = M$ and b) $L = 15$ (no tunnel barriers). The curves are drawn for $M = 13$ (solid line), $M = 15$ (solid line with circles), $M = 19$ (solid line with squares) and $M = 25$ (solid line with triangles). One can observe that the maximum amplitude is obtained roughly at $E \approx (1.5 \ldots 2.5)E_T$ and the maximum at a) does not depend on $M$ and at b) decreases with an increasing $M$. The conductances are ensemble averaged over 500 disorder realizations.

If the width $L$ of the superconductors is kept constant (Fig. 5.3b), the maximum amplitude decreases as the distance between the superconductors is increased. To find out the pace of diminution, we calculated the oscillation amplitudes for different $M$’s between 7 and 33 keeping the width $L$ constant. The amplitude maxima $\delta G_{\text{max}}$ are plotted in Fig. 5.4. An algebraic curve with $\delta G_{\text{max}} = 0.9M^{-0.65}$ fits fairly well to the points.

The decreasing amplitude can be understood by a simple geometrical argument. The increase in conductance due to the strong proximity effect mainly results from the probability for Andreev reflection (consider the usual approximation $G_\text{NL} \approx G_N$). When a quasiparticle enters the scattering region, its normal transmission probability can as a first approximation be consid-
Figure 5.4: Amplitude maxima for $M \in 7 \ldots 33$ (constant $L$) and algebraic curve $\delta G_{\text{max}} = 0.9 M^{-0.05}$ fitted to them.

... considered independent of the presence or absence of the superconductors. But the ratio between the normal and Andreev reflection probabilities depends on the ratio between the lengths of the normal and superconducting boundaries of the scattering region. Thus, when $L$ is fixed but $M$ is increased, the proportion of normal reflection increases and as a result, the conductance decreases. Since in reality also the transmission probabilities change under the proximity effect, the exponent is not strictly $-1$.

5.3 Averaged zero-energy amplitude

Let us next take a look at the oscillation amplitude $\delta G$ at $E = 0$. Some of the curves of Figs. 5.3 show a nonzero $\delta G(0)$. However, for every simulated structure $\delta G(0)$ was much smaller than the universal conductance fluctuations and the results differed by many orders of magnitude for two distinct sets of disorder realisations within the same geometry.

Still, one peculiarity in the different simulated geometries can be observed. Namely, it seems that the sign of $\delta G(0)$ depends only on the simulated geometry, not on the specific (large enough) set of impurity configur...
tions. We studied the cases $M=33$ (3 distinct simulations with 500, 2000 and 2000 realisations), 37 and 41 (1 simulation with 500 realisations for each). If the ensemble-averaged $\delta G(0)$ would be zero, one would expect at least one of the quantities be negative. Yet, each simulation produced a positive amplitude of the order of 0.01.

In conclusion, our results indicate that in the absence of tunnel barriers, the zero-energy oscillations in ensemble-averaged conductance either vanish totally or have only a tiny geometry-dependent amplitude. Moreover, this tiny amplitude would be very difficult to distinguish from the universal conductance fluctuations.

**Figure 5.5:** Ensemble-averaged conductances of structures with tunnel barriers between the diffusive region and a) both leads b) left lead: $G_0$ (solid line), $G_n$ (dashed line) and $G_N$ (solid line with circles). All the conductances are normalised by $G_N(E = 0)$. The parameters for the simulations were $\Gamma = 0.1$, $M = 35$, $L = 15$, $N = 65$. The quantities were averaged over 50 disorder realisations.
5.4 Effect of tunnel barriers

Tunnel barriers placed between the scattering region and the leads considerably change the effect of superconductors on the ensemble-averaged conductances. Figure 5.5a shows the behaviour of $G_0$, $G_\pi$ and $G_N$ for the structure with tunnel barriers of transmittivity $\Gamma = 0.1$ between the diffusive region and both leads, and Fig. 5.5b for the structure with only a single tunnel barrier between the left lead and the diffusive region.

