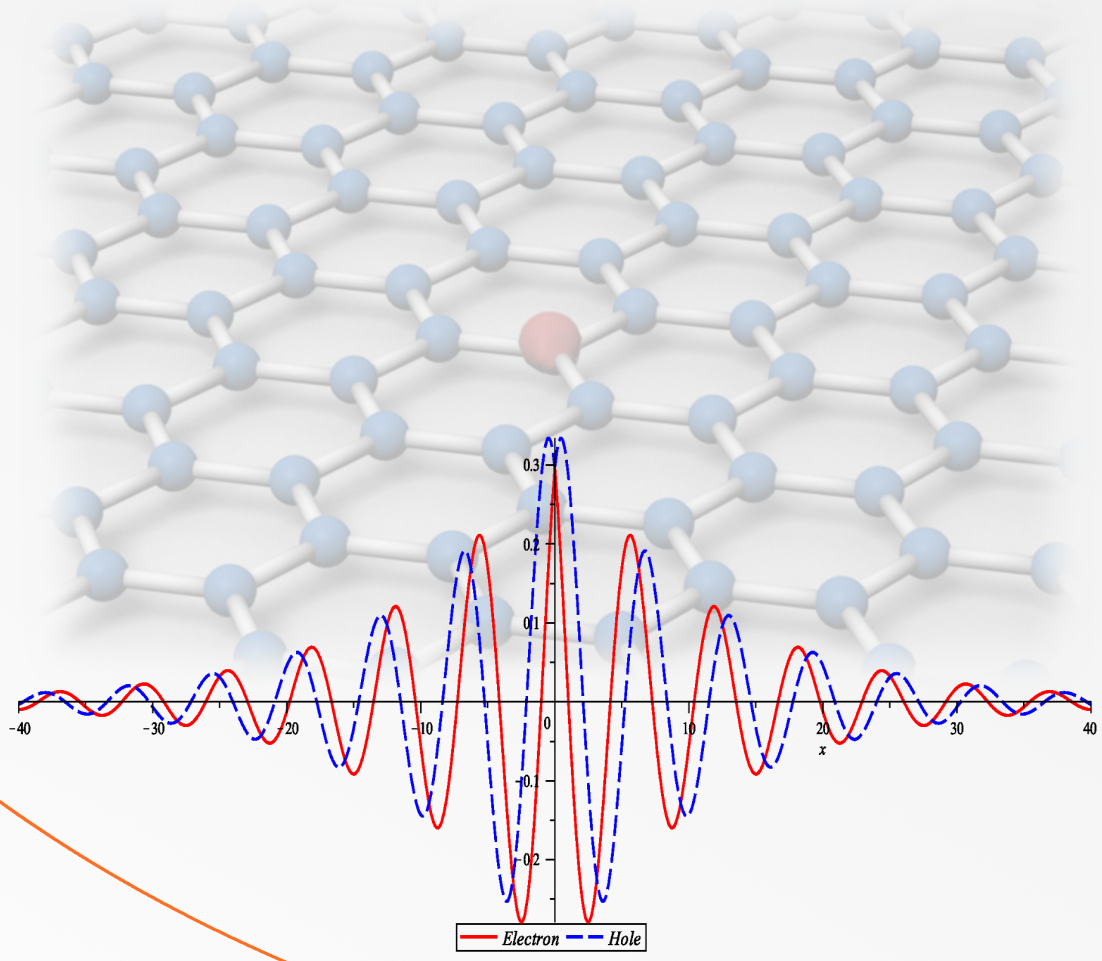
Impurity states in conventional s-wave superconductors and transport in SIS-junctions

Jan Scholtyssek
Supervisor: Jens Paaske



Niels Bohr Institute,
University of Copenhagen

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Abstract

English: After the introduction of the important tools and concepts used in many body problems, a brief introduction to the BCS-model of superconductivity will be given, including different properties of a superconductor.

The main part of this thesis is concerned with the effect of (magnetic) impurities in superconductors, where we will assume that the wave function of the superconducting system is spherical symmetric, i.e. we deal with s-wave-superconductors, and we assume that they are Type-I. The results for the impurity state energy as shown by A.I. Rusinov and P.N. Lebedev in their paper from 1969 [2] as well as the results found by other authors will be reproduced. The wave function is found and transport through a Josephson junction of zero length with superconductors with different phase of the gap parameter Δ on the right/left side is discussed.

Danish: Efter en introduktion af de vigtigste værktøjer og koncepter som bruges i flerpartikel problemer, gives en kort introduktion til BCS-teorien for superledning. I den forbindelse gennemgås nogle af superlederes egenskaber.

Størstedelen af denne rapport beskæftiger sig med effekten af (magnetiske) urenheder i superledere. Vi antager at bølge funktionen og de involverede potentialer er sfærisk symmetriske dvs. vi ser på "s-wave" superledere, og antager at superlederen er af type I. Resultaterne for urenheders tilstandsenergi som vist af A.I. Rusinov og P.N. Lebedev i deres artikel fra 1969 [2] samt resultater fra andre autorer vil blive reproduceret. Bølgefunktionen for disse tilstande bliver bestemt og elektrontransport gennem en Josephson junction af længde 0 diskuteres for superledere med forskellig fase på gab parameteren Δ for højre/venstre side.

Contents

Acknowledgement

I want to thank Jens Paaske for the whole process, which made this project possible and gave me a completely different look on research. Thanks for all the time and effort spend on this project and all the help given. Even when asking for help late at night an answer came within minutes!

1 Introduction

The main goal of this project is to explore some of the features of superconductors, the theories and different concepts involved to describe the superconducting state and the effect of impurities and constrictions. Thermodynamically superconductivity is considered a second order phase transition, which is seen in many metals, but also in other matter.

The most successful theory in describing the superconducting state, which by no means is restricted to metals and electric conductivity, but also describes superfluids like supercooled Helium, is the theory developed by Bardeen, Cooper and Schrieffer, called the "BCS-theory of superconductivity". For this theory they received the Nobel price in 1972 [1].

Some of the properties of superconductors are a gap in the conduction band of the size 2Δ, a critical temperature T_c, at which the metal changes from a normal metal for $T > T_c$ to a superconductor for $T < T_c$. Superconductors are in general affected by external magnetic fields, who destroy superconductivity when strong enough. They are subject to the Meissner-Ochsenfeld effect, i.e. they expell all magnetic flux when in the superconducting state. Superconductors are divided in two by this effect of magnetic fields, where the Type-I-superconductors have a critical field strength H_c (temperature dependent) where superconductivity is destroyed, while the Type-II-superconductors (most of them high-T_c-superconductors[2]) have two critical field strength H_{c1} and H_{c2}, where the superconductivity is destroyed at H_{c2} while the magnetic field slowly starts penetrating the superconductor for a field strength above H_{c1} and thereby destroying superconductivity in the outer regions. This strong influence of magnetic fields on the superconductor will play a crucial role in this project when we explore the behavior of the superconducting electrons in the presence of magnetic impurities. These impurities induce excitations inside the energy gap, as Sakurai ([1]), Shiba ([4]) and Rusinov ([2]) showed theoretically, after it was discovered experimentally by Abrikosov.

An important discovery was that the energy of the ground state of a superconductor is lower than that of the normal metal and was found to be due to the pairing of electrons, called Cooper pairs, through the exchange of phonons. Phonons are quasi-particles, representing vibrations in the lattice of the metal. We will explain the concept in section 1.1.2. This theoretical explanation was one of the big successes for the BCS-theory.

We will use the BCS-theory and the tools and concepts presented in section 1.1 to find the energy and wave function for the bound states induced by a impurity, fx. a different atom in the pure metal. This is done in a one dimensional case and we will then add a phase to the right side to represent a different superconductor and will find the energy for the bound states as function of the phase and will finally calculate the current through the impurity/barrier.

Different works have been published on these subjects and we will reproduce some of the results to show that our model is valid.

1.1 Tools and concepts

1.1.1 Second Quantization

A concept that we will use extensively is that of creation- and annihilation operators, which work on many body wave functions and either add or remove electrons, quasi-particles or holes. We use the conventions

[1] http://www.nobelprize.org/nobel_prizes/physics/laureates/1972/

[2] high-T_c superconductors are characterized by a critical temperature T_c well above absolute zero.

- $c^\dagger_{k\sigma}$: Creates an electron in state k and spin σ.
- $c_{k\sigma}$: Removes an electron in state k and spin σ.
- $b^\dagger_k = c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}$: Creates a Cooper pair in state k.
- $b_k = c_{k\uparrow}c_{-k\downarrow}$: Removes a Cooper pair in state k.
- $n^\dagger_{k\sigma} = c^\dagger_{k\sigma}c_{k\sigma}$: Checks if there is an electrons in state k and spin σ.
- $n_{k\sigma} = c_{k\sigma}c^\dagger_{k\sigma}$: Checks if there is a holes in state k and spin σ.
- $\gamma^\dagger_k$: Creates a Bogolon, a quasi particle introduced in section 1.1.3, in state k.
- γ_k: Removes a Bogolon in state k and spin σ.

The effect of a creation operator $c^\dagger_k$ on a wave function $|\Psi_0\rangle = |0_1 0_2 0_3 \cdots 0_k \cdots 0_N\rangle$ is

$$c^\dagger_k|0_1 0_2 0_3 \cdots 0_k \cdots 0_N\rangle = |0_1 0_2 0_3 \cdots 1_k \cdots 0_N\rangle$$

and similar for an annihilation operator on a fully filled wave function $|\Psi_1\rangle = |1_1 1_2 1_3 \cdots 1_k \cdots 1_N\rangle$

$$c_k|1_1 1_2 1_3 \cdots 1_k \cdots 1_N\rangle = |1_1 1_2 1_3 \cdots 0_k \cdots 1_N\rangle$$

Since we deal with fermions the Pauli exclusion principle applies. We define

$$\left(c^\dagger_{k\sigma}\right)^2|0_{k\sigma}\rangle = c^\dagger_{k\sigma}|1_{k\sigma}\rangle = 0$$
$$\left(c_{k\sigma}\right)^2|1_{k\sigma}\rangle = c_{k\sigma}|0_{k\sigma}\rangle = 0$$

This means that if we try to add an electron in a state that is already occupied, the system just vanishes.

