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Conductance Calculations for Semiconductor-Superconductor Majorana Structures

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Conductance Calculations for Semiconductor-Superconductor Majorana Structures

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Abstract

Conductance Calculations for
Semiconductor-Superconductor Majorana
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Majorana zero modes (MZMs), also called Majorana bound states (MBSs), are zero-energy mid-gap modes localized near boundaries and topological defects in one- and two-dimensional topological superconductors. These zero-energy modes have attracted significant attention in recent years because of their unique properties, particularly their non-Abelian exchange statistics and their ability to encode quantum information non-locally. These properties make the MZMs an ideal platform for fault-tolerant topological quantum computation. This type of quantum memory is robust against local perturbations, since the information is encoded non-locally, while the information processing, which can be done, for example, by braiding the MZMs, is topologically protected against quantum errors.

Significant theoretical steps that inspired the practical realization of MZMs were Kitaev’s model for a one-dimensional p-wave superconductor and the concrete proposals for its realization in semiconductor nanowires with strong spin-orbit coupling proximity-coupled to a standard s-wave superconductor and in the presence of a magnetic field applied along the wire. The most direct and widely used experimental method of detecting the presence of MZMs at the ends of a semiconductor-superconductor heterostructure realized in the laboratory is charge tunneling. The measured differential conductance, which is approximately related to the local density of states at the end of the wire, is predicted to exhibit a characteristic zero-bias conductance peak if a MZM is present.

This thesis describes a systematic theoretical approach to calculating the differential conductance of semiconductor-based Majorana structures that focuses on identifying the components of the theoretical model that are critical to describing the key features observed in recent experiments. It is demonstrated that, in order to properly account for the observed features, one has to treat the parent superconductor as an active component of the hybrid system, instead of a simple source of Cooper pairs. Also, the phase diagram of a non-homogeneous structure is calculated and compared with actual experimental measurements. Finally, the low-energy features of a system consisting of multiple superconductor islands separated by potential barriers are calculated and interpreted in terms of coupled MBSs.
## Contents

1 Introduction .......................... 1

2 Theoretical Background 1: Majorana’s Solution to the Dirac Equation 4
   2.1 The Dirac Equation .................. 4
   2.2 Majorana’s Solutions to The Dirac Equation .................. 12
   2.3 Possible Majorana Fermions .................. 16

3 Theoretical Background 2: Majorana Bound States in Solid State Systems 18
   3.1 Superconductors .................. 18
   3.2 Majorana Bound States in One Dimensional Spinless Superconductors .................. 24
   3.3 Braiding Majorana Bound States .................. 27
   3.4 Quantum Computation .................. 30
   3.5 A Majorana Computer .................. 32
   3.6 S-wave vs P-wave Superconductors .................. 37

4 Experimental Background .................. 41

5 Motivation .................. 47

6 Differential Conductance in Semiconductor-Superconductor Hybrid Structures .................. 49
Chapter 1

Introduction

Human kind’s desire to understand nature is something fundamental to our being. Advancement in technology has always been a happy side effect of our mysterious urge to discover the fundamental rules which determine the behavior of our world. Alan Turing is often credited as the first person to conceive of a single machine which could replicate every classical process seen in nature. Turing’s machine (which eventually lead to the modern computer) seems to be able to reproduce classical physics with the caveat that more complicated physical phenomena take more processing to replicate. If there is no symmetry the computer needs to simulate each constituent of the system separately, however, the size of the computer memory needed to simulate a classical system grows linearly with the system. The proof of this claim is simply to think of the system itself as a classical computer and various physical processes as (algorithmic) computations. If there was some physical process that could not be efficiently replicated by our machine, then our machine is incomplete and we simply need to add a drive to our computer which utilizes that physical process and therefore is capable of simulating it efficiently.

This was exactly Feynman’s idea when he realized that quantum mechanics was particularly hard to simulate on classical computers [1]. There are not enough atoms in the
known universe to build a classical computer that could simulate even relatively simple quantum systems. The number of eigenstates of a quantum system grows exponentially with the number of quantum bodies involved. In this way, quantum mechanics is fundamentally different from classical mechanics and the only way we can simulate it efficiently is to build a quantum drive.

A quantum computer consists of a number of q-bits and a set of unitary operators that act on those q-bits. The q-bits are the quantum analog of classical bits. They store one quantum of information. In other words, each q-bit can be represented by one of two quantum state vectors (e.g. \( |1\rangle \) for “on” or \( |0\rangle \) for “off”). Unlike classical bits, however, a q-bit can be in an arbitrary state of the two dimensional Hilbert space \( (\alpha |1\rangle + \beta |0\rangle) \) for arbitrary \( \alpha \) and \( \beta \). The state of the computer is then the direct product of q-bit states (e.g. \( a |0110100...\rangle + b |1001101\rangle + ... \)). At the beginning of a quantum computation, the quantum computer is set to some eigenvector of the system (e.g. \( |0110100...\rangle \)). This writes some classical information onto the quantum system. Next, a number of unitary operators act on the state of the computer. This is the quantum part of the algorithm. During this step the state of the system stores quantum information. At the end of the algorithm, the state of the computer is projected onto some eigenstate and some classical information is read off.

Much effort has been dedicated to creating a quantum computer in the last several decades. However, there are difficult basic science and engineering challenges to overcome. Perhaps the most difficult challenge is decoherence. The more quantum bodies that are involved in a computation, the harder it is to isolate those bodies from the environment. Environmental contamination is a particularly alarming concern for a quantum processor since quantum states are extremely sensitive to error. A quantum bit that is rotated by any amount from the ”on” position (e.g. the quantum state \( |1\rangle \)) has a chance of being measured
as "off" (i.e. $|0\rangle$). For this reason, it is very difficult to build a quantum computer large enough to simulate quantum systems that are too complicated to simulate on a classical computer.

On the other hand, the phase difference that results from exchanging two quantum particles is independent of outside influences. Exchanging two fermions, for example, changes the phase of the quantum state by a negative sign no matter what path the fermions use for exchange. Of course a negative sign is not extremely helpful for simulating arbitrary unitary evolutions.

However, there are exotic zero energy modes that arise in certain solid states systems known as the Majorana bound states (MBS) which can encode quantum information without the threat of decoherence. The MBS are separated from the continuum in the system and are therefore immune to small energy perturbations. Furthermore, MBS are non-Abelian meaning that braiding the bound states can change the state of the system instead of simply adding an overall sign as is the case with normal fermions.

Since Kitaev showed that MBS can be found in quantum nanowires proximity coupled to superconductors [2], much work has been done to try and detect these modes. Many of these studies measure the differential conductance in the nanowire. MBS are predicted to show up as zero bias peaks in conductance measurements. My work has been to model such conductance experiments in order to aid experimental observation.
Chapter 2

Theoretical Background 1: Majorana’s Solution to the Dirac Equation

2.1 The Dirac Equation

The Majorana fermion is the real solution of the Dirac equation [3]. For that sentence to have meaning it is necessary to first understand how the Dirac equation arises. In this section I will discuss the Dirac equation. Then in the next section the Dirac equation will be used to introduce the concept of Majorana fermions.

Let us start with the Heisenberg uncertainty principle, which states that neither the momentum and position nor the energy and time of an object can be measured simultaneously. At this point I should probably say that in most of this thesis I will be using the units in which Planck’s constant is $2\pi (\hbar = 1)$ and the speed of light is one ($c = 1$). I will continue with this convention until the results section where, I think, familiarity is more
important than style. With these conventions we have,

\[ \Delta x \Delta P \geq \frac{1}{2} \]
\[ \Delta t \Delta E \geq \frac{1}{2} \]

(2.1)

I start with the uncertainty principle because I find it to be the most intuitive aspect of quantum mechanics. In fact it could be seen as solving ancient philosophical problems. For example, it could be argued that the uncertainty principle solves Zeno’s paradox because it allows motion to happen only if space is not well defined. However, let us simply take the principle as an experimental fact. The principle can be understood by allowing objects to travel in wave packets \( \psi \). These waves can be described as functions of position and time \( \psi(x,t) \) or functions of momentum and energy \( \psi(P,E) \). With this description of nature in mind, the uncertainty principle is enforced if \( \psi(x,t) \) and \( \psi(P,E) \) are Fourier transforms of one another. Because they are Fourier transforms, we have that \( \partial_x \psi(x,t) = iP \psi(x,t) \) and \( \partial_t \psi(x,t) = -iE \psi(x,t) \). Therefore, in order to quantize an energy momentum relation all we have to do is to promote momentum and energy to operators acting on the spatial-temporal wave functions \( \psi(x,t) \).

\[ P \rightarrow -i \partial_x \]
\[ E \rightarrow i \partial_t \]

(2.2)

In this manner, the newtonian energy-momentum relation provides us with the Schrödinger equation.

\[ E = \frac{P^2}{2m} + V(x) \rightarrow \partial_t \psi(x,t) = -\frac{1}{2m} \partial^2_x \psi(x,t) + V(x) \psi(x,t) \]

(2.3)
However, we now know that the Newtonian picture is incomplete. We would like to use the relativistic energy-momentum relation.

\[ E^2 - P^2 - m^2 = 0 \rightarrow -\partial_t^2 \psi(x, t) + \partial_x^2 \psi(x, t) - m^2 \psi(x, t) = 0 \]  

(2.4)

The equation to the right of the arrow in (2.4) is known as the Klein-Gordon equation. The Klein-Gordon equation is used, at times, to describe relativistic quantum mechanics but it has a devastating consequence.

The trouble with the Klein-Gordon equation, among other things, is that it predicts negative probability densities. We can see this issue by deriving probability conservation from the Klein-Gordon equation. Just like it is done with the Schrödinger equation, we start by multiplying the conjugate field to our equation and then the normal field to the conjugate equation.

\[ -\psi^* \partial_t^2 \psi + \psi \partial_x^2 \psi - m^2 = 0 \]  

\[ -\psi \partial_t^2 \psi^* + \psi^* \partial_x^2 \psi^* - m^2 = 0 \]  

(2.5)

Then subtract these two,

\[ (\psi^* \partial_t^2 \psi - \psi \partial_t^2 \psi^*) - (\psi^* \partial_x^2 \psi - \psi \partial_x^2 \psi^*) = 0 \]  

(2.6)

\[ \partial_t i(\psi^* \partial_t \psi - \psi \partial_t \psi^*) + \partial_x i(\psi \partial_x \psi^* - \psi^* \partial_x \psi) = 0 \]  

(2.7)

which has the form

\[ \partial_t \rho + \partial_x J = 0 \]  

(2.8)

where I multiplied by \( i \) in (2.7) so that \( \rho \) and \( J \) are real and represent the probability densities.
sity and current. The problem is that since the Klein-Gordon equation is a second order equation in time, the probability density $\rho$ is a functional of $\partial_t \psi$ energy. We will see that energy can be negative which leads to a negative density.

Let us take our wave function to be $\psi = Ae^{-iP_x + iEt}$ a plane wave. Then the Klein-Gordon equation tells us that,

$$E^2 = P^2 + m^2 \quad \text{or} \quad E = \pm \sqrt{P^2 + m^2} \quad (2.9)$$

just as we would hope. However, there is a negative energy solution. On its own, energy being negative is not a problem but when we go to calculate the probability density we find,

$$\rho = i(\psi^* \partial_t \psi - \psi \partial_t \psi^*) = 2|A|^2 E = \pm 2|A|^2 \sqrt{P^2 + m^2} \quad (2.10)$$

where $|A|^2 = \psi \psi^*$. How can we interpret a negative probability density? Perhaps we could assign some meaning to this result but it is awkward. Instead of trying to force some meaning onto such a curious result we can attempt to improve upon the Klein-Gordon equation in such a way that we avoid negative density. As mentioned above the problem is that $\rho$ is a function of energy, which happens due to the Klein-Gordon equation being second order in time. To get a first order equation we might try to quantize the relativistic energy-momentum relation differently.

$$E = \sqrt{P^2 + m^2} \to i\partial_t \psi = \sqrt{-\partial_x^2 + m^2} \psi \quad (2.11)$$

Right away we see that we are going to have to somehow deal with the strange $\sqrt{-\partial_x^2 + m^2}$ operator. It is not at all clear what this operator means. Dirac realized that the meaning of $\sqrt{-\partial_x^2 + m^2}$ can be derived by starting with a generalized first order equation and then
squared that equation. The most general equation can be written as,

\[(i\gamma^\mu \partial_\mu - m\Gamma)\psi = 0\]  (2.12)

were I have switched to the convenient notation \((\gamma^\mu \partial_\mu = \gamma_t \partial_t - \gamma_x \partial_x - \gamma_y \partial_y - \gamma_z \partial_z)\). We want the parameters \(\gamma\) and \(\Gamma\) to be defined in such a way that when we square the equation we return to the Klein-Gordon equation. So let us square our first order equation.

\[(-i\gamma^\nu \partial_\nu - m\Gamma)(i\gamma^\mu \partial_\mu - m\Gamma)\psi = 0\]  (2.13)

\[(\gamma^\nu \gamma^\mu \partial_\nu \partial_\mu + im(\gamma^\nu \Gamma - \Gamma \gamma^\nu)\partial_\nu + m^2\Gamma^2)\psi = 0\]  (2.14)

From here we can make the following restrictions in order to arrive at the Klein-Gordon equation. I will use \(g^{\mu\nu} = \delta^\mu_0 \delta^\nu_0 - \delta^\mu_1 \delta^\nu_1 - \delta^\mu_2 \delta^\nu_2 - \delta^\mu_3 \delta^\nu_3\) the minkowski metric.

\[\gamma^\nu \gamma^\mu \partial_\nu \partial_\mu = g^{\nu\mu} \partial_\nu \partial_\mu\]  (2.15)

\[\gamma^\nu \Gamma - \Gamma \gamma^\nu = 0\]  (2.16)

\[\Gamma^2 = 1\]  (2.17)

By making \(\Gamma = 1\), equations 2.16 and 2.17 are satisfied. Equation 2.15 can be rewritten by noting the commutivity \((\partial_\mu \partial_\nu = \partial_\nu \partial_\mu)\) of the derivative operators.

\[\frac{1}{2}(\gamma^\nu \gamma^\mu + \gamma^\mu \gamma^\nu)\partial_\nu \partial_\mu = g^{\nu\mu} \partial_\nu \partial_\mu\]  (2.18)
Thus we have the anticommutation relation

\[ \frac{1}{2} (\gamma^\mu \gamma^\mu + \gamma^\mu \gamma^\nu) = g^{\mu\nu} \] (2.19)

In other words,

\[ \gamma^\mu \gamma^\nu = -\gamma^\nu \gamma^\mu \quad \text{for} \quad \mu \neq \nu \]

\[ \gamma^0 \gamma^0 = 1 \] (2.20)

\[ \gamma^k \gamma^k = -1 \quad \text{for} \quad k = 1, 2, 3 \]

Clearly the \( \gamma' \)'s are going to be matrices but the question is what dimension? First it will be shown that the dimension must be even and then even dimensions will be checked until one is found that works. I cannot help but point out here that (2.20) almost defines a division algebra except that \( \gamma^0 \) is not identity because it has to anticommute with the spatial components. Thus, if we include the identity matrix \( \hat{I} \) in order to make these operators into a group then division cannot be defined since \( \gamma^0 (\hat{I} + \gamma^0) = \hat{I} (\hat{I} + \gamma^0) \)

In order to show that the \( \gamma' \)'s are matrices of even dimension let a new operator be defined in terms of the other four.

\[ \gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 \] (2.21)

It is easily seen that this operator has the following properties.

\[ \gamma^5 \gamma^5 = \hat{I} \] (2.22)

\[ \gamma^\mu = -\gamma^5 \gamma^\mu \gamma^5 \]
With these properties we can look at the trace of our operators.

\[ tr(\gamma^\mu) = -tr(\gamma^5 \gamma^\mu \gamma^5) = -tr(\gamma^5 \gamma^5 \gamma^\mu) = -tr(\gamma^\mu) \]  \hspace{1cm} (2.23)

thus

\[ tr(\gamma^\mu) = 0 \]  \hspace{1cm} (2.24)

Equation (2.24) along with equation (2.20) for \( \gamma^0 \) tell us that the dimension must be even. From equation (2.20) we know that we must have \( \gamma^0 = U^T D U \) where \( U \) is some unitary operator and \( D \) is a diagonal matrix consisting of only ones and negative ones. Since the trace is zero there must be exactly as many ones as negative ones so the dimension must be even.

Now let us figure out exactly what is that dimension. I hardly would have gone through proving that the dimension is even if it was just going to be two. However, let us now take the time to prove that the dimension of the \( \gamma' \)s cannot be two. Then we will skip three dimensions as we have shown that it cannot be odd. Finally, I will present the correct four dimensional matrices and show that they satisfy equation (2.20).

