Yu-Shiba-Rusinov States in Multi-terminal Josephson Junctions

Master's Thesis

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Abstract

In this thesis I will find Yu-Shiba-Rusinov states, living in a multi terminal junction consisting of an Anderson impurity coupled to N different superconductors in the the weak coupling limit. I will examine the states and their energies, and show that the topology of the system seem to heavily involve a coupling parameter, which I will examine in detail. I will also find the supercurrents and study a simple model involving two of these junctions placed in a circuit. This is done with a perspective to outside of this thesis further the study, by considering topological properties of the states involved.

Contents

Chapter 1

Introduction

In recent years multi-terminal devices have found a resurgence in academia because of predictions of topological properties of Andreev bound states formed by the junctions as described by Riwar et al. in 2016 [1] and Heck et al. before them in 2014 [2]. These junctions made use of the scattering approach set forth by Beenakker in his paper on Superconductor-Normal metal-Superconductor (SNS) junctions [3]. From this a multitude of other papers have been written, on the topic of topological properties in multi-terminal junctions, some of which use the same scattering approach [4, 5], while others use a Hamiltonian description [6].

At the same time Josephson junctions have also been predicted to have diode characteristics, both as normal two terminal Josephson junctions [7], but also as multi-terminal devices [8, 9]. These characteristics allow for fabrications of diodes with superconducting properties, which has been previously not possible by use of conventional electrical components.

Apart from these new discoveries of Josephson junction, they are also very popular in the construction of quantum electromagnetic circuits acting as quantum bits (qubits) [10, 11]. There are three common types of qubits constructed with the use of Josephson junctions called a charge, flux or phase qubit, depending on what parameter the circuit is most robust with respect to. A proposed type consist of two different types of Josephson junctions, called 0 and π junctions, which when placed in a large superconducting loop can create a phase qubit [12, 13].

In this thesis I will follow in the footsteps of Kiršanskas et al. [14], but generalize to a multi-terminal system. This will be done with a Hamiltonian description describing a multi-terminal Josephson junctions consisting of N similar s-wave superconductors, which I will refer to as the leads. These leads will differ only in their complex phases, they will all couple to a singly occupied spin-split Anderson impurity, which I will refer to as the dot. This will be done in the weak lead-dot coupling limit, while allowing unequal couplings, with the spin of the dot polarized. In this limit I will find the type of bound states which are commonly known as Yu-Shiba-Rusinov (YSR) states [15–17], which are different to the Andreev bound states studied by most. I will in detail examine the parameters of the states and their energies, to get a sense of the topological properties of the system, and show how one might use these multi-terminal junctions in circuits to possibly create qubits.

Chapter 2

Preface

2.1 Prerequisites

Throughout this thesis I will assume that the reader in their education of quantum mechanics have learned about second quantization, to the same level of understanding as having read "Modern Quantum Mechanics" by Sakurai [11]. For a full understanding of this thesis I also recommend having read most of the book "Many-body quantum theory in condensed matter physics - an introduction" by Bruus and Flensberg [18] or any similar introductory book on theoretical condensed matter physics.

2.2 Notations

I will throughout the thesis make use of natural units, in the sense that everything is measured in units of $\hbar$, which amounts to setting $\hbar = 1$.

I will also for variables with multiple arguments write the arguments as subscripts on a compact form to minimize used space, such that for a variable v with arguments a and b, the notation v_{ab} is to be understood as $v_{a,b} = v(a,b)$. At times however the notation $v_{a,b}$ means $(v_a)_b$, like the case of the free Green's functions G_0, where $G_{0,k}$ is to be understood as the free Green's function as a function of momentum $(G_0)_k$. This should however be quite clear from the context.

I will also be working with matrices and vectors in two different bases, one for the physical system of N leads with an index $\alpha \in \{1, 2, \ldots, N\}$ running over the different superconductors coupled to the dot, and a non-physical basis of N channels with an index $\nu \in \{1, 2, \ldots, N\}$ running over respective channels. In this non-physical basis I will write the matrices and vectors with a $\sim$ above, to make it easier to differentiate between the two types. Meaning that $\tilde{\boldsymbol{M}}$ is a matrix in the non-physical basis, while $\boldsymbol{M}$ is the same matrix but written in the physical basis. This will be made more clear in chapter 5, where the non-physical base is introduced.

I will also at times, such as in chapter 4, make use of collective indices, to minimize used space, where I will write $\mu = \{\alpha, \sigma, k\}$ as a collective index, and define the negative of this as $\bar{\mu} = \{\alpha, -\sigma, -k\}$.

I will also at times work with matrices where I will neglect to write identity matrices $\mathbb{1}$ if possible, such that for a number $a \in \mathbb{C}$ and a matrix $\boldsymbol{M} \in M_{N\times N}(\mathbb{C})$, the formula $a - \boldsymbol{M}$ is to be understood as $a\mathbb{1}_{\boldsymbol{N}\times\boldsymbol{N}} - \boldsymbol{M}$. I will also neglect to write the size of the identity matrices such that the size of $\mathbb{1}$ is to understood from the context.

Chapter 3

The system

I will be examining a system comprising of $N \geq 2$ identical s-wave superconductors, as described below in section 3.1, surrounding a single quantum dot with electron-electron Coulomb repulsion and a magnetic spin splitting, which is described in section 3.2. This creates what I will call a multi-terminal quantum dot Josephson junction or in the case of a specific number of superconductors an N-terminal quantum dot Josephson junction.

While this system can be thought of as a something one can create in a lab, like in the examples of physically realized multi-terminal junctions from the experimental papers by Graziano et al. [19] and Chiles et al. [9] as seen in figures 3.1a-3.1c. An impurity coupled to N superconducting leads, is also analogous to a superconductor with an impurity embedded inside. Here the number of leads in my system would then correspond to the number of channels coupling to the impurity inside, which would depend on the type of superconductor.

In this thesis, my system will have no lead-lead coupling, even though according to paper by Klees et al. [6] it might lead to important physics. This is done for simplicity of the model, but might be a subject of later research.

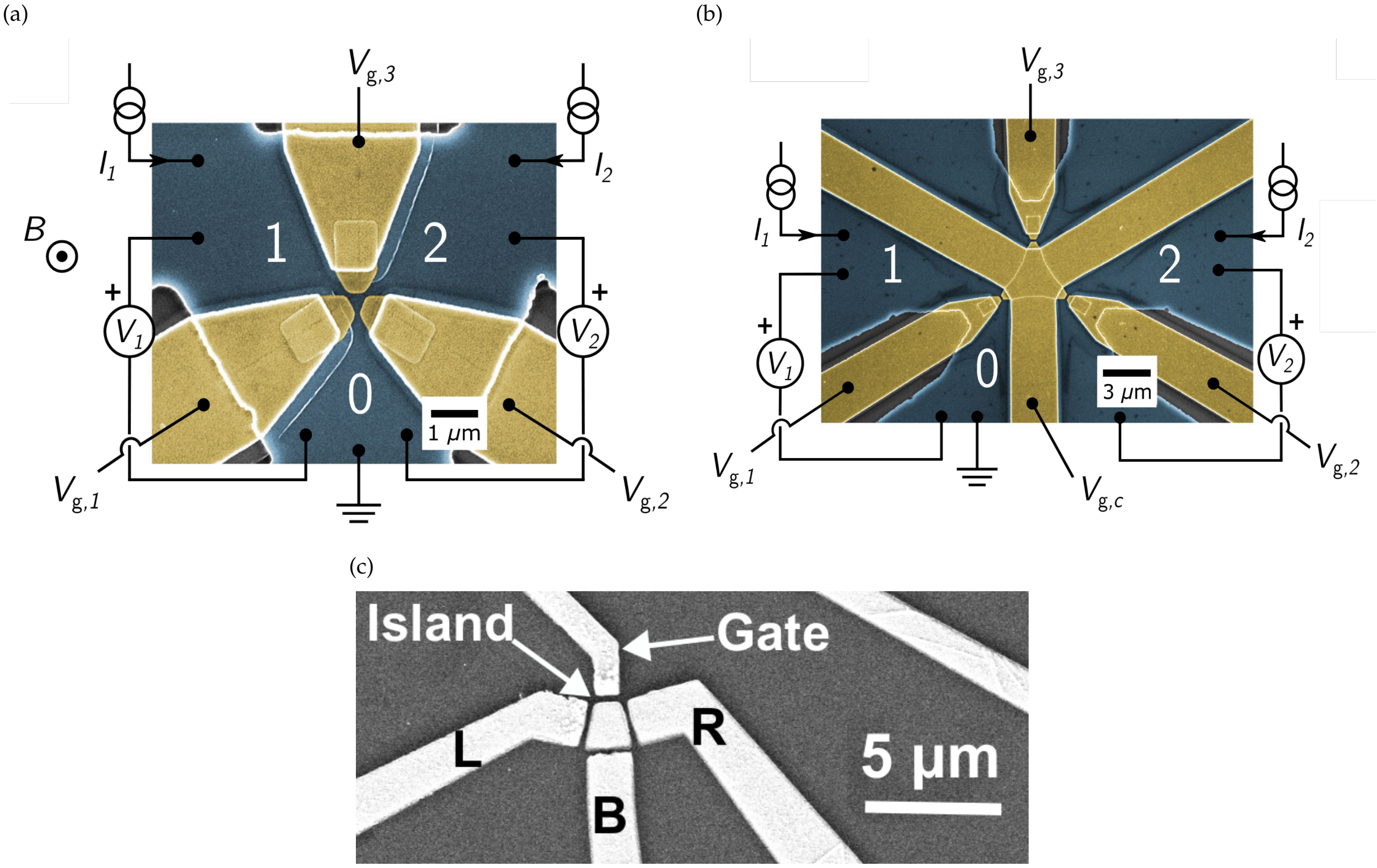


Figure 3.1: Three different physically realized three terminal junctions; (a) and (b) adapted from [19], and (c) adapted from [9]

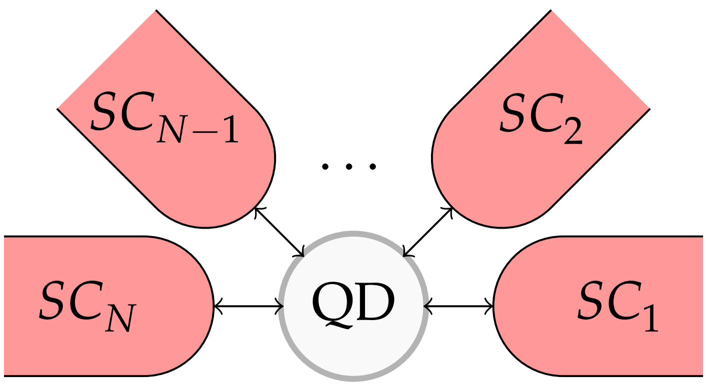


Figure 3.2: Schematic of the multi-terminal quantum dot Josephson junction, consisting of a quantum dot (QD), surrounded by N superconductors (SC_α).

3.1 Superconductors

In this section I describe superconductivity by using the model called the Bardeen-Cooper-Schrieffer (BCS) model. By applying a mean field approach this will turn into a theory describing the most common type of superconductivity. The BSC model is as follows in a momentum basis

$$H_{BCS} = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}, \tag{3.1}$$

with the biased dispersion $\xi_k = \epsilon_k - \mu$, where $\epsilon_k = \frac{k^2}{2m}$ is the usual electron dispersion relation, such that $\xi_{-k} = \xi_k$, μ is a chemical potential and $c^\dagger_{k\sigma}$ ($c_{k\sigma}$) is the usual creation (annihilation) operator for electrons with momentum k and spin σ. Note that the annihilation operator will at times be called a hole creation operator because I assume a background of filled states called the Fermi sea, such that removing an electron is the same as creating a hole.

For simplicity ξ_k is here taken to be spin independent. It is in appendix A.2 found for with spin, which will be used later on. The first term describes the energy of the single electrons, while the second term describes a potential interaction between pairs of quasi-particles called Cooper pairs, which are pairs of electrons with opposite momentum and opposite spins that behave as a composite bosonic particle. By taking this model and describing it using a Hartree-Fock mean field approach, the Hamiltonian changes to the form

$$H_{SC} \equiv H^{MF}_{BCS} = \sum_{k,\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \left(\Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \right), \tag{3.2}$$

where the so called order parameter is given as

$$\Delta_k = -\sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle . \tag{3.3}$$

With the usual notation of $\langle A \rangle$ being the expectation value of an operator A. I will throughout the rest of the thesis only consider the type of superconductors for which $V_{kk'}$ is even in k, such that $\Delta_{-k} = \Delta_k$. Further down I will restrict this even more to s-wave superconductors for which $\Delta_k = \Delta$, but for the time being I will keep it general. Also crucially note that the superconducting order parameter $\Delta_k \in \mathbb{C}$ is generally complex, which will be very important for the rest of the thesis. It can from here be shown that this will lead to zero resistivity and therefore also infinite conductance, among other things, whereby the name superconductor comes, this however is outside the scope of this thesis, but can be found in most modern condensed matter textbooks [18, 20].

Bogoliubov quasi-particles

To diagonalize this mean-field BCS Hamiltonian (3.2), quasi-particles called Bogoliubov quasi-particles or sometimes just Bogoliubons are introduced. A hint of how to define them is found by taking the commutator of the annihilation and creation operators of the electrons with the Hamiltonian to see how they evolve in time, since Heisenberg's equation of motion tells us, for an operator A

$$\frac{dA}{dt} = -i[A,H] + \frac{\partial A}{\partial t}\,. \tag{3.4}$$

By inserting the Heisenberg picture annihilation operator, it then becomes

$$i\,\frac{dc_{k\sigma}}{dt} = [c_{k\sigma}, H] = \xi_k c_{k\sigma} - \sigma\Delta_k c^{\dagger}_{-k-\sigma}\,, \tag{3.5}$$

where the commutator was found using the relation $[A, BC] = \{A,B\}C - B\{A,C\}$ together with the fermionic anti-commutator relation $\{c_\mu, c^{\dagger}_{\mu'}\} = \delta_{\mu,\mu'}$, with μ and μ' being collective indices $\mu = k,\sigma$. Since the Hamiltonian is hermitian ($H^{\dagger} = H$) it also follows that

$$i\,\frac{dc^{\dagger}_{-k-\sigma}}{dt}(t) = [c^{\dagger}_{-k-\sigma}(t), H] = -[c_{-k-\sigma}(t), H]^{\dagger} = -\xi_k c^{\dagger}_{-k-\sigma}(t) - \sigma\Delta^*_k c_{k\sigma}(t)\,. \tag{3.6}$$

This shows that electrons evolve into holes, and holes similarly evolve into electrons. Therefore stable quasi-particles will have to involve some mix of both electron and hole operators. Taking inspiration from equation (3.5) I define that the electron annihilation operator is a mix of this proposed stable quasi-particle's creation and annihilation operators.

$$c_{k\sigma} = u_k\gamma_{k\sigma} + \sigma v_k \gamma^{\dagger}_{-k-\sigma}\,. \tag{3.7}$$

These quasi-particles are defined to be fermionic particles, such that they also obey the fermionic anti-commutation relation $\{\gamma_{k\sigma}, \gamma_{k'\sigma'}\} = \{\gamma^{\dagger}_{k\sigma}, \gamma^{\dagger}_{k'\sigma'}\} = 0$ and $\{\gamma_{k\sigma}, \gamma^{\dagger}_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}$, meaning that the change from electrons to this quasi-particles is a canonical transformation. By then writing the usual anti-commutation relations for the electrons in terms of the quasi-particles, it follows that

$$\{c_{k\sigma}, c_{k'\sigma'}\} = \sigma(v_k u_{-k} - v_{-k}u_k)\delta_{k,-k'}\delta_{\sigma,-\sigma'} \stackrel{!}{=} 0 \tag{3.8}$$

$$\{c_{k\sigma}, c^{\dagger}_{k'\sigma'}\} = (|u_k|^2 + |v_{-k}|^2)\delta_{kk'}\delta_{\sigma\sigma'} \stackrel{!}{=} \delta_{kk'}\delta_{\sigma\sigma'} \tag{3.9}$$

which is most readily solved by letting $u_{-k} = u_k$ and $v_{-k} = v_k$, as well as $|u_k|^2 + |v_k|^2 = 1$. This means that for the time evolution of the quasi-particle to be stable it must hold that

$$i\,\frac{d\gamma_{k\sigma}}{dt} = [\gamma_{k\sigma}, H] \stackrel{!}{=} E_{k\sigma}\gamma_{k\sigma}\,, \tag{3.10}$$

which by calculating the commutator

$$\begin{aligned}[\gamma_{k\sigma}, H] = &\left[\xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u^*_k v^*_k + \Delta^*_k u_k v_k\right]\gamma_{k\sigma} \\ &+ \left[2\sigma\xi_k v_k u^*_k - \sigma\Delta_k (u^*_k)^2 + \sigma\Delta^*_k v_k^2\right]\gamma^{\dagger}_{-k-\sigma}\,,\end{aligned} \tag{3.11}$$

shows us that

$$E_{k\sigma} = \xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u_k^* v_k^* + \Delta_k^* u_k v_k \tag{3.12}$$

$$0 \stackrel{!}{=} 2\xi_k v_k u_k^* - \Delta_k (u_k^*)^2 + \Delta_k^* v_k^2 \,. \tag{3.13}$$

Note that even though the quasi-particle have a spin degree of freedom, from the right hand side (RHS) of equation (3.12) it follows that the energy of the quasi-particle is spin-independent $E_{k\sigma} = E_k$. This however is only true because of the assumption of the electron energy ξ_k being spin independent, the general case is considered in appendix A.2. In appendix A.1 I then find that the energy and the constants u_k and v_k must follow from the relations

$$E_k^2 = \xi_k^2 + |\Delta_k|^2 \tag{3.14}$$

$$|u_k|^2 = \frac{1}{2} + \frac{\xi_k}{2E_k} \tag{3.15}$$

$$|v_k|^2 = \frac{1}{2} - \frac{\xi_k}{2E_k} \tag{3.16}$$

$$\arg(\Delta_k) \equiv \arg(u_k) + \arg(v_k) \pmod{2\pi} \,. \tag{3.17}$$

Note that this gives two energy solutions, one positive and one negative. I can therefore define that the quasi-particle creation or annihilation operator gives either a positive or negative energy excitation. I will here consider creation operators $\gamma_{k\sigma}^\dagger$ as being positive energy excitations, such that

$$H_{SC} = \sum_{k\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + const \tag{3.18}$$

$$E_k = \sqrt{\xi_k^2 + |\Delta_k|^2} \,. \tag{3.19}$$

In the more general case shown in appendix A.2, with a spin dependent electron energy $\xi_{k\sigma} = \xi_k + \xi_\sigma$, the quasi-particle energy gain the same energy contribution as the electrons

$$E_{k\sigma} = E_k + \xi_\sigma \tag{3.20}$$

$$= \sqrt{\xi_k^2 + |\Delta_k|^2} + \xi_\sigma \,. \tag{3.21}$$

3.2 Quantum dot

Quantum dots are one of the most simple systems, one can think of. It is a point like system with just one electron level, such that the system have three different configurations: empty, singly or doubly occupied.

Physically it can be approximated by having large enough level splittings to allow for just a subset of levels to be considered. In this thesis I will consider a level with a spin splitting and a charging energy $U > 0$, accounting for effects such as Coulomb repulsion, giving the dot Hamiltonian

$$H_D = \sum_\sigma \xi_{d\sigma} d_\sigma^\dagger d_\sigma + U n_\downarrow n_\uparrow \,, \tag{3.22}$$

with the biased energies $\xi_{d\sigma} = \xi_d + \frac{\sigma g_d B}{2} = \epsilon_d + \mu_d + \frac{\sigma g_d B}{2}$ being the energy levels of an spin σ electron in a magnetic field, where g_d is the coupling factor of the electron on the dot to the magnetic field, and $n_\sigma = d_\sigma^\dagger d_\sigma$ being the electron number operator for spin σ on the dot, such that the Coulomb repulsion energy U is only experienced from having a fully filled level, such that a spin up and a spin down electron is located on the dot. The energy levels is seen in figure 3.3, where one can see that there exists a special tuning for the potential μ_d, which allow for a particle-hole symmetry to form for the singly occupied states, meaning that the energy needed to remove an electron is the same as adding one.

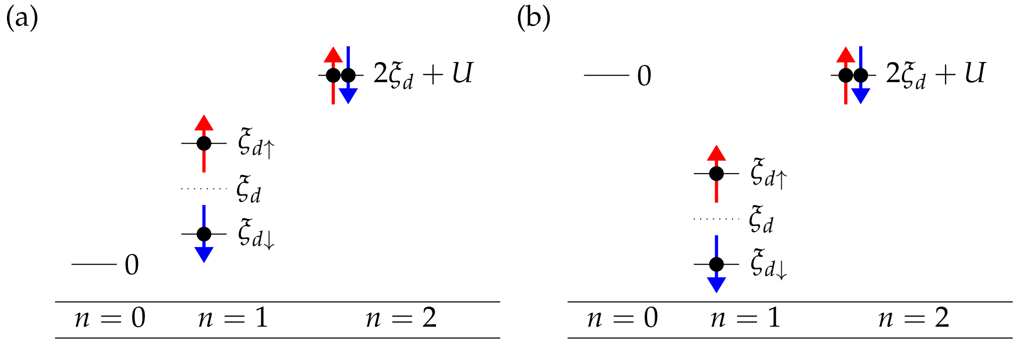


Figure 3.3: Energy levels of a quantum dot with spin splitting. In (a) level position ξ_d is larger than 0, while in (b) the level position follow the relation $2\xi_d = -U$.