In both cases one can clearly observe the suppression of $G_0$ at energies lower than $E_T$. Moreover, Fig. 5.5b indicates that the suppression cannot be explained only in terms of the proximity-induced minigap, since no real gap can appear when the other lead is in good contact with the scattering region.

![Graph](image)

**Figure 5.6:** Normalized oscillation amplitude $\delta G \equiv (G_0 - G_\pi)/G_N$ of structure with tunnel barrier between diffusive region and both (solid line) leads or only left lead (dashed line).

No big qualitative differences exist between the two cases: the behaviour of the oscillation amplitude normalized to $G_N$ (Fig. 5.6) shows that the effect is only a little more pronounced when both leads are separated from the scattering region by the barriers. Furthermore, in the simulated structure at low energies the two-barrier $G_\pi$ increases faster with energy than $G_0$,
resulting in the tiny dip downwards in the amplitude curve. However, this may only be a consequence of the specific geometry and low number of disorder realisations.

\section*{5.5 Conductance fluctuations}

The emergence of universal conductance fluctuations dependent on the particular configuration of impurities is typical for mesoscopic conductors. The magnitude of these fluctuations (usually measured by the standard deviation of an ensemble of conductances) is not dependent on the details of the structure, only the symmetry obeyed by the structure is relevant - hence the name “universal”. Superconductivity can change this symmetry: Altland and Zirnbauer [54] predicted that in the presence of a magnetic field the rms conductance fluctuations of an NS contact would increase by a factor of \(2\sqrt{2}\).
with respect to the corresponding normal case (where the superconductor is driven normal by a magnetic field exceeding its critical field).

Figure 5.7 shows the calculated rms amplitude of conductance fluctuations in an Andreev interferometer in the absence (a) or presence (b) of tunnel barriers. In this case the observation is opposite to the prediction by Altland and Zimbauer: the magnitude of fluctuations of the superconducting case falls below the corresponding normal case! Furthermore, the magnitude of the fluctuations does not depend on the phase difference between the superconducting order parameters.

The ratio $\text{rms}(G_N)/\text{rms}(G_S)$ between the mean magnitudes of fluctuations distinctly exceeds one and is in the absence of tunnel barriers 1.3 and in their presence 1.4. However, because of the small number of disorder realisations in the case of the tunnel barriers, these values are within each others error bars.
Chapter 6

Discussion

[Gathering the results, a glance at the future]
Derivation of the conductance formulae

In this appendix, the Landauer conductance formula is generalized to include the presence of Andreev scattering. The derivation utilizes the \( P \)-matrices and the Landauer-Büttiker formalism defined in Sect. 2.2. The treatment mainly follows the one used in Ref. [9].

A remarkable property of the superconducting quasiparticle picture is the possibility for a quasiparticle to be converted to a quasihole (or vice versa) in a scattering process. To ensure charge conservation, it will be shown that the chemical potential \( \mu \) for the superconductors must be chosen self-consistently. This leads to considerable modifications in the conductance formula.

The derivation begins by the observation that the current\(^1\) in lead \( i \) is composed of two parts: the particles arriving from the other reservoirs \( j \neq i \)

\[
I_{i,1} = e \frac{2}{h} \sum_{\alpha \beta} \alpha \int_0^\infty dE \sum_j P_{ij}^{\alpha \beta}(E,H) \eta_j^\beta(E)
\]

(A.1)

plus the particles coming from the reservoir \( i \) and possibly reflecting back to the lead \( i \):

\[
I_{i,2} = -e \frac{2}{h} \sum_{\alpha \beta} \alpha \int_0^\infty dE \left[ (N_i^\beta(E) \delta_{\alpha \beta} - P_{ii}^{\alpha \beta}(E,H)) \eta_i^\beta(E) \right],
\]

(A.2)

\(^1\)The direction of the current is here defined towards the scattering area, which corresponds to the electron flux towards reservoir \( i \).
where \( f_i \) is the distribution of incoming \( \alpha \)-type quasiparticles, defined in the List of symbols (p. v). The factor \( 2/\hbar \) arises from the products of the group velocities \( v_n(E) \) and densities of states \( \nu_n(E) \) for different modes in the quasi-1D lead \( i \).