The generators for \( SU(2) \) are the Pauli matrices \( \sigma^\mu \) and it is easy to show that,

\[ \gamma^k = i\sigma^k \]  \hspace{1cm} (2.25)

satisfies the spatial part of equation (2.20). For the temporal part let us try the most general matrix.

\[ \gamma^0 = a_\mu \sigma^\mu \]  \hspace{1cm} (2.26)
for arbitrary parameters $a_{\mu}$. Then from equation 2.20 we have,

$$0 = \{\gamma^0, \gamma^k\} = 2i(a_0 \sigma^k + a_k \sigma^0)$$

(2.27)

thus

$$a_{\mu} = 0 \text{ for all } \mu$$

(2.28)

However, we also need $\gamma^0 \gamma^0 = 1$ and so we need a higher dimensional matrix to satisfy the commutation relation. We could have known from the beginning that this would not work since the Pauli matrices along with the identity form a division algebra.

As promised we will skip three dimensions because it is odd. For four dimensions we could try generalized matrices and solve for the coefficients. However, this is both straightforward and cumbersome so instead I will list known $\gamma'$s and show that they satisfy equation 2.20. It turns out that there is not a unique set of $\gamma'$s. One such set is as follows:

$$\gamma^0 = \begin{pmatrix} \sigma^0 & 0 \\ 0 & -\sigma^0 \end{pmatrix} \quad \gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix}$$

(2.29)

First the spatial part of equation 2.20

$$\{\gamma^k, \gamma^l\} = \begin{pmatrix} -\{\sigma^k, \sigma^l\} & 0 \\ 0 & -\{\sigma^k, \sigma^l\} \end{pmatrix} = -2\delta_{k,l} \hat{I}$$

(2.30)

and now the time part

$$\{\gamma^0, \gamma^k\} = \begin{pmatrix} 0 & \sigma^k - \sigma^k \\ \sigma^k - \sigma^k & 0 \end{pmatrix} = 0$$

(2.31)
and

\[ \gamma^0 \gamma^0 = \begin{pmatrix} \sigma^0 & 0 \\ 0 & \sigma^0 \end{pmatrix} = \hat{I} \quad (2.32) \]

Thus with these four dimensional matrices we can write down the Dirac equation and know what we are talking about.

\[ (i \gamma^\mu \partial_\mu - m) \psi = 0 \quad (2.33) \]

At this point I would like to reflect on something that is rarely discussed. The relativistic energy momentum equation used to derive the Dirac equation comes to us from Einstein. He came to it by thinking about the consequences of the speed of light being constant. However, it does not seem absolutely clear that this is the correct energy momentum relation at all scales. It is somewhat alluring since it puts energy and momentum on equal footing (they are both second order). However, one could imagine, for example, that as energy gets smaller mass begins to lose meaning and that, perhaps, it should be replaced by an operator. At this point (the year 2017) that does not seem to be the case but it is one example of how the relativistic energy momentum relation could break down which would make the Dirac equation an incomplete description of relativistic particles.

### 2.2 Majorana’s Solutions to The Dirac Equation

Before talking about Majorana’s solution, let us examine an arbitrary solution \( \psi \) to the Dirac equation. Using the language of second quantization we can associate an operator
2.2. MAJORANA’S SOLUTIONS TO THE DIRAC EQUATION

\[ \hat{\psi}(x) = \int dp \sum_s (a_s(p)u_s(p)e^{-ipx} + b_s^\dagger(p)v_s(p)e^{ipx}) \] (2.34)

For every solution \( \psi \) there is \( \bar{\psi} \), the so-called charge conjugate solution.

\[ \bar{\psi}(x) = \int dp \sum_s (a_s^\dagger(p)\bar{u}_s(p)e^{ipx} + b_s(p)\bar{v}_s(p)e^{-ipx}) \] (2.35)

where the spinors \( u, v, \bar{u}, \) and \( \bar{v} \) are matrix functions of four-momentum, \( a_s(p) \) destroys a fermion at momentum \( p \) and spin \( s \), \( a_s^\dagger(p) \) creates a fermion, and \( b_s(p) \) and \( b_s^\dagger(p) \) destroy and create antifermions. In these equations, (2.34) and (2.35) I have left off indices in order to make the equations less cumbersome. For example \( px \) should be understood as \( p^\mu x_\mu \) a dot product.

These solutions are the normal Dirac fermions that describe such objects as electrons. Majorana wanted to find a solution \( \tilde{\psi} \) that was real [3]. In order to find a real solution of the Dirac equation, the equation itself must be real which means that the \( \gamma \) matrices must all be purely imaginary. The following choice satisfies this condition.

\[
\begin{align*}
\tilde{\gamma}^0 &= \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} \\
\tilde{\gamma}^1 &= \begin{pmatrix} i\sigma^1 & 0 \\ 0 & i\sigma^1 \end{pmatrix} \\
\tilde{\gamma}^2 &= \begin{pmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{pmatrix} \\
\tilde{\gamma}^3 &= \begin{pmatrix} i\sigma^3 & 0 \\ 0 & i\sigma^3 \end{pmatrix}
\end{align*}
\] (2.36)

Using these \( \gamma' \)'s in the Dirac equation we are guaranteed to get \( \tilde{\psi} \) a real solution. As \( \tilde{\psi} \) is real we have that \( \tilde{\psi} = \bar{\tilde{\psi}} \) it is equal to its charge conjugate. This implies the following

13
restrictions on the fermion operators from equations 2.34 and 2.35

\[ \tilde{a} = \tilde{b} \]
\[ \tilde{a}^\dagger = \tilde{b}^\dagger \]  

(2.37)

In other words the majorana particle is its own anti-particle. Furthermore, if we demand
that creating an anti-particle is the same as destroying a particle and vice-versa then we
have,

\[ \tilde{a} = \tilde{b} = \tilde{a}^\dagger \]  

(2.38)

Using this property as a restriction, we can write the Majorana operator in terms of
the Dirac operators. At this point I would like to switch from the \( \tilde{a} \) notation to the more
common \( \gamma \) notation for Majorana operators. I caution the reader not to confuse these with
the four by four matrices in the Dirac equation which I will not refer to again in this thesis.
To be perfectly clear, \( \gamma \) will no longer refer to the matrices in the Dirac equation but will
refer to Majorana operators from here on out.

There are two such operators that satisfy property 2.38.

\[ \gamma_1 = a + a^\dagger \quad \gamma_2 = i(a - a^\dagger) \]  

(2.39)

which means that we can also write the Dirac operators in terms of the two Majorana
operators.

\[ a = \frac{1}{2}(\gamma_1 - i\gamma_2) \quad a^\dagger = \frac{1}{2}(\gamma_1 + i\gamma_2) \]  

(2.40)

By looking at equation 2.40 we can try to gain some understanding of the Majorana
fermion. Clearly Dirac fermions (like electrons for example) somehow consist of two Majorana fermions. This property will become incredibly apparent in later chapters when the two Majorana operators are spatially separated and we find that the probability distribution of a single electron is split between two distant points in space. From this argument it is tempting to think of each Majorana fermion as half of an electron but that is not quite correct. Consider the second quantization states defined by,

\[
\begin{align*}
    a |0\rangle &= 0 \\
    a |1\rangle &= |0\rangle \\
    a^\dagger |0\rangle &= |1\rangle \\
    a^\dagger |1\rangle &= 0
\end{align*}
\] (2.41)

which label the number of electrons. If the Majorana fermion was half of a Dirac fermion then you would expect the Majorana operators on the ground state to give something like \( |\frac{1}{2}\rangle \). However, from equation 2.39 we find,

\[
\begin{align*}
    \gamma_1 |0\rangle &= |1\rangle \\
    \gamma_1 |1\rangle &= |0\rangle \\
    \gamma_2 |0\rangle &= -i |1\rangle \\
    \gamma_2 |1\rangle &= i |0\rangle
\end{align*}
\] (2.42)

Equation 2.42 suggests that the Majorana operators are not particle operators at all in that \((\gamma_1^\dagger \gamma_1 = \gamma_2^\dagger \gamma_2 = 1)\) they cannot define a number operator. Instead they act like two separate channels that Dirac fermions can ”travel” through to both enter and leave the
2.3. POSSIBLE MAJORANA FERMIONS

vacuum. The fact that the creation operator for Dirac fermions is written as the addition of both Majorana operators can be understood by saying that normal fermions use both Majorana channels to leave the vacuum.

2.3 Possible Majorana Fermions

There have been a few proposals as to what sort of matter can be described by Majorana’s solution. Majorana himself predicted the neutrino to be such a particle. However, at first glance the neutrino did not seem to be a its own antiparticle, therefore it could not be a Majorana fermion. Lately, however, it has been suggested that perhaps the neutrino and the anti neutrino are actually the same but with different helicity.

Take for example $\nu_\mu$ the muon neutrino. It is produced from pion decay in two different ways.

\[\pi^+ \rightarrow \nu_\mu + \mu^+\]
\[\pi^- \rightarrow \bar{\nu}_\mu + \mu^-\]  

(2.43)

The neutrino $\nu_\mu$ produced from $\pi^+$ decay can never interact with matter to produce the $\mu^+$ muon. Similarly, The neutrino $\bar{\nu}_\mu$ produced from $\pi^-$ decay can never produce the $\mu^-$ particle. This lead people to believe that $\bar{\nu}_\mu$ was the antiparticle to $\nu_\mu$ and that they were distinct.

However, there is another way to understand these decay phenomena. Perhaps the only difference between $\bar{\nu}_\mu$ and $\nu_\mu$ is that they have opposite helicity. Helicity being $h = \frac{\vec{j} \cdot \vec{P}}{|\vec{P}|}$ the direction the particles spin rotates along its path. If this is the case then the neutrino and anti-neutrino are the same particle, hence Majorana fermion.
2.3. POSSIBLE MAJORANA FERMIONS

Another suggestion is that dark matter is made up of Majorana fermions. This is not too surprising since just about everything has been suggested for dark matter. However it is likely that dark matter is neutral since it doesn’t seem to conglomerate (there are no dark matter planets).

Furthermore, Super Symmetry predicts that for every boson there is a fermion with the same internal quantum number. There is not much evidence for Super Symmetry. However, if it does hold, then Majoranas necessarily exist. Since a photon is its own anti-particle its super symmetric partner must also be its own anti-particle, hence Majorana fermion.

Out of all the suggestion, for where Majorana fermions might be found, there is one that stands above the rest as the most promising, that is, bound states within solid state systems. Excitons themselves are a mixture of electrons and holes with creation operator given by,

$$a_j^\dagger a_i + a_i^\dagger a_j$$  \hspace{1cm} (2.44)

Clearly they are their own anti-particle. However, excitons have integer spin meaning they are bosons not fermions. To find fermions that are their own anti-particle we will have to look a little bit further.
Chapter 3

Theoretical Background 2: Majorana Bound States in Solid State Systems

3.1 Superconductors

We will see in the next section that Majorana quasi particles can be found at the edge of certain types of superconductors. Before we go there I think it would be useful to motivate the Bogoliubov-de Gennes (BdG) approach [4], which I will use to describe superconductors. This method describes superconductivity at the mean-field level by introducing a pairing term that couples the electron bands and the hole bands. In this section I will demonstrate that the BdG approach arises naturally from the microscopic description of superconductivity given by Bardeen, Cooper, and Schrieffer (BCS) [5] and that it predicts the basic properties of superconductors.

There are two fundamental properties of superconductivity, zero resistance and zero magnetic penetration. Both of these properties are described by the London equation which I will now derive. Let us start with zero resistance which means that electrons are
accelerated by the electric force without friction.

\[ m\ddot{\vec{r}} = -e\vec{E} \]  

(3.1)

An acceleration of charges implies a changing current

\[ \dot{\vec{J}} = -ne\ddot{\vec{r}} = \frac{ne^2}{m}\vec{E} \]  

(3.2)

Taking the curl of both sides we have,

\[ \nabla \times \dot{\vec{J}} = -\frac{ne^2}{mc}\dot{\vec{B}} \]  

(3.3)

Where I have used Maxwell’s equations to relate the electric field to the magnetic field. Using Maxwell’s equations again and the identity \((\nabla \times \nabla \times = \nabla^2)\) we arrive at

\[ \nabla^2 \dot{\vec{B}} = \frac{4\pi ne^2}{mc^2}\dot{\vec{B}} \]  

(3.4)

which tells us that the time derivative decays exponentially into the perfect conductor. Therefore the magnetic field can be considered constant in the bulk. However, in a superconductor we have the stronger condition that the magnetic field is zero. We would have arrived at this conclusion if Eq. [3.3] had not been in terms of time derivatives. In other words zero magnetic penetration implies that,

\[ \nabla \times \vec{J} = -\frac{ne^2}{mc}\vec{B} \]  

(3.5)

This is known as the London equation and it also predicts zero resistance which can be seen by simply taking the time derivative of both sides. When I derive this equation from
3.1. SUPERCONDUCTORS

the BdG formalism it will be in terms of the vector potential.

\[ \vec{J} = -\frac{ne^2}{mc} \vec{A} \]  

(3.6)

Now we want to ask what types of interactions will get us back to the London equation \[3.6\] and therefore constitute a superconductor. I will start from the BCS Hamiltonian and on our way to the London equation I will derive the BdG Hamiltonian. The idea behind the BCS model is that resistance arises from electrons scattering off of lattice vibrations. At high temperatures these vibrations are chaotic and cause resistance, however, at low temperatures, in a perfect crystal, the main cause of vibrations is the attraction of the ion core to free electrons. This attraction causes a build up of positive charge which propagates slower than the free electrons. Thus, as an electron travels through the lattice it leaves behind an area of attractive potential which pulls in other electrons. To first order (or second order depending on how you look at it), this potential couples two electrons which we call a cooper pair. These electrons have to have opposite spin due to Pauli exclusion and they also have to have opposite wave vectors in order to not deconstructively interfere. Because they have opposite wave vector, there is no current carried by electron momentum which is subject to resistance. Instead the current is carried through the phase of the condensate generated by the vector potential. It is this current which reproduces the London equation as we will see below. Let us now write the BCS Hamiltonian based on our microscopic description.

\[ H = \sum_{k\sigma} \xi_k a_{k\sigma}^\dagger a_{k\sigma} - \sum_{k,k'} V_{k,k'} a_{k\uparrow}^\dagger a_{-k\downarrow} a_{-k'\downarrow} a_{k'\uparrow} \]  

(3.7)

The first term just counts the number of electrons where \( \xi_k \) is the energy of an electron with wave vector \( k \). The second term accounts for the interaction potential \( V_{k,k'} \). It counts
3.1. SUPERCONDUCTORS

the number of cooper pairs which are not generally diagonal in k-space (when electrons interfere they change momentum). Interacting models are typically very difficult to solve. In order to diagonalize the BCS Hamiltonian we make the following approximation [5].

$$\langle a_{k\uparrow}^\dagger a_{-k'}^\dagger a_{-k\downarrow}^\dagger a_{k'\uparrow} \rangle \approx \langle a_{k\uparrow}^\dagger a_{-k'}^\dagger \rangle a_{-k\downarrow}^\dagger a_{k'\uparrow} + a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger \langle a_{-k'\uparrow} a_{k\uparrow} \rangle$$

(3.8)

and define

$$\Delta_k = \sum_{k'} V_{kk'} \langle a_{-k'\uparrow} a_{k'\uparrow} \rangle$$

(3.9)

which gives us the BdG Hamiltonian [4]

$$H = \sum_{k\sigma} \xi_k a_{k\sigma}^\dagger a_{k\sigma} - \sum_k (\Delta_k a_{k\uparrow}^\dagger a_{-k\downarrow} + \Delta_k^* a_{-k\downarrow}^\dagger a_{k\uparrow})$$

(3.10)

I will use this BdG Hamiltonian throughout the rest of this work. The quasi particles that diagonalize this Hamiltonian are mixtures of electrons and holes. The electron creation and destruction operators can be written in terms of these operators as

$$a_{k(\uparrow\downarrow)} = u_k^* \gamma_{k(\uparrow\downarrow)} + v_k \gamma_{-k(\uparrow\downarrow)}$$

$$a_{-k(\uparrow\downarrow)}^\dagger = u_k \gamma_{-k(\uparrow\downarrow)}^\dagger - v_k^* \gamma_{k(\uparrow\downarrow)}$$

(3.11)

where $u_k$ and $v_k$ have yet to be determined except that they must obey $|u_k|^2 + |v_k|^2 = 1$ to satisfy the electron commutation relations. This further implies that $u_k = u_{-k}$ and $v_k = v_{-k}$. It should be noted that the $\gamma_{\pm k(\uparrow\downarrow)}$ and $\gamma_{\pm k(\uparrow\downarrow)}^\dagger$ obey fermionic commutation as well. Although these operators are not exactly the Majorana fermions I defined previously, I denote them by $\gamma$ in the hopes that the reader will appreciate the analogy.