3.3 Combined elements

By combining each element of the system, and allowing for tunneling between the dot and each superconductor (but not directly from superconductor to superconductor), the system is then described by the total Hamiltonian

$$H = H_{SC} + H_D + H_T \,, \tag{3.23}$$

with the elements

$$H_{SC} = \sum_{\alpha k \sigma} \xi_{\alpha k \sigma} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} - \sum_{\alpha k} \left(\Delta_\alpha c_{\alpha k \uparrow}^\dagger c_{\alpha - k \downarrow}^\dagger + \Delta_\alpha^* c_{\alpha - k \downarrow} c_{\alpha k \uparrow} \right) \tag{3.24}$$

$$H_D = \sum_\sigma \xi_{d\sigma} d_\sigma^\dagger d_\sigma + U n_\downarrow n_\uparrow \tag{3.25}$$

$$H_T = \sum_{\alpha k \sigma} \left(t_\alpha c_{\alpha k \sigma}^\dagger d_\sigma + t_\alpha^* d_\sigma^\dagger c_{\alpha k \sigma} \right) \,. \tag{3.26}$$

Where the index $\alpha \in \{1, 2, \ldots, N\}$ run over the different superconductors coupled to the dot. The superconducting order parameters $\Delta_\alpha = |\Delta_\alpha| e^{i\phi_\alpha}$ are taken to be momentum independent.

I will note that in a more in depth description [21], the phases ϕ_α need to be quantum operators which are the conjugate of the Cooper pair number operator in the large Cooper pair limit, $[\phi_\alpha, n_\alpha^{(CP)}] = i$, but here it is just considered a parameter, because of the mean field description of the order parameter in equation (3.3).

The biased electron energy dispersions $\xi_{\alpha k\sigma} = \xi_{\alpha k} + \frac{\sigma g_\alpha B}{2} \equiv \xi_{\alpha k} + \xi_{\alpha\sigma}$, are taken to be spin dependent by coupling to a magnetic field B, with coupling factors g_α. The term H_T describes the tunneling from the different superconductors to the dot with a complex coupling strength t.

Note that to be more precise, one would have to use momenta k_α which depend on the superconductor they belong to, however I will not keep track of it here and therefore implicitly assume equal sets of momenta in each superconductor $\{k_\alpha\} = \{k_{\alpha'}\} \equiv \{k\}$ for all α and α'. I immediately perform N different U(1) gauge transformation for the creation and annihilation operators of the electrons in the superconductors

$$c_{\alpha k\sigma} \to e^{i\phi_\alpha/2} c_{\alpha k\sigma} \,.$$

Which moves the phases onto the coupling constants t_α instead, giving the transformed Hamiltonians

$$H_{SC} \to \sum_{\alpha k\sigma} \xi_{k\sigma} c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma} - \sum_{\alpha k} |\Delta_\alpha| \left(c^\dagger_{\alpha k\uparrow} c^\dagger_{\alpha -k\downarrow} + c_{\alpha -k\downarrow} c_{\alpha k\uparrow} \right) \tag{3.27}$$

$$H_T \to \sum_{\alpha k\sigma} \left(t_\alpha e^{-i\phi_\alpha/2} c^\dagger_{\alpha k\sigma} d_\sigma + t^*_\alpha e^{i\phi_\alpha/2} d^\dagger_\sigma c_{\alpha k\sigma} \right) \,. \tag{3.28}$$

Which in turn also mean that the coefficients of the Bogoliubov quasi-particles $v_{\alpha k}, u_{\alpha k} \in \mathbb{R}$ can be defined to be real from equation (3.17).

Chapter 4

Schrieffer-Wolff transformation - An interaction expansion

Since the Hamiltonian for the system is quite complicated, it can be more enlightening to make use of some sort of expansion, which can be truncated to some appropriate order, to make the model simpler. The most common type is the usual perturbation theory described in most quantum mechanics textbooks [11], where by expansion in a small parameter the Hamiltonian can be truncated to some appropriate order of the parameter. Here I will follow the example of reference [14], and make use of a Schrieffer-Wolff (SW) transformation [22, 23], which is a perturbation theory that uses an expansion in interactions, much like a Feynman diagram expansions. I will do this by closely following the paper of Salomaa [24].

Mathematically the SW transformation is a unitary transformation, which is defined as

$$H_S \equiv e^S H e^{-S} \tag{4.1}$$

$$H_S^{(1)} \overset{!}{=} H_{SC} + H_D = H_0\,, \tag{4.2}$$

where $H_S^{(1)}$ is the first order expansion of H_S in terms of H_T and S, meaning that to the first order, the interaction H_T is removed. Since the transformation is unitary, it preserves the eigenenergies and has similar eigenstates $\psi_S = e^S\psi$, where ψ is the eigenstates of the original Hamiltonian. This transformation is generated by some time-independent skew-hermitian operator $S^\dagger = -S$, which is easily satisfied by defining $S = S^+ - S^-$, with $\left(S^+\right)^\dagger = S^-$. To determine the form of this operator, I start of by making use of the Baker–Campbell–Hausdorff (BCH) relation

$$e^S H e^{-S} = H + [S, H] + \frac{1}{2!}[S, [S, H]] + \mathcal{O}(S^3)\,.$$

Note that since the expansion is in terms of higher and higher orders of S, to be able to truncate it to some order, the system must be in a regime where the scale of S must be smaller than 1. As I will show this scale is related to the scale of the removed interaction compared to all other energy scales of the system.

To the first order in H_T and S the BCH expansion shows that

$$H_S^{(1)} = H_0 + H_T + [S, H_0] \stackrel{!}{=} H_0 \,. \tag{4.3}$$

Meaning that I need to find an operator S^+ such that

$$H_T + [S^+, H_0] + [S^+, H_0]^\dagger \stackrel{!}{=} 0 \tag{4.4}$$

Since a lot of indicies are involved in the description of electron in the superconductors, I will here define some collective indices $\mu = \{\alpha, k, \sigma\}$ and $\bar{\mu} = \{\alpha, -k, -\sigma\}$ and phase shifted couplings, such that the electron and Bogoliubov quasi-particle operators and the couplings are

$$c_\mu \equiv u_\mu \gamma_\mu + v_\mu \gamma_{\bar{\mu}}^\dagger \tag{4.5}$$
$$\gamma_\mu \equiv u_\mu c_\mu + v_{\bar{\mu}} c_{\bar{\mu}}^\dagger = u_\mu c_\mu - v_\mu c_{\bar{\mu}}^\dagger \tag{4.6}$$
$$u_\mu \equiv u_{\alpha k} \tag{4.7}$$
$$v_\mu \equiv \sigma v_{\alpha k} \tag{4.8}$$
$$t_\mu \equiv t_\alpha e^{-i\phi_\alpha/2}, \tag{4.9}$$

such that in terms of Bogoliubov quasi-particles the transport Hamiltonian is given as

$$H_T = \sum_\mu t_\mu \left(u_\mu \gamma_\mu^\dagger d_\sigma + v_\mu \gamma_{\bar{\mu}} d_\sigma \right) + H.C \,. \tag{4.10}$$

To find an S^+ that cancel this I will make use of the ansatz that it must be of a similar form in terms of creation and annihilation operators

$$S^+ = \sum_\mu t_\mu \left(x_\mu \gamma_\mu^\dagger d_\sigma + y_\mu \gamma_{\bar{\mu}} d_\sigma \right) \,. \tag{4.11}$$

The commutator in equation (4.4) is then given by

$$[H_0, S^+] = \left[\sum_\mu E_\mu \gamma_\mu^\dagger \gamma_\mu + \sum_\sigma \xi_{d\sigma} d_\sigma^\dagger d_\sigma + U n_\downarrow n_\uparrow, \sum_{\mu'} t_{\mu'} \left(x_{\mu'} \gamma_{\mu'}^\dagger d_{\sigma'} + y_{\mu'} \gamma_{\bar{\mu}'} d_{\sigma'} \right) \right] \,. \tag{4.12}$$

Assuming that x_μ and y_μ behaves as numbers for the operators involved, such that $[x_\mu, \mathcal{O}_{\mu'}] = [y_\mu, \mathcal{O}_{\mu'}] = 0$ for $\mathcal{O}_{\mu'} \in \{\gamma_{\mu'}, \gamma_{\mu'}^\dagger, n_{\sigma'}\}$, and making use of the relevant commutators which I have found in appendix B.1, the commutator becomes

$$[H_0, S^+] = \sum_{\mu'} t_{\mu'} \left[\left(E_{\mu'} - \xi_{d\sigma'} - U n_{-\sigma'} \right) x_{\mu'} \gamma_{\mu'}^\dagger d_{\sigma'} - \left(E_{\bar{\mu}'} + \xi_{d\sigma'} + U n_{-\sigma'} \right) y_{\mu'} \gamma_{\bar{\mu}'} d_{\sigma'} \right] \,. \tag{4.13}$$

Meaning that to solve $[H_0, S^+] \stackrel{!}{=} H_T$, I can simply define that

$$x_\mu \equiv \frac{u_\mu}{E_\mu - \xi_{d\sigma} - Un_{-\sigma}} \tag{4.14}$$

$$y_\mu \equiv \frac{-v_\mu}{E_{\bar{\mu}} + \xi_{d\sigma} + Un_{-\sigma}} \,. \tag{4.15}$$

Here the number operator in the denominator is to be understood by the Taylor expansion of the functions. Since electron number operators satisfy $\langle n_\sigma^k \rangle = \langle n_\sigma \rangle$ for $k \in \mathbb{N} \setminus \{0\}$, only two terms are involved

$$x_\mu \equiv x_\mu^{(0)} + n_{-\sigma}\tilde{x}_\mu \tag{4.16}$$

$$y_\mu \equiv y_\mu^{(0)} + n_{-\sigma}\tilde{y}_\mu \,, \tag{4.17}$$

with the number operator evaluated constants being defined as

$$x_\mu^{(0)} = x_\mu(n_{-\sigma} = 0) \tag{4.18}$$

$$\tilde{x}_\mu = x_\mu(n_{-\sigma} = 1) - x_\mu(n_{-\sigma} = 0) \,, \tag{4.19}$$

with the y constants being similarly defined. It is also important to note that since the electron energies are even in k, the operators are also even $x_{\alpha k\sigma} = x_{\alpha -k\sigma}$, $y_{\alpha k\sigma} = y_{\alpha -k\sigma}$, and because only electron number operators are involved, they are also hermitian $x_\mu = x_\mu^\dagger$ and $y_\mu = y_\mu^\dagger$.

This mean that the S^+ operator can be defined as

$$S^+ = \sum_\mu t_\mu \left((x_\mu^{(0)} + n_{-\sigma}\tilde{x}_\mu)\gamma_\mu^\dagger d_\sigma + (y_\mu^{(0)} + n_{-\sigma}\tilde{y}_\mu)\gamma_{\bar{\mu}} d_\sigma \right) \,. \tag{4.20}$$

This then sets the scale of S, which shows directly that the regime the system must be in for the truncation to some low order in S to be valid, must be one where

$$|t_\alpha| \ll |U + \xi_{d\sigma} - \xi_{\alpha\sigma} \pm E_{\alpha k}| \tag{4.21}$$

$$|t_\alpha| \ll |\xi_{d\sigma} - \xi_{\alpha\sigma} \pm E_{\alpha k}| \,, \tag{4.22}$$

meaning that the coupling between each lead and the dot must be small compared to the other energies of the system.

Since the system of $H_S^{(1)}$ is one without interaction, to regain some interesting physics I will move on to second order in S and H_T, such that I get back some effective interactions

$$\begin{aligned} H_S^{(2)} &= H_0 + H_T + [S, H_0] + [S, H_T] + \frac{1}{2}[S, [S, H_0]] \\ &= H_0 + \frac{1}{2}[S, H_T] \,. \end{aligned} \tag{4.23}$$

Then by again splitting it into S^+ and S^-, and also splitting H_T into H_T^+ and H_T^- with

$$H_T^- = \sum_\mu t_\mu^* d_\sigma^\dagger c_\mu \,, \tag{4.24}$$

and $H_T^+ = (H_T^-)^\dagger$, I get that for the part of the second order contribution involving H_T^-, I find the commutator

$$[S^+, H_T^-] = \sum_{\mu,\mu'} t_\mu t_{\mu'}^* [(x_\mu^{(0)} + n_{-\sigma}\tilde{x}_\mu)\gamma_\mu^\dagger d_\sigma + (y_\mu^{(0)} + n_{-\sigma}\tilde{y}_\mu)\gamma_{\bar{\mu}} d_\sigma \,,\, d_{\sigma'}^\dagger c_{\mu'}] \,. \tag{4.25}$$

By making use of the other commutators from appendix B.1, this simplifies to

$$\begin{aligned}[S^+, H_T^-] = \sum_{\mu,\mu'} t_\mu t_{\mu'}^* \{ &(x_\mu^{(0)} + \tilde{x} n_{-\sigma})(-u_\mu n_\sigma \delta_{\mu\mu'} + \gamma_\mu^\dagger c_{\mu'} \delta_{\sigma\sigma'}) + \tilde{x}_\mu \bar{n}_\sigma c_{\mu'} \gamma_\mu^\dagger \delta_{-\sigma\sigma'} \\ &+ (y_\mu^{(0)} + \tilde{y} n_{-\sigma})(-v_\mu n_\sigma \delta_{\mu\mu'} + \gamma_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'}) + \tilde{y}_\mu \bar{n}_\sigma c_{\mu'} \gamma_{\bar{\mu}} \delta_{\sigma'-\sigma} \} \,,\end{aligned} \tag{4.26}$$

where I have defined a dot spin flip operator as $\bar{n}_\sigma \equiv d_{-\sigma}^\dagger d_\sigma$.

By writing out the definition of the Bogoliubov operators defined by equation (4.6), the commutator in terms of the electron annihilation and creation operators become

$$\begin{aligned}[S^+, H_T^-] = \sum_{\mu,\mu'} t_\mu t_{\mu'}^* \{ &(x_\mu^{(0)} u_\mu + y_\mu^{(0)} v_\mu)(c_\mu^\dagger c_{\mu'} \delta_{\sigma\sigma'} - n_\sigma \delta_{\mu\mu'}) \\ &+ (\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu)(n_{-\sigma} c_\mu^\dagger c_{\mu'} \delta_{\sigma\sigma'} - n_{-\sigma} n_\sigma \delta_{\mu\mu'} - \bar{n}_\sigma c_\mu^\dagger c_{\mu'} \delta_{-\sigma\sigma'}) \\ &+ (\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu)(n_{-\sigma} c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} - \bar{n}_\sigma c_{\bar{\mu}} c_{\mu'} \delta_{-\sigma\sigma'}) \\ &+ (y_\mu^{(0)} u_\mu - x_\mu^{(0)} v_\mu) c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} \} \,.\end{aligned} \tag{4.27}$$

Similarly for the part of the second order contribution involving H_T^+, I find the commutator

$$[S^+, H_T^+] = \sum_{\mu,\mu'} t_\mu t_{\mu'} [(x_\mu^{(0)} + n_{-\sigma}\tilde{x}_\mu)\gamma_\mu^\dagger d_\sigma + (y_\mu^{(0)} + n_{-\sigma}\tilde{y}_\mu)\gamma_{\bar{\mu}} d_\sigma \,,\, c_{\mu'}^\dagger d_{\sigma'}] \,, \tag{4.28}$$

which by making use of the rest of the commutators from appendix B.1, reduce to

$$\begin{aligned}[S^+, H_T^+] = \sum_{\mu,\mu'} t_\mu t_{\mu'} \{ &- x_\mu^{(0)} v_\mu d_{-\sigma} d_\sigma \delta_{\mu\bar{\mu}'} + \tilde{x}_\mu d_{-\sigma} d_\sigma c_{\mu'}^\dagger \gamma_\mu^\dagger \delta_{-\sigma\sigma'} \\ &+ y_\mu^{(0)} u_\mu d_{-\sigma} d_\sigma \delta_{\mu\bar{\mu}'} + \tilde{y}_\mu d_{-\sigma} d_\sigma c_{\mu'}^\dagger \gamma_{\bar{\mu}} \delta_{-\sigma\sigma'} \} \,.\end{aligned} \tag{4.29}$$

Once again inserting the definition the Bogoliubov operators, this in terms of the electron operators gives

$$\begin{aligned}[S^+, H_T^+] = \sum_{\mu,\mu'} t_\mu t_{\mu'} \{ &(\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu) d_{-\sigma} d_\sigma c_{\mu'}^\dagger c_{\bar{\mu}} \delta_{-\sigma\sigma'} \\ &+ (\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu) d_{-\sigma} d_\sigma c_{\mu'}^\dagger c_\mu^\dagger \delta_{-\sigma\sigma'} + (y_\mu^{(0)} u_\mu - x_\mu^{(0)} v_\mu) d_{-\sigma} d_\sigma \delta_{\bar{\mu}\mu'} \} \} \,.\end{aligned} \tag{4.30}$$

By then combining each of the two commutators, the full commutator $[S, H_T] = ([S^+, H_T^+] + [S^+, H_T^-]) + ([S^+, H_T^+] + [S^+, H_T^-])^\dagger$ becomes

$$
\begin{aligned}
[S, H_T] = \sum_{\mu,\mu'} t_\mu t^*_{\mu'} \{ & (x^{(0)}_\mu u_\mu + y^{(0)}_\mu v_\mu + x^{(0)}_{\mu'} u_{\mu'} + y^{(0)}_{\mu'} v_{\mu'})(c^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} - n_\sigma \delta_{\mu\mu'}) \\
& + (\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu + \tilde{x}_{\mu'} u_{\mu'} + \tilde{y}_{\mu'} v_{\mu'})[(n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c^\dagger_\mu c_{\mu'} - n_{-\sigma} n_\sigma \delta_{\mu\mu'}] \\
& + (y^{(0)}_\mu u_\mu - x^{(0)}_\mu v_\mu) c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} + (y^{(0)}_{\mu'} u_{\mu'} - x^{(0)}_{\mu'} v_{\mu'}) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \delta_{\sigma\sigma'} \\
& + (\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu)(n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c_{\bar{\mu}} c_{\mu'} \\
& + (\tilde{y}_{\mu'} u_{\mu'} - \tilde{x}_{\mu'} v_{\mu'})(n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \} \\
+ \sum_{\mu,\mu'} t_\mu t_{\mu'} \{ & (y^{(0)}_\mu u_\mu - x^{(0)}_\mu v_\mu) d_{-\sigma} d_\sigma \delta_{\bar{\mu}\mu'} \\
& + (\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu) d_{-\sigma} d_\sigma c^\dagger_{\mu'} c_{\bar{\mu}} \delta_{-\sigma\sigma'} \\
& + (\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu) d_{-\sigma} d_\sigma c^\dagger_{\mu'} c^\dagger_\mu \delta_{-\sigma\sigma'} \} \\
+ \sum_{\mu,\mu'} t^*_\mu t^*_{\mu'} \{ & (y^{(0)}_{\mu'} u_{\mu'} - x^{(0)}_{\mu'} v_{\mu'}) d^\dagger_{-\sigma} d^\dagger_\sigma \delta_{\bar{\mu}\mu'} \\
& + (\tilde{y}_{\mu'} u_{\mu'} - \tilde{x}_{\mu'} v_{\mu'}) d^\dagger_{-\sigma} d^\dagger_\sigma c^\dagger_{\bar{\mu}'} c_\mu \delta_{-\sigma\sigma'} \\
& + (\tilde{x}_{\mu'} u_{\mu'} + \tilde{y}_{\mu'} v_{\mu'}) d^\dagger_{-\sigma} d^\dagger_\sigma c_{\mu'} c_\mu \delta_{-\sigma\sigma'} \} \, .
\end{aligned}
\tag{4.31}
$$

Since this is a very unruly quantity to work with, it is useful to combine different terms into coefficients, such that these coefficients describe amplitudes for different processes as follows

$$
\begin{aligned}
[S, H_T] = \sum_{\mu,\mu'} \{ & W_{\mu\mu'} (c^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} - n_\sigma \delta_{\mu\mu'}) \\
& + J_{\mu\mu'} [(n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c^\dagger_\mu c_{\mu'} - n_{-\sigma} n_\sigma \delta_{\mu\mu'}] \\
& + Z_{\mu\mu'} c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} + Z^\dagger_{\mu\mu'} c^\dagger_\mu c^\dagger_{\bar{\mu}'} \delta_{\sigma\sigma'} \\
& + T_{\mu\mu'} (n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c_{\bar{\mu}} c_{\mu'} + T^\dagger_{\mu\mu'} (n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'}) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \\
& + D_{\mu\mu'} d_{-\sigma} d_\sigma \delta_{\bar{\mu}\mu'} + D^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma \delta_{\bar{\mu}\mu'} \\
& + L_{\mu\mu'} d_{-\sigma} d_\sigma c^\dagger_{\mu'} c_{\bar{\mu}} \delta_{-\sigma\sigma'} + L^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma c^\dagger_{\bar{\mu}'} c_\mu \delta_{-\sigma\sigma'} \\
& + K_{\mu\mu'} d_{-\sigma} d_\sigma c^\dagger_{\mu'} c^\dagger_\mu \delta_{-\sigma\sigma'} + K^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma c_{\mu'} c_\mu \delta_{-\sigma\sigma'} \} \, .
\end{aligned}
\tag{4.32}
$$

These coefficients are defined in terms of the variables x, y, u and v as follows

$$W_{\mu\mu'} = t_\mu t^*_{\mu'}(x^{(0)}_\mu u_\mu + y^{(0)}_\mu v_\mu + x^{(0)}_{\mu'} u_{\mu'} + y^{(0)}_{\mu'} v_{\mu'}) \tag{4.33}$$

$$J_{\mu\mu'} = t_\mu t^*_{\mu'}(\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu + \tilde{x}_{\mu'} u_{\mu'} + \tilde{y}_{\mu'} v_{\mu'}) \tag{4.34}$$

$$Z_{\mu\mu'} = t_\mu t^*_{\mu'}(y^{(0)}_\mu u_\mu - x^{(0)}_\mu v_\mu) \tag{4.35}$$

$$T_{\mu\mu'} = t_\mu t^*_{\mu'}(\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu) \tag{4.36}$$

$$D_{\mu\mu'} = t_\mu t_{\mu'}(y^{(0)}_\mu u_\mu - x^{(0)}_\mu v_\mu) \tag{4.37}$$

$$L_{\mu\mu'} = t_\mu t_{\mu'}(\tilde{y}_\mu u_\mu - \tilde{x}_\mu v_\mu) \tag{4.38}$$

$$K_{\mu\mu'} = t_\mu t_{\mu'}(\tilde{x}_\mu u_\mu + \tilde{y}_\mu v_\mu)\,. \tag{4.39}$$

For the coefficients written in terms of the energies of the system, I have written them out in appendix B.2.