The electrical potentials for the reservoirs corresponding to their chemical potentials are simply given by \( e\nu_i = \mu_i \). Since a finite voltage difference between two superconductors induces a time-dependent Josephson current, the voltages in the superconductors are chosen to have a constant value \( \mu \), i.e. \( e\nu_j = \mu \) for \( j = L + 1, \ldots, L_S \). Moreover, since we are not considering thermal effects on transport, we assume a constant temperature \( T \) in each reservoir.

Expanding the sum of terms (A.1) and (A.2) to the first order in \( v_j - v \), we obtain the linear-response formula

\[
I_i = \frac{2e^2}{h} \sum_{j=1}^{L} a_{ij}(v_j - v),
\]

where

\[
a_{ij} = \int_{-\infty}^{\infty} dE \left( - \frac{\partial f}{\partial E} \right) \left[ P_{ij}^{-+}(E; \mathcal{H}) + N_i^0(E)\delta_{ij} - P_{ij}^{++}(E; \mathcal{H}) \right].
\]

Here \( f(E) \) is the Fermi function and the particle-hole symmetry relation Eq. (2.35) has been used. Note that in the absence of Andreev scattering,

\[
\sum_{j=1}^{L} a_{ij} = 0,
\]

and the contribution of \( v \) in the equation for the current vanishes. Otherwise, \( v \) acts as a Lagrange multiplier guaranteeing the conservation of total charge even in the presence of Andreev scattering.

At finite voltages, the differential conductance between reservoirs \( i \) and \( j \) is given by

\[
\frac{\partial I_i}{\partial v_j} = \frac{2e^2}{\hbar} a_{ij},
\]
where at a finite temperature,

\[ a_{ij} = \sum_{\alpha} \alpha \int_{0}^{\infty} dE \left\{ N_{i}^{\alpha}(E) \left[ -\alpha \frac{\partial f_{i}^{\alpha}(E)}{\partial E} \right] \delta_{ij} - \sum_{\beta} P_{ij}^{\alpha\beta}(E, \mathcal{H}) \left[ -\beta \frac{\partial f_{j}^{\beta}(E)}{\partial E} \right] \right\} \]

(A.7)

and for \( T = 0 \),

\[ a_{ij} = \left[ P_{ij}^{-+}(E_{j}, \mathcal{H}) + N_{i}^{+}(E_{i})\delta_{ij} - P_{ij}^{++}(E_{j}, \mathcal{H}) \right], \quad (A.8) \]

with \( E_{i} = ev_{i} - \mu \).

As an example, we consider the case with two normal leads and no superconducting leads at zero temperature. Now the linear-response formula may be written as

\[
\begin{pmatrix}
I_{1} \\
I_{2}
\end{pmatrix}
= \frac{2e^{2}}{\hbar} \begin{pmatrix}
N_{1}^{0} - P_{11}^{++} + P_{11}^{-+} & -P_{12}^{++} + P_{12}^{-+} \\
-P_{21}^{++} + P_{21}^{-+} & N_{2}^{0} - P_{22}^{++} + P_{22}^{-+}
\end{pmatrix}
\begin{pmatrix}
v_{1} - v \\
v_{2} - v
\end{pmatrix}. \quad (A.9)
\]

Here all the coefficients are calculated at zero energy. In order to ensure charge conservation, the value of \( v \) is chosen from the requirement \( I_{1} = -I_{2} \). Using this and the definitions for the normal and Andreev transmission probabilities, we obtain the linear-response conductance

\[
G = \frac{\hbar}{2e^{2} (v_{1} - v_{2})} \left( T_{0} + T_{a} \right) + 2 \left[ \frac{R_{a}R_{a}' - T_{a}T_{a}'}{R_{a} + R_{a}' + T_{a} + T_{a}'} \right]. \quad (A.10)
\]

In this thesis, the two-terminal differential conductance is also considered at finite bias voltages. In this case one could in principle use Eq. (A.6), but then the self-consistency required for the conservation of charge would be difficult to maintain. Hence, if the voltages under consideration are small compared to the Fermi energy, we may assume that the form of the conductance formula Eq. (A.10) stays unchanged, only the probabilities change with energy.