Now let us proceed with diagonalization. After plugging in the form of the electron operators in terms of our quasi particle operators we find that the only non-diagonal part
of the Hamiltonian is proportional to,

$$2\xi_k u_k v_k - \Delta_k u_k^2 + \Delta_k^* v_k^2$$

(3.12)

setting this to zero and using \(|u_k|^2 + |v_k|^2 = 1\) we get

$$|u_k|^2 = \frac{1}{2} \left( 1 + \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_k|^2}} \right)$$

(3.13)

$$|v_k|^2 = \frac{1}{2} \left( 1 - \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_k|^2}} \right)$$

with this choice the Hamiltonian is diagonal and given by

$$H = \sum_{k\sigma} \sqrt{\xi_k^2 + |\Delta_k|^2} \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + E_0$$

(3.14)

where \(E_0 = \sum_k (\xi_k - \sqrt{\xi_k^2 + |\Delta_k|^2})\) adjusts the chemical potential. From here it is clear that even when \(\xi_k = 0\) there is still a finite amount of energy \(|\Delta_k|\) needed to excite a quasi particle. Thus, \(|\Delta_k|\) defines and energy gap that protects the ground state defined by,

$$\gamma_{k\sigma} |BCS\rangle = 0$$

(3.15)

To end this section I will apply a first order electromagnetic perturbation to his ground state and see that the current driven by this perturbation satisfies the London equation and therefore is a supercurrent.

In the presence of an electromagnetic potential the momentum operator becomes \((\vec{\nabla} + \frac{e}{c} \vec{A})\) therefore the current operator is

$$\hat{J} = -e \sum_{\sigma} \int d^3r \psi_{\sigma}^\dagger(\vec{r}) \frac{1}{m}(\vec{\nabla} + \frac{e}{c} \vec{A}) \psi_{\sigma}(\vec{r})$$

(3.16)
3.1. SUPERCONDUCTORS

where I have introduced the field operator \( \psi_\sigma(r) = \sum_k e^{i\vec{k}\cdot\vec{r}} c_{\vec{k}\sigma} \). In k-space this is simply

\[
\hat{J} = -\frac{e}{m} \sum_{\vec{k}\sigma} \vec{k} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - \frac{e^2}{mc} \vec{A} \sum_{\vec{k}\sigma} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} = \hat{J}_p + \hat{J}_d
\] (3.17)

where the paramagnetic current \( \hat{J}_p \) is the term with the k-vector and the diamagnetic current \( \hat{J}_d \) is the term with the vector potential. The expectation value of the diamagnetic current is

\[
\langle \hat{J}_d \rangle = \frac{ne^2}{mc} \vec{A}
\] (3.18)

the London current. However, there is still the paramagnetic current. To first order in \( A \) all terms in the expectation value of the current are multiples of

\[
\langle l | \hat{J} | BCS \rangle
\] (3.19)

where \( \langle l \rangle \) is either some excited state or the BCS ground state. Because the superconductor ground state contains coupled electrons with opposite momentum, the paramagnetic current operator gives zero when acting on this state. To demonstrate this let us write the paramagnetic operator in terms of the BCS operators.

\[
\hat{J}_p = -\frac{e}{m} \sum_k (\vec{k} a_{\vec{k}\uparrow}^\dagger a_{\vec{k}\downarrow} - \vec{k} a_{-\vec{k}\downarrow}^\dagger a_{-\vec{k}\uparrow})
\]

\[
= -\frac{e}{m} \sum_k \vec{k} (\left[ u_{\vec{k}\uparrow} \gamma_{\vec{k}\uparrow}^\dagger + v_{\vec{k}\downarrow}^* \gamma_{-\vec{k}\downarrow} \right] \left[ u_{\vec{k}\downarrow}^* \gamma_{\vec{k}\downarrow}^\dagger + v_{\vec{k}\uparrow} \gamma_{-\vec{k}\uparrow} \right] - \left[ u_{\vec{k}\downarrow} \gamma_{-\vec{k}\downarrow}^\dagger + v_{\vec{k}\uparrow}^* \gamma_{\vec{k}\uparrow} \right] \left[ u_{\vec{k}\uparrow}^* \gamma_{\vec{k}\uparrow}^\dagger - v_{\vec{k}\downarrow} \gamma_{-\vec{k}\downarrow} \right])
\] (3.20)

In a normal metal this is nonzero and is a source of resistance, however, when this acts on
3.2 MAJORANA BOUND STATES IN ONE DIMENSIONAL SPINLESS SUPERCONDUCTORS

the superconducting ground state we find

$$\hat{J}_p |BCS\rangle = -\frac{e}{m} \sum_k k \left( u_k v_k \gamma_{k\uparrow} \gamma_{k\downarrow} |BCS\rangle + u_k v_k \gamma_{-k\downarrow} \gamma_{k\uparrow} |BCS\rangle \right) = 0 \quad (3.21)$$

Therefore, the only contribution to the total current responding to a first order perturbation of the BCS ground state is the diamagnetic current which obeys the London equation. Thus, the current flows without resistance and totally expels magnetic field. In other words the BdG Hamiltonian does indeed describe a superconductor.

3.2 Majorana Bound States in One Dimensional Spinless Superconductors

Although many of the candidates for Majorana’s seem unlikely, p-wave superconductors are very promising. The Majorana operators emerge naturally from even simple models of such superconductors \cite{2}. A thin p-wave superconducting wire can be described by discretizing the wire and considering how electrons hop from one segment to the next. The Hamiltonian can be described in three parts.

There is the energy required to raise an electron out of the continuum which is described by $\mu$ the chemical potential.

$$H_\mu = -\mu \sum_{i=1}^{N} a_i^\dagger a_i \quad (3.22)$$

Then the electrons can travel in two ways. They can travel individually with some effective mass which determines $t$ the hopping parameter.

$$H_t = -t \sum_{i=1}^{N-1} (a_i^\dagger a_{i+1} - a_i a_{i+1}^\dagger) \quad (3.23)$$
3.2. MAJORANA BOUND STATES IN ONE DIMENSIONAL SPINLESS SUPERCONDUCTORS

Alternatively they can travel as cooper pairs which in the BdG formalism can be written as,

\[ H_\Delta = \Delta \sum_{i=1}^{N-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) \]  \hspace{1cm} (3.24)

The full Hamiltonian can be written from equations 3.22, 3.23, 3.24.

\[ H = -\mu \sum_{i=1}^N a_i^\dagger a_i - \sum_{i=1}^{N-1} \left[ t(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) - \Delta(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) \right] \]  \hspace{1cm} (3.25)

The easiest way to find the Majorana modes hidden in this Hamiltonian is to take \( \mu = 0 \) and \( t = \Delta \) which gives

\[ H = -\Delta \sum_{i=1}^{N-1} [a_i^\dagger a_{i+1} - a_i^\dagger a_{i+1} + a_i^\dagger a_{i+1} - a_i^\dagger a_{i+1}] \]  \hspace{1cm} (3.26)

\[ = -\Delta \sum_{i=1}^{N-1} [(a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1})] \]

Using equation 2.40 we can rewrite the Hamiltonian in terms of the Majorana operators.

\[ H = -i\Delta \sum_{i=1}^{N-1} \gamma_i^1 \gamma_{i+1,1} \]  \hspace{1cm} (3.27)

All we have done so far is to change basis. It is not surprising that we can write this Hamiltonian in terms of Majorana operators because fermion operators can always be written in terms of Majorana operators. The surprise is still to come.

We can do another change of basis and diagonalize the Hamiltonian. Take \( b_i = \frac{1}{2} (\gamma_i^1 + i\gamma_i^2) \) and \( b_i^\dagger = \frac{1}{2} (\gamma_i^1 - i\gamma_i^2) \) to be new fermion operators. These new
operators represent electrons that are composed of Majoranas from neighboring sites like in the bottom of figure 3.1.

In this new basis the Hamiltonian is diagonalized.

\[
H = -2i\Delta \sum_{i+1}^{N-1} b_i^\dagger b_i
\]  

So the Eigan basis for the superconducting chain is simply the number of electrons that exist across the segments that I have defined. Now for the surprise. Notice that two Majorana modes \(\gamma_{N,1}\) and \(\gamma_{N,2}\) are completely left out of the Hamiltonian. These define another set of fermion operators

\[
a_M = \frac{1}{2}(\gamma_{1,1} + i\gamma_{N,2}) \\
a_M^\dagger = \frac{1}{2}(\gamma_{1,1} - i\gamma_{N,2})
\]
Since this fermion is not part of the Hamiltonian, it can be created and destroyed at zero energy. In other words we have two states defined by the number operator as

\[ a^\dagger_M a_M |0\rangle_M = 0 \]
\[ a^\dagger_M a_M |1\rangle_M = |1\rangle_M \] (3.30)

This is a fermionic state whose Majorana decomposition is non-local. We have successfully separated out the two Majorana modes. This means that we can move them about separately and even move one around the other. Since both of these states defined by the number operator are degenerate at zero energy, we can rotate from one to the other simply by exchanging the Majorana bound states. This type of exchange is called braiding and it is part of what makes Majorana modes useful in quantum computers. Since the information about the state is stored non-locally it is immune to local perturbations and since we can switch states simply by exchanging the Majoranas, unitary operators can be applied which are immune to local perturbations as long as the Majoranas are kept well separated during the exchange. I will elaborate on these points below.

3.3 Braiding Majorana Bound States

The difference between two and three dimensions is significant when considering theories of identical quantum particles. Classically the interchange of identical particles cannot have an effect on the system. However, in quantum mechanics, exchanging particles can change the state of the system. This is known as exchange statistics and it comes in only two varieties in three dimensions, no change to the wavefunction (bosons) and a rotation of the wave function by \( 2\pi \) (fermions). The natural question is why there should only be
3.3. BRAIDING MAJORANA BOUND STATES

Figure 3.2: A cartoon showing the equivalence of exchange and orbits. The exchanges on the left are equivalent to the orbits on the right. The equivalence holds because the exchange operators are necessarily path independent these two extremes. The answer, as I have hinted at, has to do with the dimensionality of space.

Consider the interchange depicted in Fig. 3.2. The double interchange is equivalent to propagating one particle in a loop around the other. Requiring that all such loops produce the same phase gives us the freedom to deform the path, however, we see fit as long as we bring the particle back to its original position at the end. This means that in three dimensions we can raise the loop out of the page and deform it into a point without intersecting the second particle. In other words, performing the interchange twice is the same as not interchanging at all. This means that there are only two possibilities for the phase change due to one interchange, either 1 or -1 corresponding to total constructive and total deconstructive interference.

Consider on the other hand what happens if we do not allow the loop to rise out of the page. Now there is no deformation that can shrink the loop to a point without crossing the second particle. Hence, there is no restriction on the double interchange and therefore no restriction on the phase change of a single interchange. This means that in two dimensions we can expect to find not just bosons and fermions but also particles with any phase upon interchange. These particles are known collectively as anyons. Similarly, anyons can exist in one dimension but the concept of interchange is a bit trickier since particles necessarily
pass through each other [6].

Alas, we live in a three dimensional world. It might seem like all this talk about two dimensions is irrelevant and that anyons are just a mad dream. However, like many mad dreams, anyons do find a place in the real world. Consider a particle trapped in a three dimensional box that is wide in two directions but is nearly flat. This produces a near continuum of long wavelength modes in the two wide directions but a very discrete set of modes in the flat direction. This means that the differences in energy between the flat direction modes are large. Therefore if the temperature is small enough that our particle cannot jump between modes in the third direction, it is effectively trapped in a two dimensional space.

We have seen that the wave function of particles confined to a low dimensional ground state can have arbitrary phase upon interchange. Now let us imagine that the ground state is degenerate. In this case, particle wave functions are described not only by their phase but also by the particular ground state that the particles occupy. Therefore, when we exchange particles their wave function can change phase as well as ground state occupation. Because of this extra freedom, exchange is not described by a complex number but a complex matrix whose size is the same as the number of degenerate ground states. These matrices do not have to commute meaning that the order in which you exchange particles matters. When particle interchange does not commute we say that the particles obey non-Abelian statistics.

At this point I think it makes sense to change our language from exchanging particles to braiding particles. The advantage being that the word braiding evokes the notion that order matters as it does for non-Abelian anyons. It is also the language used in the mathematical description of exchange. The group of exchange operators is a braid group.

Now let us return to the Majorana Fermion. I had already derived the action of the
3.4. QUANTUM COMPUTATION

Majorana operators on fermionic occupation states.

\[
\begin{align*}
\gamma_1 |0\rangle &= |1\rangle \\
\gamma_1 |1\rangle &= |0\rangle \\
\gamma_2 |0\rangle &= -i |1\rangle \\
\gamma_2 |1\rangle &= i |0\rangle
\end{align*}
\] (3.31)

Because both of the Majorana operators create a fermion from the same ground state, that state is seen as doubly degenerate to the Majorana particle. Although these operators must appear in pairs they can be spatially separated so that the electron becomes a non-local entity split between the ends of a one dimensional wire. These two ingredients, low dimensionality and a degenerate ground state are exactly the recipe for non-Abelian statistics and indeed Majoranas are non-Abelian [7].

Because they are non-Abelian, braiding Majorana fermions will give us access to a greater state space than if we exchanged Dirac fermions. We will see later on how this state space can be used for quantum computation. First let us look at the general concept of quantum computers.

### 3.4 Quantum Computation

It is useful to discuss quantum computers in general. In the simplest terms, a quantum computer uses q-bits in place of bits and unitary operators in place of logic gates. A q-bit is just a two level quantum system, like the spin of an electron which can be up or down. Thus, we can take a string of classical binary information and encode it into quantum
3.4. QUANTUM COMPUTATION

information like in the following example.

$$101001 \rightarrow |1\rangle \otimes |0\rangle \otimes |1\rangle \otimes |0\rangle \otimes |0\rangle \otimes |1\rangle \equiv |101001\rangle$$ (3.32)

However, there are states in the quantum computer that have no classical analog. We update the quantum computer by applying unitary operators. Some such operators take us into states that are not accessible using classical logic. Take for example:

$$U|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$ (3.33)

There is simply no classical logic gate that can take a computer into this state. Of course we can always represent this state in a classical computer by adding more bits of information. We could always just tell the computer to identify

- 00 means $|0\rangle$
- 10 means $|1\rangle$
- 01 means $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- 11 means $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ (3.34)

However, the amount of extra classical bits needed to encode the quantum states in this way grows exponentially with the number of q-bits. Furthermore, this type of encoding is not capable of representing states like $a |0\rangle + b |1\rangle$ where a and b are neither the same nor opposite. There are infinity many options for a and b and so it would take infinity many bits even to describe one q-bit.

Quantum computers can use these extra logic channels to arrive at solutions to certain problems much faster than classical computers. So much faster in fact that some problems
3.5 A MAJORANA COMPUTER

that simply cannot be solved on a classical computer because it would take impossibly
long amounts of time, can be solved quite quickly on a quantum computer. In this way
quantum computers are fundamentally different from classical computers.

Take for example the discrete Fourier transform of an N element list.

\[ \tilde{A}_n = \frac{1}{N+1} \sum_i \sin\left(i \frac{n \pi}{N+1}\right)A_i \]  

(3.35)

On a classical computer this takes \( N \times N \) operations. One for each element in the sum
times one for each element in the resulting list. There is a classical algorithm known
as the fast Fourier transform which reduces this to \( N \log N \) steps but that is the fastest
known method. On the other hand, the Fourier transform is a unitary operator in quantum
mechanics and thus can be performed in a single step on a quantum computer. This is
exactly the advantage used in Shor’s quantum algorithm which would be able to crack all
modern banking codes.

3.5 A Majorana Computer

One of the greatest complications with building a quantum computer is that even small
perturbations due to coupling with the environment can change the state of the computer.
This is where Majorana bound states come to the rescue. The Majorana is non-local and
is protected by the superconducting gap. Energy fluctuations smaller than the gap cannot
decoher the quantum state. As we have seen, the way to change the state of a Majorana
system is to braid one particle around another. Because the Majoranas can be separated as
far as one likes (in principle) small oscillations in position are irrelevant.