By then noting that the spin operator in a second quantized formulation can be written as

$$\boldsymbol{S}_d = \frac{1}{2}\sum_{\sigma,\sigma'} d^\dagger_\sigma \boldsymbol{\tau}_{\sigma\sigma'} d_{\sigma'} = \frac{1}{2}\sum_{\sigma,\sigma'} d^\dagger_\sigma [\delta_{-\sigma\sigma'}\,,\ -i\sigma\delta_{-\sigma\sigma'}\,,\ \sigma\delta_{\sigma\sigma'}] d_{\sigma'}\,, \tag{4.40}$$

such that

$$\boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'} = \bar{n}_\sigma \delta_{-\sigma\sigma'} + \frac{1}{2}(n_\sigma - n_{-\sigma})\delta_{\sigma\sigma'}\,, \tag{4.41}$$

some of the terms in the commutator can be rewritten in the form of the spin operator of the dot

$$n_{-\sigma}\delta_{\sigma\sigma'} - \bar{n}_\sigma \delta_{-\sigma\sigma'} = \frac{1}{2}(n_\sigma + n_{-\sigma})\delta_{\sigma\sigma'} - \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma\sigma'}\,. \tag{4.42}$$

This mean that the commutator can be written in terms of the dot spin operator as

$$\begin{aligned}
[S, H_T] = \sum_{\mu,\mu'} \{ & W_{\mu\mu'}(c^\dagger_\mu c_{\mu'}\delta_{\sigma\sigma'} - n_\sigma \delta_{\mu\mu'}) \\
& + J_{\mu\mu'}\left[\left(\frac{n_\sigma + n_{-\sigma}}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'}\right) c^\dagger_\mu c_{\mu'} - n_{-\sigma} n_\sigma \delta_{\mu\mu'}\right] \\
& + Z_{\mu\mu'} c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} + Z^\dagger_{\mu\mu'} c^\dagger_\mu c^\dagger_{\bar{\mu}'} \delta_{\sigma\sigma'} \\
& + T_{\mu\mu'}\left(\frac{n_\sigma + n_{-\sigma}}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'}\right) c_{\bar{\mu}} c_{\mu'} + T^\dagger_{\mu\mu'}\left(\frac{n_\sigma + n_{-\sigma}}{2}\delta_{\sigma\sigma'} - \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'}\right) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \\
& + D_{\mu\mu'} d_{-\sigma} d_\sigma \delta_{\bar{\mu}\mu'} + D^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma \delta_{\bar{\mu}\mu'} \\
& + L_{\mu\mu'} d_{-\sigma} d_\sigma c^\dagger_{\mu'} c_{\bar{\mu}} \delta_{-\sigma\sigma'} + L^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma c^\dagger_{\bar{\mu}'} c_\mu \delta_{-\sigma\sigma'} \\
& + K_{\mu\mu'} d_{-\sigma} d_\sigma c^\dagger_{\mu'} c^\dagger_\mu \delta_{-\sigma\sigma'} + K^\dagger_{\mu\mu'} d^\dagger_{-\sigma} d^\dagger_\sigma c_{\mu'} c_\mu \delta_{-\sigma\sigma'} \}
\end{aligned} \tag{4.43}$$

4.1 Hamiltonian subspace and other approximations

I will for the rest of the thesis instead of working with a Hamiltonian in terms of a general dot level, constrict this to a subspace of the Hamiltonian in which the dot is singly occupied, such that $n_\sigma + n_{-\sigma} = 1$. For this to be physically realised, the singly occupied levels will have to be much lower than the empty and doubly occupied configurations. Meaning that the approximations $\xi_{d\sigma} \ll 0$ and $\xi_{d\sigma} \ll 2\xi_d + U$ must hold. In particular, this forces the signs of the energies to be negative $\xi_d < 0$, with respect to some reference potential, and for the electron-electron interaction on the dot to be repulsive as previous assumed $U > 0$.

By these approximations a lot of terms drop from the commutator

$$[S, H_T]_{(eff)} = \sum_{\mu,\mu'} \Bigg\{ \left(W_{\mu\mu'} + \frac{J_{\mu\mu'}}{2}\right) c^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} - J_{\mu\mu'} \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'} c^\dagger_\mu c_{\mu'} \\ + \left(Z_{\mu\mu'} + \frac{T_{\mu\mu'}}{2}\right) c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} + \left(Z^\dagger_{\mu\mu'} + \frac{T^\dagger_{\mu\mu'}}{2}\right) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \delta_{\sigma\sigma'} \\ - T_{\mu\mu'} \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'} c_{\bar{\mu}} c_{\mu'} - T^\dagger_{\mu\mu'} \boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'} c^\dagger_\mu c^\dagger_{\bar{\mu}'} \Bigg\} . \tag{4.44}$$

I will also follow the example of reference [14], and tacitly assume that the dot spin can be written as

$$\boldsymbol{S}_d = S\hat{\boldsymbol{z}} , \tag{4.45}$$

where $\hat{\boldsymbol{z}} = (0,0,1)^T$ is defined to be the unit vector in a direction which I define as the z-direction. This assumption is therefore a spin polarization approximation, which also at times is called a classical spin approximation. By this approximation it follows that $\boldsymbol{S}_d \cdot \boldsymbol{\tau}_{\sigma,\sigma'} = \sigma S \delta_{\sigma\sigma'}$, giving the commutator

$$[S, H_T]_{(eff)} = \sum_{\mu,\mu'} \Bigg\{ \left(W_{\mu\mu'} + \frac{J_{\mu\mu'}}{2} - \sigma S J_{\mu\mu'}\right) c^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} \\ + \left(Z_{\mu\mu'} + \frac{T_{\mu\mu'}}{2} - \sigma S T_{\mu\mu'}\right) c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} \\ + \left(Z^\dagger_{\mu\mu'} + \frac{T^\dagger_{\mu\mu'}}{2} - \sigma S T^\dagger_{\mu\mu'}\right) c^\dagger_\mu c^\dagger_{\bar{\mu}'} \delta_{\sigma\sigma'} \Bigg\} \tag{4.46}$$

Given the new form of the commutator, it is useful to redefine the coefficients as follows

$$2W'_{\mu\mu'} = W_{\mu\mu'} + \frac{J_{\mu\mu'}}{2} \tag{4.47}$$
$$2J'_{\mu\mu'} = -J_{\mu\mu'} \tag{4.48}$$
$$2Z'_{\mu\mu'} = Z_{\mu\mu'} + \frac{T_{\mu\mu'}}{2} \tag{4.49}$$
$$2T'_{\mu\mu'} = -T_{\mu\mu'}\,, \tag{4.50}$$

giving the full effective Hamiltonian for the system to second order in terms of electron operators as

$$\begin{aligned} H_S^{(2)} &= \sum_{\mu} \xi_\mu c_\mu^\dagger c_\mu - \sum_{\mu} \frac{\sigma\Delta_\alpha}{2}\left(c_\mu^\dagger c_{\bar{\mu}}^\dagger + c_{\bar{\mu}} c_\mu\right) \\ &+ \sum_{\mu,\mu'} \left\{ \left(W'_{\mu\mu'} + \sigma S J'_{\mu\mu'}\right) c_\mu^\dagger c_{\mu'} \delta_{\sigma\sigma'} + \left(Z'_{\mu\mu'} + \sigma S T'_{\mu\mu'}\right) c_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} + \left(Z'^\dagger_{\mu\mu'} + \sigma S T'^\dagger_{\mu\mu'}\right) c_\mu^\dagger c_{\bar{\mu}'}^\dagger \delta_{\sigma\sigma'} \right\} \end{aligned} \tag{4.51}$$

Lastly to get the Hamiltonian to a more familiar form, as seen in reference [14], with no creation-creation and annihilation-annihilation terms as well as no momentum or spin dependence, it is assumed that

$$|E_{\alpha k}| \ll |\xi_{\alpha\sigma} - \xi_{d\sigma} - U| \tag{4.52}$$
$$|E_{\alpha k}| \ll |\xi_{\alpha\sigma} - \xi_{d\sigma}| \tag{4.53}$$
$$\left|\frac{\sigma B}{2}(g_\alpha - g_d)\right| \ll |\xi_d + U| \tag{4.54}$$
$$\left|\frac{\sigma B}{2}(g_\alpha - g_d)\right| \ll |\xi_d|\,. \tag{4.55}$$

These assumptions both remove these terms ($Z'_{\mu\mu'} \approx 0$ and $T'_{\mu\mu'} \approx 0$), and makes the remaining coefficients of the form

$$W'_{\mu\mu'} \approx -\frac{t_\mu t^*_{\mu'}}{2}\left(\frac{1}{\xi_d + U} + \frac{1}{\xi_d}\right) \tag{4.56}$$
$$J'_{\mu\mu'} \approx t_\mu t^*_{\mu'}\left(\frac{1}{\xi_d + U} - \frac{1}{\xi_d}\right) \tag{4.57}$$

Note that these coefficients are the same as the coefficients one would get from a SW transformation of normal metals (cf. the textbook [18]), but here used in the context of superconductors. This is because of the assumption from equation (4.52), is a very strong assumption which in essence forces the dot level to be far from the BCS energy gap Δ. For future work this assumption might very well be relaxed, but for the remainder of the thesis I will work within this regime.

Introducing the dimensionless distance from the particle-hole symmetric point $x = 1 + \frac{2\xi_d}{U}$, which by the earlier assumption is forced to be in the interval $|x| < 1$, this can be simplified even further as

$$W'_{\mu\mu'} \approx t_\mu t^*_{\mu'} \frac{2x}{U(1-x^2)} \equiv \hat{t}_\mu \hat{t}^*_{\mu'} W \tag{4.58}$$

$$J'_{\mu\mu'} \approx t_\mu t^*_{\mu'} \frac{4}{U(1-x^2)} \equiv \hat{t}_\mu \hat{t}^*_{\mu'} J \tag{4.59}$$

with $\hat{t}_\mu \equiv \frac{t_\alpha e^{-i\phi_\alpha/2}}{\sqrt{\sum_\alpha |t_\alpha|^2}} \equiv \hat{t}_\alpha e^{-i\phi_\alpha/2} \equiv \check{t}_\alpha$, such that W and J are real and proportional to the summed tunnelling rate $\Gamma = \sum_\alpha \Gamma_\alpha = \sum_\alpha \pi\nu_F |t_\alpha|^2$.

Note that as one approach the particle-hole symmetric case for the dot $x \to 0$ the potential W disappears $W \to 0$.

Lastly I will for simplicity assume that all of the superconductors are expressed by the same quantities, and are therefore all of the same type, such that $\Delta_\alpha = \Delta$ and $\xi_{\alpha k\sigma} = \xi_{k\sigma}$.

Chapter 5

Lead summed basis

Given all of the approximations from the chapter above, an effective Hamiltonian of the system is found as

$$H = \sum_{\alpha k \sigma} \left[\xi_{k\sigma} c^{\dagger}_{\alpha k \sigma} c_{\alpha k \sigma} - \frac{\sigma \Delta}{2} \left(c^{\dagger}_{\alpha k \sigma} c^{\dagger}_{\alpha -k -\sigma} + c_{\alpha -k -\sigma} c_{\alpha k \sigma} \right) \right] \\ + \sum_{\alpha \alpha' k k' \sigma} \left(W + \sigma S J \right) \check{t}_{\alpha} \check{t}^{*}_{\alpha'} c^{\dagger}_{\alpha k \sigma} c_{\alpha' k' \sigma} , \tag{5.1}$$

where one sees that since the coefficient in the new spin term is positive $J > 0$, this is in essence an anti-ferromagnetic interaction between the dot spin S and the superconductor electrons, meaning for $\sigma S < 0$ the energy is lower. One also notes that the new terms have the operators $c^{\dagger}_{\alpha k \sigma} c_{\alpha' k' \sigma}$, taking electrons from a superconductor α and creating a new electron in any superconductor, making this an effective scattering interaction. Since the dot taken to effectively always be singly occupied, this scattering is cotunneling, meaning that transport is of the form of two virtual tunnelling processes, one to and one from the dot.

Because of this $(\alpha, k) \rightarrow (\alpha', k')$ scattering it is useful to work in a new basis, in which the scattering interaction term become diagonal

$$H_V = \sum_{kk'\sigma} \left(W + \sigma S J \right) \left(\sum_{\alpha} \check{t}_{\alpha} c^{\dagger}_{\alpha k \sigma} \right) \left(\sum_{\alpha'} \check{t}^{*}_{\alpha'} c_{\alpha' k' \sigma} \right) \tag{5.2}$$

$$\equiv \sum_{kk'\sigma} \left(W + \sigma S J \right) \tilde{c}^{\dagger}_{Nk\sigma} \tilde{c}_{Nk'\sigma} . \tag{5.3}$$

Note that from here on out I use the notation that vectors and matrices written in this lead summed basis have a $\sim$ above, such that a vector $\tilde{\boldsymbol{v}}$ is to be understood as being in this new basis, with $\boldsymbol{v}$ corresponding to the vector in the usual basis.

This change of basis is defined by a unitary transformation matrix $\boldsymbol{U}$, such that the new fermion operators become

$$\tilde{c}_{\nu k\sigma} = \sum_{\alpha} U_{\nu\alpha} c_{\alpha k\sigma}\,, \tag{5.4}$$

with the condition defined by equation (5.2), that

$$(U^{\dagger})_{\alpha N} U_{N\alpha'} = \check{t}_{\alpha} \check{t}^{*}_{\alpha'}\,. \tag{5.5}$$

This corresponds to diagonalizing the matrix defined by the phase shifted tunnel couplings

$$\Theta_{\alpha\alpha'} = \check{t}_{\alpha} \check{t}^{*}_{\alpha'} = (\check{\boldsymbol{t}} \otimes \check{\boldsymbol{t}}^{\dagger})_{\alpha\alpha'}\,, \tag{5.6}$$

where the vector of phase shifted tunnel couplings $\check{\boldsymbol{t}}$ is defined by the elements $\check{t}_{\alpha} = \hat{t}_{\alpha} e^{-i\phi_{\alpha}/2}$, and the $\otimes$ being the outer product without complex conjugation, sometimes called the Kronecker product. Because $\boldsymbol{\Theta}$ can be written as a outer product as above, its eigenvalues must be 0 and 1, where $N-1$ of the eigenvalues are 0 and only one eigenvalue is 1. Meaning that the transformation used above is

$$\boldsymbol{U}\boldsymbol{\Theta}\boldsymbol{U}^{\dagger} = \delta_{N}\,, \tag{5.7}$$

where $\boldsymbol{\delta}_{N}$ is a matrix with elements $(\delta_{N})_{\nu\nu'} = \delta_{\nu N}\delta_{\nu' N}$, such that only the (N,N)'th element is filled.

I then define that the transformation matrix $\boldsymbol{U}$ is given as

$$\boldsymbol{U}^{\dagger} = \begin{pmatrix} \boldsymbol{v_1} & \dots & \boldsymbol{v_N} \end{pmatrix}\,, \tag{5.8}$$

where the vectors $\boldsymbol{v_{\alpha}}$ are N linearly independent eigenvectors of $\boldsymbol{\Theta}$, such that $\boldsymbol{U}^{\dagger}\boldsymbol{U} = \mathbb{1}$.

In particular I will choose that the N'th eigenvector is $\boldsymbol{v_N} = e^{i\psi}\check{\boldsymbol{t}}$, such that the eigenvalue is 1, where the overall phase $\psi \in \mathbb{R}$ can be chosen arbitrarily. This new phase ψ allows for an overall U(1) gauge-choice, such that only phase differences between the superconductors are gauge invariant. This restricts the parameter space from being N dimensional to instead an $N-1$ dimensional. This is to be expected, since one could have just as easily absorbed the phase into the $c_{\alpha k\sigma}$ operators.

All the other eigenvectors with eigenvalue 0 can be chosen if needed from the unit tangent space defined by the vector $\boldsymbol{v_N} = \check{\boldsymbol{t}}e^{i\psi} \in S^{N-1}(\mathbb{C}) = S^{2N-1}$, meaning that the $N-1$ other eigenvectors are $\boldsymbol{v_{\alpha\neq N}} \in UT_{\boldsymbol{v_N}}S^{2N-1}$.

If needed, it would be possible to write the unitary matrix $\boldsymbol{U}$ in terms of hyper-spherical coordinates, but as one might suspect, the choices of the vectors $\boldsymbol{v_{\alpha\neq N}}$, correspond to a choice of gauge, and will not contribute to any meaningful quantity, so I will leave it abstract for now.

Now that I have crated a transformation matrix, I will use this to construct a Nambu space in this lead summed basis. The reason for going to a Nambu space is useful, is because of the off-diagonal terms in the Hamiltonian. In this Nambu space the transformation between the the usual and the lead summed basis then become

$$\tilde{\boldsymbol{C}}^\dagger_{k\sigma} \equiv \begin{pmatrix} \tilde{c}^\dagger_{1k\sigma} & \dots & \tilde{c}^\dagger_{Nk\sigma} & -\sigma\tilde{c}_{1-k-\sigma} & \dots & -\sigma\tilde{c}_{N-k-\sigma} \end{pmatrix} \tag{5.9}$$

$$= \begin{pmatrix} \boldsymbol{c}^\dagger_{k\sigma}\boldsymbol{U}^\dagger & -\sigma\boldsymbol{c}^T_{-k-\sigma}\boldsymbol{U}^T \end{pmatrix} \tag{5.10}$$

$$= \boldsymbol{C}^\dagger_{k\sigma} \begin{pmatrix} \boldsymbol{U}^\dagger & 0 \\ 0 & \boldsymbol{U}^T \end{pmatrix}, \tag{5.11}$$

where the usual Nambu basis is defined as

$$\boldsymbol{C}^\dagger_{k\sigma} = \begin{pmatrix} \boldsymbol{c}^\dagger_{k\sigma} & -\sigma\boldsymbol{c}^T_{-k-\sigma} \end{pmatrix}. \tag{5.12}$$

In this Nambu space, the interaction in Nambu space become diagonal

$$H_V = \frac{1}{2}\sum_{kk'\sigma} \boldsymbol{C}^\dagger_{k\sigma} \begin{pmatrix} (W+\sigma SJ)\,\boldsymbol{\Theta} & 0 \\ 0 & -(W+(-\sigma)SJ)\,\boldsymbol{\Theta}^T \end{pmatrix} \boldsymbol{C}_{k'\sigma} \tag{5.13}$$

$$= \frac{1}{2}\sum_{kk'\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \begin{pmatrix} (\sigma SJ + W)\,\boldsymbol{\delta}_N & 0 \\ 0 & (\sigma SJ - W)\,\boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{C}}_{k'\sigma} \tag{5.14}$$

$$\equiv \frac{1}{2}\sum_{kk'\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \begin{pmatrix} V_{\sigma+}\boldsymbol{\delta}_N & 0 \\ 0 & V_{\sigma-}\boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{C}}_{k'\sigma} \tag{5.15}$$

$$\equiv \frac{1}{2}\sum_{kk'\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \tilde{\boldsymbol{\mathcal{V}}}_\sigma \tilde{\boldsymbol{C}}_{k'\sigma}. \tag{5.16}$$

Here I have defined the spin dependent potentials $V_{\sigma\pm} = \sigma SJ \pm W$, since it makes it easier to generalize later if needed.

Similarly in this Nambu space the freely moving part of the Hamiltonian become

$$H_0 = \frac{1}{2}\sum_{k\sigma} \boldsymbol{C}^\dagger_{k\sigma} \begin{pmatrix} \xi_{k\sigma} & \Delta \\ \Delta & -\xi_{-k-\sigma} \end{pmatrix} \boldsymbol{C}_{k\sigma} \tag{5.17}$$

$$= \frac{1}{2}\sum_{k\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \begin{pmatrix} \xi_k + \xi_\sigma & \Delta\boldsymbol{U}\boldsymbol{U}^T \\ \Delta\boldsymbol{U}^*\boldsymbol{U}^\dagger & -\xi_k + \xi_\sigma \end{pmatrix} \tilde{\boldsymbol{C}}_{k\sigma} \tag{5.18}$$

$$\equiv \frac{1}{2}\sum_{k\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \begin{pmatrix} \xi_k + \xi_\sigma & \Delta\boldsymbol{P} \\ \Delta\boldsymbol{P}^\dagger & -\xi_k + \xi_\sigma \end{pmatrix} \tilde{\boldsymbol{C}}_{k\sigma} \tag{5.19}$$

$$\equiv \frac{1}{2}\sum_{k\sigma} \tilde{\boldsymbol{C}}^\dagger_{k\sigma} \tilde{\boldsymbol{\mathcal{H}}}_{0,k\sigma} \tilde{\boldsymbol{C}}_{k\sigma}, \tag{5.20}$$

where the new unitary matrix $\boldsymbol{P} = \boldsymbol{U}\boldsymbol{U}^T$ is defined to save space, since the $\boldsymbol{U}$ matrices from here on always appear in pairs.

All in all this mean that the full Hamiltonian in the lead summed basis is given as

$$H = \frac{1}{2} \sum_{kk'\sigma} \tilde{\boldsymbol{C}}^{\dagger}_{k\sigma} \left[\tilde{\boldsymbol{\mathcal{H}}}_{0,k\sigma} \delta_{kk'} + \tilde{\boldsymbol{\mathcal{V}}}_{\sigma} \right] \tilde{\boldsymbol{C}}_{k'\sigma} \,. \tag{5.21}$$

The usefulness of this transformation will be made clear in the next section.

Chapter 6

Bound states and their energies

From the Hamiltonian that I have found in chapter 5, I will now determine the energies of any possible bound states in the system as well as finding a description of the actual states themselves. Because of the type of dot I have made use of, the states will be generalizations of the states first found by Yu, Shiba and Rusinov in the case of particle hole symmetry and without phase difference [15–17]. Even though my states are technically generalized states I will still call them Yu-Shiba-Rusinov (YSR) states.