The different conductance formulae are considered in detail in Refs. [9, 21]. Furthermore, thermoelectric effects induced by varying temperature are considered in Ref. [31]. One example of the effect of superconductivity on the thermoelectric properties of materials is the breakdown of the Wiedemann - Franz law in the presence of Andreev scattering.
Generalised Fisher-Lee relation

In this appendix we define the relation between the $s$-matrix and the Green's function corresponding to the Bogoliubov-de Gennes equation, satisfying

$$(E - \mathcal{H}(\mathbf{r}) \pm i\eta) \mathcal{G}^\pm = \delta(\mathbf{r} - \mathbf{r}').$$  

(B.11)

Here the infinitesimal imaginary term $i\eta$ is used to choose the correct initial condition: the retarded Green's function (plus-sign in Eq. (B.11)) corresponds to the response of a delta-like excitation, while the advance Green's function (minus-sign) corresponds to a source wave with a delta-like response. Moreover, for simplicity the Hamiltonian $\mathcal{H}(\mathbf{r})$ is chosen local; a nonlocal potential would only correspond to one additional integration.

The derivation is made in the nearly free electron approximation, where the Bogoliubov-de Gennes Hamiltonian can be written as

$$\mathcal{H}(\mathbf{r}) = \begin{pmatrix}
-\frac{\hbar^2}{2m} \left( \nabla - \frac{ieA(\mathbf{r})}{\hbar c} \right)^2 - E_F + U(\mathbf{r}) & \Delta(\mathbf{r}) \\
\Delta(\mathbf{r})^* & -\frac{\hbar^2}{2m} \left( \nabla - \frac{ieA(\mathbf{r})}{\hbar c} \right)^2 + E_F - U(\mathbf{r})
\end{pmatrix}.$$  

(B.12)

The $s$-matrix elements describe the correlation between amplitudes of different $\alpha$-type transverse modes $a$ in leads $i$. Ideal leads external to the scattering region can be described by the kinetic Hamiltonian $h(\mathbf{r})$ obtained from (B.12) by setting $\Delta(\mathbf{r}) = 0$, $A(\mathbf{r}) = 0$ and from $U(\mathbf{r})$ retaining only the part describing the transverse boundaries of the leads. The eigenfunctions of $h(\mathbf{r})$ corresponding to a unit quasiparticle flux of type $\alpha$ at energy $E$, incident along channel $a$ of lead $i$ are plane waves of type (2.29). These eigenfunctions form a basis for the Hilbert space of quasiparticle states in
the leads and, thus, any quasiparticle state in the leads can be expressed in terms of these functions.

Consider first an ideal translationally invariant wire consisting of two semi-infinite leads $i$ and $j$ of an equal cross section, connected at $x = x'$. Now the term $\delta(r - r')$ of Eq. (B.11) ($r = (\rho, x)$) describes a delta-type excitation at $r = r'$.\(^2\) The Green’s function $G^+_W(r, r')$ is the response to this source at the system described by $h(r)$:

$$G^+_W(r, r') = \sum_{a \in i} A^\alpha_a \phi^\alpha_{i,a}(\rho) \exp(k^\alpha_a |x - x'|) + \sum_{b \in j} B^\beta_b \phi^\beta_{j,b}(\rho) \exp(k^\beta_b |x - x'|).$$

(B.13)