A process for braiding Majorana zero modes is depicted in Figure 3.3. The idea is
to switch \( \gamma_u \) the Majorana at the left end of the upper chain with \( \gamma_L \) the Majorana at the
3.5. A MAJORANA COMPUTER

Figure 3.3: An example of a braiding procedure from [7]. Gray circles (labeled by $s_i$) are Dirac fermions while the smaller blue, red, and black circles (labeled by $\gamma^{(u,l)}_{(L,R)}$) are Majorana fermions (only the left most Majorana’s are labeled in this figure). The gray bars represent normal hopping (labeled by $J_{u,l,\perp}$) and superconductor hopping (labeled by $\Delta$). Each step of the process corresponds to turning on a particular Hamiltonian.

left end of the lower chain. The magic happens in the first step. It is not obvious why this step switches the Majorania states so let us explore it in detail. Here we turn off all coupling between sites $s_3$ and $s_4$ and between sites $s_1$ and $s_2$ as they are labeled in Figure 3.3. At the same time we turn on the normal type coupling between the $s_1$ and $s_3$ sites. The Hamiltonian during this process looks as follows.

$$H_I(t) = \cos(\frac{\pi}{2t_f}t)[H_{N,(1,2)} + H_{S,(1,2)} + H_{N,(3,4)} + H_{S,(3,4)}] + \sin(\frac{\pi}{2t_f}t)H_{S,(1,3)}$$ (3.36)

where $H_N$ is the normal type hopping.

$$H_{N,(i,j)} = a_i^{\dagger}a_j + a_j^{\dagger}a_i$$ (3.37)

and $H_S$ is the superconductor type hopping.

$$H_{S,(i,j)} = a_i^{\dagger}a_j + a_j a_i^{\dagger}$$ (3.38)

Now we want to know how the eigenstates evolve. For this, I solve the Heisenberg
3.5. A MAJORANA COMPUTER

equation of motion for the two Majorana operators.

\[
\begin{align*}
[\gamma^u_L(t), H_I(t)] &= 0 \\
[\gamma^l_L(t), H_I(t)] &= 0
\end{align*}
\] (3.39)

with the condition that at \( t = 0 \) we have \( \gamma^u_L(0) = \gamma_{s1,1} \) and \( \gamma^l_L(0) = \gamma_{s3,1} \). Solving Equation 3.39 we find,

\[
\begin{align*}
\gamma^u_L(t) &= \frac{2\cos\left(\frac{\pi}{2f_t} t\right)\gamma_{s1,1} - \sin\left(\frac{\pi}{2f_t} t\right)\gamma_{s4,1}}{\sqrt{4\cos^2\left(\frac{\pi}{2f_t} t\right) + \sin^2\left(\frac{\pi}{2f_t} t\right)}} \\
\gamma^l_L(t) &= \frac{2\cos\left(\frac{\pi}{2f_t} t\right)\gamma_{s3,1} - \sin\left(\frac{\pi}{2f_t} t\right)\gamma_{s2,1}}{\sqrt{4\cos^2\left(\frac{\pi}{2f_t} t\right) + \sin^2\left(\frac{\pi}{2f_t} t\right)}}
\end{align*}
\] (3.40)

So it is clear that during the process in step one the upper Majorana goes to the lower chain while the lower Majorana goes to the upper chain. This is a somewhat clever method of braiding where the Majorana’s somehow pass through each other without interfering. The fact that they do not interfere is guaranteed by the gap which does not close during the entire process.

The rest of the steps are straightforward. In step two the coupling between sites \( \vec{s}_3 \) and \( \vec{s}_4 \) are turned back on and the hopping between sites \( \vec{s}_1 \) and \( \vec{s}_3 \) is turned on the rest of the way. This allows \( \gamma^u_L \) to travel to site \( \vec{s}_1 \) which is now the end of the lower wire. In step three, a potential is turned on at site \( \vec{s}_1 \) and the \( \vec{s}_1 \) to \( \vec{s}_3 \) hopping is turned off. This pushes \( \gamma^u_L \) down to the \( \vec{s}_3 \) site. In the last step the \( \vec{s}_1 \) to \( \vec{s}_2 \) hopping is turned back on which allows \( \gamma^l_L \) to travel to the \( \vec{s}_1 \) site. The final result is that \( \gamma^u_L \rightarrow \gamma^l_L(0) \) and \( \gamma^l_L \rightarrow -\gamma^u_L(0) \). This result can be checked in a similar manner as was done for step one. However, I think the
3.5. A MAJORANA COMPUTER

last three steps are intuitive. For more detail see [7].

Besides a procedure for braiding we also need q-bits. The most obvious q-bit is a pair of Majoranas which can either be $|1\rangle$ occupied by an electron or $|0\rangle$ empty. However, all observable operators have parity symmetry since $a^\dagger a = \mathcal{P} a^\dagger a \mathcal{P}$. Therefore, it is meaningless to superimpose states of different parity because no observer will be able to tell. For that reason we take our q-bit to be four Majorana bound states confined to $|00\rangle$ and $|11\rangle$ the even parity states. Next we want to see what operations we can do to our q-bit via braiding.

It has been shown that to have a universal quantum computer you must be able to perform these three gates; the Hadamard gate $H$, the controlled-Z gate $Z$, and the $\frac{\pi}{8}$-phase gate $T$ [8].

$$H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} \hat I & 0 \\ 0 & -\hat I \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$$

In order to preform these gates on our Majorana computer let me remark that the operator $\gamma_i \gamma_j$ acts as a braiding operator since $\gamma_i \gamma_j \gamma_j = \gamma_i$ and $\gamma_i \gamma_j \gamma_i = -\gamma_j$. I will also use the parity operator $(1 - i \gamma_i \gamma_j)$ which measures the parity of the electron state $|1\rangle = 1/2(\gamma_i - i \gamma_j) |0\rangle$. In other words, $(1 - i \gamma_i \gamma_j) |0\rangle = |0\rangle$ while $(1 - i \gamma_i \gamma_j) |1\rangle = -|1\rangle$ which can be easily checked. Therefore, checking the parity involves braiding the Majoranas.

We can preform the Hadamard gate on a q-bit by measuring the parity of the second and third particles [8].

$$\begin{align*} (1 - i \gamma_2 \gamma_3) |00\rangle &= |00\rangle + |11\rangle \\ (1 - i \gamma_2 \gamma_3) |11\rangle &= |11\rangle - |00\rangle \end{align*}$$
The controlled-Z gate entangles two sets of q-bits and is a bit more complicated but can be carried out as follows. We take our first q-bit to be Majoranas 1-4 and our second q-bit to be Majoranas 5-8. The first step is to measure the parity of the electron composed of the 4th and 5th Majorans and drop odd parity states. Then we perform the braid $6 \rightarrow 3$ which gives us the desired operation but we are no longer in the q-bit basis. To fix this, we reintroduce the 4th and 5th Majoranas, measure the parity of the second q-bit, and drop odd parity states. This description is given in more detail as follows.

A general state of the 2 q-bit system is:

$$\Phi = a |00, 00\rangle + b |00, 11\rangle + c |11, 00\rangle + d |11, 11\rangle$$

We measure the parity $(1 - i\gamma_4\gamma_5)$ and throw out odd parity states. This reduces our basis to 6 Majorana modes and allows us to entangle the two q-bits,

$$\Phi \rightarrow a |000\rangle + b |011\rangle + c |110\rangle + d |101\rangle$$

Now we braid the remaining middle two Majorana modes,

$$(i\gamma_3\gamma_6)\Phi = a |000\rangle - b |011\rangle - c |110\rangle + d |101\rangle$$

At this point we have entangled the two q-bits in the desired way but we still need to go back to the 4 Majorana per q-bit encoding. Therefore we reintroduce $\gamma_4$ and $\gamma_5$ in the even parity state,

$$\Phi \rightarrow a(|0000\rangle + |0110\rangle) - b(|0101\rangle + |0011\rangle)$$

$$-c(|1010\rangle + |1100\rangle) + d(|1111\rangle + |1001\rangle)$$
Finally, we want both q-bits to be in the even parity state. To achieve this we can make a measurement of the second q-bit’s parity \((1 - i \gamma_5 \gamma_6)(1 - i \gamma_7 \gamma_8)\) and drop odd parity,

\[
\Phi \rightarrow a |00, 00\rangle - b |00, 11\rangle - c |11, 00\rangle + d |11, 11\rangle
\]

which is the action of the controlled-Z gate on \(\Phi\).

Unfortunately there is no way to enact the \(\frac{\pi}{8}\) gate by braiding Majoranas. To act with this gate one can bring two Majoranas close together so that their energy is split by \(\Delta E\). If they are left there for a time \(t = \frac{\pi}{i \Delta E}\) and then pulled apart once more then we have achieved the desired phase shift. However, this is completely unprotected. This unprotected operation is troubling at first glance but as long as we can do error correction using topologically protected braiding operations then there is no trouble.

### 3.6 S-wave vs P-wave Superconductors

When we looked at the Kitaev model for Majorana bound states, we ignored spin. In conventional superconductors we have a spin degeneracy of states. Because of the spin degeneracy, we cannot isolate a single electron which is necessary for the creation of the MBS. Thus, we would like to lift the spin degeneracy. This degeneracy arises due to the symmetry of the pairing potential \(\Delta(k)\) which couples the electrons. Conventional superconductors (known as s-wave) have a pairing potential whose phase is independent of the direction of \(k\). Because \(\Delta(k) = \Delta(-k)\) we have time reversal symmetry and thus spin degeneracy. On the other hand, theoretical p-wave superconductors have pairing potentials whose phase does depend on the direction of \(k\) and therefore they break time reversal symmetry which lifts the spin degeneracy.

Unfortunately, p-wave superconductors do not exist in nature. So in order to realize the
Majorana bound state we will need to manufacture single particle superconductivity. As I have said, the problem with conventional superconductors is that they are spin degenerate which prevents us from having single particle states. The most obvious way to lift the degeneracy would be to apply a magnetic field. The problem is that once you have a strong enough magnetic field to lift the spin degeneracy, you destroy the superconductivity. A conventional superconductor couples spin up at positive $k$ with spin down at negative $k$. What we need is a single band which has different spin for positive $k$ than it does for negative $k$ so that we can have single particle superconducting states.

To that end, we can bring a semiconductor with high spin orbit interaction in proximity to a normal s-wave superconductor. The spin orbit interaction gives us exactly the property that we want. It splits the bands so that one has spin left (for example) for positive $k$ and spin right for negative $k$ while the other band has the opposite. The only problem
3.6. **S-WAVE VS P-WAVE SUPERCONDUCTORS**

Figure 3.5: A depiction of the semiconductor-superconductor device. The gray box represents a normal s-wave superconductor, the blue cylinder represents the semiconducting nanowire which has strong spin orbit coupling, the black arrow represent the magnetic field.

is that there is still a degeneracy point at \( k=0 \) where the bands cross. Finally to lift this degeneracy we add a magnetic field. With both spin orbit coupling and magnetic field we have not quite opposite spin for positive and negative \( k \) but there is some component that is opposite so that the superconductivity can be induced in the semiconductor nanowire.

Figure 3.5 depicts the semiconductor-superconductor (SM-SC) hybrid device that has been described in this section. Superconductivity is induced on the semiconductor by its proximity to the parent superconductor. A method for probing this device is to tunnel current into the semiconductor from a normal metallic lead. The current \((I)\) will increase every time the bias \((V)\) on the lead crosses a states of the SM-SC device that lives near the tunnel barrier. Therefore, the conductance \((dI/dV)\) will have a peak whenever the bias

Figure 3.6: A color map of a typical differential conductance calculation as a function of bias potential and Zeeman (magnetic) field.
potential crosses a state near the tunnel barrier. If the tunnel barrier is put at one end of
the semiconductor nanowire then one of the MBS which live at the ends of the wire will
be clearly visible in the differential conductance.

Figure 3.6 shows a typical \(\frac{dI}{dV}\) color map as a function of bias potential and mag-
netic field. Each state in the SM-SC device shows up as a peak in the color map with
the intensity of the curve being determined by the weight of the state at the tunnel barrier
which is at the end of the semiconductor wire. The MBS shows up, after the gap closes
and then reopens, as a zero bias peak (ZBP). The ZBP oscillates as the magnetic field is
increased due to finite size effects.
Chapter 4

Experimental Background

Let us review some of the experimental findings in the field of Majorana bound states in one dimensional semiconductor-superconductor devices. In 2012 a group from the Netherlands \[9\] showed the first experimental evidence of Majorana bound states in a proximity coupled semiconductor-superconductor nanowire. Fig. 4.1 shows a scanning electron microscope image of their device. Superconductivity is induced on an InSb nanowire by coupling to a superconductor. The system is atop several back gates which control the potential in the nanowire. A magnetic field is applied parallel to the wire. The states of the semiconductor-superconductor hybrid system are probed by tunneling electrons from a normal metal contact through a barrier potential generated from the gate marked with the green line in Fig. 4.1.

When the bias potential difference between the metallic lead and the superconductor (which is grounded) crosses an energy eigenstate of the hybrid system the current steps up. The electrons from the metal need states in the semiconductor to tunnel into in order for current to flow. As the bias crosses a new state, electrons can tunnel through the barrier more often which results in a step like increase in the current. Therefore, the differential conductance \((dI/dV_{\text{bias}})\) shows peaks when the bias potential crosses a state. Since the
Figure 4.1: A scanning electron microscope image of one of the first experimental setups [9]. The normal metal lead is labeled N and the proximity coupled superconductor is labeled S. There are a number of back gates labeled 1 through 4 and a barrier gate marked with the green line. A magnetic field is applied along the wire. InSb is used for the nanowire as it is known to have a spin orbit interaction ($\alpha = 0.2 \, eVÅ$).

Majorana bound state exists at zero energy, it will show up as a conduction peak with height ($2e^2/h$) see appendix A.5 for details on why the Zero bias peak is normalized.

Figure 4.2: Overlay of many conductance curves as a function of bias potential taken from the device in Fig 4.1 [9]. The magnetic field is scanned from 0 mT to 490 mT with each trace offset in $dI/dV$ for clarity. Green arrows mark the induced gap.

Fig. 4.2 shows experimental results from the device in Fig. 4.1. Here we see an overlay of differential conductance curves as a function of bias potential as the magnetic field is increased. The exciting result is that there is indeed a zero bias peak. However,
there are several concerns regarding this data. First, the zero bias peak is not even close to normalized. We know that temperature will broaden the peak keeping it from being perfectly normalized, however, the zero bias peak in Fig 4.2 is smaller than one would expect even considering the nominal temperature of the device.

Another striking concern is that there is weight beneath the induced gap. The gap induced on the semiconductor is marked with green arrows in Fig. 4.2. One would expect zero density of states below the gap and therefore zero differential conductance. However, the conductance strength dies off smoothly below the induced gap. This phenomenon is known as the soft gap and is a problem when considering the protection of the Majorana
bound state which is guaranteed because it is separated from the continuum by the superconducting gap.

Finally, as the magnetic field increases the induced gap should close, leave behind the ZBP, then reopen. There is no signature of the gap closing in Fig. 4.2. This is not very surprising, however, since the states associated with the closing of the gap have very little weight at the barrier making it hard for electrons to tunnel into those states. This point will be discussed further in the results section 6.4.

Since these initial results were published, there has been a great deal of effort to improve the interface between the semiconductor and the parent superconductor. It is believed that the main cause of the soft gap (a non-zero density of states below the induced gap) is an disordered coupling to the superconductor. The energy of the induced gap is de-
Figure 4.5: Top: Scanning electron micrograph used in the work [12]. A Pd lead is in contact with an InSb nanowire proximity coupled to a NbTiN superconductor. Several gates are used to control the potential along the nanowire. Bottom: Color plot of the differential conductance as a function of bias and the potential over BG1. The magnetic field is off and one can see the induced gap marked by white arrows. Above the induced gap several resonance lines are visible. The first is marked with a solid line and the second by a dashed line. None of the resonance lines are particle hole symmetric.

termined by this coupling. If the coupling is inhomogeneous along the wire (for example) then the induced gap becomes smeared. Fig. 4.3 shows results from a similar device to that in 4.1 except that great effort was taken to make the interface between the semiconductor and the superconductor very clean [10].

The upper left panel of Fig. 4.3 shows a false color electron micrograph of the device. Once again there is a nanowire coupled to a superconducting drain and a metallic lead. Here there are only three gates: one for the barrier potential, one for the hybrid device, and one for the normal metal. A magnetic field is again turned on parallel to the nanowire. For comparison I include both an overlay plot (Fig. 4.3 bottom left) and a color plot (Fig. 4.3 right). Here we see a sharper induced gap in both plots. Although the gap is still not
perfect. Furthermore, they were able to capture the closing of the gap. However, there does not appear to be any signature of the gap reopening, as is expected. The zero bias peak is still much smaller than it should be.

Advances in growing techniques mark a new class of Majorana nanowires. A group in Denmark [11] has been able to grow a thin layer of superconducting aluminum directly onto the semiconductor. In Fig. 4.4-a you see the geometry of these wires. This method greatly increases the coupling between the semiconductor and the superconductor so that the gap is very sharp Fig 4.4-c. As far as the theoretical model is concerned these devices require a different description and should be considered to be in a new, high-coupling regime. The increase in coupling also increases the energy of the induced gap and it is not totally clear if we are seeing the induced gap or the bulk gap of the parent superconductor. This question will be considered in detail in the results section 6.4.

There is one more issue with all these results that I have not yet mentioned. A simple theoretical model of the system predicts particle hole symmetry which amounts to a reflection symmetry across zero bias. This asymmetry is very apparent in the bottom panel of Fig 4.5. Here we see several discrete resonance lines corresponding to states in the nanowire. The magnetic field is turned off so we do not expect to see a ZBP. However, one would expect to see both particle and hole states which would amount to a reflection across zero bias. Very near the induced gap (marked by white arrows) both particle and holes states seem to be visible but the hole states die off quite quickly away from the induced gap while the particle states do not. An explanation for this anti-symmetric behavior is given in the results section 6.4.
Chapter 5

Motivation

In the previous chapter we saw some examples of semiconductor-superconductor (SM-SC) devices that seem to host Majorana bound states (MBS). Although there are a variety of devices that are predicted to host MBS [2] [13–22], the semiconductor nanowire with spin orbit coupling proximity coupled to a superconductor has attracted the most experimental attention [9–12, 23–31]. While in short nanowires the Majorana edge modes can overlap destroying the topological protection, long nanowires are predicted to host well protected zero energy MBS are stable against disorder [32 [33], interactions [34–36], and multi-sub-band effects [20 [37].