The energies will first be found by use of a Green's functions formalism, following the example set by reference [14], and then reconfirmed in a Bogoliubov-de Gennes (BdG) formalism in which I also will find the states following the example of Pientka et al. [25].

6.1 Green's function formalism - The bound state energies

I start of by writing the formula for the full retarded Green's function, in terms of the retarded Green's function of freely moving fermions

$$G^R = [\mathbb{1} - G_0^R V]^{-1} G_0^R \,, \tag{6.1}$$

where G_0^R is a general Green's function for non-interacting moving particles, and V is some interaction. For my system this correspond to a Green's function for the superconductors and the effective potential at the dot respectively.

Since I am concerned with the states which are bound by the dot, I will only make use of the subspace in which the Green's functions are local

$$G_{0,local}^R = \sum_k G_{0,k}^R \,. \tag{6.2}$$

The reason why this is a local Green's function can be seen by remembering the definition of Fourier transforms, which shows that since $f(r) = \sum_k f_k e^{ikr}$, the Green's function is $G^R_{0,local} = G^R_0(\delta x = 0)$. This mean that it describes transport of particles right next to one another.

From equation (5.20) the retarded local Green's functions for the non-interacting fermions is then found as a matrix

$$\boldsymbol{\mathcal{G}}^R_{0,\sigma,local} = \sum_k \left[\omega_\sigma - \boldsymbol{\mathcal{H}}_{0,k\sigma}\right]^{-1} \equiv \sum_k \left[\Omega_\sigma - \boldsymbol{\mathcal{H}}_{0,k}\right]^{-1} , \tag{6.3}$$

where I have defined the magnetically shifted energy $\Omega_\sigma = \omega_\sigma - \xi_\sigma$.

Inverting the matrix is quite simple because of the structure of $\boldsymbol{\mathcal{H}}_{0,k}$, giving

$$\boldsymbol{\mathcal{G}}^R_{0,\sigma,local} = \sum_k \begin{pmatrix} \Omega_\sigma - \xi_k & -\Delta \boldsymbol{P} \\ -\Delta \boldsymbol{P}^\dagger & \Omega_\sigma + \xi_k \end{pmatrix}^{-1} \tag{6.4}$$

$$= \sum_k \frac{1}{\Omega_\sigma^2 - \Delta^2 - \xi_k^2} \begin{pmatrix} \Omega_\sigma + \xi_k & \Delta \boldsymbol{P} \\ \Delta \boldsymbol{P}^\dagger & \Omega_\sigma - \xi_k \end{pmatrix} . \tag{6.5}$$

To be able to calculate the sum I will approximate it as an integral

$$\sum_k \approx \frac{L}{2\pi} \int dk = \int_{-D}^{D} d\xi_k \left(\frac{L}{2\pi} \frac{dk}{d\xi_k} \right) = \int_{-D}^{D} d\xi_k D(\xi_k) \approx \nu_F \int_{-D}^{D} d\xi_k . \tag{6.6}$$

Where $D(\xi_k)$ is the density of states, and the integration boundary D defines the bandwidth of the superconductors. I will make use of the wide-band approximation, such that $|\Omega_\sigma|, |\Delta| \ll D$ and the density of states is assumed to be constant $D(\xi_k) \approx \nu_F$. The integral is performed using a contour integral assuming $|\Delta| > |\Omega_\sigma|$, since it can be shown that there are no consistent solutions for either assuming $|\Delta| < |\Omega_\sigma|$ or $|\Delta| = |\Omega_\sigma|$. Meaning that there are no bound states in the continuum (BIC) in this system. The non-interacting local Green's function therefore become

$$\boldsymbol{\mathcal{G}}^R_{0,\sigma,local} = \frac{-\pi \nu_F}{\sqrt{\Delta^2 - \Omega_\sigma^2}} \begin{pmatrix} \Omega_\sigma & \Delta \boldsymbol{P} \\ \Delta \boldsymbol{P}^\dagger & \Omega_\sigma \end{pmatrix} . \tag{6.7}$$

These energies will be those for which the full retarded Green's function have poles, which is the same places where the matrix $\mathbb{1} - \boldsymbol{\mathcal{G}}^R_{0,\sigma,local} \tilde{\boldsymbol{\mathcal{V}}}_\sigma$ is singular. This mean that I can find the energies from the determinant equation

$$\det\left(\mathbb{1} - \boldsymbol{\mathcal{G}}^R_{0,\sigma,local} \tilde{\boldsymbol{\mathcal{V}}}_\sigma\right) \stackrel{!}{=} 0 . \tag{6.8}$$

Here it is now clear why the lead summed basis is useful

$$\mathbb{1} - \boldsymbol{\mathcal{G}}^R_{0,\sigma,local} \tilde{\boldsymbol{\mathcal{V}}}_\sigma = \begin{pmatrix} \mathbb{1} + \hat{\Omega}_\sigma \hat{V}_{\sigma+} \boldsymbol{\delta}_N & \hat{\Delta}_\sigma \hat{V}_{\sigma-} \boldsymbol{P} \boldsymbol{\delta}_N \\ \hat{\Delta}_\sigma \hat{V}_{\sigma+} \boldsymbol{P}^\dagger \boldsymbol{\delta}_N & \mathbb{1} + \hat{\Omega}_\sigma \hat{V}_{\sigma-} \boldsymbol{\delta}_N \end{pmatrix} , \tag{6.9}$$

where $\hat{V}_{\sigma\pm} \equiv \pi\nu_F V_{\sigma\pm} = \sigma g \pm w$, with the dimensionless potentials defined as $g \equiv \pi\nu_F SJ$ and $w \equiv \pi\nu_F W$. And for convenience in intermediate calculations I have also defined the dimensionless energy ratio $\hat{\Delta}_\sigma = \frac{\Delta}{\sqrt{\Delta^2-\Omega_\sigma^2}}$, and similarly for $\hat{\Omega}_\sigma$.

The form of this matrix makes finding the determinant easy, as it reduces quite nicely as seen in appendix C, to the form

$$\det\left(\mathbb{1} - \mathcal{G}^R_{0,local}\tilde{\mathcal{V}}_\sigma\right) = \begin{vmatrix} 1+\hat{\Omega}_\sigma\hat{V}_{\sigma+} & \hat{\Delta}_\sigma\hat{V}_{\sigma-}P_{NN} \\ \hat{\Delta}_\sigma\hat{V}_{\sigma+}P^\dagger_{NN} & 1+\hat{\Omega}_\sigma\hat{V}_{\sigma-} \end{vmatrix} . \tag{6.10}$$

Writing this out and multiplying all terms by $\sqrt{\Delta^2-\Omega_\sigma^2}$ the energies of the bound states, must follow the formula

$$\left(\sqrt{\Delta^2-\Omega_\sigma^2} + \Omega_\sigma\left(\sigma g + w\right)\right)\left(\sqrt{\Delta^2-\Omega_\sigma^2} + \Omega_\sigma\left(\sigma g - w\right)\right) - \Delta^2 u\chi \stackrel{!}{=} 0\,. \tag{6.11}$$

Where the lead parameter $\chi = P_{NN}P^\dagger_{NN}$ and the potential $u = \hat{V}_{\sigma+}\hat{V}_{\sigma-} = g^2 - w^2$ were introduced. From my earlier assumptions one can see from equations (4.58) and (4.59) that this potential is positive $u > 0$. Note that I choose to define u with a different sign than reference [14] and [26], since it is more natural to have it be defined as $\hat{V}_{\sigma+}\hat{V}_{\sigma-}$.

Solving for the magnetically shifted bound state energies Ω_σ, I find that

$$\Omega_{\sigma\pm} = \frac{\mathrm{sgn}(\Omega_{\sigma\pm})\Delta}{\sqrt{(1-u)^2+4g^2}}\left[(1-u)(1-u\chi)+2g^2 \pm 2|g|\sqrt{g^2-u(1-\chi)(1-u\chi)}\right]^{1/2} . \tag{6.12}$$

The sign of $\Omega_{\sigma\pm}$ can then be found directly by the determinant equation (6.11), giving the relation

$$\mathrm{sgn}(\Omega_{\sigma\pm}) = \mathrm{sgn}\left(-\sigma\frac{\Omega^2_{\sigma\pm}(u-1)+\Delta^2(1-u\chi)}{2g\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}}\right) , \tag{6.13}$$

which after simplification gives two different signs, depending on the value of $\pm$

$$\mathrm{sgn}(\Omega_{\sigma+}) = -\sigma\,\mathrm{sgn}(S) \tag{6.14}$$
$$\mathrm{sgn}(\Omega_{\sigma-}) = -\sigma\,\mathrm{sgn}(S)\,\mathrm{sgn}(1-u\chi)\,. \tag{6.15}$$

This means four different bound state energies are found to have the form

$$\omega_{\sigma\pm} = \frac{-\sigma\,\mathrm{sgn}(S)c_\pm\Delta}{\sqrt{(1-u)^2+4g^2}}\left[(1-u)(1-u\chi)+2g^2 \pm 2|g|\sqrt{g^2-u(1-\chi)(1-u\chi)}\right]^{1/2} + \xi_\sigma\,. \tag{6.16}$$

where the signs $c_\pm$ are $c_+ = 1$ and $c_- = \operatorname{sgn}(1-u\chi)$.

These energies are plotted in figure 6.1, in the case of equal lead-dot couplings ($t_\alpha = t_\beta \, \forall \, \alpha, \beta$).

I will for the rest of the thesis without loss of generality assume that $S = \frac{1}{2}$, such that spin is chosen to be positive in the direction $\hat{z}$. The spin σ, stemming from the superconductor electrons, should then be considered as aligned for $\sigma = 1$ and anti-aligned for $\sigma = -1$, instead of up and down.

Note that the energies depends on many parameters, some of which are not controllable and some of which are. I will consider the particle-hole symmetry distance x of the dot as controllable, by coupling a gate to the dot, as in figure 3.1c, and thereby changing the potential μ_d, which changes ξ_d and therefore also x. This however might prove difficult to realize in practice, without introducing couplings to the gate, and therefore putting the situation outside of my model.

I will also consider χ as controllable, since as shown below it depends on the phase differences of the different superconductors, which are controllable by use of magnetic fluxes i loops created by connecting the leads.

Interestingly the energies of the bound states with spin up are related to the down states by a sign flip

$$\omega_{\sigma\pm} = -\omega_{-\sigma\pm} \equiv -\sigma\omega_\pm \tag{6.17}$$

In the case of no phase difference the lead parameter $\chi = 1$, the energies become

$$\Omega_{\sigma\pm}(\chi = 1) = \frac{-\sigma c_\pm \Delta}{\sqrt{(1-u)^2 + 4g^2}} \left[2g^2 + (1-u)^2 \pm 2g^2\right]^{1/2} \tag{6.18}$$

$$= \begin{cases} -\sigma\Delta & \text{for} \quad \pm = + \\ -\sigma\Delta \operatorname{sgn}(1-u)\sqrt{\frac{(1-u)^2}{(1-u)^2+4g^2}} & \text{for} \quad \pm = - \end{cases} \tag{6.19}$$

Meaning that the two + state energies have moved out into the superconductor energies, such that they no longer are bound states, while two other states remain. In the particle hole symmetric case $x = 0$, these two remaining states recover the well known Yu-Shiba-Rusinov energies

$$\Omega_{\sigma-}(\chi = 1, x = 0) = -\sigma\Delta\frac{1-g^2}{1+g^2}\,. \tag{6.20}$$

In the opposite end of the spectrum of lead parameters, the cancellation of the lead parameter $\chi = 0$, can happen in certain scenarios, which will be discussed in detail in section 6.2. For now I find the energies in this case

$$\Omega_{\sigma\pm}(\chi = 0) = \frac{-\sigma\Delta}{\sqrt{(1-u)^2 + 4g^2}} \left[(1-u) + 2g^2 \pm 2|g||w|\right]^{1/2}\,. \tag{6.21}$$

It is then clear that in the $x = 0$ case, the $+$ states and $-$ states, become doubly degenerate, with the energies

$$\Omega_{\sigma+}(\chi = 0, x = 0) = \Omega_{\sigma-}(\chi = 0, x = 0) = \frac{-\sigma\Delta}{\sqrt{1+g^2}}, \tag{6.22}$$

which can be seen in figure 6.1. Where for the two lead systems as seen in figures 6.1a and 6.1b, it occurs at phase difference $\phi_{12} = \pi$, while for the three leads in figure 6.1d, it occurs at phase differences $(\phi_{12}, \phi_{13}) = \pm\left(\frac{2\pi}{3}, \frac{-2\pi}{3}\right)$. The reason that $\chi = 0$ for exactly these phase differences will be discussed in great detail below in section 6.2.

Lastly as seen in the figures, there can also be points for which $\omega_{\uparrow-} = \omega_{\downarrow-}$, like in figure 6.1a, however from 6.1b it is clear that this is not always the case. I will find these in the case of $B = 0$, such that the sign factor $\operatorname{sgn}(1 - u\chi) = 0$ determine when this happens, such that

$$\omega_{\uparrow-}\left(B = 0, \chi = \frac{1}{u}\right) = \omega_{\downarrow-}\left(B = 0, \chi = \frac{1}{u}\right) = 0 \tag{6.23}$$

For $B \neq 0$, the formula becomes more complicated, but it follows from setting $\omega_{\sigma-} = 0$. Whether or not there exist a point such that $\chi = \frac{1}{u}$ will be examined in the discussion in section 6.2.

Note that in the limit $\frac{\Gamma}{U} \to \infty$ as well as for the limit $g \to 0$ while w is held constant, the energies reduce to an expression similar to the usual Andreev bound state energies [3]

$$\omega_{\pm}^{ABS} = \pm\Delta\sqrt{1 - T\sin^2(2\theta)}, \tag{6.24}$$

with T being a transmission coefficient. Here they are of the forms

$$\Omega_{\sigma\pm}\left(\frac{\Gamma}{U} \to \infty\right) \to \mp\sigma\Delta\sqrt{\chi} \overset{N=2}{=} \mp\sigma\Delta\sqrt{1 - 2\sin^2(2\theta)\sin^2\left(\frac{\phi}{2}\right)} \tag{6.25}$$

$$\Omega_{\sigma\pm}(g = 0) = -\sigma\Delta\sqrt{\frac{1 + w^2\chi}{1 + w^2}} \overset{N=2}{=} -\sigma\Delta\sqrt{1 - \frac{w^2\sin^2(2\theta)}{1 + w^2}\sin^2\left(\frac{\phi}{2}\right)}, \tag{6.26}$$

with θ being the angle defined by $(\cos(\theta), \sin(\theta)) = (|\hat{t}_1|, |\hat{t}_2|)$. Note that these limits are not a part of my model, since they break the approximations I have used. It however shows that a Hamiltonian of the form in equation (5.1) can give the normal Andreev bound states, if the potentials J and W are defined in some different way than mine.

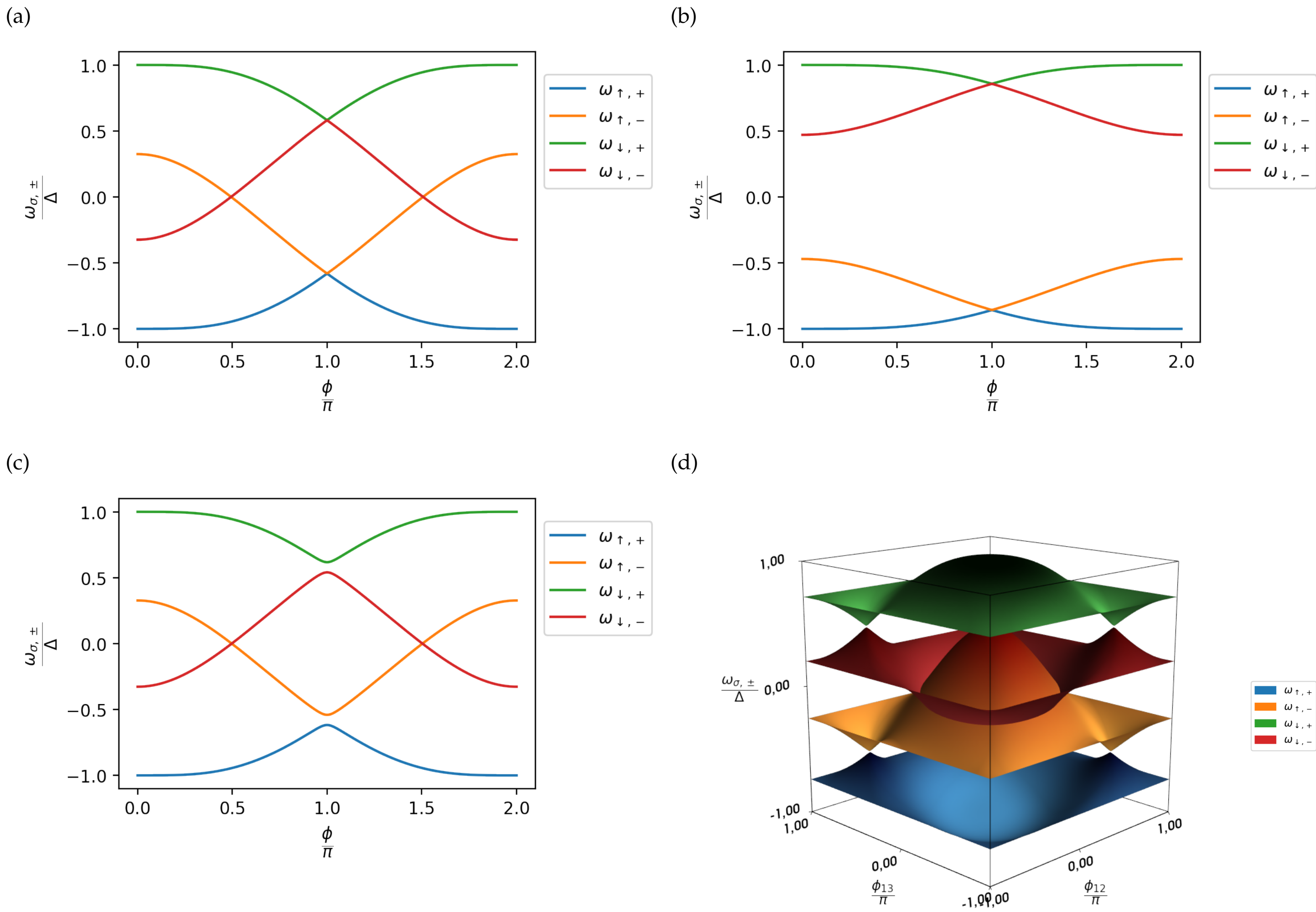


Figure 6.1: The bound state energies of an N terminal quantum dot Josephson junction with equal lead-dot couplings $t_\alpha = t_\beta \,\forall\, \alpha, \beta$, and no magnetic field $B = 0$. For (a)-(c) $N = 2$ and for (d) $N = 3$. In subfigures (a), (b) and (d) there is particle hole symmetry $x = 0$, while in (c) $x = 0.1$. The potential strengths $\frac{\Gamma}{U}$ are in (a),(c) and (d) 0.7, while in (b) it is 0.3

6.2 Analysis of lead parameter χ

I have found that the energies of the bound states are dependent on some parameter χ, which I have shown to encode some kind of properties of symmetric points like for $\omega_{\sigma+} = \omega_{\sigma+}$. This parameter seem to also be the one to encode the information about the amount of superconductors that are coupled to the dot, up to a scaling of Γ. Starting with the definition of χ, it can be written as

$$\chi = P_{NN}P_{NN}^{\dagger} = (\boldsymbol{U}\boldsymbol{U}^T)_{NN}(\boldsymbol{U}^*\boldsymbol{U}^{\dagger})_{NN} = \sum_{\alpha\alpha'} \left(U_{\alpha N}^{\dagger}U_{N\alpha'}\right)^2 \tag{6.27}$$

$$= \mathrm{Tr}\left[\boldsymbol{\Theta}\boldsymbol{\Theta}^T\right] \tag{6.28}$$

$$= \sum_{\alpha\alpha'} \hat{t}_{\alpha}^2 (\hat{t}_{\alpha'}^*)^2 e^{-i\phi_{\alpha\alpha'}}\,, \tag{6.29}$$

where $\phi_{\alpha\alpha'} = \phi_\alpha - \phi_{\alpha'}$.

By then writing the normalized coupling vector components as $\hat{t}_\alpha = |\hat{t}_\alpha|e^{i\theta_\alpha}$, since they in general can be complex, and using the fact that the summands $s_{\alpha\alpha'}$ are related by $s_{\alpha\alpha'}^* = s_{\alpha'\alpha}$, meaning that the imaginary parts sum to zero, the parameter simplifies as

$$\chi = \sum_{\alpha\alpha'} |\hat{t}_\alpha|^2|\hat{t}_{\alpha'}|^2 e^{-i(\phi_{\alpha\alpha'}+2\theta_{\alpha\alpha'})} = \sum_{\alpha\alpha'} |\hat{t}_\alpha|^2|\hat{t}_{\alpha'}|^2 \cos\left(\phi_{\alpha\alpha'} + 2\theta_{\alpha\alpha'}\right). \tag{6.30}$$

Which by using the cosine sum formula, can be split into two separate sums

$$\chi = \left(\sum_{\alpha} |\hat{t}_\alpha|^2 \cos(\phi_\alpha + 2\theta_\alpha)\right)^2 + \left(\sum_{\alpha} |\hat{t}_\alpha|^2 \sin(\phi_\alpha + 2\theta_\alpha)\right)^2 \tag{6.31}$$

One can recognize this as being distance from a sum of vectors, such that if I write the square distance of a 2-dimensional vector $\boldsymbol{r}$, which is a sum of some other vectors $\{\boldsymbol{v}_\alpha\}$, it is of the form

$$|\boldsymbol{r}|^2 = \left|\sum_{\alpha} \boldsymbol{v}_\alpha\right|^2 = \left(\sum_{\alpha} |v_\alpha| \cos(\varphi_\alpha)\right)^2 + \left(\sum_{\alpha} |v_\alpha| \sin(\varphi_\alpha)\right)^2 \tag{6.32}$$

with $|v_\alpha|$ and φ_α being the polar coordinates of the vectors $\boldsymbol{v}_\alpha$. This also mean that by scaling each vector by a factor of N, the equation (6.32) become a center of mass equation, such that by plotting $|v_\alpha| = N|\hat{t}_\alpha|^2$ as radii and $\varphi_\alpha = \phi_\alpha + 2\theta_\alpha$ as angles, the distance to the center of mass of the plot gives the value of $\sqrt{\chi}$, as seen in figure 6.2. This allows for an easy understanding, of what possible values χ can take for different phase differences $\phi_{\alpha\alpha'} + 2\theta_{\alpha\alpha'}$, without having to calculate it directly.