Since at $r \neq r'$ $G^+_W$ is a strong solution to Eq. (B.11), only singularities it may contain are at the point of excitation. At this point its second derivative is infinite. Moreover, integrating (B.11) twice we find that its first derivative is here discontinuous by $2m/h^2$ and the function itself is continuous:

$$[G^+_W(\rho, x; \rho', x')]_{x = x'} = [G^+_W(\rho, x; \rho', x')]_{x = x'} - \frac{2m}{h^2} \delta(\rho - \rho').$$

(B.14)

Substituting Eq. (B.13) into Eq. (B.15) we obtain

$$\sum_{a \in i} A^\alpha_a \phi^\alpha_{i,a} = \sum_{b \in j} B^\beta_b \phi^\beta_{j,b}$$

(B.16)

$$\sum_{a \in i} ik^\alpha_a A^\alpha_a \phi^\alpha_{i,a} + \sum_{b \in j} ik^\beta_b B^\beta_b \phi^\beta_{j,b} = \frac{2m}{h^2} \delta(\rho - \rho').$$

(B.17)

Multiplying by $(\phi^\beta_{j,b})^\dagger(\rho)$, integrating over $\rho$, denoting the corresponding transverse modes at leads $i$ and $j$ with the same letters and using the or-

\(^2\)Note that the junction between the leads can always be chosen such that its $x$-coordinate coincides with the point of excitation.
thogonality of $\{\phi_{\alpha a}^\alpha\}$ we find

$$A_a^\alpha = B_a^\alpha \text{ and } ik_a^\alpha [A_a^\alpha + B_a^\alpha] = \frac{2m}{\hbar^2} v_a^\alpha \phi_{i,a}^\alpha (\rho').$$

Here the term $v_a^\alpha = \hbar k_a^\alpha / m$ arises from the normalization of the transverse wavefunctions. Hence, the amplitudes are

$$A_a^\alpha = B_a^\alpha = -\frac{i}{\hbar} \phi_{i,a}^\alpha (\rho'). \quad (B.18)$$

The Green’s function for an ideal normal-metal wire could now be obtained by substituting Eq. (B.18) into Eq. (B.13). At this point we transform the system adiabatically to a multi-probe structure containing the scattering region between the leads. Far away from this region the excitations can still be expressed in terms of the transverse quasiparticle modes. Consider now a delta-type excitation at point $\rho' = (\rho', x')$ in lead $i$. The limiting form of the retarded Green’s function in lead $j$ long way off from the scattering region can now be expressed as

$$G^{\dagger}_{ji}(\rho; \rho') = \sum_{\alpha} \sum_{\substack{a \in i \\beta \in j}} \left[ \delta_{\alpha\beta} \phi_{\alpha a}^a (\rho') \phi_{\beta b}^b (\rho) \right] . \quad (B.19)$$

Here we have chosen both $x$ and $x'$ in the leads $j$ and $i$, respectively, far away from the scattering region. The $x$-dependent exponential term would only yield an unimportant phase factor, which cancels out from the observables.

Recalling the form for $A_a^\alpha$ (Eq. (B.18)), we get the limiting retarded Green’s function in lead $j$:

$$G^{\dagger}_{ji}(\rho; \rho') = \sum_{\alpha} \sum_{\substack{a \in i \\beta \in j \\beta \in j \\beta \in j}} \left[ \delta_{\alpha\beta} \phi_{\alpha a}^a (\rho') \phi_{\beta b}^b (\rho) \right] . \quad (B.20)$$

To simplify notation, we denote the $\alpha$-type transverse state $a$ of lead $i$ by

$$| a, \alpha, i \rangle = \left( \begin{array}{c} 1 \\ \phi_{\alpha a}^a (\rho) \end{array} \right) .$$
To find the individual $s$-matrix elements, we multiply Eq. (B.20) by $\phi_{i,a}^{\alpha}(\rho')\phi_{j,b}^{\beta}(\rho)$ and integrate over $\rho$ and $\rho'$. Recalling the normalization and orthogonality of the eigenfunctions $\phi_{i,a}^{\alpha}$, we arrive at the equation

$$
\delta_{\beta a}^{\alpha} = -\delta_{j,b}^{\beta} \langle i,a | \mathcal{G}_{ji}^+ | a,\alpha, i \rangle.
$$