There are, however, still major difficulties with these SM-SC devices. As pointed out in the last section, the zero bias peak (ZBP) (which signals the presence of the MBS) is accompanied by a soft induced gap in experiments. This soft gap is deadly for quantum computation since the ZBP is not separated from the continuum. In other words, it is no longer protected against small local perturbations. We also saw that there has been a lot of effort put into improving the SM-SC coupling in order to sharpen the induced gap [10, 11]. Although these devices show a hard gap at low magnetic field, in the Majorana regime the soft gap reappears.
Related to the soft-gap is the broadening of the ZBP \([10, 21, 30]\) and the fact that its height is not quantized to \((2e^2/h)\), as predicted \([38-40]\), see A.5 for more details. Some broadening is expected in experiments due to finite temperature and coupling to the states in the metallic lead, however, experimentally observed ZBPs are always smaller and broader than expected.

Both of these effects (the soft induced gap and the broadening of the ZBP) could be explained by a finite density of sub-gap states in the parent superconductor. Most simple models of the SM-SC device treat the parent superconductor by introducing a pairing term in the semiconductor Hamiltonian. Recently, the parent superconductor has been treated as an active component of the SM-SC system \([41]\). However, the effect of explicitly incorporating the parent SC on the differential conductance was not studied. The first section of my work is devoted to calculating the differential conductance in SM-SC devices treating the parent superconductor as an active component.

Until recently \([12]\), the measurement of the topological phase diagram was another outstanding experimental problem. The presence of the MBS signifies a transition between a topologically trivial state and a topological superconducting state. The phase diagram has been established theoretically for an infinite nanowire \([18, 19, 21, 22]\). However, the experiments carried out in \([12]\) were for an intermediate length wire. The second part of my work was to supplement that experimental study with a calculation of the phase diagram for a finite sized nanowire.

Since there was striking experimental evidence of MBS in these finite sized nanowires it was suggested that the protection of the MBS could be increased by attaching several of these short wires to effectively create a long wire. In the final section of my work I study simulations of these multi-island devices and explore the challenges of using them in practice.
Chapter 6

Differential Conductance in
Semiconductor-Superconductor Hybrid Structures

6.1 Model Hamiltonian

As discussed in the last section, in order to realize a Kitaev chain one needs a semiconductor with moderate to strong spin orbit coupling proximity coupled to a normal s-wave superconductor. A common way of probing these devices is through tunneling experiments and so I also model a metallic lead. The Hamiltonians for all three systems are shown below,

\[ H_m = - \sum_{i,\delta} t_m^{\delta} a_i^{\dagger} a_{i+\delta} - \mu_m \sum_i a_i^{\dagger} a_i \]  

\[ H_{sc} = - \sum_{i,\delta} t_{sc}^{\delta} a_i^{\dagger} a_{i+\delta} - \mu_{sc} \sum_i a_i^{\dagger} a_i + \Delta_0 \sum_i (a_{i\uparrow}^{\dagger} a_{i\downarrow} + a_{i\downarrow} a_{i\uparrow}) \]
6.1. MODEL HAMILTONIAN

\[ H_{sm} = -\sum_{i,\delta} t_{sm}^{\delta} c_i^{\dagger} c_{i+\delta} + \sum_{i} (-\mu_{sm} + V_i) c_i^{\dagger} c_i + \sum_{i} \left( \frac{i\alpha_x}{2} c_{i+d_y}^{\dagger} \hat{\sigma}_y c_i - \frac{i\alpha_y}{2} c_{i+d_y}^{\dagger} \hat{\sigma}_x c_i + \text{h.c.} \right) + \Gamma \sum_{i} c_i^{\dagger} \hat{\sigma}_x c_i \]

(6.3)

where \( V_i \) and \( \Gamma \) are external field parameters for the strength of the gate potential under site \( i \) and the Zeeman splitting from a magnetic field pointed along the wire respectively.

The fermionic destruction operators \( a_i = (a_{i\uparrow}, a_{i\downarrow}) \), \( a_i = (a_{i\uparrow}, a_{i\downarrow}) \), and \( c_i = (c_{i\uparrow}, c_{i\downarrow}) \) destroy electrons in the metal, superconductor, and semiconductor respectively while \( i = (i_x, i_y, i_z) \) is the site index for the sub-system in context. The metal has \( N_m \) sites labeled by \( i_x \) and \( N_y \) chains labeled by \( i_y \) and only one layer in \( i_z \), the semiconductor has \( N_s m \) sites labeled by \( i_x \), the same \( N_y \) chains labeled by \( i_y \) and one layer in \( i_z \), the superconductor

Figure 6.1: Cartoon of the hybrid structure. Current is sent in through the metallic lead which is coupled to the semiconductor. At the tunnel junction there is a confining barrier potential. A magnetic field is applied along the semiconductor which is proximity coupled to the superconductor. The superconductor is grounded and therefore acts as the drain.
6.2. DIFFERENTIAL CONDUCTANCE

has $N_{sc}$ sites labeled by $i_x$, $N_y$ chains labeled by $i_y$, and $N_z$ layers. The parameters $t_n$ and $\mu_n$ are the nearest neighbor hopping strength and chemical potential labeled by the sub-system. $\delta = (\delta_x, \delta_y)$ indexes the sites between nearest neighbors. $\Delta_0$ is the gap of the parent superconductor and $(\alpha_x, \alpha_y)$ are the spin orbit coupling strengths.

The full Hamiltonian for the system is given by the Hamiltonian of all three subsystems and their respective couplings.

$$H = H_m + T_m + H_{sm} + T_{sc} + H_{sc} \quad (6.4)$$

The tunneling between the metal and the semiconductor happens across a single site from the left end of the metal to a site at the right end of the semiconductor.

$$T_m = -\tilde{t}_m \sum_{i_y} (a^\dagger_{(N_m, i_y)} c_{(1, i_y)} + h.c.) \quad (6.5)$$

The coupling to the superconductor on the other hand happens over most of the length of the semiconductor.

$$T_{sc} = -\tilde{t}_{sc} \sum_{i=N_0}^{N_{sc}} \sum_{i=1}^{N_y} (c^\dagger_i a_i + h.c.) \quad (6.6)$$

where $N_0$ is a small number of uncovered $i_x$ indexed sites at the beginning of the semiconductor.

6.2 Differential Conductance

As discussed in section 5 many recent experiments have used the differential conductance to probe semiconductor-superconductor hybrid structures. In such experiments the Majorana mode is predicted to appear as a peak in the conductance at zero bias, since the MBS are fundamentally zero energy excitations.
I explore two different methods of calculating the differential conductance of these Majorana systems. As I will show later on, both methods give very similar results. On the other hand, the formalisms are quite different and there are situations where one is more convenient than the other. Here I will present both methods. The first involves imposing propagator boundary conditions and solving for the reflection and transmission coefficients. It was introduced in a paper by Blonder, Tinkham, and Klapwijk \cite{42} in the context of standard s-wave superconductors. I will refer to this method as the BTK formalism. The second method uses the non-equilibrium Green’s function formalism introduced by Mstislav Keldysh. I will refer to this method as the Keldysh formalism.

6.2.1 BTK Formalism

In the BTK formalism we will be solving for the reflection coefficients for an incoming plane wave just like we would do in an introductory quantum mechanics course except that we are dealing with a tight binding Hamiltonian. Let us start with the Schrödinger equation for our full Hamiltonian.

\[
\sum_{n=1}^{N} (H_{n,n'} - \omega \delta_{n,n'}) \Psi_n = 0 \quad \text{for } n' = 1, \ldots, N
\]  

(6.7)

Now I want to send in and take out plane waves at the leads and drains. For this I set boundary conditions on the wave functions each of which will make one of the equations
6.2. DIFFERENTIAL CONDUCTANCE

in (6.10) redundant.

\[
\Psi_{\nu,\sigma}^{(1,i_y,1)} = \phi_{\nu}(i_y) \begin{pmatrix} \delta_{\sigma,\uparrow} \\ \delta_{\sigma,\downarrow} \\ 0 \\ 0 \end{pmatrix} + \sum_{\nu'} \phi_{\nu'}(i_y) \begin{pmatrix} r_N(\sigma,\nu;\nu') \\ r_N(\sigma,\nu;\nu') \\ r_A(\sigma,\nu;\nu') \\ r_A(\sigma,\nu;\nu') \end{pmatrix}
\]

\[
\Psi_{\nu,\sigma}^{(2,i_y,1)} = \phi_{\nu}(i_y) \begin{pmatrix} \delta_{\sigma,\uparrow} \\ \delta_{\sigma,\downarrow} \\ e^{ik_x a} \end{pmatrix} + \sum_{\nu'} \phi_{\nu'}(i_y) \begin{pmatrix} r_N(\sigma,\nu;\nu') e^{-ik_y a'} \\ r_N(\sigma,\nu;\nu') e^{-ik_y a'} \\ r_A(\sigma,\nu;\nu') e^{ik_y a'} \\ r_A(\sigma,\nu;\nu') e^{ik_y a'} \end{pmatrix}
\]

\[
\Psi_{\nu,\sigma}^{(N_{sc}-1,i_y,i_z)} = \sum_{\nu'} \theta_{\nu'}(i_y,i_z) \begin{pmatrix} u_0 t_N(\sigma,\nu;\nu') e^{-iq_y a'} + u_0 t_A(\sigma,\nu;\nu') e^{iq_y a'} \\ u_0 t_N(\sigma,\nu;\nu') e^{iq_y a'} - u_0 t_A(\sigma,\nu;\nu') e^{-iq_y a'} \\ u_0 t_A(\sigma,\nu;\nu') e^{iq_y a'} - v_0 t_N(\sigma,\nu;\nu') e^{-iq_y a'} \\ u_0 t_A(\sigma,\nu;\nu') e^{iq_y a'} + v_0 t_N(\sigma,\nu;\nu') e^{-iq_y a'} \end{pmatrix}
\]

\[
\Psi_{\nu,\sigma}^{(N_{sc},i_y,i_z)} = \sum_{\nu'} \theta_{\nu'}(i_y,i_z) \begin{pmatrix} u_0 t_N(\sigma,\nu;\nu') + v_0 t_A(\sigma,\nu;\nu') \\ u_0 t_N(\sigma,\nu;\nu') - v_0 t_A(\sigma,\nu;\nu') \\ u_0 t_A(\sigma,\nu;\nu') - v_0 t_N(\sigma,\nu;\nu') \\ u_0 t_A(\sigma,\nu;\nu') + v_0 t_N(\sigma,\nu;\nu') \end{pmatrix}
\]
6.2. DIFFERENTIAL CONDUCTANCE

\[ \sum_{i=1}^{N} (H_{i,y} - \omega \delta_{i,y}) \Psi_i = 0 \quad \text{for } \sigma' = \pm 1, \quad i'_y = 1, ..., N_y, \quad i'_z = 1, ..., N_z \]

\[ i'_z = \begin{cases} 
2, ..., N_{sm} & \text{if } i'_z = 1 \\
1, ..., N_{sc} - 1 & \text{if } i'_z > 1
\end{cases} \quad (6.10) \]

where \( \phi_{\nu}(i_y) = \sqrt{\frac{2}{N_y+1}} \sin(i_y \frac{\nu \pi}{N_y+1}) \) is the transverse wave function in the semiconductor and \( \theta_{\nu}(i_y, i_z) \) is the wave function in the superconductor. The coefficients \( r_N, r_A \) are the normal and anomalous reflection coefficients while \( t_N, t_A \) are the normal and anomalous transmission coefficients. The lattice constant \( a \) is for the metallic lead while \( a' \) is for the superconducting drain. The wave vector in the lead is given as,

\[ k_{e,h}^{\nu}(\omega) = \frac{1}{a} \cos^{-1}\left[ \frac{\mu + 2t_{ym} \cos\left(\frac{n \pi}{N_y+1}\right) \mp \omega}{2t_{ym}} \right] \quad (6.11) \]

and in the drain,

\[ q_{e,h}^{\nu}(\omega) = \frac{1}{a'} \cos^{-1}\left[ \frac{\mu + 2t_{ym} \cos\left(\frac{n \pi}{N_y+1}\right) \mp \sqrt{\omega^2 - \Delta^2}}{2t_{ym}} \right] \quad (6.12) \]

and the BSC coherence factors \( u_0 \) and \( v_0 \) are \[42\]

\[ u_0(\omega)^2 = 1 - v_0(\omega)^2 = \frac{1}{2} \left( 1 + \frac{\sqrt{\omega^2 - \Delta^2}}{\omega} \right) \quad (6.13) \]

I can rewrite these equations as the matrix equation (for details see the appendix \[A.1\]),

\[ \tilde{\Psi}(\omega) = (\tilde{H} + Q(\omega) - \omega)^{-1} J(\omega) \quad (6.14) \]
where \( Q(\omega) \) and \( J(\omega) \) depend on the boundary conditions. \( \bar{H} \) is the Hamiltonian with the redundant sites removed and \( \bar{\Psi} \) is the wave vector with redundancies removed, \( \bar{\Psi} \) still contains the reflection and transmission coefficients which are used to define the current.

\[
I = \sum_{\sigma,\nu,\sigma',\nu'} \int_{-\mu_{\text{lead}}}^{V} d\omega \left( 1 - |r_{N,\sigma,\nu,\sigma',\nu'}(\omega)|^2 + |r_{A,\sigma,\nu,\sigma',\nu'}(\omega)|^2 \right)
\]  
(6.15)

which makes the conductance

\[
\sigma(V,0) = \frac{dI}{dV} = \sum_{\sigma,\nu,\sigma',\nu'} (1 - |r_{N,\sigma,\nu,\sigma',\nu'}(V)|^2 + |r_{A,\sigma,\nu,\sigma',\nu'}(V)|^2)
\]  
(6.16)

If I want to allow for finite temperature then I simply broaden with the derivative of the Fermi function.

\[
\sigma(V,T) = \int de \frac{\sigma(V,0)}{4T \cosh^2 \left( \frac{V-e}{2T} \right)}
\]  
(6.17)

### 6.2.2 Keldysh Formalism

In the Keldysh formalism we want to solve for the propagator

\[
\langle \Psi_0 | c_{1,i_y}^\dagger a_{N_m,i_y} | \Psi_0 \rangle
\]  
(6.18)

where \( a_{N_m,i_y} \) destroys an electron in chain \( i_y \) on the last site of the metallic lead and \( c_{1,i}^\dagger \) creates an electron in chain \( i \) on the first site of the semiconductor. The state \( |\Psi_0\rangle \) is the equilibrium quantum state of the entire system.

The differential conductance is taken from the propagator as follows. The current is
6.2. DIFFERENTIAL CONDUCTANCE

given by the time derivative of the number operator.

\[ I = e \langle \Psi_0 | \dot{N}_{sm} | \Psi_0 \rangle = \frac{i e}{\hbar} \langle \Psi_0 | [N_{sm}, H] | \Psi_0 \rangle \]  

(6.19)

where the number operator \( N_{sm} = \sum_{i,j} c_{i,j}^\dagger c_{i,j} \) is for the semiconductor subsystem. The only way \( N_{sm} \) can change is if some electrons cross the junction and so the current is reduced to the following,

\[ I = \frac{i e}{\hbar} \sum_{l,r} T_m Im[\langle \Psi_0 | c_{1,j}^\dagger a_{N_{m,j}} | \Psi_0 \rangle] \]  

(6.20)

where \( T_m \) is the part of the Hamiltonian that couples the semiconductor to the metal. Finally, the differential conductance will be extracted by taking the derivative of the current \( \frac{dI}{dV} \) with respect to the bias voltage in the lead.