As it can be seen from the definition of the counting operators $n^\dagger_k$ and n_k, the creation and annihilation operators generally do not commute. From the above definition it is easy to see that $c^\dagger_k c_k|1_k\rangle = c^\dagger_k|0_k\rangle = |1_k\rangle$ is not the same as $c_k c^\dagger_k|1_k\rangle = c_k \cdot 0 = 0$. Generally we have

$$\left[c_{k\sigma}, c^\dagger_{k'\sigma'}\right] = \delta_{kk'}\delta_{\sigma\sigma'}$$
$$[c_{k\sigma}, c_{k'\sigma'}] = 0 \left[c^\dagger_{k\sigma}, c^\dagger_{k'\sigma'}\right] = 0$$

Physically this is easy to understand: The first commutator expresses that the difference between the electron counting operator $n^\dagger_{k\sigma} = c^\dagger_{k\sigma}c_{k\sigma}$ and the hole counting operator $n_{k\sigma} = c_{k\sigma}c^\dagger_{k\sigma}$ is 1, i.e. there is either a hole or an electron but not both at the same time. The two other commutators say that it is not important whether you first add a hole/electron in state k and then in k' or first in k' and then in k. If $k = k'$ the product is 0 anyway.

1.1.2 Quasi-particles

Quasi-particles are the representation of different phenomena by a particle. Fx. a sound wave through a solid, which is a displacement of the atoms, can be modeled as a particle traveling through the solid. The quasi-particle is a superposition of many particles and

hence not a particle by itself, but it often makes calculations easier. One example is the center of mass of two or more objects. The center of mass is not by itself an object, but by treating it as one, we can calculate its trajectory without having to calculate the trajectory for each of the objects, which can be rather troublesome or impossible. The center of mass is a quasi-particle. We will use different quasi-particles in this project but the most important is the Bogolon, which we introduce now.

1.1.3 Transformations

When working with the Hamiltonian of a superconducting system in the BCS-theory, expressed in creation/annihilation operators for electrons it turns out that the Hamiltonian is not diagonal and hence it is hard to determine the eigenenergies for the electrons. We introduce a transformation that will diagonalize the BCS-Hamiltonian. This transformation is called Bogoliubov-transformation. We introduce a new quasi-particle, the Bogolon, which is a combination of an electron and a hole in the "opposite" state. By "opposite" we mean a hole that is in state $-k$ and has spin $\downarrow$ for an electron in state k and spin $\uparrow$. The transformation is given by (see also ch. 10 of [6])

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k^* & -v_k \\ v_k^* & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

The coefficients u_k, v_k will play a crucial role for us. We determine them when introducing the BCS-theory. To find the inverse transformation and hence get an expression for the c_k's in terms of the Bogolon-operator γ_k, we have to invert the matrix. We will use the formula

$$A^{-1} = \frac{1}{\det A}\mathrm{adj}A$$

The determinant for our matrix is

$$\det \begin{pmatrix} u_k^* & -v_k \\ v_k^* & u_k \end{pmatrix} = |u_k|^2 + |v_k|^2$$

It turns out that we get a useful expression by looking at the commutator $\left[\gamma_{k\uparrow}, \gamma^\dagger_{k\uparrow}\right]$. The Bogolon is a fermion, so it has to satisfy the anticommutation relations for fermions. We hence have ((10.9) of [6])

$$\begin{aligned}
\left[\gamma_{k\uparrow}, \gamma^\dagger_{k\uparrow}\right] =& 1 \\
\left[\gamma_{k\uparrow}, \gamma^\dagger_{k\uparrow}\right] =& \gamma_{k\uparrow}\gamma^\dagger_{k\uparrow} + \gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} \\
=& u_k^* u_k c_{k\uparrow} c^\dagger_{k\uparrow} - u_k^* v_k^* c_{k\uparrow} c_{-k\downarrow} - v_k u_k c^\dagger_{-k\downarrow} c^\dagger_{k\uparrow} + v_k u_k^* c^\dagger_{-k\downarrow} c_{-k\downarrow} \\
&+ u_k u_k^* c^\dagger_{k\uparrow} c_{k\uparrow} - u_k v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - v_k^* u_k^* c_{-k\downarrow} c_{k\uparrow} + v_k^* v_k c_{-k\downarrow} c^\dagger_{-k\downarrow} \\
=& |u_k|^2 \left[c_{k\uparrow}, c^\dagger_{k\uparrow}\right] - u_k^* v_k^* \left[c_{k\uparrow}, c_{-k\downarrow}\right] - v_k u_k \left[c^\dagger_{-k\downarrow}, c^\dagger_{k\uparrow}\right] + |v_k|^2 \left[c^\dagger_{-k\downarrow}, c_{-k\downarrow}\right] \\
=& |u_k|^2 + |v_k|^2
\end{aligned}$$

So we have $|u_k|^2 + |v_k|^2 = 1$ and hence we have the inverse transformation

$$\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix}$$

1.1.4 Mean-field theory

When introducing the BCS-theory, we will rewrite the Hamiltonian using mean field theory. In this approach we assume, that the actual value of the creation/annihilation operators are close to their mean values. The number of electrons in the superconducting state is not constant but we assume that the fluctuations are small, which justifies that the operators are close to their average. We then use

$$AB = (A - \langle A \rangle)(B - \langle B \rangle) + A\langle B \rangle + \langle A \rangle B - \langle A \rangle \langle B \rangle$$

We note that $(A - \langle A \rangle)(B - \langle B \rangle)$ is small since the deviation from the average is small and hence this factor will be removed and we get

$$AB = A\langle B \rangle + \langle A \rangle B - \langle A \rangle \langle B \rangle \tag{1.1}$$

1.1.5 Scattering theory: S-matrices and phase shift

Scattering theory deals with the effect of potentials on passing particles, fx. an electron passing an atom. We restrict our considerations to the 1 dimensional case, since we will deal with spherical symmetric potentials and wave functions and hence only have to calculate the radial part.

When working with free particles the strategy is to determine the effect of the potential on the free particle wave function of the form $Ae^{ikx}+Be^{-ikx}$, where the first part represents a particle moving to the right and the second part a particle moving to the left, both with wavenumber k. We are interested in the transmission and reflection due to the potential, so we introduce a wave function for the left and the right side of the potential (which is supposed to be located around $x = 0$). Then the amplitudes can be calculated, giving us the transmission and reflection. This is done by applying continuity requirements:

- $\Psi(x)$ has to be continuous for all x.
- $\frac{d\Psi}{dx}$ has to be continuous for all x, except where the potential is infinite.

When the potential is infinite and has the form $V(x) = -\alpha\delta(x)$ then $\Psi(x)$ has to satisfy

$$\frac{d\Psi_R}{dx} - \frac{d\Psi_L}{dx} = -\frac{2m\alpha}{\hbar^2}\Psi(0)$$

(cf. equation 2.125 in [7]).

Let the left and right wave functions be

$$\Psi_L = Ae^{ikx} + Be^{-ikx}$$
$$\Psi_R = Fe^{ikx} + Ge^{-ikx}$$

then the continuity requirements lead to two equations that can be written on matrix form

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}$$

The matrix is called the "scattering matrix" or short "S-matrix". While the S-matrix tells us the outgoing amplitude in terms of the ingoing, we can also express the right side amplitude in terms of the left side amplitudes by rewriting the S-matrix. The new matrix is called the "transfer matrix" or short "T-matrix".

A powerful tool in working with scatterings is the phase shift. When an electron passes the potential it will experience a change in its phase. When solving for the eigenvalues of the S-matrix we obtain the phase shift due to the potential.

2 The superconducting system

As mentioned superconductivity is most widely known for its ability to conduct charges without resistance for temperatures below a critical temperature T_c. This was discovered when it became possible to liquefy Helium and thus cool matter down to a few degrees Kelvin. The resistivity for Mercury was observed to drop almost instantaneously at around 4,1 K. This was the discovery of the first conventional superconductor. But Mercury was found not to be the only element with this property. Actually 53 of the pure elements in the periodic table become superconducting under some circumstances (a combination of temperature, pressure and the absence of a magnetic field). The definition of conventional superconductivity is that it "result from an attractive interaction between electrons for which phonons play a dominant role." ([6], p. 8).

We will have a brief look on the properties that characterize a superconductor. Some of these properties will be used to derive and justify approximations for the Hamiltonian and the behavior in the presence of an impurity. We start with taking a look on the microscopic properties, like the interaction of electrons through phonons and the origin of the energy gap.

2.1 Microscopic properties

Microscopic a conventional (Type-I-)superconductor is characterized by the forming of Cooper pairs, i.e. electrons of opposite spin with energy near the Fermi energy (in k-space the electrons located near the Fermi surface) interact and create pairs, which are energetically preferable to the unpaired electrons. The thickness of this shell around the Fermi surface is of the order of $10^{-4}eV$ for the most pure elements that become superconducting. This is also the order of the energy gap Δ that is thereby created. The Cooper pairs are not stable. They will emerge and will be destroyed thus the count of Cooper pairs is not constant, but the fluctuation is small and we will hence call the average number of Cooper pairs N and treat it as constant. The electrons that are not paired (those beneath the Fermi surface in the normal state[3]) constitute a reservoir from which the Cooper pairs are created and in which the electrons return when the Cooper pair is broken. The size of the Cooper pairs, i.e. the average distance between the paired electrons, is called the coherence length and is denoted ξ_0. This length emerges when treating superconductivity in a thermodynamic framework, where superconductivity is viewed as a phase transition. This is done in the Ginzburg-Landau-theory of superconductivity (see [10]) which also provides us with other useful relations regarding the critical temperature T_c and flux quantization. In this project we only use the coherence length when evaluating Rusinovs result for the radial wave function of the impurity states.