Equation (B.21) is the generalisation of the Fisher - Lee formula [27] for systems involving Andreev scattering. Alternative derivations for it can be found in Refs. [55, 56].
Derivation of lead Green’s functions

To derive the Green’s function $G_L$ for the isolated leads (Eq. (3.2)), we start from the spectral representation of the retarded Green’s function of a system with eigenmodes $|m\rangle$ and eigenenergies $\epsilon_m$:

$$G = \sum_m \frac{|m\rangle \langle m|}{E - \epsilon_m + i\eta}. \quad (C.22)$$

Since the leads are not coupled with each other and there is no particle-hole coupling, the Green’s function falls into four parts $G_{LD}^\alpha \equiv (EI - \mathcal{H}_{DL}^\alpha)^{-1}$ describing the behaviour of different quasiparticles $\alpha \in \{+1, -1\}$ in the two isolated leads $D \in \{L, D\}$. The eigenfunctions of the isolated lead in the nearly free electron approximation are given by

$$|a, \alpha\rangle = \begin{pmatrix} \delta_{\alpha,+1} \\ \delta_{\alpha,-1} \end{pmatrix} \sqrt{\frac{2}{L}} \chi_0^a(\rho) \sin(\kappa x),$$

where $x = 0$ is chosen to be the boundary of the lead. Because the lead is infinite in the $x$-direction, $\kappa$ is continuous and the sum over $\kappa$’s can be changed into an integral according to the rule $\sum_\kappa \rightarrow \frac{L}{\pi} \int d\kappa$. Moreover, since we are now interested only in the sites near $x \approx 0$, we may set $x = x' \approx 0$. Thus substituting to Eq. (C.22) and recalling the dispersion relation yields

$$G_{LL}^\alpha = \frac{1}{2\pi} \sum_a \chi_0^a(\rho) \chi_m(\rho') \int_0^\infty \frac{\sin^2(\kappa x)}{E - \epsilon_a^L - \frac{\hbar^2 k^2}{2m} + i\eta} d\kappa. \quad (C.24)$$
CHAPTER 6. DISCUSSION

Noting that \( \sin^2(\kappa x) = \frac{1}{4}(2 - e^{i2\kappa x} - e^{-i2\kappa x}) \) and applying the calculus of residues we finally obtain

\[
\mathcal{G}^0_{LL} = - \sum_a \frac{2 \sin(k_a^0 x)}{hv_a^0} \chi_a^0(\rho) e^{i k_a^0 x} \chi_a^0(\rho'),
\]

(C.25)

where \( k_a^0 = \frac{1}{\hbar} \sqrt{2m(E - \varepsilon_a^0)} \) and \( v_a^0 = \frac{\hbar k_a^0}{m} \). To obtain the corresponding Green’s function in the tight-binding model, we may change the group velocity accordingly (see List of symbols). Thus the total retarded Green’s function \( \mathcal{G}_L \) for the isolated leads \( L \) and \( R \) in the tight-binding model at the surface slide \( x = a \) is

\[
\mathcal{G}_L = \begin{pmatrix}
\mathcal{G}_{LL}^+ & 0 & 0 & 0 \\
0 & \mathcal{G}_{RL}^+ & 0 & 0 \\
0 & 0 & \mathcal{G}_{LL}^- & 0 \\
0 & 0 & 0 & \mathcal{G}_{RL}^-
\end{pmatrix},
\]

(C.26)

where the individual elements are given by

\[
\mathcal{G}_{DL}^0 = \frac{1}{\gamma} \sum_a \chi_{D,a}(\rho) e^{i k_a^D \cdot x} \chi_{D,a}^0(\rho').
\]

(C.27)
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