Now we have to evaluate the propagator in equation 6.18. You might notice that this is different from the normal, time ordered propagator.

\[ \langle \Psi_f | T c_{i,j}^\dagger a_{N_{m,j}} | \Psi_i \rangle \]  

(6.21)

where \( T \) is the time ordering operator. Of course the initial wave function \( \Psi_i \) can always be given by the equilibrium wave function but when the system is out of equilibrium \( \Psi_f \) is in general different. Taking the time boundaries to infinity, equation 6.21 appears as

\[ \langle \Psi(\infty) | T S(\infty, t) c_{1,j}^\dagger(t) S(t, t') a_{N_{m,j}}(t') S(t', -\infty) | \Psi(-\infty) \rangle \]  

(6.22)

where \( S(t, t') = T e^{-i \int_{t_1}^{t'} dt_1 H(t_1)} \) is the time evolution operator. Equation 6.22 can be interpreted as starting at the equilibrium wave function at time \( t_1 = -\infty \), progressing to \( t_1 = t' \) (assuming \( t > t' \)), destroying an electron in the lead, progressing to time \( t_1 = t \),
creating and electron in the semiconductor, progressing to \( t = \infty \), then projecting onto some final state. This progression is shown in figure [6.2]

![Progression of the time ordered propagator](image)

Figure 6.2: Progression of the time ordered propagator. The system starts in a state \(|\Psi(\infty)\rangle\) an electron is destroyed at position \(N\) and time \(t'\) then an electron is created at position 1 and time \(t\) then we find the probability that the state is in \(\langle \Psi(\infty) | \). The problem is that we do not know \(\Psi(\infty)\). The Kedlysh formalism has a simple solution to this problem in that \(\Psi(\infty) = \Psi(-\infty)S(-\infty, \infty)\). With this replacement equation [6.22] becomes,

\[
\langle \Psi(-\infty) | T_c S(-\infty, \infty) S(\infty, t) c_{1j}^\dagger(t) S(t, t') c_{Nj}(t') S(t', -\infty) | \Psi(-\infty) \rangle \tag{6.23}
\]

Where \(T_c\) is the contour time ordering operator which follows the time contour shown in figure [6.3]

Now there are several orientations for the field operators. Each of these orientations are prescribed their own Green function. Let \(C_+\) be the forward branch of the Keldysh time contour and \(C_-\) be the backwards branch. Then the four orientations called \(G^T\) time
6.2. DIFFERENTIAL CONDUCTANCE

Figure 6.3: Progression of the contour time ordered propagator. The system starts in a state $|\Psi(-\infty)\rangle$ an electron is destroyed at position $N$ and time $t'$ then we go out to infinity and back along the contour to create an electron at position 1 and time $t$ then we find the probability that the system is still in its initial state. This progression might be altered depending on which branch of the contour $c$ and $c^\dagger$ are on which is taken care of by $T_c$ the contour time ordering operator.

ordered, $G^<$ lesser, $G^>$ greater, and $G^\tilde{T}$ anti-time ordered Green functions are given by,

$$
G^T(j,t,t') = i \langle \Psi_0 | T c^\dagger_{1,j}(t)a_{N,m,j}(t') | \Psi_0 \rangle \quad \text{for } t, t' \in C_+
$$

$$
G^<(j,t,t') = i \langle \Psi_0 | c^\dagger_{1,j}(t)a_{N,m,j}(t') | \Psi_0 \rangle \quad \text{for } t \in C_+, t' \in C_-
$$

$$
G^>(j,t,t') = -i \langle \Psi_0 | a_{N,m,j}(t')c^\dagger_{1,j}(t) | \Psi_0 \rangle \quad \text{for } t \in C_-, t' \in C_+
$$

$$
G^\tilde{T}(j,t,t') = i \langle \Psi_0 | \tilde{T} c^\dagger_{1,j}(t)a_{N,m,j}(t') | \Psi_0 \rangle \quad \text{for } t, t' \in C_-
$$
where $\tilde{T}$ is the anti-time ordering operator. Therefore, the full propagator is a matrix.

$$G = \begin{pmatrix} G^T & G^< \\ G^> & G^\tilde{T} \end{pmatrix} \quad (6.25)$$

However, we would like to use the retarded and advanced Green functions which we know how to calculate.

$$G^+(t - t' = 0) = \int \frac{d\omega}{2\pi} G^+(\omega) = \int \frac{d\omega}{2\pi} [\omega - H + i0^+]^{-1}$$
$$G^-(t - t' = 0) = \int \frac{d\omega}{2\pi} G^-(\omega) = \int \frac{d\omega}{2\pi} [\omega - H - i0^+]^{-1} \quad (6.26)$$

We can rotate the full propagator into a basis that contains these Green functions,

$$\tilde{G} = \frac{1}{2}(\sigma_0 - i\sigma_2) \sigma_3 G(\sigma_0 + i\sigma_2^\dagger) = \begin{pmatrix} G^+ & G^K \\ 0 & G^- \end{pmatrix} \quad (6.27)$$

where $G^K$ is known as the Keldysh Green’s function. These can be written in terms of the lesser, greater, and time ordered Green’s functions,

$$G^+(i_y, t - t') = i\Theta(t - t') \langle \Psi_0 | [c_{1,i_y}^\dagger(t), a_{N_m,i_y}(t')]_+ | \Psi_0 \rangle = G^T(i_y, t, t') - G^<(i_y, t, t')$$
$$G^-(i_y, t - t') = -i\Theta(t' - t) \langle \Psi_0 | [c_{1,i_y}^\dagger(t), a_{N_m,i_y}(t')]_+ | \Psi_0 \rangle = G^T(i_y, t, t') - G^>(i_y, t, t')$$
$$G^K(i_y, t - t') = -i \langle \Psi_0 | [c_{1,i_y}^\dagger(t), a_{N_m,i_y}(t')]_+ | \Psi_0 \rangle = G^>(i_y, t, t') + G^<(i_y, t, t') \quad (6.28)$$

Here I should point out that the propagator we are after in equation 6.18 is the lesser Green function at $t = t' = 0$. It is clear from equations 6.24 and 6.28 that $G^<(i_y, 0, 0) =$
6.2. DIFFERENTIAL CONDUCTANCE

\( G^\uparrow(i_y, 0, 0) = \frac{1}{2}G^k(i_y, 0, 0) \). Now we can return to our current. Equation 6.20 becomes

\[
I = \frac{-2e}{\hbar} \sum_j T_m \text{Re} \left[ \frac{1}{2}G^k(j, 0, 0) \right] = \frac{e}{\hbar} \int d\omega \text{Re} \text{Tr} T_m (G^k(\omega)) \tag{6.29}
\]

The last step is to expand \( G^K \) in terms of the left and right systems.

\[
\begin{pmatrix}
G^+ & G^K \\
0 & G^-
\end{pmatrix}
= G = G_{sm} T_m G_m + G_{sm} T_m G_m T_m G_{sm} T_m G_m + \ldots \tag{6.30}
\]

For completeness I should point out that the entire point of collecting the greens functions into a matrix like (6.30) is to perform expansions correctly. I have tried to motivate the form of this matrix although I have not really shown that it reproduces the correct expansion. For a nice explanation see \[43\] or the appendix A.2. Collecting the terms in this expansion gives (see appendix A.3),

\[
T_m G^K = \left[ 1 - G_{sm}^+ T_m G_{m}^+ T_m \right]^{-1} (G_{sm}^+ T_m G^K_m + G_{sm}^- T_m G_{m}^-) \left[ 1 - G_{sm}^- T_m G_{m}^- T_m \right]^{-1} \tag{6.31}
\]

In thermal equilibrium, we have that \( G^k_{m,sm}(\omega) = (1 - 2f_{m,sm}(\omega))(G^+_{m,sm}(\omega) - G^-_{m,sm}(\omega)) \) \[44\]. Now we can take the derivative with respect to the bias voltage in the lead. I assume that the lead is scanned by the bias voltage \( f_m(\omega) = f(\omega - eV) \) but that the semiconductor is not \( f_{sm}(\omega) = f(\omega) \). I further assume that the properties of the lead
vary slowly with bias voltage and keep only derivatives on the fermi distribution.

\[ \sigma(V) = \frac{dI}{dV} = -\frac{2e^2}{h} \int d\omega \frac{df(\omega - eV)}{dV} Re[Tr[(1 - G_R^+ T_m G_L^+ T_m)^{-1}G_R^+ T_m (G_L^- - G_R^-)(1 - G_R^- T_m G_L^- T_m)^{-1}] ] \]

(6.32)

Finite temperature conductance can be calculated for the Keldysh model in the same as the BTK model, by convolving with the derivative of the Fermi distribution.

### 6.3 SC Self Energy

In both formalisms the relevant entities are zero time Green functions. Either the retarded and advanced Green functions

\[ G^\pm(\omega) = (\omega - H \pm i0^+)^{-1} \]

(6.33)

or (to coin a term) the boundary Green function

\[ G^Q(\omega) = -(\omega - H - Q)^{-1} \]

(6.34)

This allows us to use Dyson equations to integrate out the irrelevant superconductor degrees of freedom and rewrite the Green functions in terms of a superconductor self energy.

\[ \Sigma_{sc}^{\pm,Q}(\omega) = T_{sc} G_{sc}^{\pm,Q}(\omega) T_{sc} \]
So that the total Green functions are

\[ G^\pm(\omega) = (\omega - H_0 - \Sigma^\pm(\omega) \pm i0^+)^{-1} \]  \quad (6.35) 

\[ G^Q(\omega) = -(\omega - H_0 - \Sigma^Q_{sc}(\omega) - Q_m)^{-1} \]  \quad (6.36) 

where \( H_0 = H_m + T_m + H_{sm} \) and \( Q_m \) is the boundary conditions in the metallic lead.

Below the bulk gap of the parent superconductor where the transmission coefficients are zero, we have

\[ \Sigma^Q_{sc}(\omega) = \Sigma^+_{sc}(\omega) = -\tilde{t}_{sc}^2 \nu_{sc}(\frac{\omega \tau_0 + \Delta_0 \tau_x}{\sqrt{\Delta_0^2 - \omega^2}} + \zeta \tau_z) \]  \quad (6.37) 

where \( \nu_{sc} \) is the surface density of states for the parent superconductor and \( \zeta \) is a proximity-induced shift of the SM chemical potential see Appendix [A.4] for details.

### 6.4 Results

#### 6.4.1 Conductance and Density of States

As a first step we need to make sure that the codes are working and that the differential conductance tells us something about the states in the semiconducting wire. One check is to make sure that the probability of reflection plus the probability of transmission is unity. This check was done for a wide range of parameters and always holds. Another check is to compare the two methods which were coded independently. The BTK and Keldysh methods are compared in figure [6.4] Even though the approaches are quite different, one can see that calculated conductance maps in figure [6.4](c-d) are nearly identical.
6.4. RESULTS

Figure 6.4: Differential conductance \(\frac{dI}{dV}\), density of states (DOS), and local density of states (LDOS) at the end of the proximitized wire adjacent to the tunnel barrier as functions of the chemical potential and bias voltage/energy. The differential conductance is calculated using both the BTK [panel (c)] and Keldysh [panel (d)] methods. Note that \(\frac{dI}{dV}\) reflects (qualitatively) the local density of states near the barrier [panel (b)], rather than the total DOS [panel (a)]. The length of the wire is \(L = 1\ \mu\text{m}\), the parent superconductor gap is \(\Delta_0 = 2\ \text{meV}\), and the induced gap is \(\Delta_{\text{ind}} = 0.25\ \text{meV}\).

The second point, that the differential conductance tells us something about the semiconductor states, is also addressed in figure 6.4. It is clear that the differential conductance is a good measure of the local density of states near the barrier where electrons tunnel into the semiconductor. This tells us that the differential conductance can be used to probe the semiconductor states near the barrier. However, the total density of states looks quite different from the differential conductance as there are many states in the semiconductor that the electrons cannot reach because they are located away from the tunnel barrier.

The parabolic features in figure 6.4 are due to the finite size of the nanowire. For an infinite size nanowire, the maps would be a continuum starting at \((\mu = 0)\) the bottom of the
band. Notice that while the total density of states has a clear maximum at the bottom of the band, there is no corresponding maximum in the local density of states or the conductance. In fact the conductance strength grows with chemical potential. At the bottom of the band, the group velocity of states is small and hence there is little barrier penetration. As the chemical potential is increased so is the group velocity and thus so is the density of states that live near the barrier.

The only major difference between the local density of states and the differential conductance is that the local density of states extends away from the induced gap ($\Delta_i = 0.25$ in figure 6.4) while the conductance dies off quickly. Below the bulk gap of the parent superconductor, there is no normal transmission and the differential conductance is proportional to the anomalous reflection probability. Anomalous reflection requires both a particle and a hole so that at the induced gap, where the semiconductor states are perfect blends of particle and hole, anomalous reflection happens easily. On the other hand, away from the induced gap states become either particle like or hole like and the anomalous reflection is suppressed.

These conclusions, that the conductance is a good measure of the local density of states and that the BTK and Keldysh methods calculate nearly identical conductance values, have been verified for a wide range of parameters and seem to be generic properties for high tunnel barriers.

### 6.4.2 The Superconductor Proximity Effect

Now that we understand what the differential conductance is measuring, we want to explore the superconductor proximity effect. As mentioned in section 6.3 the parent superconductor can be modeled as a constant pairing potential in the semiconductor if the coupling between the two sub-systems is much smaller than the bulk gap of the super-
Figure 6.5: Differential conductance as a function of bias potential for a wire of length $L = 1 \mu m$ in the presence of a finite magnetic field $\Gamma = 0.5 \, meV$ for different ratios $\gamma/\Delta_0$ that correspond to a constant induced gap $\Delta_{ind} \approx 0.25 \, meV$. (a) Weak coupling regime with $\gamma = 0.25 \, meV$ and $\Delta_0 = 10 \, meV$. The conductance curve is nearly identical to that calculated based on the effective pairing approximation. (b) System with $\Delta_0 = 1 \, meV$ and $\gamma = 0.32 \, meV$. (c) $\Delta_0 = 0.5 \, meV$ and $\gamma = 0.44 \, meV$. In the lower panels the location of peaks is shifted and the weight of each peak is reduced, revealing the effects of the proximity-induced low-energy renormalization.
6.4. RESULTS

Figure 6.6: (a) Differential conductance calculated using the BTK formalism and including only anomalous reflection processes. (b) Differential conductance that includes both Andreev reflection processes and contributions from the normal transmission through the parent superconductor. Blue (darker gray) represents features below the bulk superconductor gap, while orange (light gray) marks contributions above the gap. The model parameters are: $L = 0.3 \, \mu m$, $\Gamma = 0$, $\Delta_0 = 2$ meV, $\gamma = 1.5$ meV, and $k_B T = 0.002$ meV.

So far we have a full description of the proximity effect below the parent superconductor’s bulk gap where all current through the parent superconductor is supercurrent. However, above the parent bulk gap, electrons can travel normally through the superconductor. In this case, we must model the full superconductor with transmission boundary condition at its ends. In figure 6.6 the results of modeling without the transmission boundary conditions (a) and with the boundary conditions (b) are shown. Clearly the boundary conditions are needed in order to see the full conductance response. When they are included one notices a conductance peak at the bulk gap of the parent superconductor which decays smoothly. Above the bulk gap, the semiconductor states merge with the continuum in the superconductor. This continuum has a maximum conductance at the gap edge where
6.4. RESULTS

Figure 6.7: Differential conductance in the weak tunneling limit as a function of the bias voltage for different values of the effective SM-SC coupling $\gamma$. The model parameters are $L = 1 \ \mu m$, $\Delta_0 = 2 \ \text{meV}$, $\Gamma = 0$, and $k_B T = 0.005 \ \text{meV}$. The induced gap increases with $\gamma$, approaching $\Delta_0$ in the strong coupling limit $\gamma/\Delta_0 \to \infty$, while the spacing between energy eigenstates decreases. The conductance peak associated with the bulk gap edge (orange/light gray) becomes more pronounced in the strong coupling regime.

The resistance is minimum. As the cooper pairs break above the parent superconducting gap, the resistance increases and the conductance decreases.

The presence of the resonance peak at the bulk gap begs the questions; how does one know if they are looking at the induced gap or the bulk gap? In figure 6.7, the dependence on coupling between the semiconductor and the superconductor is shown. As the coupling is increased the states in the semiconductor begin to merge with those in the superconductor. In other words, the semiconducting wire begins to look more and more like a continuation of the parent superconductor. The resonance peak at the bulk gap becomes sharper and the induced gap gets closer in energy to the bulk gap. At intermediate to large coupling, the induced gap is close enough to the bulk gap that one might mistake the two.

Figure 6.8 shows the conductance plots for two different lengths of the nanowire and
6.4. RESULTS

Figure 6.8: Differential conductance as a function of the bias voltage for different values of the potential barrier and wire length. Increasing the length of the semiconductor wire increases the number of sub-gap states (blue/darker gray), but does not affect the feature associated with the parent superconductor (orange/light gray). Increasing the potential barrier suppresses the differential conductance, but the sub-gap features are significantly more affected than the bulk contribution. The model parameters are: $\Gamma = 0$, $\Delta_0 = 2$ meV, $\gamma = 1.5$ meV, and $k_B T = 0.002$ meV.

three different values of the barrier potential. Longer wires have denser states, eventually becoming a continuum if the wire is long enough. Increasing the barrier potential decreases the probability that electrons will be able to tunnel through into the semiconductor. This decrease in tunneling means that the conductance will decrease as the barrier potential increases. However, the conductance above the bulk gap of the parent superconductor decreases slower than the conductance inside the parent bulk gap. So if the coupling is strong and the barrier is high (both desirable situations) then one might miss the induced gap when scanning through bias potential especially if the wire is long (also desirable) in which case the semiconductor states can look like a small decay of the par-
6.4. RESULTS

Figure 6.9: Differential conductance as function of chemical potential and bias voltage for a hybrid system containing (a) a “clean” superconductor and (b) a parent superconductor with sub-gap states. The finite density of sub-gap states is modeled as a finite imaginary part in the retarded Green function of the parent superconductor corresponding to $\delta = 20 \mu\text{eV}$. The model parameters are: $L = 400 \text{ nm}$, $\Delta_0 = 2 \text{ meV}$, $\gamma = 0.3 \text{ meV}$, $\Gamma = 0$, and $k_B T = 2 \mu\text{eV}$.

ent bulk gap. This issue can be resolved by doing scans of the barrier potential to make sure both features are present. If the coupling is strong both features should appear within similar regions of bias potential so by scanning the barrier potential one ought to see some states that decay faster than others and then one knows that those states are the semiconductor states. If all states decay at the same rate than it is likely that the semiconductor states are simply not visible.