2.2 Quantum mechanic description

We will now derive the BCS-Hamiltonian for the superconducting system, like it is presented by Mattuck ([5]) and Timm ([6]).

2.2.1 BCS-potential, Coulomb-potential, screening electrons, phonon-interaction

We start with the Hamiltonian, presented by Mattuck, which takes into account different interactions in the system. By approximations and transformations we will end up with

[3]The sphere in k-space that is restricted by the Fermi surface is often called the Fermi sea and the electrons beneath the surface are said to come lie deep down in the Fermi sea.

the BCS-Hamiltonian in a reduced form, which then will be our starting point for deriving the effects of impurities on the system.

Mattucks Hamiltonian reads

$$
\begin{aligned}
H &= H_{free\ electron} + H_{Coulomb} + H_{free\ phonon} + H_{electron-phonon} \\
H_{free\ electron} &= \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} = \sum_{k,\sigma} \epsilon_k n^\dagger_{k\sigma} \\
H_{Coulomb} &= \frac{1}{2} \sum_{k,k',Q,\sigma,\sigma'} V_Q c^\dagger_{k'-Q,\sigma'} c^\dagger_{k+Q,\sigma} c_{k\sigma} c_{k'\sigma'} \\
H_{free\ phonon} &= \sum_q \Omega_q (B^\dagger_q B_q + \frac{1}{2}) \\
H_{electron-phonon} &= \sum_{k,k',q,\sigma} g_q (B_q + B^\dagger_{-q}) c^\dagger_{k'\sigma} c_{k\sigma}
\end{aligned}
$$

where $B^\dagger_q$ is the phonons creation operator, Ω_q is the phonon frequency and g_q is a couling strength for electrons and phonons.

This can be transformed into (also we use the symbol H as the resulting Hamiltonian in both cases, it must be noted that there are done some approximations along the way and hence they are not equal).

$$
\begin{aligned}
H &= H_{quasi-electron} + H_{shielded\ Coulomb} + H_{el-ph-el} + H_{dressed\ phonon} \\
H_{quasi-electron} &= \sum_{k,\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} = \sum_{k,\sigma} \xi_k n_{k\sigma}, \qquad \xi_k = \frac{\hbar^2 k^2}{2m_{eff}} - \epsilon_F \\
H_{dressed\ phonon} &= \sum_q \hbar\omega_k (B^\dagger_q B_q + \frac{1}{2}) \\
H_{shielded\ Coulomb} + H_{el-ph-el} &= \frac{1}{2} \sum_{k,k',q,\sigma,\sigma'} \mathcal{V}_{kq} c^\dagger_{k'-q,\sigma'} c^\dagger_{k+q,\sigma} c_{k\sigma} c_{k'\sigma'}
\end{aligned}
$$

Here $\mathcal{V}_{kq}$ is the so called "BCS interaction" and is given by

$$
\mathcal{V}_{kq} = \frac{4\pi e^2}{q^2 + \lambda^2} + \frac{2\hbar\omega_q |M_q|^2}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}
$$

The first term is the shielded Coulomb interaction and the second term is the shielded interaction between two electrons through the exchange of a phonon.

M_q is the coupling strength between electron and phonon and $\hbar\omega_q$ is the energy of the phonon. For a normal metal the coupling strength is rather weak, but as the metal is cooled down and the lattice vibration gets more important, M_q gets bigger.

This potential is attractive when the electron-phonon-electron interaction dominates, since $\hbar\omega_q$ is bigger than $\epsilon_k - \epsilon_{k+q}$ and hence the potential gets negative (=attractive). This transformation hence show us where the electron-phonon-electron interaction, the origin of Cooper pairs comes in.

Cooper showed that two electrons in the state $k\uparrow$ and $-k\downarrow$ would form a bound state (a pair) which energy is lower than the sum of the unpaired electrons' energy. When the electrons near the Fermi surface get paired they lower their energy and leave a gap in the energy band with a width of 2Δ. We will explain Δ in a moment, when we derive the BCS-Hamiltonian.

The point in the BCS theory is, that instead of having a linear combination of all electron states (like in a normal metal, where the total wave function is given by a Slater determinant) only the states, where the electrons are paired contribute to the total wave function. They were then able to write the Hamiltonian in a simple form, that we want to derive now.

2.2.2 BCS ground state and BCS-Hamiltonian

Our[4] strategy is to use the variational principle to determine the BCS ground state and calculate the coefficients by minimizing the energy. Our trial-wave function is

$$|\psi_{BCS}\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle$$

We normalize this wave function and get a relation that we already used to determine the inverse Bogoliubov transform:

$$\begin{aligned}
1 &= \langle\psi_{BCS}|\psi_{BCS}\rangle \\
&= \langle 0|\prod_k (u_k^* + v_k^* c_{k\uparrow} c_{-k\downarrow}) \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle \\
&= \langle 0|\prod_k \left(|u_k|^2 + u_k v_k^* c_{k\uparrow} c_{-k\downarrow} + u_k^* v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + |v_k|^2 \underbrace{(c_{k\uparrow} c_{-k\downarrow} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})}_{=1}\right)|0\rangle \\
&= \prod_k \left(|u_k|^2 + |v_k|^2\right)
\end{aligned}$$

We have used that $(c^\dagger_{k\uparrow})^* = c_{k\uparrow}$ and that the creation/annihilation operators alter the "ket"-vacuum which then is orthogonal to the "bra" state.

We can now see, what we already saw in section 1.1.3, that $|u_k|^2 + |v_k|^2 = 1$. While there is no a priori reason to think that this is the case (it could be possible that there are pairs $k_1,\ k_2$ such that $|u_{k1}|^2 + |v_{k1}|^2$ is the reciprocal of $|u_{k2}|^2 + |v_{k2}|^2$ which also would satisfy the above equation), but we end up with reasonable results when choosing $|u_k|^2 + |v_k|^2 = 1$ which justifies this choice.

We use the variational principle with the Hamiltonian

$$H = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} + V_{int}$$

where V_{int} is an interaction potential (containing all the interactions that we mentioned in the last section). We want the interaction to be as simple as possible and hope to be able to replace it by a constant interaction. We require the potential to satisfy

1. only electrons close to the Fermi surface of the normal metal contribute to the potential, i.e. $|\xi_k| < \omega_D$ where ω_D is the Debye frequency.

2. the lowering of the electrons energy relative to the Fermi surface of the normal metal, and hence the destruction of the Fermi surface, is mainly due to the electron-phonon-electron interaction which creates the Cooper pairs.

[4]This derivation of the Hamiltonian was originally done in this way by Bardeen, Cooper and Schrieffer.

To account for the last requirement, we choose

$$V_{int} = \frac{1}{N} \sum_{k,k'} V_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} c_{k'\uparrow} c_{-k'\downarrow}$$

where N is the average total particle count. This represents an interaction that takes a Cooper pair in state k' and kicks it to state k.

To account for the first requirement, we let $V_{kk'}$ be defined by

$$V_{kk'} = \begin{cases} -V_0 & \text{for } |\xi_k|, |\xi_{k'}| < \omega_D \\ 0 & \text{otherwise} \end{cases} \tag{2.1}$$

We want to minimize the energy of the system by varying u_k and v_k. We hence have to calculate $\langle \psi_{BCS} | H | \psi_{BCS} \rangle$. This is done in detail by Timm ([6], p. 86) and the result is

$$\langle \psi_{BCS} | H | \psi_{BCS} \rangle = 2 \sum \xi_k |v_k|^2 + \frac{1}{N} \sum_{k,k'} V_{kk'} v_k^* u_k u_{k'}^* v_{k'}$$

The energy has to be real and hence the arguments/phases of u_k and v_k^* have to be equal. Adding a phase factor $e^{i\phi_k}$ to u_k and v_k^* has no effect as it vanishes. We can hence choose u_k and v_k to be real. Since they have to satisfy $u_k^2 + v_k^2 = 1$ we choose the obvious solution

$$u_k = \cos\theta_k$$
$$v_k = \sin\theta_k$$

and then get (after some calculations, we refer to [6] for details)

$$\langle \psi_{BCS} | H | \psi_{BCS} \rangle = \sum_k \xi_k (1 - \cos 2\theta_k) + \frac{1}{4N} \sum_{k,k'} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'}$$

To minimize the energy $\langle \psi_{BCS} | H | \psi_{BCS} \rangle$, we differentiate with respect to θ_k, equate to 0 and define

$$\sin 2\theta_k =: \frac{\Delta_k}{\sqrt{\xi_k^2 + \Delta_k^2}}$$

Δ_k can then be expressed as

$$\Delta_k = -\frac{1}{2N} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}$$

This is called the *gap equation*, since it defines the gap-parameter Δ_k for a given potential. Δ first occured as the order parameter in the Ginzburg-Landau theory, describing the phase transition from normal to superconducting phase, since Δ is temperature dependent and goes to 0 for the temperature approaching the critical temperature T_c. But Δ also describes the approximate thickness of the shell around the normal states Fermi surface, where the electrons will pair up as Cooper pairs and hence also describes the width of the energy gap.

For our potential (2.1) the solution to the gap equation is obtained by using a variational ansatz of the same form as $V_{kk'}$ with $\Delta > 0$ instead of $-V_0$. In terms of the density of states for the Fermi energy in the normal state, $D(E_F) = \rho_F$, it is

$$\Delta = \omega_D \sinh\left(\frac{1}{V_0 D(E_F)}\right)^{-1} \cong 2\omega_D \exp\left(-\frac{1}{V_0 D(E_F)}\right)$$

where the last expression is valid for $V_0 D(E_F) \to 0$.