Note that this mean that for any two leads α and α', if one were to fix the phases to be equal $\phi_{\alpha\alpha'} + 2\theta_{\alpha\alpha'} = 0$, then they would behave as a collective lead, with a scaled coupling strength $|\hat{t}^{(collective)}|^2 = |\hat{t}_\alpha|^2 + |\hat{t}_{\alpha'}|^2$. Meaning that even though I have not explicitly considered what would happen if each lead couple to the dot via multiple channels, it is still the same model as long as the phases of the channels in the leads are equal.

From this center of mass picture it is therefore clear that the maximum must occur when all phases differences are set to zero, such that all of the vectors lie on top of one another, and the value become

$$\max(\chi) = \left(\sum_\alpha |\hat{t}_\alpha|\right)^2 = 1\,, \tag{6.33}$$

which is independent on the number of leads, and the magnitude of each individual $\hat{t}_\alpha$ since the sum is defined to be normalized.

The minimum however must depend on the magnitude and number of tunnel couplings. As can be seen in 6.2c as soon as $t_1 \neq t_2$ for an $N = 2$ lead system the minimum of χ can no longer be zero, whereas for a $N = 3$ lead system, there is a range for the magnitudes of the couplings $\hat{t}_\alpha$ where the minimum can still be zero as seen in 6.2d.

The reason for this is relatively easy to see because if one radius $|v_\alpha|$ become larger than the sum of all other radii, then the minimum can no longer be zero, since the minimum then instead become the one where all other radii lie opposite the large $|v_\alpha|$, such that $\min(\chi) = (|v_\alpha| - \sum_{\beta\neq\alpha} |v_\beta|)^2$.

By writing out the inequality for which the minimum is non-zero, and using the fact that $\hat{\boldsymbol{t}}$ is normalized, one finds that

$$\min(\chi) \neq 0 \quad \text{if} \quad |\hat{t}_\alpha|^2 > \sum_{\beta\neq\alpha} |\hat{t}_\beta|^2 = 1 - |\hat{t}_\alpha|^2\,. \tag{6.34}$$

Meaning that the minimum of χ must be as follows

$$\min(\chi) = \begin{cases} N^2(2|\hat{t}_\alpha|^2 - 1)^2 & \text{if } \exists\, t_\alpha : |\hat{t}_\alpha| > \frac{1}{\sqrt{2}} \\ 0 & \text{otherwise} \end{cases} \tag{6.35}$$

This way of thinking allows finding the geometry of the points for which $\chi = 0$. By assuming that the couplings are such that $|\hat{t}_\alpha| < \frac{1}{\sqrt{2}}$ for all α , meaning $\min(\chi) = 0$. Then by the construction of the plots, it follows that for 2 leads there is only one point for which $\chi = 0$, which is then for $\phi_{12}^* = \pi$. Where * signifies that it is the point for which $\chi(\phi_{12}^*) = \min(\chi)$.

For 3 leads there must be two points, since if $\chi = 0$ at one point $(\phi_{12}^*, \phi_{13}^*)$, then by an inversion the value of χ is preserved, while the angles must change to $(-\phi_{12}^*, -\phi_{13}^*)$. This can be thought of as two points which describe a winding of phase, going either clockwise or counterclockwise.

For 4 leads because of the much larger freedom, it is possible to do continuous movements of the two vectors such that the points form a line. For example if $t_1 = t_3$ and $t_2 = t_4$ then the transformation $(\phi^*_{12}, \phi^*_{13}, \phi^*_{14}) \rightarrow (\phi^*_{12} + x, \phi^*_{13}, \phi^*_{14} + x)$ leave $\chi = 0$ invariant.

Note however that this invariance most likely will be broken if one consider the more physical model with nearest neighbor superconductor-superconductor coupling as in reference [6], since this breaks the lead labeling/positioning invariance, which is the part of my model that allows for any lead to cancel the contribution of any other. If one include the interaction, it will most likely break into a two point case once again, with clockwise and counterclockwise winding. However this is purely speculation and, will have to be examined properly in detail in later works.

In my system the generalization of the two cases considered above, is such that if there exist a point $\boldsymbol{\phi}^*$ in the phase difference space $\mathbb{P} = T^{N-1} = [-\pi, \pi)^{N-1}$ for which $\chi = 0$ and there are $N > 2$ leads in the system, then that point is a part of an $N-3$ dimensional space $S^* \subset [-\pi, \pi)^{N-1}$ for which any point $\boldsymbol{\phi}^* \in S^*$ give the value $\chi(\boldsymbol{\phi}^*) = 0$.

A reason for why this generalization must hold, is that there are placed two restrictions for these points, they have a specific value $\chi(\phi^*) = 0$ and since they are minima they must also have no gradient $(\nabla_{\boldsymbol{\phi}} \chi)(\phi^*) = \mathbf{0}$. Note that even though such conditions must be true for all extrema of χ, for any given set of couplings $\boldsymbol{t}$, not all extrema define a $N-3$ dimensional space. Since for certain points under inversion they transform into themselves $\boldsymbol{\phi}^{(trivial)}_{max/min} \equiv -\boldsymbol{\phi}^{(trivial)}_{max/min} \pmod{2\pi}$. These points will be $\boldsymbol{\phi}_{max/min} = [\eta_1 \pi, \eta_2 \pi, \ldots, \eta_{N-1} \pi]^T$ with $\eta_i = \{0, 1\}$, meaning that the space S^* is just points. In the center of mass plots, these correspond to either all vectors on top of one another or some opposite all others. Another reason that $\chi = 0$ is so special, is that as shown earlier $\omega_{\sigma+} = \omega_{\sigma-}$ at these points for $x = 0$, which mean that these points might have topologically interesting properties. Since they are the point for which the energies touch in conical intersections for $N = 3$, meaning they might be either Weyl or Dirac points. For higher N these become nodal lines and other $N-3$ hypersurfaces.

Similarly I will find the points for which two of the bound state energies go to zero, which I in the case of $B = 0$ have shown to be the ones for which $\chi = \frac{1}{u}$. Here since this condition is satisfied by one restriction, if the points exist they must lie in either a 0 dimensional or an $N-2$ dimensional surface of points. Note that the case of a 0 dimensional surface is a highly tuned situation. The surfaces can be seen in figure 6.1. The interval of χ allows the existence of such points if

$$\min(\chi) \leq \frac{1}{g^2 - w^2} \leq 1\,, \tag{6.36}$$

which by writing out the definitions of g and w become

$$4\min(\chi) \leq (1 - x^2)\left(\frac{\Gamma}{U}\right)^{-2} \leq 4\,. \tag{6.37}$$

Meaning that the inequality sets an interval for the potential strength, where the points exist

$$\frac{1}{2}\sqrt{1 - x^2} \leq \frac{\Gamma}{U} \leq \frac{1}{2}\sqrt{\frac{1 - x^2}{\min(\chi)}}\,. \tag{6.38}$$

In the case $\min(\chi) = 0$, the upper limit is to be ignored.

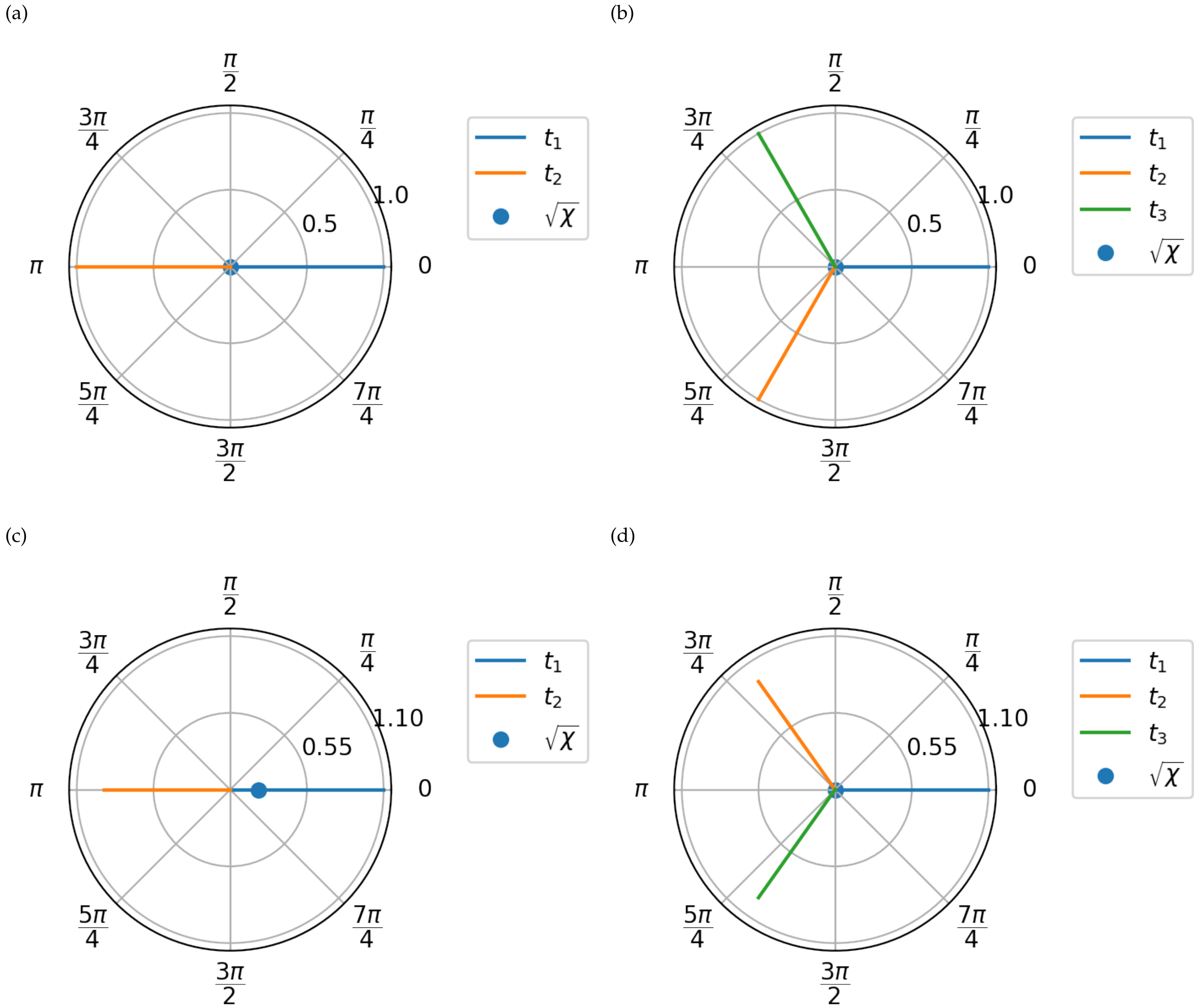


Figure 6.2: Visualizations of the minimum value of χ for 2 and 3 leads, rotated such that $\phi_1 = 0$: (a) is for two leads with equal tunnel couplings $t_1 = t_2$; (c) is for two leads with unequal tunnel couplings $t_1 > t_2$, whereby $\min(\chi) \neq 0$; (b) is for three leads with equal tunnel couplings $t_1 = t_2 = t_3$ and (d) is for three leads with unequal tunnel couplings $t_1 > t_2 = t_3$, but still $\min(\chi) = 0$

6.3 Bogoliubov-de Gennes formalism - The bound states

Now that I have shown in section 6.1 that, there exists in general four different bound states with energies $\omega_{\pm\sigma}$ as defined in equation (6.16), I will follow Pientka et al. [25], to find the eigenspinors associated with the states. Starting from the Bogoliubov-de Gennes Hamiltonian in the lead summed basis (5.21), I assume a eigenspinor decomposition as

$$\tilde{\boldsymbol{\mathcal{H}}}_{kk'\sigma} = \sum_{\pm} \omega_{\sigma\pm} \tilde{\boldsymbol{\psi}}_{\sigma\pm k} \otimes \tilde{\boldsymbol{\psi}}^{\dagger}_{\sigma\pm k'} + \tilde{\boldsymbol{\mathcal{H}}}^{NBS}_{kk'\sigma}, \tag{6.39}$$

where the product $\tilde{\boldsymbol{\psi}}_{\sigma\pm k} \otimes \tilde{\boldsymbol{\psi}}^{\dagger}_{\sigma\pm k'}$ is to be understood as an outer product of two $2N$ component vectors, leading to a $2N \times 2N$ matrix. Here $\tilde{\boldsymbol{\mathcal{H}}}^{NBS}_{kk'\sigma}$ is the part of the Hamiltonian describing any other state than the bound states. Multiplying both sides by $\tilde{\boldsymbol{\psi}}_{\sigma\pm' k'}$, and using the orthogonality properties $\tilde{\boldsymbol{\psi}}^{\dagger}_{\sigma\pm k'} \cdot \tilde{\boldsymbol{\psi}}_{\sigma\pm' k'} = |\tilde{\boldsymbol{\psi}}_{\sigma\pm k'}|^2 \delta_{\pm\pm'}$ and $\tilde{\boldsymbol{\mathcal{H}}}^{NBS}_{kk'\sigma} \cdot \tilde{\boldsymbol{\psi}}_{\sigma\pm' k'} = 0$, and then summing over momentum the eigenspinors $\tilde{\boldsymbol{\psi}}_{\sigma\pm' k'}$ must satisfy

$$\sum_{k'} \left[\tilde{\boldsymbol{\mathcal{H}}}_{0,k\sigma} \delta_{kk'} + \tilde{\boldsymbol{\mathcal{V}}}_{\sigma} \right] \tilde{\boldsymbol{\psi}}_{\sigma\pm' k'} = \omega_{\sigma\pm'} \tilde{\boldsymbol{\psi}}_{\sigma\pm' k} \sum_{k'} |\tilde{\boldsymbol{\psi}}_{\sigma\pm' k'}|^2 . \tag{6.40}$$

I define that these spinors are normalized in momentum space, such that this reduces to finding the solution to the equation

$$(\omega_{\sigma\pm} - \tilde{\boldsymbol{\mathcal{H}}}_{0,k\sigma}) \tilde{\boldsymbol{\psi}}_{\sigma\pm k} = \tilde{\boldsymbol{\mathcal{V}}}_{\sigma} \tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{r} = \boldsymbol{0}) . \tag{6.41}$$

Where $\tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{r} = \boldsymbol{0}) = \sum_k \tilde{\boldsymbol{\psi}}_{\sigma\pm k}$ is the Fourier transform defining the spinors value at the placement of the dot $\boldsymbol{r} = \boldsymbol{0}$. This equation neatly determines the full momentum dependent eigenspinors in terms of the value at the dot. Writing it out

$$\begin{aligned} \tilde{\boldsymbol{\psi}}_{\sigma\pm k} &= \begin{pmatrix} \Omega_{\sigma\pm} - \xi_k & -\Delta \boldsymbol{P} \\ -\Delta \boldsymbol{P}^{\dagger} & \Omega_{\sigma\pm} + \xi_k \end{pmatrix}^{-1} \cdot \begin{pmatrix} V_{\sigma+} \boldsymbol{\delta}_N & 0 \\ 0 & V_{\sigma-} \boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{0}) \\ &= \frac{1}{\Omega^2_{\sigma\pm} - \xi^2_k - \Delta^2} \begin{pmatrix} (\Omega_{\sigma\pm} + \xi_k) V_{\sigma+} \boldsymbol{\delta}_N & V_{\sigma-} \Delta \boldsymbol{P} \boldsymbol{\delta}_N \\ V_{\sigma+} \Delta \boldsymbol{P}^{\dagger} \boldsymbol{\delta}_N & (\Omega_{\sigma\pm} - \xi_k) V_{\sigma-} \boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{0}) . \end{aligned} \tag{6.42}$$

By a Fourier transform using the wide-band approximation and constant density of states once again this becomes the eigenequation

$$\tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{0}) = \sum_k \tilde{\boldsymbol{\psi}}_{\sigma\pm k} \approx \frac{-\pi\nu_F}{\sqrt{\Delta^2 - \Omega^2_{\sigma\pm}}} \begin{pmatrix} V_{\sigma+} \Omega_{\sigma\pm} \boldsymbol{\delta}_N & V_{\sigma-} \Delta \boldsymbol{P} \boldsymbol{\delta}_N \\ V_{\sigma+} \Delta \boldsymbol{P}^{\dagger} \boldsymbol{\delta}_N & V_{\sigma-} \Omega_{\sigma\pm} \boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{\psi}}_{\sigma\pm}(\boldsymbol{0}) , \tag{6.43}$$

which written in a collective side is

$$\boldsymbol{0} = \begin{pmatrix} \mathbb{1} + \hat{V}_{\sigma+} \hat{\Omega}_{\sigma\pm} \boldsymbol{\delta}_N & \hat{V}_{\sigma-} \hat{\Delta}_{\sigma\pm} \boldsymbol{P} \boldsymbol{\delta}_N \\ \hat{V}_{\sigma+} \hat{\Delta}_{\sigma\pm} \boldsymbol{P}^{\dagger} \boldsymbol{\delta}_N & \mathbb{1} + \hat{V}_{\sigma-} \hat{\Omega}_{\sigma\pm} \boldsymbol{\delta}_N \end{pmatrix} \tilde{\boldsymbol{\psi}}^0_{\sigma\pm} . \tag{6.44}$$

Where for notation I have defined $\tilde{\boldsymbol{\psi}}^0_{\sigma\pm} = \tilde{\boldsymbol{\psi}}_{\sigma\pm}(\mathbf{0})$. Here it again show how it is helpful to work in this lead-summed basis, since writing out what the eigenequation shows the simple relations

$$\tilde{\psi}^0_{\sigma\pm\nu} = -\hat{V}_{\sigma-}\hat{\Delta}_{\sigma\pm}P_{\nu,N}\tilde{\psi}^0_{\sigma\pm 2N} \quad \text{for} \quad \nu \in [1, N-1] \cap \mathbb{Z} \tag{6.45}$$

$$\tilde{\psi}^0_{\sigma\pm\nu} = -\hat{V}_{\sigma+}\hat{\Delta}_{\sigma\pm}P^\dagger_{(\nu-N),N}\tilde{\psi}^0_{\sigma\pm N} \quad \text{for} \quad \nu \in [N+1, 2N-1] \cap \mathbb{Z} \tag{6.46}$$

$$\tilde{\psi}^0_{\sigma\pm N} = \frac{-\hat{V}_{\sigma-}\hat{\Delta}_{\sigma\pm}P_{NN}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}\tilde{\psi}^0_{\sigma\pm 2N} \tag{6.47}$$

$$\tilde{\psi}^0_{\sigma\pm 2N} = \frac{-\hat{V}_{\sigma+}\hat{\Delta}_{\sigma\pm}P^\dagger_{NN}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}\tilde{\psi}^0_{\sigma\pm N}\,. \tag{6.48}$$

From (6.47) and (6.48), it follows that

$$0 = \left(1 - \frac{\hat{V}_{\sigma+}\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}\chi}{(1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})(1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})}\right)\tilde{\psi}^0_{\sigma\pm N}\,. \tag{6.49}$$

This gives precisely the same equation as (6.11), which therefore also gives the bound state energies as expected.

By writing the eigenspinors as vectors with 2N elements it become of the form

$$\tilde{\boldsymbol{\psi}}^0_{\sigma\pm} = \begin{bmatrix} -\hat{V}_{\sigma-}\hat{\Delta}_{\sigma\pm}\boldsymbol{P}_{(1\to N-1),N}\tilde{\psi}^0_{\sigma\pm 2N} \\ \tilde{\psi}^0_{\sigma\pm N} \\ -\hat{V}_{\sigma+}\hat{\Delta}_{\sigma\pm}\boldsymbol{P}^\dagger_{(1\to N-1),N}\tilde{\psi}^0_{\sigma\pm N} \\ \tilde{\psi}^0_{\sigma\pm 2N}\end{bmatrix} = \begin{bmatrix} \boldsymbol{P}_{(1\to N-1),N}\frac{\hat{V}_{\sigma+}\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}P^\dagger_{NN}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}\tilde{\psi}^0_{\sigma\pm N} \\ \tilde{\psi}^0_{\sigma\pm N} \\ \boldsymbol{P}^\dagger_{(1\to N-1),N}\frac{\hat{V}_{\sigma+}\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}P_{NN}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}\tilde{\psi}^0_{\sigma\pm 2N} \\ \tilde{\psi}^0_{\sigma\pm 2N}\end{bmatrix}, \tag{6.50}$$

where the vectors $\boldsymbol{P}_{(1\to N-1),N}$ and $\boldsymbol{P}^\dagger_{(1\to N-1),N}$ are to be understood as the N-1'st entries in the N'th column of the matrices $\boldsymbol{P}$ and $\boldsymbol{P}^\dagger$.