So far I have modeled the parent superconductor as a perfect superconductor with no states below its bulk gap. This is probably not the case in most experiments. Figure 6.9a shows the conductance as a function of chemical potential and bias potential at zero magnetic field with a clean parent superconductor. The nanowire is rather short (about 400 nm) so that discrete resonance peaks are distinguishable. These peaks are strongest at the induced gap where states are in equal part particle and hole and they die of symmetrically away from the induced gap. This is how things work for an ideal superconductor but in real
6.4. RESULTS

Figure 6.10: Majorana-induced zero-bias conductance peaks for two different values of the potential barrier. The solid lines correspond to a clean system, while the dashed lines are for a parent superconductor with a finite density of sub-gap states corresponding to $\delta = 20\ \mu\text{eV}$. Note that the quantization of the zero-bias peak is broken in the presence of a finite density of sub-gap states in the parent superconductor.

In general, the picture is more like figure 6.9-b. Here, there is a finite density of states below the bulk gap in the parent superconductor. These states provide a channel for incoming electrons to tunnel through the superconductor as normal current even below the parent bulk gap. For this reason, the differential conductance does not die off along the electron branch of the resonance parabolas. Instead there are extended asymmetric stripes. This is how some experimental conductance maps look as will be discussed further in the next section.

So the question becomes; what happens to the ZBP when there are sub-gap states in the parent superconductor? Figure 6.10 shows a ZBP for two different values of the barrier potential. The solid lines are without sub-gap states. Notice that the ZBP remains normalized but the weight under the peak is reduced when the barrier potential increases.
Figure 6.11: Dependence of the zero-bias conduction peak on relevant parameters. (a) The area of the ZBP as a function of the potential barrier height for two different barrier widths. The barrier potential is modeled as a Gaussian with a standard deviation $\sigma$. Note that for $T = 0, \delta = 0$ the peaks are quantized (at $2e^2/h$). (b) The height of the ZBP as a function of temperature for $\Delta = 0$ and various widths and heights of the tunnel barrier potential. Note that the area of the ZBP is independent of $T$. (c) The height of the ZBP as a function of $\delta$ for $T = 0$ and various widths and heights of the barrier potential. The ZBP area is $\delta$-independent.

Now I turn on the sub-gap states and get the dotted lines. The sub-gap states act to broaden the peak while keeping the weight constant. Thus, by increasing the barrier potential I now decrease the height of the peak.

The effect of sub-gap states is similar to the effect of temperature. Figure 6.11 shows the height of the ZBP as a function of temperature (6.11-b) and density of sub-gap states (6.11-c). While the temperature is responsible for some of the broadening in experiments, the ZBP is consistently shorter than would be expected from the nominal temperature of the device. The extra broadening could be due to sub-gap states in the parent superconductor.
Chapter 7

Calculation of the Phase Diagram

7.1 Model

Figure 7.1: Left: Scanning electron micrograph of the device used by the experimental group [12]. An InSB nanowire is half-covered by a superconductor NbTiN, and is in contact with a normal metal Pd lead. The nanowire is placed on FG and BG metal gates. Right: Model schematics. A nanowire is contacted by a superconductor and a normal metal. The potential profile is shown by the black curve. A plane wave coming from the normal metal can tunnel into the nanowire through the barrier above FG. The chemical potential above BG1 $\mu_{BG1}$ is tunable while potentials above BG2 and BG3 are fixed. The probability distributions for the zero-energy states are shown in red and blue.

Using the theoretical tools developed in the previous chapter I model an experimen-
7.2. RESULTS

tal device used by the Frolov group (U. Pitt.) to map out the topological phase diagram [12]. The experimental device is shown in figure 7.1-a and a representation of our model is depicted in 7.1-b. They have a nanowire (InSb) proximity coupled to an s-wave superconductor (NbTiN) and a metallic lead (Lb). This system is atop several back gates. The gate labeled FG2 is used to create the barrier potential and BG1 is scanned to map out the phase diagram in the plane defined by the chemical potential (more precisely, the BG1 potential) and the Zeeman field. Not depicted, a magnetic field can be turned on parallel to the nanowire. What is different from the classic Kitaev picture is that there are these regions over BG2 and BG3 that are not tuned during the phase diagram scan.

The model Hamiltonian for the device can be described by Eq. 6.1-6.6 with the exception that $V_i$ now describes both the barrier potential and the potential profile of the back gates. I calculate the differential conductance using the BTK method. The incoming plane wave boundary condition is depicted in figure 7.1-b. These boundary conditions are put on a normal metallic lead which is coupled to our semiconductor wire. I use parameters which mimic the low energy InSb band structure: $t_{\delta x}^{\delta x} = 9.5 \text{ meV}$, $t_{\delta x}^{\delta y} = 1.1 \text{ meV}$, $\alpha_{\delta x} = 0.2 \text{ meV}$, $\alpha_{\delta y} = 0.7 \text{ meV}$, $\tilde{t}_m = 2.3 \text{ meV}$. As all of these calculations are done far below the bulk gap of NbTiN, I use an effective pairing potential $\Delta = 0.25 \text{ meV}$. The potential profile is shown as the black curve in 7.1-b and is a rough estimate of the potential profile for the experimental device. The barrier potential (FG) and the chemical potential (BG1) are controlled separately. An example pair of MBSs are calculated and shown in the red and blue curves sitting on top of the potential profile.

7.2 Results

One major difference between this setup and the classic Kitaev chain is that here the electrochemical potential is not uniform, having different values in the BG1 region as com-
7.2. RESULTS

Figure 7.2: Top: Comparison between the spatial dependence of the amplitudes of the lowest energy states corresponding to a long wire with a step-like potential (a) and a short wire of length equal to the BG1 region (b). Bottom: Zeeman field dependence of the low energy spectrum for a long wire with step like potential (c) and a short wire corresponding to the BG1 segment (d). The amplitude of the zero energy splitting oscillations show a qualitatively different dependence on the Zeeman field.

pared to the BG2/BG3 region. Because the BG1/BG2 potential is set to zero the BG2 and BG3 regions are in the normal phase and so the MBS is trapped in the BG1 region. However, the situation is different from a short wire of length equal to the length of BG1. The normal phase regions allow the Majorana at the right end of BG1 to bleed out which increases the protection of the Majorana phase. The protection is observed as an increase in the pinning to zero energy. In figure 7.2 both the situation with and without the depletion region are shown. The top panels 7.2-a,b show the probability amplitude for the zero bias state with a depletion region (a) and in a short wire (b). Notice that in panel-a there is a nonzero decay into the trivial regions. The bottom two panels 7.2-c,d show the energy bands as a function of Zeeman splitting. In the case where there is a trivial region (c), the
ZBP sticks closer to zero energy then in the case where there is not (d).

Figure 7.3 shows the experimental measurement of differential conductance as a function of bias potential and the potential from BG1. There are many discrete resonance peaks consistent with a short nanowire and an induced gap of about 0.25 mV. Unlike the case with a perfect superconductor, these peaks are asymmetric and they extend away from the induced gap. These results suggest that there are sub-gap states in the NbTiN superconductor. Furthermore, the slope of the conductance lines increases from the first resonance peak (solid red line) to the second peak (dashed red line). This result suggests that the chemical potential responds non-linearly to BG1.

Another discrepancy between calculation and experiment is the strength of the first resonance (solid red line in 7.3) compared to the second (dotted red line in 7.3). In the cal-
7.2. RESULTS

Figure 7.4: (a) Simulated conductance map of bias vs. $\mu_{BG1}$ for a homogeneous potential. (b) differential conductance map of bias vs. $\mu_{BG1}$ for a non-homogeneous potential. (c) potential profile $V_E$ along the nanowire used to generate the map in (a). (d) potential profile $V_E$ along the nanowire used to generate the map in (b). Both conductance maps are taken at zero Zeeman energy.

culation, the strength of the conductance increases with group velocity as this increases the penetration through the barrier. However, in 7.3 the first conductance peak is stronger than the second. The strength of the first conduction peak could be explained by a nonuniform potential in the BG1 region. Figure 7.4 compares a uniform BG1 potential to a nonuniform potential. In the nonuniform case a low energy state becomes trapped in the potential well just to the right of the barrier. This state has high barrier penetration due to its location and so it shows a strong conductance response. The exact shape of the gate potential is unknown and is very difficult to calculate. However, it is likely to be inhomogeneous. Figure 7.4 demonstrates that an inhomogenous potential can have significant effects for the conductance. It would be worth exploring the potential profile in detail in future work.

The experimental formation of the ZBP is shown in figure 7.5. In the first three panels
7.2. RESULTS

Figure 7.5: Experimental conductance maps in bias voltage $V$ vs. BG1 at different magnetic fields indicated in the lower right corner of each panel. Arrows in panel (f) mark the ZBP onset gate voltages plotted in Figure 7.8. The dashed line in panel (h) is obtained by tracing the visible maximum in sub-gap conductance and flipping the resulting trace around $V=0$.

The gap closes as the magnetic field parallel to the wire is increased. The closing of the gap at $B = 0.32T$ corresponds to the phase transition into the quasi topological regime. As the magnetic field is increased further, the conductance at zero bias broadens and oscillates. The broadening is consistent with the parabolic shape of the topological phase diagram. The oscillations are consistent with overlapping MBS hence the use of the "quasi topological" terminology.

This experimental ZBP formation is consistent with the calculated formation shown in 7.6. Here I have assumed a finite sized nanowire. Thus we see discrete states at zero Zeeman splitting and an oscillating ZBP inside the quasi topological phase. The only major discrepancy between the experimental conductance maps in figure 7.5 and the theoretical maps in 7.6 is that the experimental conductance is asymmetric across zero bias. Above
7.2. RESULTS

Figure 7.6: Left: Low energy spectrum as a function of $\mu_{BG1}$ for three different values of $E_Z$ the Zeeman field. Right: Calculated conductance maps as functions of bias voltage $V$ and $\mu_{BG1}$ for the same Zeeman field as the left panels. A small thermal broadening of 0.02 meV is used here.

the induced gap this can be explained by sub-gap states in the parent superconductor like in figure 6.9. However, at zero bias all states are equal parts particle and hole. This begs the question, how far from zero bias is the asymmetry noticeable?

The sub-gap states are turned on in figure 7.7 and I have zoomed into the ZBP. It is clear that sub-gap states can cause asymmetry even very close to zero bias. Although, the shape of the asymmetry is a little different from the shape in figure 7.5, the fact that the ZBP is not particle hole symmetric is consistent with theory given that the superconductor has a finite density of sub-gap states.

In figure 7.8 the phase diagram of the zero bias peak is mapped. The black squares are data collected from figure 7.5 while the blue circles are additional data points. The two data sets are consistent with the square root dependence $E_Z = \sqrt{\Delta^2 + \mu^2}$ predicted
7.2. RESULTS

Figure 7.7: Calculated conductance map for a nonezero density of states below the bulk gap in the parent superconductor. Even states quite close to zero bias can be asymmetric.

for an infinite nanowire except that the magnetic field onset is shifted to higher Zeeman splitting. Based on figure 7.8 the bottom of the band appears to be at \( BG1 = -0.4 \text{ V} \). The minimal onset field occurs at \( B = 0.33 \text{ T} \) or \( E_Z = 0.4 \text{ meV} \) where the g-factor (\( g=40 \)) can be extracted from the data. The shift of the onset field is expected for overlapping MBSs which tend to split at the topological transition point.

In figure 7.9 a calculated zero bias conductance map is plotted. I include a significant thermal broadening of 50 \( \mu \text{eV} \). Therefore, we see conductance at zero bias even when the lowest energy states are somewhat split in bias voltage. Notice that the onset field is above the induced gap just as in the experiment. The close match between the experimental and calculated phase diagrams strongly supports the interpretation of the observed ZBPs as signatures of overlapping MBS.
7.2. RESULTS

Figure 7.8: Phase diagram of zero bias peak. Zero bias peak onset points are collected from data in Figure 7.5 (black squares) and other data (blue circles), with error bars judged by deviation of the peak from zero bias within 1/2 of the full width of half maximum of ZBPs. Data marked with blue circles are offset by +0.02 V in BG1 to compensate for a systematic shift due to a charge switch. The top axis $E_Z$ is calculated from magnetic field using $g=40$. The right axis $\mu$ is calculated from BG1 according to 10 meV/V, and set to be zero at the parabolic vertex, $BG1=-0.395$ V. The theoretical phase boundary for an infinite wire $E_Z > \sqrt{\Delta^2 + \mu^2}$ is plotted as a solid red line using $\Delta = 0.25$ mV.
7.2. RESULTS

Figure 7.9: Calculated conductance map as a function of back gate potential and Zeeman splitting taken at zero bias. The red curve corresponds to a plot of the infinite wire phase boundary $E_Z > \sqrt{\Delta^2 + \mu^2}$. Notice that just like the experimental data the onset of the zero bias peak is pushed back from that of an infinite wire.
Chapter 8

Majorana Zero Modes in Coupled Semiconductor-Superconductor Islands

As seen in the last chapter, experimental groups have had success with short Majorana wires. A natural question is to ask whether the separation of the Majorana modes could be increased by combining several short wires in a chain. In this way, one could use the short wire devices that have already been tested to realized well protected Majorana zero modes. In 2012, some theoretical work was carried out on chains of topological islands \[45\]. Here I look at these chains in more detail to examine whether they are practical.

Fig. 8.1 depicts the devices that will be studied in this chapter. The setup is similar to previous chapters except that instead of covering the entire nanowire with a superconductor I attach several superconductors and use gates to control the barrier between the covered regions. In this way, I create superconducting islands in the semiconductor nanowire. The Hamiltonian for this device can be described by Eq. \[6.1\]-\[6.6\] except that \(T_{SC}\) is site dependent and \(V_i\) describes the barriers between the islands as well as the tunnel barrier.

In order to understand the device it is useful to look at the location of states in the nanowire. Figs. 8.2, 8.3, and 8.4 show where the states live in a two covered region.
Figure 8.1: A cartoon of the multi-island device. A semiconductor nanowire is proximity coupled to several (three in this picture) s-wave superconductors. A metallic lead is used for tunnel calculations and a magnetic field can be applied along the wire. There is a barrier potential at the tunnel barrier and between each covered region.

nanowire. The left side of Fig. 8.2 shows the local density of states along the wire as a function of energy for different lengths of the barrier region. There is zero density of states in the covered regions below 0.25 meV meaning that the covered regions have an induced superconducting gap of about $\Delta = 0.25 \text{ meV}$. On the right side of Fig. 8.2 I plot the lowest energy state in a short range of barrier strength. The barrier strength is varied in order to find the smallest gap. Since the states in the covered region all have an energy of at least $E = 0.25 \text{ meV}$, the gap depicted in these figures can be understood as the gap of the barrier region.

There is a finite gap induced in the barrier region regardless of the length of that region. However, when the region is long enough (around $L = 0.4 \mu m$) it can be considered to be non-superconducting for practical purposes. Below, (unless otherwise stated) I use lengths that are shorter than $L = 0.4 \mu m$ in order to emphasize some of the effects that become very weak for longer barriers.

Fig. 8.3 shows the local density of states along the nanowire was a function of the
barrier strength for four different values of the magnetic field. The phase transition for the covered region occurs at $E_z = \Delta_c$, however, the barrier region has a smaller induced gap. At $E_z = 0.2 \text{ meV}$ we see low-energy modes in the barrier region when the barrier strength is low. At $E_Z = \Delta_c = 0.25$, the low-energy modes jump to the ends of the wire at low barrier strengths. Above the covered region phase transition, at high barrier strength there are two pairs of low-energy modes which live at the ends of the covered regions. The transition between one pair of low-energy modes and two pair depends on both the magnetic field and the barrier strength.

Fig. 8.4 shows the local density of states along the wire as a function of barrier region length for different barrier region lengths. The barrier height is chosen to minimize the energy of the lowest energy barrier region state. Right: the energy of the two states nearest to zero energy as a function of barrier height for various barrier region lengths. Notice that the superconducting gap induced on the uncovered barrier region decreases with barrier length. For a large enough barrier region the gap is effectively zero. The magnetic field is turned off in these plots.
Figure 8.3: Local density of states at zero energy as a function of position and barrier strength for different magnetic field strengths. At a magnetic field of $E_Z = 0.2 \text{ (meV)}$ the SC gap of the covered region has not yet closed, however, the smaller gap in the barrier region is closed. Here we see low-energy modes in the barrier region for small barrier potentials. At $E_Z = \Delta_c = 0.25 \text{ (meV)}$ we see the topological phase transition in the covered region. Whether or not the barrier region is topological depends on both the barrier strength and the magnetic field strength.