By further exploiting the variational principle one ends up with an expression for the energy difference between the energy for the BCS wave function and the normal metal

$$E_S - E_N \cong -\frac{1}{2} N D(E_F) \Delta^2 < 0$$

This agrees with the observation that the forming of Cooper pairs lowers the energy.

Our last step is now to transform the BCS-Hamiltonian

$$H = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} + \frac{1}{N} \sum_{k,k'} V_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} c_{k'\uparrow} c_{-k'\downarrow}$$

to a form that we will use in the rest of this thesis and is convenient when working with superconductivity.

We now use equation (1.1) with $A = c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}$ and $B = c_{-k\downarrow} c_{k\uparrow}$. We get

$$\begin{aligned} H =& \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} \\ &+ \frac{1}{N} \sum_{k,k'} V_{k,k'} (c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle + \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle c_{-k'\downarrow} c_{k'\uparrow} - \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle) \end{aligned} \tag{2.2}$$

The last factor in the parenthesis is a constant, which we will hide in the energy ξ_k.

By defining

$$\Delta^*_k = -\frac{1}{N} \sum_{k'} V_{kk'} \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \tag{2.3}$$

$$\Delta_k = -\frac{1}{N} \sum_{k'} V_{kk'} \langle c_{k\uparrow} c_{-k\downarrow} \rangle \tag{2.4}$$

we get

$$H_{BCS} = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} - \sum_k (\Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \Delta^*_k c_{-k\downarrow} c_{k\uparrow}) \tag{2.5}$$

We will assume, where appropriate, that Δ is real and hence $\Delta^*_k = \Delta_k$ and we use, as before, $\Delta_k = \Delta$ for the electrons with energy below the Debye frequency. We end up with the form

$$\boxed{H_{BCS} = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} - \Delta \sum_k (c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow})} \tag{2.6}$$

Bogoliubov-de Gennes equation This Hamiltonian can be diagonalized using the Bogoliubov transform and then reads

$$H^{\text{transf}}_{BCS} = E_0 + \sum_{k,\sigma} \epsilon_k \gamma^\dagger_{k\sigma} \gamma_{k\sigma}$$

The Bogoliubov-de Gennes equations (BdG) are the Bogoliubov-transformed version of the Schrödinger equation $H\psi = E\psi$ and are obtained in the following way:

We add a constant potential to the Hamiltonian (2.6) by replacing $\xi_k \to \xi_k + U$. We first find the commutator $[c_{k\uparrow}, H_{BCS}]$ and $[c_{k\downarrow}, H_{BCS}]$:

$$\begin{aligned}[c_{k\uparrow}, H_{BCS}] &= c_{k\uparrow}H_{BCS} - H_{BCS}c_{k\uparrow} \\ &= \sum_k (\xi_k + U)c_{k\uparrow} + \Delta c^\dagger_{k\downarrow} \qquad (2.7)\\ [c_{k\downarrow}, H_{BCS}] &= c_{k\downarrow}H_{BCS} - H_{BCS}c_{k\downarrow} \\ &= \sum_k (\xi_k + U)c_{k\downarrow} + \Delta c^\dagger_{k\uparrow} \qquad (2.8)\end{aligned}$$

Using the Bogoliubov transform $c_{k\uparrow}$ and $c_{k\downarrow}$ are replaced by $\gamma_{k\uparrow}u_k - \gamma^\dagger_{k\downarrow}v^*_k$ and $\gamma_{k\downarrow}u_k + \gamma^\dagger_{k\uparrow}v^*_k$, respectively.

We can thus rewrite the above commutators. We first transform the left side of the commutator $[c_{k\uparrow}, H_{BCS}]$:

$$\begin{aligned}[\gamma_{k\uparrow}u_k - \gamma_{k\downarrow}v^*_k, H^{\text{transf}}_{BCS}] =& \sum_k \epsilon_k \Big(u_k(\gamma_{k\uparrow}\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma_{k\uparrow}\gamma^\dagger_{k\downarrow}\gamma_{k\downarrow} - \gamma^\dagger_{k\uparrow}\gamma_{k\uparrow}\gamma_{k\uparrow} - \gamma^\dagger_{k\downarrow}\gamma_{k\downarrow}\gamma_{k\uparrow}) \\ &+v^*_k(-\gamma^\dagger_{k\downarrow}\gamma^\dagger_{k\downarrow}\gamma_{k\downarrow} - \gamma^\dagger_{k\downarrow}\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{k\downarrow}\gamma_{k\downarrow}\gamma^\dagger_{k\downarrow} + \gamma^\dagger_{k\uparrow}\gamma_{k\uparrow}\gamma^\dagger_{k\downarrow})\Big) \\ =& \sum_k \epsilon_k \Big(u_k\gamma_{k\uparrow} + u_k\gamma_{k\uparrow}\gamma^\dagger_{k\downarrow}\gamma_{k\downarrow} - u_k\gamma_{k\uparrow}\gamma^\dagger_{k\downarrow}\gamma_{k\downarrow} \\ &-v^*_k\gamma^\dagger_{k\downarrow}\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + v^*_k\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow}\gamma^\dagger_{k\downarrow}\Big) \\ =& \sum_k \epsilon_k u_k\gamma_{k\uparrow}\end{aligned}$$

The right side of (2.7) after transformation reads

$$\sum_k (\xi_k + U)\left(\gamma_{k\uparrow}u_k - \gamma^\dagger_{k\downarrow}v^*_k\right) + \Delta\left(\gamma^\dagger_{k\downarrow}u^*_k + \gamma_{k\uparrow}v_k\right)$$

By now comparing the coefficients for $\gamma_{k\uparrow}$ we get the first BdG-equation

$$\epsilon_k u_k = (\xi_k + U)u_k + \Delta v_k$$

In the same way we can obtain the second equation by solving the other commutator and comparing the coefficients of $\gamma_{k\downarrow}$

$$\epsilon_k v_k = -(\xi_k + U)u_k + \Delta u_k$$

The BCS u- and v-functions Earlier we assumed that the phase of u_k and v^*_k is the same and have assumed that they were real. In general they can be written as

$$u_k = \sqrt{\frac{1}{2} + \frac{\xi_k}{2\sqrt{\xi_k^2 + \Delta_k^2}}} \qquad (2.9)$$

$$v_k = \sqrt{\frac{1}{2} - \frac{\xi_k}{2\sqrt{\xi_k^2 + \Delta_k^2}}} \qquad (2.10)$$

For the detailed derivation, that also gives us some useful relations between u_k and v_k, we refer to Timm ([6]). It is easily obtained, with $\xi^2 = E^2 - \Delta^2$, that

$$|u_k| = |v_k| = \sqrt{\frac{\Delta}{E}} \qquad (2.11)$$

$$\text{Arg}(u_k) = -\text{Arg}(v_k) = \arctan\left(\sqrt{\frac{\Delta - E}{\Delta + E}}\right) \qquad (2.12)$$

In particular this means that u_k and v_k are each others complex conjugate.

3 Impurities in superconductors

Conventional superconductivity is a result of an unstable lowering of the electrons energy by forming Cooper pairs through the exchange of phonons. This instability is affected by external potentials, especially magnetic fields. This makes the superconductor vulnerable to spin-impurities. The effect of a spin impurity in a superconducting metal is studied in this section. Our starting point is the article of Rusinov and Lebedev from 1969 ([2]), which, together with the work of Yu ([3]) and Shiba ([4]) had an important impact on the field.

3.1 Shiba states

Shiba was one of the first to publish a theoretical paper on the effect of a spin-impurity on a superconductor, after the initial paper of Yu ([3]) in 1965. Shiba showed that there exist bound states with an energy located inside the superconductors energy gap, after there had been some discussion with other researchers who don't believed that there are subgap states. Shiba used Green functions and related concepts to show that the bound state has the energy

$$E_{Shiba} = \pm\Delta\frac{1-\zeta^2}{1+\zeta^2}, \qquad \zeta = \frac{JS}{2}\rho\pi$$

where J is the strength of the spin-orbit-coupling, S is the spin and ρ is the density of states for a normal metal for ϵ_F.

Short after Rusinov did the same for a more general potential, as Yu had done. He used a spherical symmetric potential that includes a spin-independent and a spin-dependent part

$$V(r) = \frac{2\pi}{m}\left(U(r) + J(r)\sigma\vec{S}\right)$$

Both $U(r)$ and $J(r)$ involve δ-functions and hence $V(r)$ is a point potential.

Rusinov expanded this potential in its spherical harmonics and used only the first coefficient $(U_0 \pm J_0 S)$, which is a good approximation since the potential is spherical symmetric and where the spin matrix is replaces by its eigenvalues ± 1.

He then used the Bogoliubov-de Gennes equations to obtain an expression for the BCS u- and v-functions and by integrating them with respect to the energy ξ he obtained the expression for the energy E of the subgap states:

$$E = \pm\Delta\frac{1+\rho_F^2(U_0^2-(J_0S)^2)}{\sqrt{(1+\rho_F^2(U_0^2-(J_0S)^2))^2+4(J_0S)^2}}$$

which can be written in terms of the scattering phase shift ϕ.

$$E = \pm\Delta\cos(\phi)$$

The phase shift is the difference of the electron- and the hole-phase shifts ϕ_0^+ and ϕ_0^-. The potential can then be written

$$(U_0 \pm J_0 S) = \tan\phi_0^{\pm}$$

We will show this later. Also we drop the 0-subscript.