By using the energy relation from equaitons (6.16) and (6.49), and defining the basis vector of the N'th elements as $\vec{\boldsymbol{\delta}}_N = \hat{\boldsymbol{e}}_N = [0,\ldots,0,1]^T$, the eigenspinor can be written on the compact form

$$\tilde{\boldsymbol{\psi}}^0_{\sigma\pm} = \begin{bmatrix} ((1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\frac{\boldsymbol{P}}{P_{NN}} - \hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm N} \\ ((1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})\frac{\boldsymbol{P}^\dagger}{P^\dagger_{NN}} - \hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm 2N}\end{bmatrix}. \tag{6.51}$$

Where the element $P^\dagger_{NN}$ is as follows

$$P^\dagger_{NN} = \sum_\alpha (U^\dagger_{\alpha N})^2 = \sum_\alpha \check{t}^2_\alpha = \sum_\alpha \hat{t}^2_\alpha e^{-i\phi_\alpha} = \check{\boldsymbol{t}}\cdot\check{\boldsymbol{t}}\,, \tag{6.52}$$

and similarly for $P_{NN} = (P^\dagger_{NN})^* = \check{\boldsymbol{t}}^*\cdot\check{\boldsymbol{t}}^*$.

The leftover factors $\tilde{\psi}^0_{\sigma\pm N}$ and $\tilde{\psi}^0_{\sigma\pm 2N}$, must be determined by normalization of the spinors

$$1 \stackrel{!}{=} \sum_k |\tilde{\psi}_{\sigma\pm k}|^2 \approx \nu_F \int d\xi |\tilde{\psi}_{\sigma\pm}(\xi)|^2 . \tag{6.53}$$

For finding the normalization factors, I make use of equation (6.42), such that

$$|\tilde{\boldsymbol{\psi}}_{\sigma\pm k}|^2 = \frac{1}{D^2_{\sigma\pm k}} (\tilde{\boldsymbol{\psi}}^0_{\sigma\pm})^\dagger \begin{pmatrix} V^2_{\sigma+}((\Omega_{\sigma\pm}+\xi_k)^2+\Delta^2)\delta_N & 2V_{\sigma+}V_{\sigma-}\Delta\Omega_{\sigma\pm}P_{NN}\delta_N \\ 2V_{\sigma+}V_{\sigma-}\Delta\Omega_{\sigma\pm}P^\dagger_{NN}\delta_N & V^2_{\sigma-}((\Omega_{\sigma\pm}-\xi_k)^2+\Delta^2)\delta_N \end{pmatrix} \tilde{\boldsymbol{\psi}}^0_{\sigma\pm} . \tag{6.54}$$

Where the denominator is defined as $D_{\sigma\pm k} \equiv \Omega^2_{\sigma\pm} - \xi^2_k - \Delta^2$. Expanding out the matrix product this reduces to

$$|\tilde{\boldsymbol{\psi}}_{\sigma\pm k}|^2 = \frac{1}{D^2_{\sigma\pm k}} \Big[V^2_{\sigma+}((\Omega_{\sigma\pm}+\xi_k)^2+\Delta^2)|\tilde{\psi}^0_{\sigma\pm N}|^2 + 2V_{\sigma+}V_{\sigma-}\Delta\Omega_{\sigma\pm}P_{NN}(\tilde{\psi}^0_{\sigma\pm N})^*\tilde{\psi}^0_{\sigma\pm 2N}$$
$$+ 2V_{\sigma+}V_{\sigma-}\Delta\Omega_{\sigma\pm}P^\dagger_{NN}\tilde{\psi}^0_{\sigma\pm N}(\tilde{\psi}^0_{\sigma\pm 2N})^* + V^2_{\sigma-}((\Omega_{\sigma\pm}-\xi_k)^2+\Delta^2)|\tilde{\psi}^0_{\sigma\pm 2N}|^2 \Big] . \tag{6.55}$$

By approximating the sum as an integration, and once again making use of the wide-band approximation and constant density of states, the normalization condition becomes

$$1 \stackrel{!}{=} \frac{\pi\nu_F}{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}^3} \Big[\Delta^2 (V^2_{\sigma+}|\tilde{\psi}^0_{\sigma\pm N}|^2 + V^2_{\sigma-}|\tilde{\psi}^0_{\sigma\pm 2N}|^2) \tag{6.56}$$
$$+ V_{\sigma+}V_{\sigma-}\Delta\Omega_{\sigma\pm}(P_{NN}(\tilde{\psi}^0_{\sigma\pm N})^*\tilde{\psi}^0_{\sigma\pm 2N} + P^\dagger_{NN}\tilde{\psi}^0_{\sigma\pm N}(\tilde{\psi}^0_{\sigma\pm 2N})^*) \Big] .$$

By converting to the unit-less variables $\hat{V}_{\sigma\pm}$, $\hat{\Omega}_{\sigma\pm}$ and $\hat{\Delta}_{\sigma\pm}$ this can be written as

$$1 \stackrel{!}{=} \frac{(\pi\nu_F)^{-1}}{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}} \Big[\hat{\Delta}^2_{\sigma\pm} (\hat{V}^2_{\sigma+}|\tilde{\psi}^0_{\sigma\pm N}|^2 + \hat{V}^2_{\sigma-}|\tilde{\psi}^0_{\sigma\pm 2N}|^2) \tag{6.57}$$
$$+ \hat{V}_{\sigma+}\hat{V}_{\sigma-}\hat{\Delta}_{\sigma\pm}\hat{\Omega}_{\sigma\pm}(P_{NN}(\tilde{\psi}^0_{\sigma\pm N})^*\tilde{\psi}^0_{\sigma\pm 2N} + P^\dagger_{NN}\tilde{\psi}^0_{\sigma\pm N}(\tilde{\psi}^0_{\sigma\pm 2N})^*) \Big] .$$

By inserting from equation (6.47), this must be the same as

$$\frac{1}{|\tilde{\psi}^0_{\sigma\pm 2N}|^2} \stackrel{!}{=} \frac{\hat{\Delta}^2_{\sigma\pm}\hat{V}^2_{\sigma-}(\pi\nu_F)^{-1}}{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}} \left[\frac{\hat{V}^2_{\sigma+}\hat{\Delta}^2_{\sigma\pm}\chi}{(1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})^2} + 1 - \frac{2\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}\chi}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}} \right] . \tag{6.58}$$

Which by use of equation (6.49) tells that the normalization must have the size

$$|\tilde{\psi}^0_{\sigma\pm 2N}| \stackrel{!}{=} \sqrt{\frac{1}{\hat{V}_{\sigma-}(1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})}}\sqrt{\frac{\pi\nu_F\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}}{\frac{\hat{V}_{\sigma+}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}+\frac{\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}-2\hat{\Omega}_{\sigma\pm}}}. \tag{6.59}$$

Now that I have the normalization constant up to some arbitrary phase, I will find the bound states in momentum space using equation (6.42) and (6.51)

$$\tilde{\boldsymbol{\psi}}_{\sigma\pm k} = \frac{1}{D_{\sigma\pm k}}\begin{pmatrix}(\Omega_{\sigma\pm}+\xi_k)V_{\sigma+}\boldsymbol{\delta}_N & V_{\sigma-}\Delta\boldsymbol{P}\boldsymbol{\delta}_N \\ V_{\sigma+}\Delta\boldsymbol{P}^\dagger\boldsymbol{\delta}_N & (\Omega_{\sigma\pm}-\xi_k)V_{\sigma-}\boldsymbol{\delta}_N\end{pmatrix} \begin{bmatrix}((1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\frac{\boldsymbol{P}}{P_{NN}}-\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm N} \\ ((1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})\frac{\boldsymbol{P}^\dagger}{P^\dagger_{NN}}-\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm 2N}\end{bmatrix}. \tag{6.60}$$

By matrix multiplication this is the same as

$$\tilde{\boldsymbol{\psi}}_{\sigma\pm k} = \frac{1}{D_{\sigma\pm k}}\begin{bmatrix}(\Omega_{\sigma\pm}+\xi_k)V_{\sigma+}\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm N}+V_{\sigma-}\Delta\boldsymbol{P}\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm 2N} \\ V_{\sigma+}\Delta\boldsymbol{P}^\dagger\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm N}+(\Omega_{\sigma\pm}-\xi_k)V_{\sigma-}\vec{\boldsymbol{\delta}}_N\tilde{\psi}^0_{\sigma\pm 2N}\end{bmatrix}. \tag{6.61}$$

Now that it is of a simple form, I will transform back to the physical Nambu space, by use of the transformation defined by equation (5.11)

$$\boldsymbol{\psi}_{\sigma\pm k} = \begin{bmatrix}\boldsymbol{U}^\dagger & 0 \\ 0 & \boldsymbol{U}^T\end{bmatrix}\tilde{\boldsymbol{\psi}}_{\sigma\pm k} = \frac{1}{D_{\sigma\pm k}}\begin{bmatrix}(\Omega_{\sigma\pm}+\xi_k)V_{\sigma+}\tilde{\psi}^0_{\sigma\pm N}\check{\boldsymbol{t}}+V_{\sigma-}\Delta\tilde{\psi}^0_{\sigma\pm 2N}\check{\boldsymbol{t}}^* \\ V_{\sigma+}\Delta\tilde{\psi}^0_{\sigma\pm N}\check{\boldsymbol{t}}+(\Omega_{\sigma\pm}-\xi_k)V_{\sigma-}\tilde{\psi}^0_{\sigma\pm 2N}\check{\boldsymbol{t}}^*\end{bmatrix}. \tag{6.62}$$

Inserting from equation (6.47) and equation (6.59), this becomes

$$\boldsymbol{\psi}_{\sigma\pm k} = \frac{e^{i\Theta}}{D_{\sigma\pm k}}\sqrt{\frac{\hat{V}_{\sigma-}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}}\sqrt{\frac{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}}{\pi\nu_F\left[\frac{\hat{V}_{\sigma+}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}+\frac{\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}-2\hat{\Omega}_{\sigma\pm}\right]}} \begin{bmatrix}-(\Omega_{\sigma\pm}+\xi_k)\frac{\hat{V}_{\sigma+}\hat{\Delta}_{\sigma\pm}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}P_{NN}\check{\boldsymbol{t}}+\Delta\check{\boldsymbol{t}}^* \\ -\Delta\frac{\hat{V}_{\sigma+}\hat{\Delta}_{\sigma\pm}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}P_{NN}\check{\boldsymbol{t}}+(\Omega_{\sigma\pm}-\xi_k)\check{\boldsymbol{t}}^*\end{bmatrix}. \tag{6.63}$$

Here Θ is the complex phase of $\tilde{\psi}^0_{\sigma\pm 2N}$ such that $\tilde{\psi}^0_{\sigma\pm 2N} = |\tilde{\psi}^0_{\sigma\pm 2N}|e^{i\Theta}$, which I will choose later. I will then once again make use of equation (6.49), such that the spinor can be rewritten as

$$\boldsymbol{\psi}_{\sigma\pm k} = \frac{e^{i\Theta}}{D_{\sigma\pm k}}\sqrt{\frac{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}}{\pi\nu_F\left[\frac{\hat{V}_{\sigma+}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}+\frac{\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}-2\hat{\Omega}_{\sigma\pm}\right]}} \begin{bmatrix}-(\Omega_{\sigma\pm}+\xi_k)\sqrt{\frac{\hat{V}_{\sigma+}}{(1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\chi}}P_{NN}\check{\boldsymbol{t}}+\Delta\sqrt{\frac{\hat{V}_{\sigma-}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}}\check{\boldsymbol{t}}^* \\ -\Delta\sqrt{\frac{\hat{V}_{\sigma+}}{(1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})\chi}}P_{NN}\check{\boldsymbol{t}}+(\Omega_{\sigma\pm}-\xi_k)\sqrt{\frac{\hat{V}_{\sigma-}}{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}}\check{\boldsymbol{t}}^*\end{bmatrix} \tag{6.64}$$

Note however by equation (6.49) as $\chi \to 0$ to get something finite $\frac{(1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm})(1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm})}{\hat{V}_{\sigma+}\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}\chi} \to 0$ as well, meaning that to avoid $\frac{0}{0}$ expressions the relation

$$\frac{\hat{V}_{\sigma\pm'}}{1+\hat{V}_{\sigma\pm'}\hat{\Omega}_{\sigma\pm}} = \frac{\hat{V}_{\sigma\pm'}(1+\hat{V}_{\sigma\mp'}\hat{\Omega}_{\sigma\pm})}{(1+\hat{V}_{\sigma\pm'}\hat{\Omega}_{\sigma\pm})(1+\hat{V}_{\sigma\mp'}\hat{\Omega}_{\sigma\pm})} = \frac{1+\hat{V}_{\sigma\mp'}\hat{\Omega}_{\sigma\pm}}{\hat{V}_{\sigma\mp'}\hat{\Delta}^2_{\sigma\pm}\chi}, \tag{6.65}$$

can be usefull some places. Then by inserting equation (6.47) and the normalization (6.59)

$$\boldsymbol{\psi}_{\sigma\pm k} = \frac{e^{i\Theta}}{D_{\sigma\pm k}}\sqrt{\frac{\chi\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}}{\pi\nu_F\left[\frac{\hat{V}_{\sigma+}+\hat{V}_{\sigma-}}{\hat{V}_{\sigma+}\hat{V}_{\sigma-}}+2\hat{\Omega}_{\sigma\pm}(1-\chi)\right]}} \begin{bmatrix} -(\Omega_{\sigma\pm}+\xi_k)\sqrt{\frac{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}{\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}\chi^2}}P_{NN}\check{\boldsymbol{t}} + \Delta\sqrt{\frac{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}{\hat{V}_{\sigma+}\hat{\Delta}^2_{\sigma\pm}\chi}}\check{\boldsymbol{t}}^* \\ -\Delta\sqrt{\frac{1+\hat{V}_{\sigma-}\hat{\Omega}_{\sigma\pm}}{\hat{V}_{\sigma-}\hat{\Delta}^2_{\sigma\pm}\chi^2}}P_{NN}\check{\boldsymbol{t}} + (\Omega_{\sigma\pm}-\xi_k)\sqrt{\frac{1+\hat{V}_{\sigma+}\hat{\Omega}_{\sigma\pm}}{\hat{V}_{\sigma+}\hat{\Delta}^2_{\sigma\pm}\chi}}\check{\boldsymbol{t}}^* \end{bmatrix} \tag{6.66}$$

Converting $\hat{\Omega}_{\sigma\pm}$ and $\hat{\Delta}_{\sigma\pm}$ back to the quantities with units, and simplifying this gives the final expression for the momentum eigenspinor

$$\boldsymbol{\psi}_{\sigma\pm k} = \frac{1}{D_{\sigma\pm k}}\sqrt{\frac{\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}^3}{\pi\nu_F\left[(\hat{V}_{\sigma+}+\hat{V}_{\sigma-})\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}+2\Omega_{\sigma\pm}\hat{V}_{\sigma+}\hat{V}_{\sigma-}(1-\chi)\right]}}$$
$$\begin{bmatrix} -\frac{\Omega_{\sigma\pm}+\xi_k}{\Delta}\sqrt{\hat{V}_{\sigma+}(\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}+\hat{V}_{\sigma-}\Omega_{\sigma\pm})}\check{\boldsymbol{\tau}} + \sqrt{\hat{V}_{\sigma-}(\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}+\hat{V}_{\sigma+}\Omega_{\sigma\pm})}\check{\boldsymbol{\tau}}^* \\ -\sqrt{\hat{V}_{\sigma+}(\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}+\hat{V}_{\sigma-}\Omega_{\sigma\pm})}\check{\boldsymbol{\tau}} + \frac{\Omega_{\sigma\pm}-\xi_k}{\Delta}\sqrt{\hat{V}_{\sigma-}(\sqrt{\Delta^2-\Omega^2_{\sigma\pm}}+\hat{V}_{\sigma+}\Omega_{\sigma\pm})}\check{\boldsymbol{\tau}}^* \end{bmatrix} \tag{6.67}$$

where I have chosen the phase $-2\Theta = \arg\left(\sqrt{\frac{P^2_{NN}}{\chi}}\right) = \arg\left(\sqrt{\frac{P_{NN}}{P^\dagger_{NN}}}\right) = \arg\left(P_{NN}\right) = \arg\left(\check{\boldsymbol{t}}^*\cdot\check{\boldsymbol{t}}^*\right)$, such that I define $\check{\boldsymbol{\tau}} \equiv e^{-i\Theta}\check{\boldsymbol{t}} = \left(\frac{\check{\boldsymbol{t}}^*\cdot\check{\boldsymbol{t}}^*}{\check{\boldsymbol{t}}\cdot\check{\boldsymbol{t}}}\right)^{1/4}\check{\boldsymbol{t}}$.

It is possible to now write out the bound state annihilation and creation operators, from equation (5.21) and (6.39), it is clear that I can define some operators

$$\gamma^{BS}_{\sigma\pm k} \equiv \tilde{\boldsymbol{\psi}}^\dagger_{\sigma\pm k'}\cdot\boldsymbol{C}_{k'\sigma} \tag{6.68}$$

which diagonalize the bound state part of the full Hamiltonian, and have the energies $\omega_{\sigma\pm}$. However I will not make further use of these states in this thesis, and instead leave them for use outside of this thesis.

6.4 Ground state energy and many body energies

Now that I have found the bound states and energies for single particle excitations, I will make use of the Bogoliubov-de Gennes formalism to find the ground state energy up to a constant. This can be done by using $\omega_{gs} = \frac{1}{2}\sum_{\omega<0}\omega$, which when written out by using the fact that $\omega_{\sigma\pm} = -\sigma\omega_{\pm}$ gives

$$\omega_{gs} = -\sum_{\pm}\frac{|\omega_{\pm}|}{2}. \tag{6.69}$$

This shows that there are four different non-interacting many body cotunnelling states for which this ground state can become [26]. The fact that these are cotunnelling states, as explained earlier, stems from the assumption that the dot must be singly occupied, such that any dynamics of the system must be governed by processes where as soon as one electron leaves the dot, another must enter. The energies of these many body states are therefore up to a common constant given by

$$\omega_{s0} = \frac{\omega_{\uparrow+} + \omega_{\downarrow-}}{2} = \frac{\Omega_{\uparrow+} + \Omega_{\downarrow-}}{2} \tag{6.70}$$

$$\omega_{s1} = \frac{\omega_{\downarrow+} + \omega_{\uparrow-}}{2} = \frac{\Omega_{\downarrow+} + \Omega_{\uparrow-}}{2} \tag{6.71}$$

$$\omega_{u0} = \frac{\omega_{\uparrow+} + \omega_{\uparrow-}}{2} = \frac{\Omega_{\uparrow+} + \Omega_{\uparrow-}}{2} + \xi_{\uparrow} \tag{6.72}$$

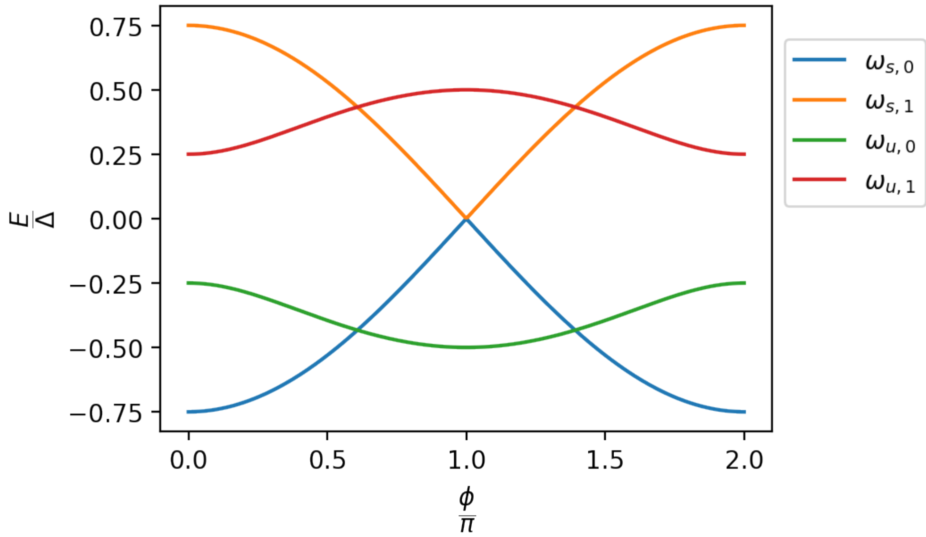
$$\omega_{u1} = \frac{\omega_{\downarrow+} + \omega_{\downarrow-}}{2} = \frac{\Omega_{\downarrow-} + \Omega_{\downarrow+}}{2} + \xi_{\downarrow}. \tag{6.73}$$

These can be seen in figure 6.3, in the case of two and three leads. Note that the conical intersections still exist for these states. The energies are split into two types, ω_s the screened many body state energies which are independent on the magnetic field B, and ω_u the unscreened energies which do depend on B.

Since the ground state for some given phase differences is the the same as the lowest of the four many body state energies seen in figure 6.3, there are for $B = 0$ two possibilities for the energy state, either ω_{s0} or ω_{u0}. As seen in figure 6.4, for the case of larger coupling like $\frac{\Gamma}{U} = 0.7$ (figure 6.4a), the ground can undergo a transition between the states with energies ω_{s0} and ω_{u0} corresponding to a spin-flip, while for lower couplings like $\frac{\Gamma}{U} = 0.45$ (figure 6.4b), the state remain in the state with energy ω_{u0}.

It is easy to see that the condition of this change of the ground state, is the same as finding when $\omega_{s0} \stackrel{?}{=} \omega_{u0}$, which by the definition of these energies for $B = 0$ is the same condition as $\omega_{\uparrow-} \stackrel{?}{=} \omega_{\downarrow-}$, which I have already shown to be $\chi = 1/U$. Equation (6.38) therefore explain why for $x = 0$ as in figure 6.4, a transition can occur for figure 6.4a where $\frac{\Gamma}{U} = 0.7 > 0.5$, while no transition can occur in figure 6.4b where $\frac{\Gamma}{U} = 0.45 < 0.5$.