The energy of the subgap states/Shiba states as function of the spin potential JS is plotted in figure 1:

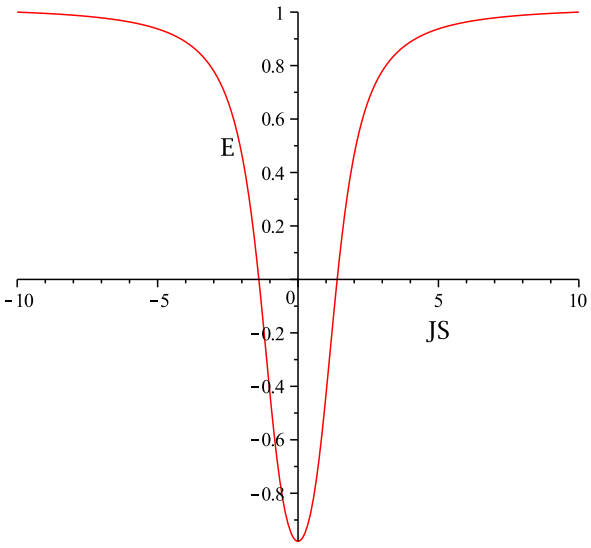


Figure 1: *Subgap energy as function of the spin potential JS. The energy is in units of* Δ.

3.1.1 Excitation energy and wave function for interactions with classical spin - S-matrix method

Our strategy is now to study the scattering (reflection/transmission) by the impurity potential for incoming electrons and holes to reproduce the above results. We restrict ourselves to the 1 dimensional case, as the problem is spherical symmetric and we therefore just have to study the radial behavior. For the 1 dimensional case we have the impurity at x=0 and have a right and a left side. In the study of superconductors it is convenient to work with 4-dimensional spinors as wave functions, i.e. a separate wave function for an electron/hole with spin $\uparrow/\downarrow$, respectively. We restrict our calculation to 2-spinors with an wavefunction for electron- and hole-like-particles, respectively, without introducing a separate u- and v-function for the spin.

We let our wave function be the sum of wave functions for free electrons with wave number k_+ and holes with wave number k_- traveling either left (e^{ikx}) or right (e^{-ikr}). The probability amplitude for each of these 4 cases are labeled a_i, b_i, c_i and d_i where $i = L, R$ denoting the coefficients for the left and the right side, respectively. We thus have the wave function of the form

$$\Psi(x) = \begin{cases} a_L \begin{pmatrix} u \\ v \end{pmatrix} e^{-ik_+x} + b_L \begin{pmatrix} u \\ v \end{pmatrix} e^{ik_+x} + c_L \begin{pmatrix} v \\ u \end{pmatrix} e^{-ik_-x} + d_L \begin{pmatrix} v \\ u \end{pmatrix} e^{ik_-x} & x < 0 \\ a_R \begin{pmatrix} u \\ v \end{pmatrix} e^{-ik_+x} + b_R \begin{pmatrix} u \\ v \end{pmatrix} e^{ik_+x} + c_R \begin{pmatrix} v \\ u \end{pmatrix} e^{-ik_-x} + d_R \begin{pmatrix} v \\ u \end{pmatrix} e^{ik_-x} & x \geq 0 \end{cases} \tag{3.1}$$

We have hence chosen that

	$\leftarrow$	$\rightarrow$
Electron-like	a	b
Hole-like	c	d

Table 1: *The convention for the coefficients in (3.1).*

The functions u and v in the spinor $\begin{pmatrix} u \\ v \end{pmatrix}$ are the functions (2.9) and (2.10). We choose them, since they represent the probability amplitude for the state with the energy $E \sim k$ to be electron-like (u) or hole-like (v). As it can be seen from table 1 the first terms of the left/right side are that for an electron-like particle. The last two terms represent a hole-like particle. Further the wave functions are separated by the spinor. The first (upper) term in the spinor is related to the electron-like particle and the second (lower) term is related to the hole-like particle. In a normal metal we would have

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The electron-like and the hole-like particle are hence completely separated in a normal metal. This is due to the fact that the normal metal has a well defined Fermi surface and hence it is completely determined whether a particle is inside or outside the Fermi surface. In the superconducting state this is not the case. The analog to the electron in the normal case is the Bogolon for the superconducting system (the particle that diagonalizes the Hamiltonian).

We have to make sure that $\Psi(x)$ satisfies the continuity requirements presented in section 1.1.5. $\frac{d\Psi}{dx}$ is clearly continuous for $x < 0$ and $x > 0$. For $x = 0$ our potential is infinite (since it is given by a δ-function) and hence has to satisfy

$$\Psi'_L - \Psi'_R = -\frac{2m}{\hbar^2} \begin{pmatrix} U + JS & 0 \\ 0 & -(U - JS) \end{pmatrix} \Psi(0)$$

where m is the electron mass and $U \pm JS$ is the first coefficient in the spherical harmonic expansion of the potential, where the + is used for spin $\uparrow$ and - for spin $\downarrow$ as before. We discard the factor $\frac{2m}{\hbar^2}$ and use it implicit when needed.

When looking for solutions we are not interested in the trivial $\vec{0}$ solution. We hence demand the determinant of the resulting 4x4 system to be 0.

Before writing out the 4 equations on matrixform, we take a look on the wave numbers $k_\pm$. They are the (positive) solution to the equation

$$E = \sqrt{\left(\frac{k^2}{2m} - \frac{k_F^2}{2m}\right)^2 + \Delta^2} \tag{3.2}$$

which is the quasi-particle energy for Cooper pairs relative to the Fermi surface of the normal state. When solving for k we get 4 solutions:

$$\pm k_F \sqrt{1 \pm \frac{\sqrt{E^2 - \Delta^2}}{\mu}}$$

where $\mu = \frac{2m}{k_F^2}$ is the chemical potential. k_+ is the solution where both signs are positive and k_- the solution where the outer sign is positive and the inner sign is negative.

We will later assume that $E < \Delta$ to find that there are bound states induced by the impurity, the mentioned subgap states or Shiba states. Right now we only assume that $\mu \gg \Delta$, and we hence can replace $k_\pm$ by k_F. This assumption is justified by the observation that the electrons involved in the superconducting state lie in a thin shell around the normal metals Fermi surface, with a thickness of about $10^{-4}eV$, while k_F normally is of the order of some eV.

When applying the assumption $E < \Delta$ the wave numbers $k_\pm$ will have an imaginary part and hence the plane waves will decay/grow exponentially. k_+ has a positive imaginary

part and k_- a negative one. Using this fact we can rule out 4 of the 8 coefficients (2 on each side). Fx. (we skip the spinor) $b_L e^{ik_+ x}$ goes to ∞ for $x \to -\infty$ and hence $b_L = 0$. We hence have

$$b_L = c_L = a_R = d_R = 0 \tag{3.3}$$

We then have the system of continuity equations in matrixform

$$\begin{pmatrix} u & v & -u & -v \\ v & u & -v & -u \\ u(-ik_F) + (U + JS)u & v(ik_F) - (U + JS)v & -u(ik_F) & -v(-ik_F) \\ v(-ik_F) + (U - JS)v & u(ik_F) - (U - JS)u & -v(ik_F) & -u(-ik_F) \end{pmatrix} \begin{pmatrix} a_L \\ d_L \\ b_R \\ c_R \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{3.4}$$

When equating the determinant of the matrix to 0 and substituting u and v by (2.9) and (2.10), we get

$$\frac{E^2((JS)^2 - 4k_F^2 - U^2) + (-(JS)^2 + 4k_F^2 + U^2)\Delta^2 + 4iEJSk_F\sqrt{E^2 - \Delta^2}}{E^2} = 0$$

solving for E we get the 4 solutions

$$E = \pm\Delta$$

$$E = \pm\frac{((JS)^2 - 4k_F^2 - U^2)\Delta}{\sqrt{(JS)^4 + 8(JS)^2k_F^2 + 16k_F^4 - 2(JS)^2U^2 + 8k_F^2U^2 + U^4}} \tag{3.5}$$

$$= \mp\Delta\frac{\alpha}{\sqrt{1 + \alpha^2}} \tag{3.6}$$

where

$$\alpha = \frac{1 + p_F^2(U^2 - JS^2)}{2p_FJS}$$

with p_F the Fermi momentum. This is the same result that Rusinov found by using the BdG-equations.

We observe that

$$\frac{\alpha}{\sqrt{1 + \alpha^2}} \leq 1$$

Hence the energy is inside the gap. We define

$$\cos(\phi) = \frac{\alpha}{\sqrt{1 + \alpha^2}} \tag{3.7}$$

and have the desired form

$$E = \Delta\cos(\phi) \tag{3.8}$$

We can then confirm that the potential can then be written

$$(U \pm JS) = \tan\phi^{\pm} \tag{3.9}$$

by confirming that (3.8) and (3.9) are consistent and remember that $\phi = \phi^+ - \phi^-$. We absorb p_F into the potential and get

$$\alpha = \frac{1 + \tan(\phi^+)\tan(\phi^-)}{\tan(\phi^+) - \tan(\phi^-)} = \frac{1}{\tan(\phi^+ - \phi^-)}$$

Passing this back into (3.6) we get

$$\begin{aligned}\frac{E}{\Delta} &= \frac{\alpha}{\sqrt{1+\alpha^2}} = \frac{1}{\tan(\phi^+-\phi^-)\sqrt{1+\frac{1}{\tan(\phi^+-\phi^-)^2}}} \\ &= \frac{1}{\sqrt{\tan(\phi^+-\phi^-)^2+1}} = \frac{1}{\sqrt{\frac{\sin(\phi^+-\phi^-)^2}{\cos(\phi^+-\phi^-)^2}+1}} = \frac{\cos(\phi^+-\phi^-)}{\sqrt{\sin(\phi^+-\phi^-)^2+\cos(\phi^+-\phi^-)^2}} \\ &= \cos(\phi^+-\phi^-)\end{aligned}$$

In Ref. [8] Balatsky et al. come up with a solution for the impurity wave function using the variational principle. The variational ansatz differs from the BCS-system, where all electrons are paired, by a single, unpaired electron with opposite spin compared to the impurity and the electron hence screens the impurity. They also give the variational wave function Ψ_{-1} which has the form

$$\Psi_{-1} = \gamma_{-1}^\dagger \prod_n (u_n + v_n b_n^\dagger)|0\rangle = \gamma_{-1}^\dagger |\Psi_0\rangle$$

They note that $\gamma_1^\dagger|\Psi_0\rangle$ has much larger energy than the gap and hence is of no interest for us. This is important, since $\gamma_{-1}^\dagger$ adds a holelike Bogolon (hence removes an electron) while $\gamma_1^\dagger$ adds a Bogolon (adds a single electron), hence it justifies that the impurity breaks an electron pair to get a screening electron instead of attracting a new electron from the reservoir.

The breaking of a Cooper pair near the impurity can be understood as a local suppression of the superconducting state by the magnetic impurity. We may then think of it as being a SNS-junction, which experimentally mainly is obtained by connect two superconductors of the same or different elements (or compounds) with another metal that is not superconducting. The normal region between the superconductors can even be modified with some impurities, giving rise to different effects and properties. We will study our system in terms of a SNS- and SIS-junction in the next section.

We now remove the assumption that $\mu \gg \Delta$ to find the wave function. The normalized wave function is (see appendix A)

$$\Psi(x) = \frac{1}{\sqrt{4}} \begin{cases} \begin{pmatrix} u \\ v \end{pmatrix} e^{-ik_+ x} + \begin{pmatrix} v \\ u \end{pmatrix} e^{ik_- x} & x < 0 \\ \begin{pmatrix} u \\ v \end{pmatrix} e^{ik_+ x} + \begin{pmatrix} v \\ u \end{pmatrix} e^{-ik_- x} & x \geq 0 \end{cases} \tag{3.10}$$

When plotting this wave function (figure 2) we see that it has both the form that characterizes a bound state of a delta potential and it has an oscillatory part. Rusinov proposed that the wave functions $u_{k\uparrow}$ and $v_{k\downarrow}$ have the form

$$u_{k\uparrow},\ v_{k\downarrow} = \frac{\sin(p_F r - \phi^\pm)}{p_F r} \exp\left(-\frac{r}{\xi_0}|\sin(\phi)|\right) \tag{3.11}$$

we can obtain a similar result when substituting the expression for $u,\ v$ and $k_\pm$ into $\Psi(x)$. We do this for the left side for both the electron-like and the hole-like part. We note that $k_\pm$ can be written

$$k_\pm = k_F \left(\overbrace{\sqrt{\frac{1}{2}}\sqrt{\sqrt{1+\frac{\Delta^2-E^2}{\mu^2}}+1}}^{X} \pm i \overbrace{\sqrt{\frac{1}{2}}\sqrt{\sqrt{1+\frac{\Delta^2-E^2}{\mu^2}}-1}}^{Y} \right) \tag{3.12}$$

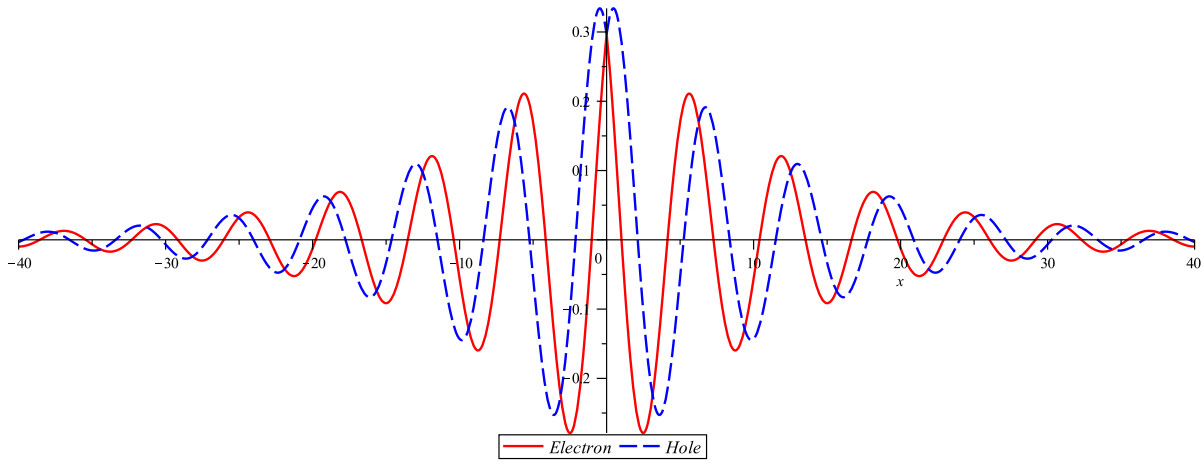


Figure 2: *The normalized wave functions for an electron and a hole due to the impurity potential as function of the position.*

Using (2.11) and (2.12) with $\theta_u := \mathrm{Arg}(u_k)$ we get for the electron-like part

$$\begin{aligned}\Psi_e(x) &= ue^{-ik_+x} + ve^{ik_-x} = \sqrt{\frac{\Delta}{E}}\left(e^{i\theta_u}e^{-i(Xk_F+iYk_F)x} + e^{-i\theta_u}e^{i(Xk_F-iYk_F)x}\right)\\ &= \sqrt{\frac{\Delta}{E}}e^{Yk_Fx}\left(e^{-i(Xk_Fx-\theta_u)} + e^{i(Xk_Fx-\theta_u)}\right)\\ &= 2\sqrt{\frac{\Delta}{E}}e^{Yk_Fx}\cos(Xk_Fx-\theta_u) \qquad (3.13)\end{aligned}$$

for $x < 0$. Similarilty for the hole-like part:

$$\Psi_h(x) = 2\sqrt{\frac{\Delta}{E}}e^{Yk_Fx}\cos(Xk_Fx+\theta_u) \qquad (3.14)$$

This is not Rusinovs result in its exact form but we can tell that the electron wave function and the hole wave function are phase shifted relative to each other by

$$\phi_+ - \phi_- = 2\theta_u = 2\arctan\left(\sqrt{\frac{\Delta-E}{\Delta+E}}\right)$$

and decays with a decaylength λ with

$$\lambda = \frac{1}{Yk_F} = \sqrt{\frac{2\mu}{k_F^2(\sqrt{\mu^2+\Delta^2-E^2}-\mu)}} \qquad (3.15)$$

3.2 Current through Josephson junction with two (different) superconductors

3.2.1 Junctions

In this last section we will leave the case of a bulk superconductor with an impurity (atom) and study the excitation energies in the case of a SNS[5]-/SIS[6]-junction, both for

[5]A junction with superconductors on both sides and a normal region separating them.
[6]A superconductor-junction with two superconductors separated by some sort of point-potential.

the same superconductor on both sides and for the case where the phase of one of the superconductors is changed by a phase θ. When $\theta = 0$ and the potential separating the two superconductors is as before given by a spin-dependent part and a δ-function, we have the results found in the last section. In our case the junction is of 0 length because of the δ-function, so the junction is more a SIS-junction than a SNS-junction, however the SNS-junction-model is of some interest.

Some general notes on junctions For two superconductors separated by a tunneling region (i.e. the distance between the superconductors is short enough for the wave functions to have a non-vanishing overlap), the junction is often called a Josephson junction. Junctions between two superconductors have some interesting properties, depending on the setup. For a Josephson junction there are roughly 3 cases to consider:

1. The DC tunneljunction, where there is no potential between the two superconductors. In this case there is a tunneling current, that flows due to Cooper pairs tunneling between the two sides. It is of order $I = I_c \sin(\theta)$. We will reproduce this current in a moment by applying a phase to the BCS u-function (representing a phase on the order parameter).

2. If a constant potential is applied over the junction we observe that the current oscillates. We will not condsider this time dependent effect.

3. When an oscillating current is applied over the junction, a constant potential over the junction is induced. We are not interested in this effect in this project.

Another effect that is relevant in a SNS-junction is the Andreev reflection. In a superconductor all conduction electrons are paired and hence an incoming electron from the normal metal is either reflected or, when getting paired and continuing in the superconductor, a hole is reflected in the normal metal. When there are superconductors on both sides of the normal region (for a SNS-junction) or if the superconductors have a different phase, fx. by applying a potential between them (in a SIS-junction), an electron can be reflected multiple times and in the limit where the probability of forming a Cooper pair goes to zero, the electron is captured inside the normal region, forming a bound state. An extension to this thesis could be to investigate if an impurity gives rise to Andreev reflections.

3.2.2 Subgap states for a SIS-junction

We will now add the phase θ to the BCS u-function.

For $\Psi(x) = \begin{pmatrix} u \\ v \end{pmatrix} e^{ikx}$ the BdG-equations are satisfied. When adding the phase θ to u and Δ the Schrödinger equation reads

$$\begin{aligned} E \begin{pmatrix} ue^{i\theta} \\ v \end{pmatrix} e^{ikx} &= \begin{pmatrix} -\frac{\hbar}{2m}\frac{d^2}{dx^2} & \Delta e^{i\theta} \\ \Delta^* e^{-i\theta} & \frac{\hbar}{2m}\frac{d^2}{dx^2} \end{pmatrix} \begin{pmatrix} ue^{i\theta} \\ v \end{pmatrix} e^{ikx} \\ &= \begin{pmatrix} \frac{\hbar}{2m}k^2 ue^{i\theta} + \Delta e^{i\theta} v \\ \frac{\hbar}{2m}k^2 v + \Delta^* e^{-i\theta} ue^{i\theta} \end{pmatrix} e^{ikx} \\ &= \begin{pmatrix} \epsilon_F ue^{i\theta} + \Delta e^{i\theta} v \\ -\epsilon_F v + \Delta^* u \end{pmatrix} e^{ikx} \end{aligned}$$

This are exactly the BdG-equations.