(a)



(b)

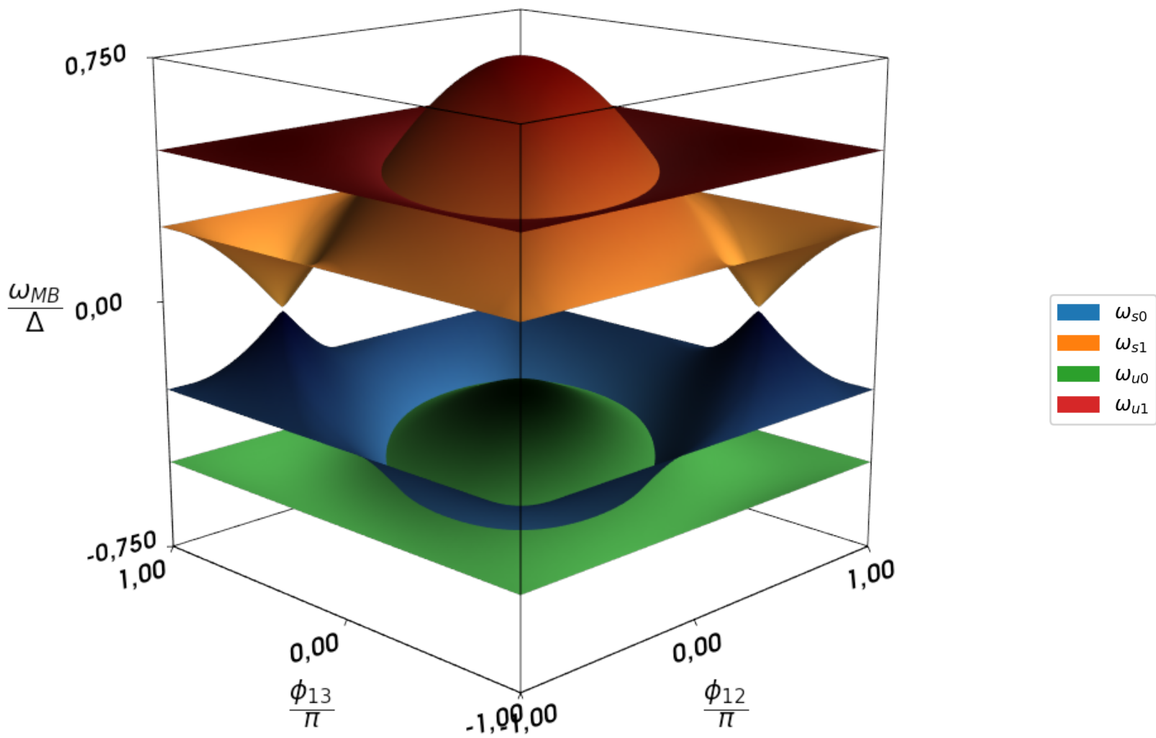


Figure 6.3: The many body energies of the quantum dot Josephson junction with equal tunneling amplitudes $t_\alpha = t_{\alpha'}$ as well as particle hole symmetry $x = 0$, zero magnetic field $B = 0$, and potential strength $\frac{\Gamma}{U} = 0.7$, (a) in the case of two leads and (b) the case of three leads

(a)

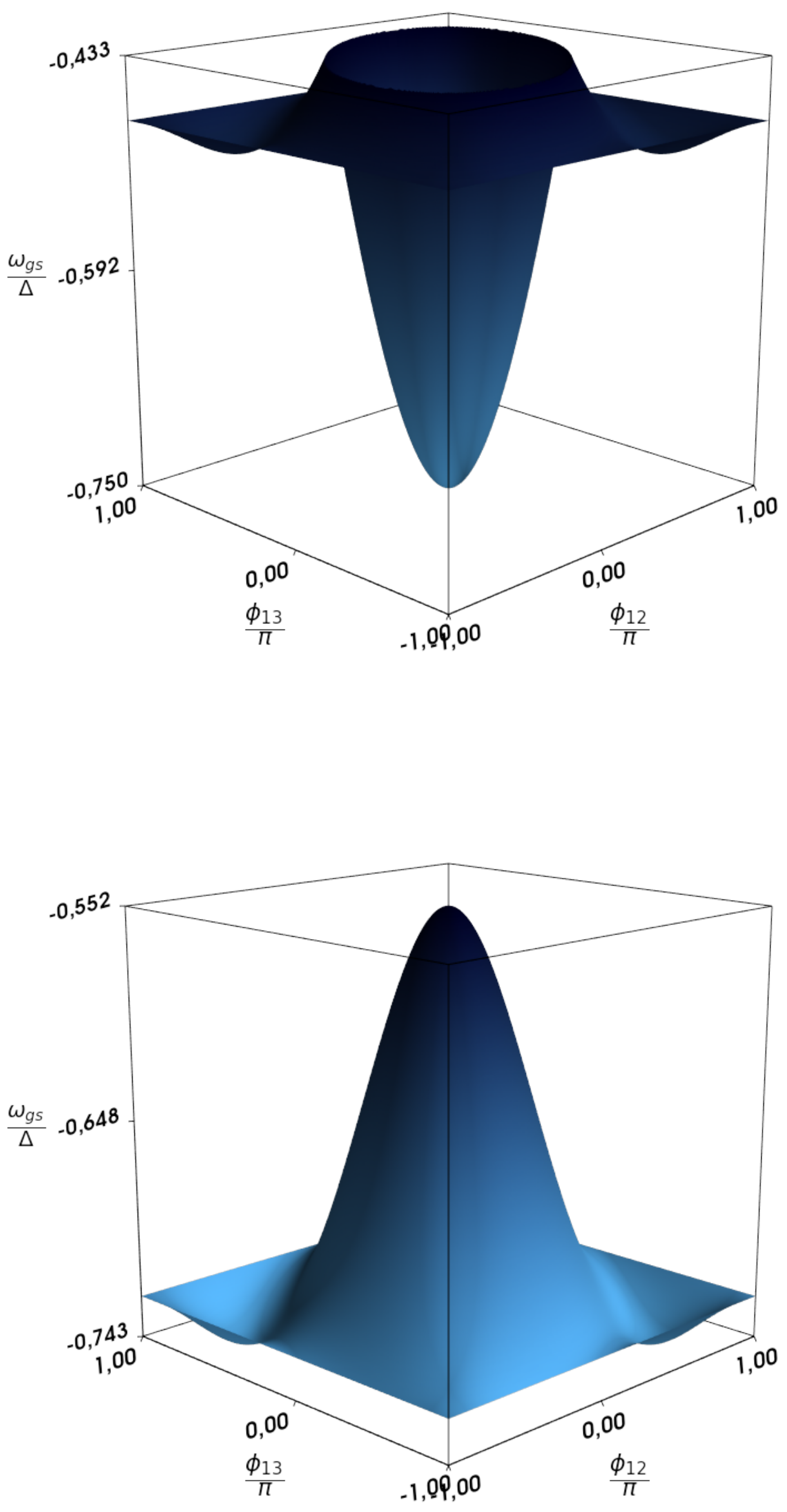


Figure 6.4: The ground state energies for a three terminal junction, with equal tunneling amplitudes $t_1 = t_2 = t_3$ as well as particle hole symmetry $x = 0$, zero magnetic field $B = 0$, and for (a) a potential strength of $\frac{\Gamma}{U} = 0.7$, while for (b) $\frac{\Gamma}{U} = 0.45$

6.5 Supercurrent and Ground state minima

From the ground state energy it is possible find the supercurrent flowing between the different leads. Such that the supercurrent flowing from a lead α' to another lead α follow the formula

$$I^S_{\alpha\alpha'} = 2e\frac{\partial \omega_{gs}}{\partial \phi_{\alpha\alpha'}}\,, \tag{6.74}$$

where e is the electron charge. This can be determined from something like a Green's function, T- and S-matrix formalism, but I will tacitly assume it to be true as in reference [14]. However since I have N different leads, it is more useful to define the current flowing from the dot into a lead α

$$I^S_{\alpha} = 2e\frac{\partial \omega_{gs}}{\partial \phi_{\alpha}}\,. \tag{6.75}$$

Note that current conservation immediately follows

$$\sum_\alpha I^S_\alpha = 2e\left(\sum_\alpha \frac{\partial}{\partial \phi_\alpha}\right)\omega_{gs} = 2e\hat{0}\omega_{gs}\,, \tag{6.76}$$

where $\hat{0}$ is the null operator, since the phases sum as $\sum_\alpha \phi_\alpha \equiv 0 \pmod{2\pi}$.

Since $\omega_{\sigma\pm}$ only have a phase dependence in the variable χ, by use of the chain rule it follows that

$$\frac{\partial \omega_{gs}}{\partial \phi_\alpha} = \frac{\partial \chi}{\partial \phi_\alpha}\frac{\partial \omega_{gs}}{\partial \chi}\,. \tag{6.77}$$

Showing both that the extrema of ω_{gs} corresponds to either places of discontinuities in the derivative $\frac{\partial \omega_{gs}}{\partial \phi_\alpha}$ or maxima and minima of χ, and that for these extrema of χ no current can flow since $\frac{\partial \chi}{\partial \phi_\alpha} = 0$ for any α there.

Whether the minima of ω_{gs} corresponds to minima of χ or maxima of χ, is decided by the values of B, $\frac{\Gamma}{U}$, x and the largest relative coupling $\hat{t}_\alpha$, in the two cases shown in figure 6.4, both types are shown. For figure 6.4a the minima of ω_{gs} corresponds to maxima of χ, while in figure 6.4b the minima of ω_{gs} corresponds to minima of χ.

From the discussion in section 6.2, it is understood that χ can have two different types of minima depending on the size of the largest relative coupling strengths $\hat{t}_\alpha$. If $\hat{t}_\alpha < \frac{1}{\sqrt{2}}$ for all α, then the minimum of χ is for the three lead junction is doubly degenerate, and for the $N > 3$ lead junction it is infinitely degenerate as $\min(\chi)$ is in a $N-3$ dimensional space.

Because of these different types of minima of the ground state energy ω_{gs}, it has become commonplace in the case of a two lead junction to classify it depending on where the

Naming	Value of χ	location of minimum for ω_{gs}
0	$\chi = 1$	$\boldsymbol{\phi} = \mathbf{0}$
$\boldsymbol{\pi}$	$\chi = N^2(2\lvert\hat{t}_\alpha\rvert^2 - 1)^2$	$\phi_\alpha = \pi$ and $\phi_\beta = 0$ for all other
$\boldsymbol{\chi}$	$\chi = 0$	$\boldsymbol{\phi} = \boldsymbol{\phi}^* \in S^*$ where $\dim(S^*) = N - 3$

Table 6.1: The classifications of a N lead junction

minimum is. Which for two leads gives rise to the names **0** and $\boldsymbol{\pi}$ junctions where in the case of $\min(\omega_{gs}) = \omega_{gs}(\phi = 0)$ and $\min(\omega_{gs}) = \omega_{gs}(\phi = \pi)$ respectively. Some people also classify whether or not discontinuities in the current occur by adding a $'$ to the respective names giving $\mathbf{0}'$ and $\boldsymbol{\pi}'$ junctions.

Expanding this naming scheme for a general N lead junction gives six types, which I here choose to call **0**, $\mathbf{0}'$, $\boldsymbol{\pi}$, $\boldsymbol{\pi}'$, $\boldsymbol{\chi}$ and $\boldsymbol{\chi}'$, where $'$ still signifies a discontinuity of the current. This naming convention is summed up in table 6.1.

Note that the discontinuities of the supercurrent, happen whenever the ground state switches its state, which as explained earlier corresponds to a spin-flip in the state. This happens at the places where the single bound state excitation energies $\omega_{\sigma-}$ cross zero energy, which as pointed out in equation (6.23) happens at $\chi = \frac{1}{u}$, in the case of zero magnetic field $B = 0$, if the condition of equation (6.38) is fulfilled. An example of this discontinuity can be seen in figure 6.5, where the supercurrent corresponds to the ground state energy of figure 6.4a.

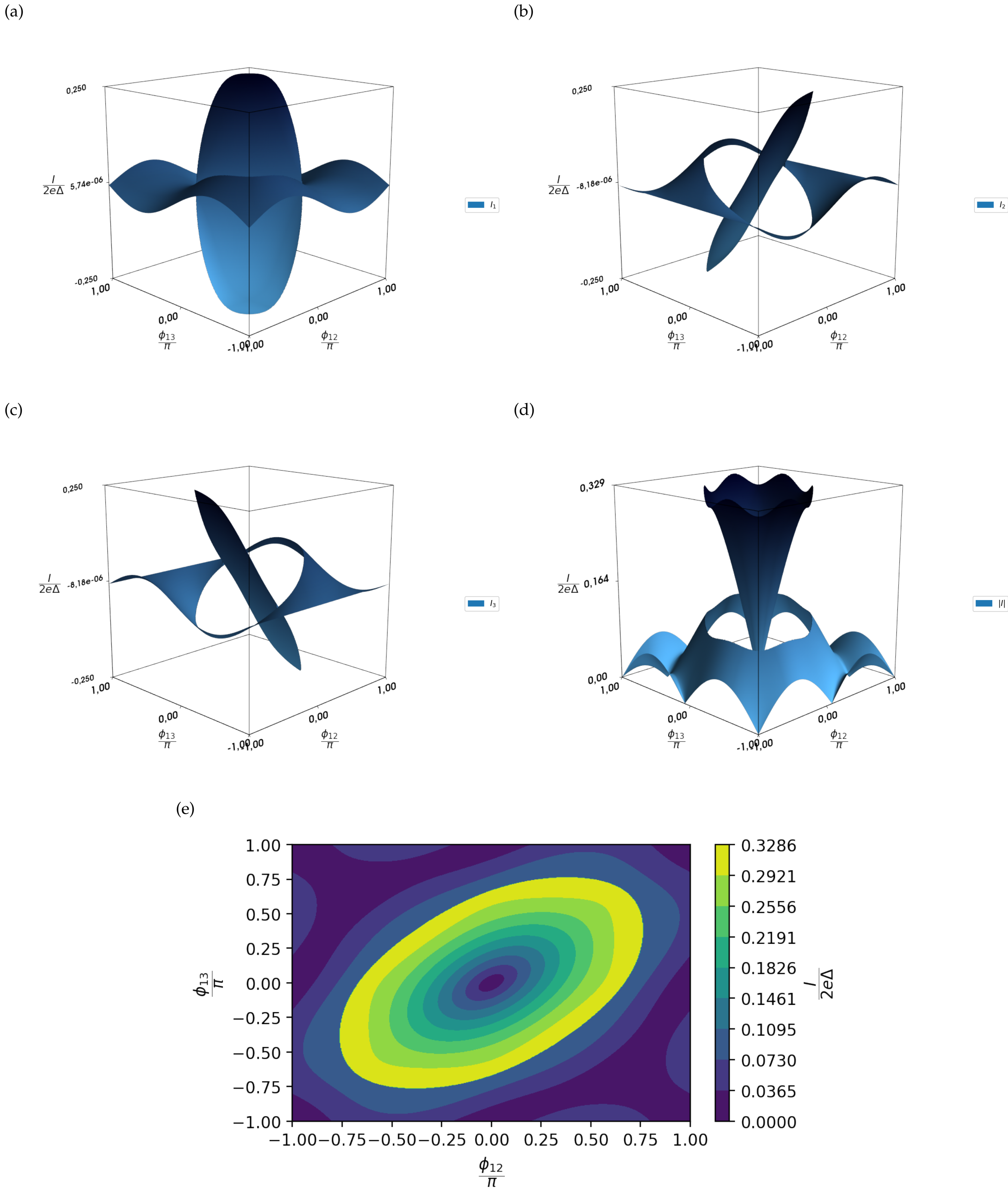


Figure 6.5: Plots of the supercurrents in a three lead quantum dot Josephson junction with equal tunneling amplitudes $t_1 = t_2 = t_3$ as well as particle hole symmetry $x = 0$, zero magnetic field $B = 0$, and potential strength $\frac{\Gamma}{U} = 0.7$: (a) shows the current flowing into lead 1; (b) shows the current flowing from into lead 2; (a) shows the current flowing from into lead 3; and (d) and (e) shows the total magnitude $|I| = \sqrt{I_1^2 + I_2^2 + I_3^2}$ of the current flowing.

Chapter 7

Circuits

In this section I will describe a scenario in which one can use two of these multi-terminal Josephson junctions in a circuit. The type of circuit which I will use here have already been shown to allow for the creation of qubits in the case of two terminals [12, 13].

7.1 Types of Josephson circuits

When building circuits there are 3 major effects to take into account inductive, capacitive and resistive effects. In building Josephson junction circuits however because the leads are superconductors resistance can be neglected.

Instead one might consider circuits build of just junctions and superconductors where the circuit interacts inductively and capacitively. This mean that one can set up the Hamiltonian

$$\mathcal{H} = 2e^2 \left(\boldsymbol{n} - \boldsymbol{n}_g\right)^T \boldsymbol{C}^{-1} \left(\boldsymbol{n} - \boldsymbol{n}_g\right) + \frac{1}{2}\boldsymbol{I}^T \boldsymbol{M} \boldsymbol{I} + U_J(\boldsymbol{\phi}) \,, \tag{7.1}$$

where $\boldsymbol{C}$ is the capacitance matrix between all superconductors, $\boldsymbol{n}$ is the vector of copper pair number operators n_α for each superconductor and $\boldsymbol{n}_g$ is the vector of gate biases or charge offsets $n_{g\alpha}$ for each superconductor. $\boldsymbol{I}$ is the vector of currents flowing in the superconductors and $\boldsymbol{M}$ is the inductance matrix which contains both mutual- and self-inductance. The last term $U_J(\boldsymbol{\phi})$ is the Josephson energy potential part of the circuit, which is a sum of ground state energies (6.69) for each junction in the circuit. The phase differences for each superconductor at the dots is then determined by the inductances and the geometry of the circuit, because of the wavefunction single-valuedness relation [21]

$$\sum_{l \in \text{loop}} \Delta\phi_l + 2\pi \left(\frac{\Phi_{loop}}{\Phi_0} + k\right) = 0 \tag{7.2}$$

where $\Delta\phi_l$ is the phase differences in the loop, $\Phi_0 = \frac{h}{2e}$ is the magnetic flux quantum, and Φ_{loop} is the total magnetic flux penetrating the loop, which is the sum of the flux induced by any flowing current as well as any externally supplied flux $\Phi = \Phi_{ind} + \Phi_{ext}$. Lastly k is some integer, which only have influence on something like the Little-Parks effect which will not be covered in this thesis [21, 27].

For the purposes of this thesis, I will assume that the capacitance contribution is irrelevant, meaning that the circuit is large enough such that $|\boldsymbol{C}^{-1}|$ is small, meaning that the system can be described as

$$\mathcal{H} \approx U_{ind}(\Phi_{ind}) + U_J(\boldsymbol{\phi}) \tag{7.3}$$

7.2 Double junction system

I will be considering a generalization of the circuit considered in reference [12], but here with two multi-terminal Josephson junctions connected to each other by some amount of terminals, such that the full circuit consists of two quantum dots, D and $\bar{D}$, and N superconducting wires as seen in figure. Here the total energy can then be written as

$$U_{tot} = U_D(\boldsymbol{\phi}) + U_{\bar{D}}(\bar{\boldsymbol{\phi}}) + U_{ind}(\boldsymbol{\Phi}_{ind})\,, \tag{7.4}$$

Then by the single-valuedness, it follows that

$$\phi_{i,i+1} + \bar{\phi}_{i+1,i} + 2\pi\left(\frac{\Phi_{i,i+1}}{\Phi_0} + l_{i,i+1}\right) = 0 \tag{7.5}$$

Which can be written on a vector form as

$$\boldsymbol{\phi} - \bar{\boldsymbol{\phi}} + 2\pi\left(\frac{\boldsymbol{\Phi}}{\Phi_0} + \boldsymbol{l}\right) = \boldsymbol{0}\,, \tag{7.6}$$

where the elements $\boldsymbol{\phi}_i = \phi_{i,i+1}$, and similarly for $\bar{\boldsymbol{\phi}}$ and $\boldsymbol{\Phi}$. This relation fixes $N-1$ of the variable since there are $N-1$ loops, meaning I can write the total energy in terms of the fluxes, and the phase differences at one of the dots

$$U_{tot} = U_D(\bar{\boldsymbol{\phi}}, \boldsymbol{\Phi}) + U_{\bar{D}}(\bar{\boldsymbol{\phi}}) + U_{ind}(\boldsymbol{\Phi}_{ind})\,. \tag{7.7}$$

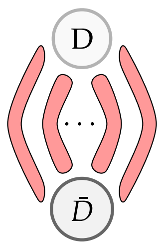


Figure 7.1: A sketch of a two dot - N lead cicuit. Superconducting leads are red and the dots signify the $N-4$ other leads)

Where the inductive energy term can be written as

$$U_{ind}(\boldsymbol{\Phi}_{ind}) = \frac{1}{2}\boldsymbol{I}^T\boldsymbol{M}\boldsymbol{I} = \frac{1}{2}\boldsymbol{\Phi}_{ind}^T\tilde{\boldsymbol{M}}^{-1}\boldsymbol{M}\tilde{\boldsymbol{M}}^{-1}\boldsymbol{\Phi}_{ind}\,, \tag{7.8}$$

where $\tilde{\boldsymbol{M}}$ is the self inductances, which is the same as the diagonal of $\boldsymbol{M}$. To then minimize with respect to either the phases or the fluxes (depending on what one is most interested in), the differential equation

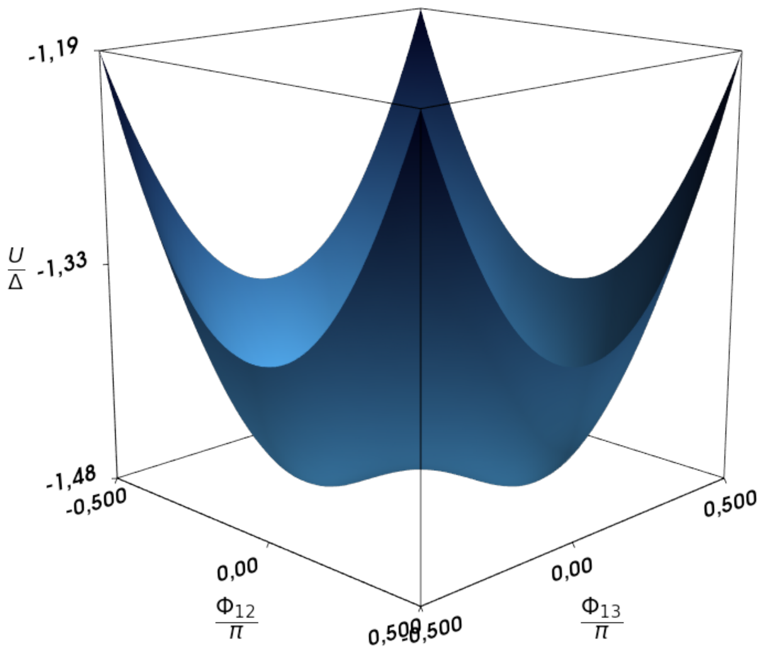
$$\frac{\partial U_{tot}}{\partial \boldsymbol{\Phi}} = \frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{\Phi}}\frac{\partial U_D}{\partial \boldsymbol{\phi}}(\boldsymbol{\phi}) + \frac{\partial U_{ind}}{\partial \boldsymbol{\Phi}}(\boldsymbol{\Phi}_{ind}) \overset{!}{=} \boldsymbol{0}\,, \tag{7.9}$$

is set up.