The energy for this system is obtained in the exact same way as in the last section. The continuity equation matrix reads

$$\begin{pmatrix} u & v & -u\mathrm{e}^{i\theta} & -v \\ v & u & -v & -u\mathrm{e}^{-i\theta} \\ u\left(-ik_F + (U+JS)\right) & v\left(ik_F - (U+JS)\right) & -iu\mathrm{e}^{i\theta}k_F & ivk_F \\ v\left(-ik_F - (U-JS)\right) & u\left(ik_F + (U-JS)\right) & -ivk_F & iu\mathrm{e}^{-i\theta}k_F \end{pmatrix} \tag{3.16}$$

The spinor $\begin{pmatrix} v \\ u \end{pmatrix}$ is the complexconjugated version of $\begin{pmatrix} u \\ v \end{pmatrix}$. We hence have complexconjugated the added phase in row 2 and 4.

When equating the determinant to zero and solving for E we get 4 very long expression for the energy. They are most easily explored in a computer algebra system like Maple. The energy as function of the phase θ is shown on figure 6.

First we see that the function is 2π-periodic as we would expect. Second we see that the energy function is converging to a constant line for $U \to \infty$, while an increase in the spin-coupling JS bends the function more and lets the minimum (for $E/\Delta > 0$) move towards $E/\Delta = 0$ until it crosses this value for $JS = U$. When increasing JS further (with fixed U) the levels cross as it can be seen on figure 6(c). Further increment of JS leads to the energy levels separating again, converging to a constant function.

As it is seen, there are some jumps in the energy functions. The origin of this jumps could not be completely determined. It doesn't look like it is a numerical problem or a random jump, since we can obtain an analytic expression for the energy functions. When calculating the energy as mentioned above we get the expression

$$E(\theta) = -\Delta \frac{X^2 - 1}{X^2 + 1} \tag{3.17}$$

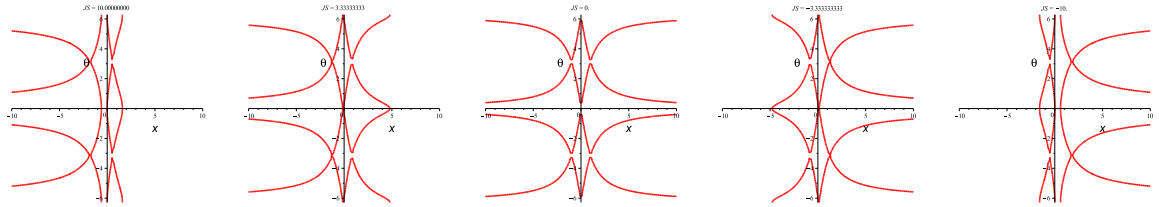
where X is one of the solutions for the polynomial equation

$$\begin{aligned} &(\cos(\theta)k_F^2 - k_F^2)x^4 - 4k_F JSx^3 \\ &+ (2\cos(\theta)k_F^2 - 2JS^2 + 2U^2 + 6k_F^2)x^2 \\ &+ 4k_F JSx + \cos(\theta)k_F^2 - kF^2 = 0 \end{aligned} \tag{3.18}$$

where we have to solve for x. A contourplot of this equation versus the phase and x for $U = 1,\ k_F = 8$ and different values of JS are seen on figure 3. These plots do not have any discontinuities or zero-crossings for the values were we see the jumps. When equating the determinant of the system to 0 and solving for the energy while passing in values for $U,\ k_F$ and JS, we get an expression that has the jumps but has a continuous form. For $k_F = 8,\ JS = 1$ and $U = 5$ we have two positive solutions of the form

$$\frac{1}{1241}\sqrt{835193 + 347480e^{-i\theta} + 347480e^{i\theta}} \\ \pm(9928i)e^{-i\theta}\sqrt{16 - 45e^{2i\theta} + 6e^{3i\theta} + 16e^{4i\theta} + 6e^{i\theta}}$$

they are plotted in figure 4. The jumps occurs at $\theta = \pm\pi$ which is necessary for the energy to be 2π-periodic. But when plotting the same function without using the explicit expression, as done in figure 6, Maple outputs the energy functions with jumps not at $\theta = \pm\pi$, but the functions are still 2π-periodic.



(a) $JS = 10$ (b) $JS = 3$ (c) $JS = 0$ (d) $JS = -3$ (e) $JS = -10$

Figure 3: *Contourplot for the equation (3.18) with* $U = 1$, $k_F = 8$. *The variable* x *is on the first axis, the phase* θ *on the second.*

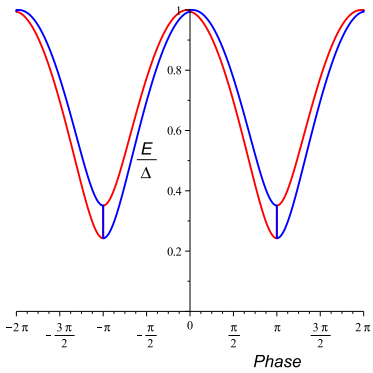


Figure 4: *Two solutions for the energy with* $k_F = 8$, $JS = 1$ *and* $U = 5$. *The jump occurs at* $\theta = \pm\pi$.

It can be observed, when varying the parameters, that the the values of θ where the jumps occur are dependent on JS and U. Increasing U moves the jumps to the left while an increase in JS moves them to the right. After all this is more a problem of choosing a solution, rather than discontinuities in the energy levels.

In [9] (3.8) is rewritten for a SNS-junction in the limit $JS \to 0$ as

$$E^{\pm} = \pm\Delta\sqrt{1 - T\sin(\frac{\theta}{2})^2} \tag{3.19}$$

which is valid for a SNS-junction of length shorter than the coherence length ξ_0. T is the transmission coefficient through the junction in limit $\Delta \to 0$ (the normal state) and depends on the potential U:

$$T = \frac{1}{1 + \frac{U^2}{2k_F^2}}$$

The energy is plotted in figure 5(a) for different values of T.

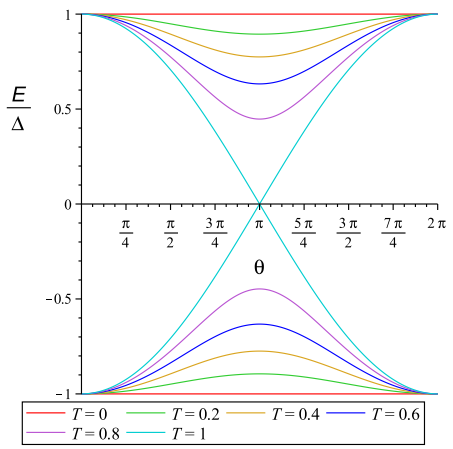
When solving (3.18) using a formula published by Cardano and derived by Ferrari in 1540, we obtain for $JS = 0$

$$X = \frac{\sqrt{-\cos(\theta)\,k_F^2 - 3k_F^2 + \sqrt{U^2 + 4k_F^2}\sqrt{U^2 + 2\cos(\theta)\,k_F^2 + 2k_F^2} - U^2}}{k_F\sqrt{\cos(\theta) - 1}}$$

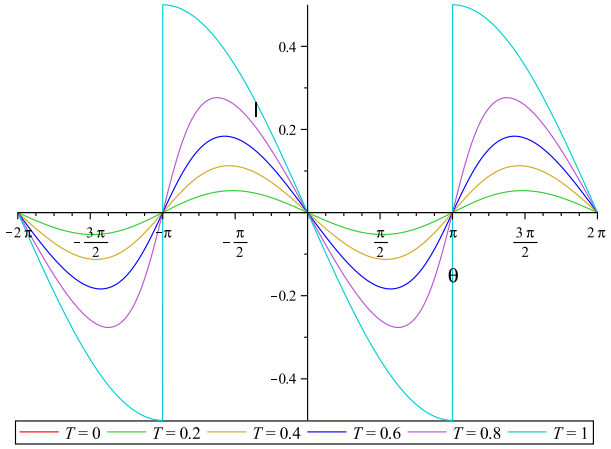
passing this into (3.17), we get exactly (3.19).

The above form of the energy formula can also be obtained by starting with the determinant of (3.16) equated to and simplifying the expression by using (3.7) and the corresponding equation

$$\sin(\phi) = \sqrt{\frac{1}{1 + \alpha^2}} \tag{3.20}$$



(a) *Energy as function of the phase θ for different values of the transmission coefficient T.*



(b) *The supercurrent as function of the phase θ for different values of the transmission coefficient T.*

Figure 5: *The energy (a) and the corresponding supercurrent (b) for the expression (3.19)*

We then get

$$\frac{E^2}{\Delta^2} = \cos(\phi)^2 - \cos(\phi)\sin(\phi)\sin\left(\frac{\theta}{2}\right)^2 \frac{k_F}{JS} + \frac{\sin(\phi)}{2}\left(1-\cos\left(\frac{\theta}{2}\right)\sqrt{1+\left(\frac{2k_F}{JS}\right)^2\sin\left(\frac{\theta}{2}\right)^2+\left(\frac{U}{JS}\right)^2\tan\left(\frac{\theta}{2}\right)^2}\right)$$

In the limit $JS \to 0$ we have $\cos(\phi) \to 1$ and $\sin(\phi) \to 0$ since $\alpha \to \infty$. We then get the above formula for the energy.

$$\begin{aligned}\frac{E^2}{\Delta^2} &= 1 - \frac{1}{1+\left(\frac{U}{2k_F}\right)^2}\frac{1-\cos(\theta)}{2} \\ &= 1 - \frac{1}{1+\left(\frac{U}{2k_F}\right)^2}\sin\left(\frac{\theta}{2}\right)^2\end{aligned}$$

3.2.3 Supercurrent through impurity/SIS-junction

Finally we will find the current that flows through our junction/quantum dot as function of the phase θ. The current through a SNS-junction, with the length of the normal region much smaller than the coherence length ξ_0, is

$$I(\theta) = \frac{2e}{\hbar}\frac{\partial E}{\partial \theta} \tag{3.21}$$

(cf. (22) in [9]) for the occupied bound states. This is a simplification, that we will use to estimate the effect of the chosen potential on the current. A more general formula, that includes the effect of the phase dependence of the order parameter Δ and the density of states, can be found in the paper of P. Bagwell ([12]). Bagwell splits up the current in a continuum part and a discrete part. The continuum part is the current due to the electrons in the conduction bands, i.e. the electrons with energy less than $-\Delta$ or greater than Δ. The discrete part is due to the subgap states. He notes that when the length L

of the normal region is much smaller than the coherence length, as in our case, then the contribution from the continuum is neglectable.

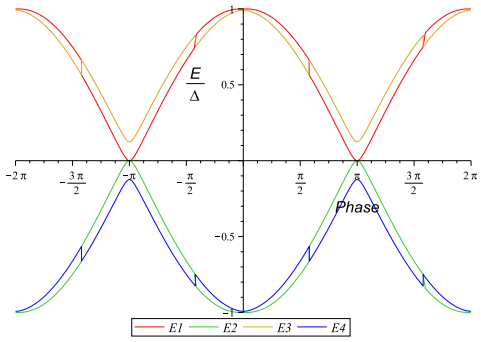
We can use the above formula for the current, even if it is derived for a SNS-junction, because of the impurity inducing a region that can be treated as being normal, due to the breaking of Cooper pairs near it. The decay of the wave function for the impurity bound state is of the order of the coherence length.

The current through a normal SIS-junction with a δ-function (Josephson junction) separating the two superconductors is

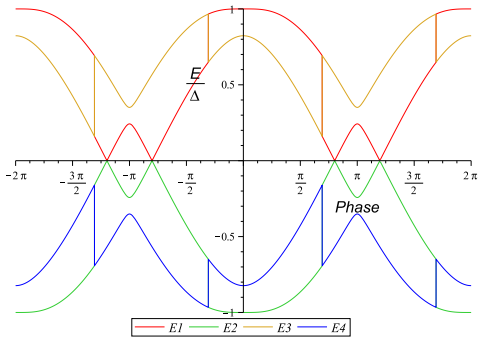
$$I(\theta) = I_c \sin(\theta)$$

This is in full agreement with (3.21) for our impurity bound state energy, where $E = \Delta \cos(\theta)$.

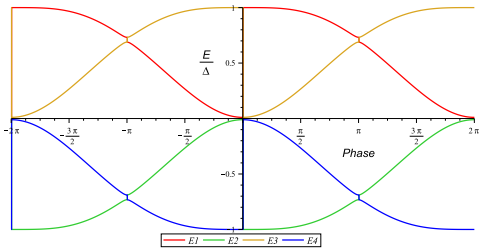
In figure 7 the current is plotted for the energy functions shown in figure 6. We can see that they are no longer clean sinus-oscillations but instead have their maximum close to the energy minimum at $\theta = \pm\pi$ but go sharply to zero for θ converging to $\pm\pi$. For $U \to 0$, the current has a discontinuity at $\theta = \pm\pi$, where it shifts sign, as seen in figure 5(b) for $T = \frac{1}{1-\frac{0}{k_F^2}} = 1$.



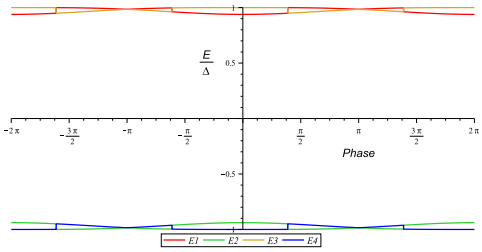
(a) $U = 1,\ JS = 1,\ k_F = 8,\ \Delta = 1$



(b) $U = 1,\ JS = 5,\ k_F = 8,\ \Delta = 1$

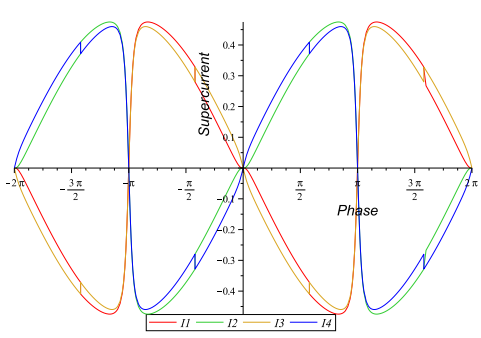


(c) $U = 1,\ JS = 16.2,\ k_F = 8,\ \Delta = 1$

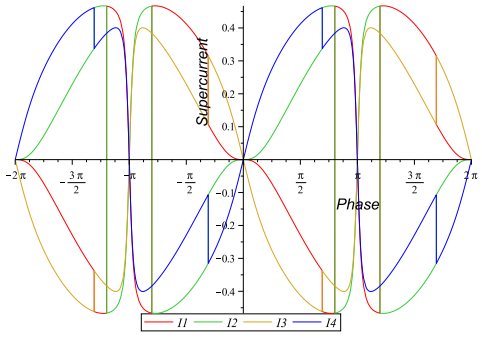


(d) $U = 1,\ JS = 90,\ k_F = 8,\ \Delta = 1$

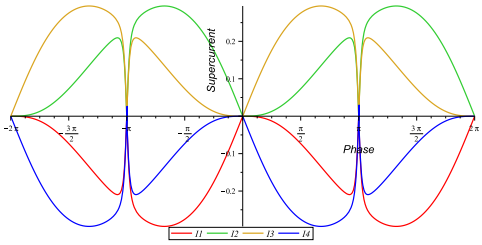
Figure 6: *Energy for the different bound states as function of the phase θ. The jumps are of no physical relevance.*



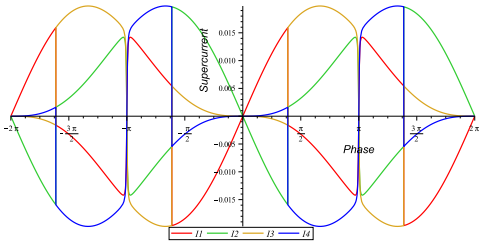
(a) $U = 1,\ JS = 1,\ k_F = 8,\ \Delta = 1$



(b) $U = 1,\ JS = 5,\ k_F = 8,\ \Delta = 1$



(c) $U = 1,\ JS = 16.2,\ k_F = 8,\ \Delta = 1$



(d) $U = 1,\ JS = 90,\ k_F = 8,\ \Delta = 1$

Figure 7: *Supercurrent through the different occupied bound states as function of the phase θ. The jumps are of no physical relevance.*

4 Conclusion and references to the results of others

We have introduced the BCS-theory of superconductivity and have derived the energy and the wave function, that was found by Rusinov, in terms of scattering theory where we reduced our considerations to the one dimensional case with the impurity at $x = 0$ and a left and a right side. We then added a phase to right side to study the energy dependence on this phase and thereby modeling a SIS-junction or a quantum dot. Our method and results reassemble that of section "III. JOSEPHSON CURRENT THROUGH A QUANTUM POINT CONTACT" in [12]. Beenakker and Houten include some more details to the supercurrent by not only taking into account the energy eigenvalue dependence of the phase but also that for the density of states and the order parameter Δ versus the phase. They also argue that adding a constant phase is a good model in the case of a SIS- or S-QD-S-junction:

> *"The characterization of the reservoirs by a constant phase is not strictly correct. The phase of the pair potential has a gradient in the bulk if a current flows. The gradient is* $1/\xi_0$ *when the current density equals the critical current density in the bulk. In our case the critical current is limited by the point contact, so that the gradient of the phase in the bulk is much smaller than* $1/\xi_0$ *[..]. Since the excitation spectrum is determined by the region within* ξ_0 *from the junction, one can safely neglect this gradient in calculating* $I(\delta\phi)$ *from Eq. (2.17)."*

We could reproduce several results as special cases, fx. the result for the energy versus the phase

$$E^{\pm} = \pm\Delta\sqrt{1 - T\sin(\frac{\theta}{2})^2}$$

as presented in [9].

5 Appendices

Appendix A - Normalized impurity wave function

We have to find the coefficient $a_L,\ d_L,\ b_R,\ c_R$ to find the resulting wave function for our impurity bound state. We have to solve the system of continuity equations (3.4):

$$\begin{pmatrix} u & v & -u & -v \\ v & u & -v & -u \\ u(-ik_F)+(U+JS)u & v(ik_F)-(U+JS)v & -u(ik_F) & -v(-ik_F) \\ v(-ik_F)+(U-JS)v & u(ik_F)-(U-JS)u & -v(ik_F) & -u(-ik_F) \end{pmatrix} \begin{pmatrix} a_L \\ d_L \\ b_R \\ c_R \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Evaluating the first two rows (they lead to the same equation when interchanging u and v) we get

$$(a_L - b_R)u + (d_L - c_R)v = 0$$

and hence

$$\begin{aligned} a_L &= b_R \\ d_L &= c_R \end{aligned}$$

Evaluating the third row we get

$$((-ik_F + U + JS)a_L + (-ik_F)b_R)u + ((ik_F - (U+JS))d_L + (ik_F)c_R)v = 0$$

By comparing the coefficients for $U + JS$ we have

$$-a_L u + d_L v = 0$$

This must especially hold for $u = v$ and we hence have

$$a_L = d_L = b_R = c_R$$

We finally have to normalize the wave function. We do this for the left side by calculating the inner product and choosing to set $a_L = d_L = b_R = c_R = 1$.

$$\begin{aligned} &\left((u,v)e^{-ik_+x} + (v,u)e^{ik_-x}\right)\left(\begin{pmatrix} u \\ v \end{pmatrix} e^{-ik_+x} + \begin{pmatrix} v \\ u \end{pmatrix} e^{ik_-x}\right) \\ &= (u^2+v^2) + 2uve^{-i(k_+-k_-)x} + 2uve^{i(k_+-k_-)x} + (v^2+u^2) \\ &= 2 + 2\frac{\Delta}{E}\cos(k_+ - k_-) = 4 \end{aligned}$$

So we have to multiply the coefficients by $\frac{1}{\sqrt{4}}$ and hence have

$$a_L = d_L = b_R = c_R = \frac{1}{\sqrt{4}}$$

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