This can be numerically solved with respect to the phases $\boldsymbol{\phi}$, and then reinserted this into the energy equation. This can be seen in figure 7.2, for a circuit with three wires. Here one can see that for this specific case the circuit give two degenerate minima, much like the two lead system in reference [12].

This suggests that it might be possible to construct a qubit using this new system, but further work outside of this thesis will be needed to properly describe how this would work, and how robust this might be compared to other types of qubits.

(a)



(b)

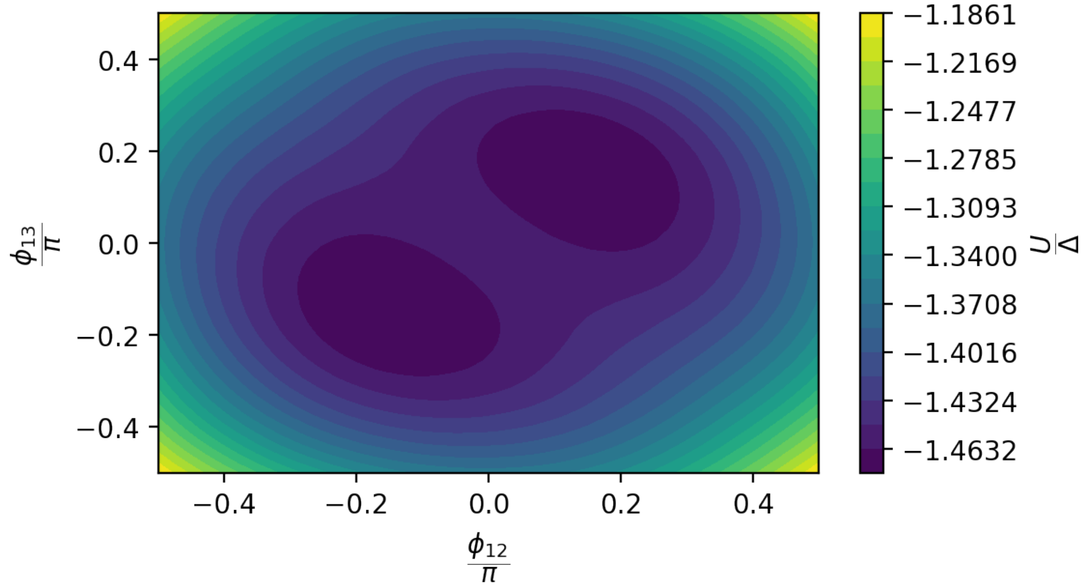


Figure 7.2: The numerically minimized circuit energies, for a 3 wire 2 dot circuit, with a $\mathbf{0}'$ junction and a χ junction, with strong self inductances.

Chapter 8

Discussion

While I have found the bound states and their energies, as well as tried to insert this new type of junction into an existing circuit, I have have simply laid the groundwork for further work. I will here summarize further work which I expect could be interesting.

8.1 Multi-terminal/junction circuit correspondence

Circuits have been studied theoretically in the case of circuit with two terminal junctions, to create artificial topological matter in an paper by Fatemi et al. [28]. In that paper they find that for a three Josephson junction circuit, where the three terminals are connected by an upper and lower common line, that for an offset of cooper pair charge being $n = 0.5$, there exist two Weyl nodes. These nodes seem to be located close to the same phase differences as the $x = 0$ conical intersections as in my three terminal Josephson junctions for equal coupling $t_{\alpha} = t_{\alpha'}$. Suggesting that there might be the same symmetries in both systems for these parameters, which might mean that there exist some N-terminal junction/N junction circuit correspondence for some set of parameters.

8.2 Topological matter

In chapter 6 I found the bound states and their energies. Where I have hinted that there might be something interesting happening in terms of topological quantities. However I have not in any details studied the actual topological properties which Riwar et al. in their paper [1] have pointed out as interesting. It therefore might be really interesting in further works, to determine these with an in depth description of the topology involved in the system.

Chapter 9

Conclusion

I have found that by having N superconductors weakly coupling to a single spin split Anderson impurity, bound states appear in the form of Yu-Shiba-Rusinov states. These states can be described as depending a parameter χ which lives in a $N-1$ dimensional quasi-momentum space of phase differences.

I have found these states and their energies, and have extensively examined the symmetries and other properties of the parameter χ. I found that it encodes the information of lead asymmetry, and depends on both the individual lead-dot coupling strengths as well as differences in phases between leads. I have found that the extrema of the energies of the states must also be at the extrema of this parameter χ. Here I have shown that the parameter allows for extrema which are in a certain interval, meaning that for these N terminal junctions the 0 and π junction classification has to be generalized to allow for a new type, which I have chosen to call a χ junction.

I have then found the supercurrents that form in these N terminal junction, and have used these in a simple example of a quantum electromagnetic circuit, which might have characteristics needed for creating a quantum bit.

Lastly I have given an overview of two areas of research, within an overarching topic of topology and symmetries, where I suspect this thesis might be of further use.

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Appendix A

Finding the energy of a Bogoliubov quasi-particle

A.1 The energy of a Bogoliubov quasi-particle without a magnetic field

From the main text it was found that (in equations (3.12) and (3.13))

$$E_k = \xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u_k^* v_k^* + \Delta_k^* u_k v_k \tag{A.1}$$

$$0 \stackrel{!}{=} 2\xi_k v_k u_k^* - \Delta_k (u_k^*)^2 + \Delta_k^* v_k^2 \tag{A.2}$$

Note that since $E_{k\sigma} \in \mathbb{R}$ either $\Delta_k u_k^* v_k^*$, $\Delta_k^* u_k v_k \in \mathbb{R}$ or $\Delta_k u_k^* v_k^* + \Delta_k^* u_k v_k = 0$ (while I will not show it here, the second case is a special case of the first, meaning that the first is the most general). This means that I can find a real number r, such that

$$u_k^* v_k^* = \Delta_k^* \frac{r}{|\Delta_k|^2} \tag{A.3}$$

by then multiplying equation (A.2) by $u_k v_k^*$, it follows that

$$0 \stackrel{!}{=} (2\xi_k v_k u_k^* - \Delta_k (u_k^*)^2 + \Delta_k^* v_k^2) u_k v_k^* = 2\xi_k \frac{r^2}{|\Delta_k|^2} - |u_k|^2 r + |v_k|^2 r \tag{A.4}$$

I then see that by squaring equation (A.3), it also follows that

$$r^2 = |u_k|^2 |v_k|^2 |\Delta_k|^2 \tag{A.5}$$

Inserting this new relation it follows that

$$0 \stackrel{!}{=} 2\xi_k |u_k|^2 |v_k|^2 - |u_k|^2 r + |v_k|^2 r \tag{A.6}$$

Meaning the real number must be

$$r = 2\xi_k \frac{|u_k|^2|v_k|^2}{|u_k|^2 - |v_k|^2} \tag{A.7}$$

Substituting the real number into equation (A.1), then shows that

$$\begin{aligned} E_k &= \xi_k(|u_k|^2 - |v_k|^2) + 2r \\ &= \xi_k(|u_k|^2 - |v_k|^2) + 4\xi_k \frac{|u_k|^2|v_k|^2}{|u_k|^2 - |v_k|^2} \\ &= \frac{\xi_k(|u_k|^2 + |v_k|^2)^2}{|u_k|^2 - |v_k|^2} \\ &= \frac{\xi_k}{|u_k|^2 - |v_k|^2} \end{aligned}$$

By then once again using that $|u_k|^2 + |v_k|^2 = 1$ I get the relations that

$$|u_k|^2 = \frac{1}{2} + \frac{\xi_k}{2E_k} \tag{A.8}$$

$$|v_k|^2 = \frac{1}{2} - \frac{\xi_k}{2E_k} \tag{A.9}$$

where the complex phases of u_k and v_k can be chosen semi arbitrarily such that $\arg(u_k) + \arg(v_k) \equiv \arg(\Delta_k) \pmod{2\pi}$. Which shows that

$$|u_k|^2 - |v_k|^2 = \frac{\xi_k}{E_k} \tag{A.10}$$

Inserting this into equations (A.7) and squaring (A.5) and also dividing by $|u_k|^2|v_k|^2$, I find the energy from

$$4E_k^2|u_k|^2|v_k|^2 = E_k^2\left(1 - \frac{\xi_k^2}{E_k^2}\right) = |\Delta_k|^2 \tag{A.11}$$

Meaning that I get the energy as

$$E_k^2 = \xi_k^2 + |\Delta_k|^2 \tag{A.12}$$

A.2 The energy of a Bogoliubov quasi-particle in magnetic field

By adding a spin index to the energy for the electrons, such that $\xi_{k\sigma} = \xi_k + \xi_\sigma$, I find that the commutator of the quasi-particle in equation (3.11) now instead gives

$$E_{k\sigma} = \xi_{k\sigma}|u_k|^2 - \xi_{k-\sigma}|v_k|^2 + \Delta_k u_k^* v_k^* + \Delta_k^* u_k v_k \tag{A.13}$$

$$0 \stackrel{!}{=} (\xi_{k\sigma} + \xi_{k-\sigma})v_k u_k^* - \Delta_k (u_k^*)^2 + \Delta_k^* v_k^2 \tag{A.14}$$

which simplifies to

$$E_{k\sigma} = \xi_\sigma + \xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u_k^* v_k^* + \Delta_k^* u_k v_k \tag{A.15}$$

$$0 \stackrel{!}{=} 2\xi_k v_k u_k^* - \Delta_k (u_k^*)^2 + \Delta_k^* v_k^2 \tag{A.16}$$

This mean that the only change is that the energy of the quasi-particle now also have the same spin energy as the electrons.

$$E_{k\sigma} = E_k + \xi_\sigma \tag{A.17}$$

where the energy $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$ following the same arguments as in appendix A.1.

Appendix B

Schrieffer-Wolff quantities

B.1 Commutators of the Schrieffer-Wolff transformation

Below is a list of all the involved commutators of the first order SW transformation

$$\left[\gamma^\dagger_\mu \gamma_\mu, \gamma^\dagger_{\mu'} d_{\sigma'}\right] = \gamma^\dagger_\mu d_\sigma \delta_{\mu\mu'} \tag{B.1}$$

$$\left[\gamma^\dagger_\mu \gamma_\mu, \gamma_{\bar{\mu}'} d_{\sigma'}\right] = -\gamma_\mu d_{-\sigma} \delta_{\mu\bar{\mu}'} \tag{B.2}$$

$$\left[d^\dagger_\sigma d_\sigma, \gamma^\dagger_{\mu'} d_{\sigma'}\right] = -\gamma^\dagger_{\mu'} d_\sigma \delta_{\sigma\sigma'} \tag{B.3}$$

$$\left[d^\dagger_\sigma d_\sigma, \gamma_{\bar{\mu}'} d_{\sigma'}\right] = -\gamma_{\bar{\mu}'} d_\sigma \delta_{\sigma\sigma'} \tag{B.4}$$

$$\left[n_\downarrow n_\uparrow, \gamma^\dagger_{\mu'} d_{\sigma'}\right] = -n_{-\sigma'} \gamma^\dagger_{\mu'} d_{\sigma'} \tag{B.5}$$

$$\left[n_\downarrow n_\uparrow, \gamma_{\bar{\mu}'} d_{\sigma'}\right] = -n_{-\sigma'} \gamma_{\bar{\mu}'} d_{\sigma'} \tag{B.6}$$

For the second order I make use of the commutators below

$$[\gamma^\dagger_\mu d_\sigma\, ,\, d^\dagger_{\sigma'} c_{\mu'}] = \gamma^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} - u_\mu n_\sigma \delta_{\mu\mu'} \tag{B.7}$$

$$[n_{-\sigma}\, ,\, d^\dagger_{\sigma'} c_{\mu'}] = d^\dagger_{-\sigma} c_{\mu'} \delta_{-\sigma\sigma'} \tag{B.8}$$

$$[n_{-\sigma} \gamma^\dagger_\mu d_\sigma\, ,\, d^\dagger_{\sigma'} c_{\mu'}] = n_{-\sigma}(\gamma^\dagger_\mu c_{\mu'} \delta_{\sigma\sigma'} - u_\mu n_\sigma \delta_{\mu\mu'}) + \bar{n}_\sigma c_{\mu'} \delta_{-\sigma\sigma'} \gamma^\dagger_\mu \tag{B.9}$$

$$[\gamma_{\bar{\mu}} d_\sigma\, ,\, d^\dagger_{\sigma'} c_{\mu'}] = \gamma_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} - v_\mu n_\sigma \delta_{\mu\mu'} \tag{B.10}$$

$$[n_{-\sigma} \gamma_{\bar{\mu}} d_\sigma\, ,\, d^\dagger_{\sigma'} c_{\mu'}] = n_{-\sigma}(\gamma_{\bar{\mu}} c_{\mu'} \delta_{\sigma\sigma'} - v_\mu n_\sigma \delta_{\mu\mu'}) + \bar{n}_\sigma c_{\mu'} \gamma_{\bar{\mu}} \delta_{-\sigma\sigma'} \tag{B.11}$$

$$[\gamma_\mu^\dagger d_\sigma\,,\,c_{\mu'}^\dagger d_{\sigma'}] = -v_\mu d_{-\sigma} d_\sigma \delta_{\mu\bar{\mu}'} \tag{B.12}$$

$$[n_{-\sigma}\gamma_\mu^\dagger d_\sigma\,,\,c_{\mu'}^\dagger d_{\sigma'}] = d_{-\sigma} d_\sigma c_{\mu'}^\dagger \gamma_\mu^\dagger \delta_{-\sigma\sigma'} \tag{B.13}$$

$$[\gamma_{\bar{\mu}} d_\sigma\,,\,c_{\mu'}^\dagger d_{\sigma'}] = u_\mu d_{-\sigma} d_\sigma \delta_{\mu\bar{\mu}'} \tag{B.14}$$

$$[n_{-\sigma}\gamma_{\bar{\mu}} d_\sigma\,,\,c_{\mu'}^\dagger d_{\sigma'}] = d_{-\sigma} d_\sigma c_{\mu'}^\dagger \gamma_{\bar{\mu}} \delta_{-\sigma\sigma'} \tag{B.15}$$

B.2 Schrieffer-Wolff transformation coefficients

$$W_{\mu\mu'} = t_\mu t_{\mu'}^* \left(\frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} + \frac{\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - E_{\alpha' k'}}{(\xi_{\alpha'\sigma'} - \xi_{d\sigma'})^2 - E_{\alpha' k'}^2} \right) \tag{B.16}$$

$$\begin{aligned} J_{\mu\mu'} = t_\mu t_{\mu'}^* \Bigg(& \frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - U - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} - \frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \\ & + \frac{\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - U - E_{\alpha' k'}}{(\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - U)^2 - E_{\alpha' k'}^2} - \frac{\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - E_{\alpha' k'}}{(\xi_{\alpha'\sigma'} - \xi_{d\sigma'})^2 - E_{\alpha' k'}^2} \Bigg) \end{aligned} \tag{B.17}$$

$$Z_{\mu\mu'} = t_\mu t_{\mu'}^* \frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \tag{B.18}$$

$$T_{\mu\mu'} = t_\mu t_{\mu'}^* \left(\frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} - \frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \right) \tag{B.19}$$

$$D_{\mu\mu'} = t_\mu t_{\mu'} \frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \tag{B.20}$$

$$L_{\mu\mu'} = t_\mu t_{\mu'} \left(\frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} - \frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \right) \tag{B.21}$$

$$K_{\mu\mu'} = t_\mu t_{\mu'} \left(\frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - U - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} - \frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \right) \tag{B.22}$$

The special redefined coefficients read as

$$\begin{aligned} W'_{\mu\mu'} = \frac{t_\mu t_{\mu'}^*}{4} \Bigg(& \frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - U - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} + \frac{\xi_{\alpha\sigma} - \xi_{d\sigma} - E_{\alpha k}}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \\ & + \frac{\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - U - E_{\alpha' k'}}{(\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - U)^2 - E_{\alpha' k'}^2} + \frac{\xi_{\alpha'\sigma'} - \xi_{d\sigma'} - E_{\alpha' k'}}{(\xi_{\alpha'\sigma'} - \xi_{d\sigma'})^2 - E_{\alpha' k'}^2} \Bigg) \end{aligned} \tag{B.23}$$

$$Z'_{\mu\mu'} = \frac{t_\mu t_{\mu'}^*}{4} \left(\frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma} - U)^2 - E_{\alpha k}^2} + \frac{\Delta_\alpha}{(\xi_{\alpha\sigma} - \xi_{d\sigma})^2 - E_{\alpha k}^2} \right) \tag{B.24}$$

the others trivially follow from the ones above this.

Under the approximation of the main text for $\Delta_\alpha = \Delta$ the other redefined coefficients become

$$Z'_{\mu\mu'} \approx \frac{t_\mu t^*_{\mu'}}{4} \left(\frac{\Delta}{\xi_d^2} + \frac{\Delta}{(\xi_d + U)^2} \right) = 2 t_\mu t^*_{\mu'} \frac{\Delta(1+x^2)}{U^2(1-x^2)^2} \propto \frac{\Delta\Gamma}{U^2} \tag{B.25}$$

$$T'_{\mu\mu'} \approx \frac{t_\mu t^*_{\mu'}}{2} \left(\frac{\Delta}{\xi_d^2} - \frac{\Delta}{(\xi_d + U)^2} \right) = 8 t_\mu t^*_{\mu'} \frac{\Delta x}{U^2(1-x^2)^2} \propto \frac{\Delta\Gamma}{U^2} \tag{B.26}$$

Appendix C

Determinant of special block matrices

For a 2N x 2N block matrix $\boldsymbol{M}$ of the form

$$M = \begin{pmatrix} \mathbb{1} + a\boldsymbol{\delta}_N & \boldsymbol{V}\boldsymbol{\delta}_N \\ \boldsymbol{W}\boldsymbol{\delta}_N & \mathbb{1} + b\boldsymbol{\delta}_N \end{pmatrix} = \begin{pmatrix} [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,1)} & [\mathbf{0}]^{(N-1,N-1)} & [\boldsymbol{v}']^{(N-1,1)} \\ [\mathbf{0}]^{(1,N-1)} & 1+a & [\mathbf{0}]^{(1,N-1)} & v_{NN} \\ [\mathbf{0}]^{(N-1,N-1)} & [\boldsymbol{w}']^{(N-1,1)} & [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,1)} \\ [\mathbf{0}]^{(1,N-1)} & w_{NN} & [\mathbf{0}]^{(1,N-1)} & 1+b \end{pmatrix} \tag{C.1}$$

Where $[\_]^{(i,j)}$ signifies that the block is a $i \times j$ matrix, with its elements described by what is inside of the parenthesis, and the vectors $\boldsymbol{v}'$, $\boldsymbol{w}'$ are the first N-1 entries in the vector $\boldsymbol{v}_i = (\boldsymbol{V}\boldsymbol{\delta}_N)_{i,N}$. The following simplification of the determinant then takes place

$$\det(M) = (1+a)\begin{vmatrix} [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,N-1)} & [\boldsymbol{v}']^{(N-1,1)} \\ [\mathbf{0}]^{(N-1,N-1)} & [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,1)} \\ [\mathbf{0}]^{(1,N-1)} & [\mathbf{0}]^{(1,N-1)} & 1+b \end{vmatrix} + (-1)^N v_{NN}\begin{vmatrix} [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,1)} & [\mathbf{0}]^{(N-1,N-1)} \\ [\mathbf{0}]^{(N-1,N-1)} & [\boldsymbol{w}']^{(N-1,1)} & [\mathbb{1}]^{(N-1,N-1)} \\ [\mathbf{0}]^{(1,N-1)} & w_{NN} & [\mathbf{0}]^{(1,N-1)} \end{vmatrix} \tag{C.2}$$

$$= (1+a)(1+b)\begin{vmatrix} [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,N-1)} \\ [\mathbf{0}]^{(N-1,N-1)} & [\mathbb{1}]^{(N-1,N-1)} \end{vmatrix} + (-1)^N v_{NN}(-1)^{N-1} w_{NN}\begin{vmatrix} [\mathbb{1}]^{(N-1,N-1)} & [\mathbf{0}]^{(N-1,N-1)} \\ [\mathbf{0}]^{(N-1,N-1)} & [\mathbb{1}]^{(N-1,N-1)} \end{vmatrix} \tag{C.3}$$

$$= (1+a)(1+b) - v_{NN}w_{NN} \tag{C.4}$$

Showing that

$$\begin{vmatrix} \mathbb{1} + a\boldsymbol{\delta}_N & \boldsymbol{V}\boldsymbol{\delta}_N \\ \boldsymbol{W}\boldsymbol{\delta}_N & \mathbb{1} + b\boldsymbol{\delta}_N \end{vmatrix} = \begin{vmatrix} 1+a & \boldsymbol{V}_{NN} \\ \boldsymbol{W}_{NN} & 1+b \end{vmatrix} \tag{C.5}$$