Because there is a small but finite gap in the barrier region, at zero potential the entire wire is topological. For long barriers the topology is easily destroyed. The length at which four low-energy modes emerge depends on the barrier height. For short regions it takes quite a large barrier in order to destroy the full-wire topology.

In Fig. 8.5 we see the differential conductance as a function of magnetic field and bias potential ($V_B$) for six different values of the barrier potential. At $V_1 = 0.0$ we have a phase transition at $E_Z = 0.25 \text{ meV}$ and a rather well protected ZBP. As $V_1$ increases the oscillations of the ZBP increase as well as the Zeeman energy required for the phase transition. Just above $V_1 = 0.8 \text{ meV}$ the two covered regions behave as if they were totally uncoupled (of course there is always some finite coupling). I will refer to these $V_1$
values as the uncoupled regime. For all practical purposes the uncoupled regime behaves as if the two covered regions were simply two separate short wires. Below the uncoupled regime but above $V_1 = 0.0$ there is an intermediate regime where the protection of the ZBP is stronger than if the wire was half as long but not as strong as if there was no barrier at all. Below $V_1 = 0.0$ the Zeeman energy of the phase transition starts to increase again. Here the barrier region does not act like a barrier at all but like a potential well. Notice at $V_1 = -0.8 \text{ meV}$ there is an Andreev crossing just above $E_Z = 0.6 \text{ meV}$. This crossing is due to a state trapped in the potential well created by $V_1$. Although there is potential for further study, I will not discuss the well regime any further.

Fig. 8.6 depicts the differential conductance for a wire with two barrier regions as a function of magnetic field and bias potential for several values of both barrier strengths. When both barriers are turned off the ZBP extends across the entire length of the wire. In this case the phase transition occurs at the gap of the covered regions $E_Z = \Delta_c = 0.25 \text{ meV}$ and there are no noticeable oscillations. When the first barrier gets into the
Figure 8.5: Differential conductance as a function of magnetic field and bias potential for various barrier potential strengths. Above $V_1 = 0.8 \text{ meV}$ the two regions separate and the protection of the ZBP is that of a wire half the size of the original. However, the protection increases smoothly as the barrier potential decreases to zero. Furthermore, the protection decreases again as the barrier becomes a potential well. Notice an Andreev crossing in the $V_1 = -0.8 \text{ meV}$ plot.

In the uncoupled regime there are now four low-energy modes, however, only one pair is strongly visible in the differential conductance. If the wires were perfectly uncoupled one would not see a conductance response from the second set of partially-separated Majorana modes at all. However, a very narrow peak is visible in the rightmost graphs in Fig. 8.6. Looking closely at this narrow peak one sees that its oscillations grow as $V_2$ is increased. On the other hand, the strongly visible peak is unaffected by $V_2$ when $V_1$ is in the uncoupled regime. Similarly, when $V_1$ is turned off there is hardly any effect on the ZBP conductance as $V_2$ is increased. Hence, the first two covered regions are long enough to host a strongly protected ZBP. Even when $V_2$ is in the uncoupled regime, at $V_1 = 0.0$ there is hardly any change to the ZBP that is visible in tunneling conductance. Contrary to both the uncoupled regime and the case when $V_1 = 0.0$, when $V_1$ is in the intermediate regime then $V_2$ has a sizable effect on the ZBP. Unlike $V_1 = 0.0$ when the first two Majorana modes are well separated and the uncoupled regime where the first two partially separated Majorana modes are uncoupled from the rest, in the intermediate regime the first two Majorana modes
Figure 8.6: Differential conductance as a function of magnetic field and bias potential for various barrier potential strengths. Here there are three covered regions and two barrier regions. The barrier $V_1$ is closer to the tunneling edge than the $V_2$ barrier. The wire is long enough that when $V_1$ is turned off the value of $V_2$ does not have much of an effect on the ZBP protection. Interestingly the effect of $V_2$ on ZBP protection increases at intermediate values of the $V_1$ potential. At large values of $V_1$ the first covered region is effectively disconnected from the other regions and $V_2$ once again has a negligible effect on the tunneling conductance.

are close together and they are coupled to the other four partially separated Majorana modes. Therefore, increasing the gap between the second and third covered regions has a noticeable effect on the low-energy density of states at the tunneling edge.

In Fig. 8.7 there are still three covered regions, however, the second barrier is kept at zero. Here we see how the two lowest energy states behave as the first barrier is increased from zero into the uncoupled regime. The top row of graphs are plots of the differential conductance as a function of magnetic field and bias voltage. The next row (green border) depicts the probability distribution along the wire for the second lowest energy state. The third row (red border) shows the probability distribution for the lowest state. When $V_1$ is off, the lowest energy state is composed nearly separated Majorana modes located at

88
Figure 8.7: Top: differential conductance as a function of magnetic field and bias potential for various strengths of the first barrier potential. Bottom: The lowest visible energy state probability distribution (red border/lower) and second lowest visible state probability distribution (green border/upper). When $V_1$ is turned off the lowest state is composed of two nearly separated Majorana modes located at either end of the wire and the second lowest state is a bulk state that is barely visible at the tunnel barrier. As $V_1$ is increased, the first state loses weight at the tunnel barrier shifting its weight to the edges of the combined second/third covered region. Meanwhile the second state lowers in energy and shifts its weight to the edges of the first covered region.

either end of the wire. The wire is fairly short, so there are some visible oscillations in the ZBP even when both potentials are off. The second state is a bulk state of the wire. It has very little weight at the ends of the wire and is therefore very weakly observed in tunnel conductance. Going right, the next two rows show that both states have weight at all four edges (the ends of the wire and the sides of the first barrier region). These probability distributions define the intermediate regime. Here all four edges are coupled and even though the lowest energy state starts to lose protection, it is still more protected than in the uncoupled regime. Furthermore, both energy states are clearly visible in the differential conductance because both states have weight at the end of the wire. In the last row, the
Figure 8.8: Right: probability distribution as a function of position for the first two energy levels at an intermediate barrier strength (upper) and an uncoupled barrier strength (lower). These distributions are taken at a magnetic field of $E_Z = 0.5 \text{ meV}$. Left: Energy levels as a function of magnetic field for the same two barrier strengths. Here there are two covered regions and one barrier region. When the barrier potential is strong (bottom) the covered regions are effectively disconnected and the lowest energy levels act like two independent and highly overlapping edge modes. At intermediate values of the barrier potential, the two covered regions are coupled so that the two lowest energy modes avoid crossing. The coupling (or splitting) pushes one of the modes down so that it is pinned closer to zero energy.

The lowest energy state has very little weight at the left end of the wire and has therefore lost most of its visibility in the conductance. On the other hand, the second state has gained visibility as its weight has shifted to the edges of the first covered region. The first region is very small meaning its low-energy mode acts like an Andreev bound state which is why this state does not resemble a ZBP.

For Fig. 8.8 I once again have a single barrier region that cuts the wire in half. On the left we see the probability distribution for the lowest and second lowest energy levels. On the right we see the energy levels as a function of magnetic field. When the barrier is in the uncoupled regime (bottom) the energy levels are uncorrelated. The lowest two levels act like partially separated Majorana modes at the ends of two short wires. On the other hand, when the barrier is in the intermediate regime the two lowest energy levels anti-cross. The
splitting of these two levels pushes one of them down closer to zero bias. It is this splitting effect that is responsible for the apparent increase in protection of the ZBP in conductance calculations. In some sense, the low-energy modes in the intermediate regime are more protected than the uncoupled case. The states are further from the continuum. However, it would be very difficult (perhaps impossible in practice) to braid the lowest energy state without picking up the second lowest state. Therein lies the major difficulty with these many region devices. Although one could easily see exponential protection by lowering the barrier potential, in order for the device to be useful in a quantum computer, one has to be sure that the potential barrier is all the way off. Being certain that the potential barrier is off can be challenging since the exact potential profile in the wire is typically unknown. One way to attempt to find the “off” potential is to systematically scan the external potentials until one finds the maximum protection of the ZBP. This, however, does not guarantee that the low-energy state has no (or even very small) weight at the barrier regions as inhomogeneities in the transverse spacial profile of the potential can create intrinsic barriers at the covered-uncovered interface.

Although it is not always possible to remove the weight of the low-energy state at the island barriers, it is possible to decompose the low-energy modes into maximally separated Majorana modes. It is not always possible to fully separate the Majorana modes if the uncovered regions are short or if the magnetic field has not crossed the critical value. However, there is always some maximum possible separation. In the top left panel of Fig. [8.9] we see the spatial profile of the first two energy states. Not depicted in Fig. [8.9] but needed for the decomposition are the corresponding hole states. I will use the labels $\psi_{\epsilon_1}$ and $\psi_{\epsilon_2}$ for the two particle states and $\psi_{-\epsilon_1}$ and $\psi_{-\epsilon_2}$ for the hole states. In order for a state
Figure 8.9: The coupled low-energy modes can be decomposed into four maximally separated Majorana modes. Top left: the probability distributions for the first (blue) and second (green) lowest energy levels. Bottom left: maximally separated Majorana decomposition of the four low-energy modes. Right: the space of possible Majorana decomposition is the surface of a sphere. The decomposition which maximally separates the Majorana modes, like in the bottom left graph, is a unique point on any octant of the spherical surface.

$\gamma_i$ to be a Majorana states it must have the property

$$\gamma_i \rightarrow \gamma_i^\ast \; \text{when} \; \epsilon \rightarrow -\epsilon$$  \hspace{1cm} (8.1)

the normal Majorana decomposition is,

$$\gamma_{1a} = \psi_{\epsilon_1} + \psi_{-\epsilon_1}$$
$$\gamma_{1b} = i(\psi_{\epsilon_1} - \psi_{-\epsilon_1})$$
$$\gamma_{2a} = \psi_{\epsilon_2} + \psi_{-\epsilon_2}$$
$$\gamma_{2b} = i(\psi_{\epsilon_2} - \psi_{-\epsilon_2})$$  \hspace{1cm} (8.2)

In order to maximally separate the Majorana modes I will have to mix the two energy levels. The following mixed states still satisfy Eq. (8.1) and are orthogonal and normalized.
\( \gamma_w = \cos[\phi] \gamma_{1a} + \sin[\phi] \gamma_{2a} \)

\( \gamma_x = -\sin[\phi] \gamma_{1a} + \cos[\phi] \gamma_{2a} \)

\( \gamma_y = \cos[\theta] \gamma_{1b} + \sin[\theta] \gamma_{2b} \)

\( \gamma_z = -\sin[\theta] \gamma_{1b} + \cos[\theta] \gamma_{2b} \)

(8.3)

The unspecified parameters \( \theta \) and \( \phi \) define a unit 2-sphere as in Fig. 8.9, however, only one octant of the sphere is unique up to an overall sign. The rule is for \( \phi \to \phi + \pi/2 \): \( \gamma_w \to \gamma_x \) and \( \gamma_x \to -\gamma_w \) and for \( \theta \to \theta + \pi/2 \): \( \gamma_y \to \gamma_z \) and \( \gamma_z \to -\gamma_y \). In other words, braiding \( \gamma_w \) and \( \gamma_x \) shifts \( \phi \) by \( \pi/2 \) while braiding \( \gamma_y \) and \( \gamma_z \) shifts \( \theta \) by \( \pi/2 \). Every point on the octant is a unique collection of Majorana modes but there is only a single point which separates the modes as in the bottom left panel of Fig. 8.9. Using these states one can understand why the low-energy modes in the intermediate regime are not useful in quantum computations. Braiding these modes does not simply switch from an occupied to an unoccupied state as in the normal Majorana braiding prescription but also exchange energy levels. This can be seen by writing the particle and hole states in terms of the maximally separated modes.

\[
\psi_{\epsilon_1} = \frac{1}{2} (\cos[\phi] \gamma_w - \sin[\phi] \gamma_x - i \cos[\theta] \gamma_y + i \sin[\theta] \gamma_z)
\]

\[
\psi_{-\epsilon_1} = \frac{1}{2} (\cos[\phi] \gamma_w - \sin[\phi] \gamma_x + i \cos[\theta] \gamma_y - i \sin[\theta] \gamma_z)
\]

\[
\psi_{\epsilon_2} = \frac{1}{2} (\sin[\phi] \gamma_w + \cos[\phi] \gamma_x - i \sin[\theta] \gamma_y - i \cos[\theta] \gamma_z)
\]

\[
\psi_{-\epsilon_2} = \frac{1}{2} (\sin[\phi] \gamma_w + \cos[\phi] \gamma_x + i \sin[\theta] \gamma_y + i \cos[\theta] \gamma_z)
\]

(8.4)

Take for example \( \gamma_x \to -\gamma_w \), \( \gamma_w \to \gamma_x \) and \( \gamma_z \to -\gamma_y \), \( \gamma_y \to \gamma_z \). This double braid
takes $\psi_{e_1} \rightarrow \psi_{e_2}$. On the other hand, $\gamma_y \rightarrow \gamma_w$, $\gamma_w \rightarrow -\gamma_y$ and $\gamma_z \rightarrow \gamma_x$, $\gamma_x \rightarrow -\gamma_z$ takes $\psi_{e_2} \rightarrow \psi_{-e_1}$ only if $\theta = \phi$ which is the case when the barrier is turned off and when the two energy levels are degenerate (i.e. the uncoupled regime).

A general number of low-energy modes can be decomposed in a similar way. One needs to use the same number ($n$) of energy levels as covered regions. To figure out the number of parameters that need to be specified in order to decompose the low-energy modes, consider the number of conditions on these states. There are $n$ particle wave functions, $n$ hole wave functions, and $2n$ edge modes that can be decomposed. This gives a total of $2n \times 2n$ parameters. The Majorana condition (Eq. 8.1) drops $n$ terms (one per energy level) in each of the $2n$ equations which cuts the number of parameters in half. Then there are $2n$ normalization conditions and $2 \sum_{m=1}^{n}(n - m)$ orthogonality conditions for a total of $2 \sum_{m=0}^{n}(n - m) = n(n + 1)$ conditions. Therefore, the total number of parameters is $2n \times n - n \times (n + 1) = n \times (n - 1)$.

To solve for these $n \times (n - 1)$ parameters one requires that each maximally separated Majorana mode vanish at every edge (or have as little weight there as possible) except
for one. There are 2\( n \) Majorana modes and 2\( n \) edges. However any overlap between particle hole symmetric modes and antisymmetric modes (i.e. between \( a(\psi_{\epsilon_1} + \psi_{-\epsilon_1}) + b(\psi_{\epsilon_2} + \psi_{-\epsilon_2}) + \ldots \) and \( c(\psi_{\epsilon_1} - \psi_{-\epsilon_1}) + d(\psi_{\epsilon_2} - \psi_{-\epsilon_2}) + \ldots \) for arbitrary \( a, b, c, \) and \( d \)) is not removed in this procedure. In the topological phase, this overlap is identically zero. Therefore, the number of equations is cut in half. Furthermore, requiring that the mode associated with edge \( A \) vanish at edge \( B \) gives the same information as requiring that the mode at edge \( B \) vanish at edge \( A \). These two considerations reduce the number of equations to \( 2 \sum_{m=1}^{n}(n - m) = n \times (n - 1) \) the same as the number of parameters.

In Fig. 8.10 I have six covered regions separated by five barrier regions. On the left we see the tunnel conductance and on the right we see the spatial probability profile of the ZBP at four different magnetic fields. Notice that the conductance shows a very well pinned ZBP even though the wave function certainly does not represent end modes separated by the length of the wire. By using the first six particle and hole states the twelve maximally separated Majorana bound states could be decomposed similar to the bottom left panel of Fig. 8.9. It is important to note that the ZBP has the strongest conductance response of the six lowest states. It would be very easy to mistake it for well separated end modes which it is not. One give away is that the lowest state pins to zero around 0.4 meV which is larger than the predicted topological phase transition. However, the magnetic g factor is often unknown in these hybrid devices and is taken from the slope of the lowest energy mode as a function of the external field. In other words, the Zeeman energy is related to the external magnetic field by assuming that the ZBP emerges at the induced gap. Therefore, there would be no way to tell that this is not the case unless if there is a reference device that does host end modes (as opposed to several low-energy modes located at the edge of each covered region).
Chapter 9

Summary and Outlook

I have carried out several theoretical differential conductance studies on semiconductor-superconductor hybrid systems. These studies include the development of the general theoretical approach by explicitly treating the superconductor as an active component of the hybrid system, the modeling of an experimental hybrid device and calculation of the corresponding topological phase diagram, and an analysis of systems of coupled superconducting islands.

In the first study I show that it is essential to treat the superconductor explicitly in order to capture all experimentally-relevant, low-energy features of the system. These features include the exact location of the induced gap, a resonance peak in the conductance at the bulk gap of the superconductor, and the relative conductance strength of states below and above the bulk gap. I also find that some experimentally observed features in the differential conductance, such as the height of the ZBP and the ”stripy” features above the induced gap, can be explained by having sub-gap states in the parent superconductor.

In the second study, I was able to successfully model the phase diagram of an experimental device. Our toy model not only captures the main features of the phase diagram but is also able to explain many observed features of the differential conductance profile.
at zero magnetic field.

Finally, I turned to the investigation of coupled superconducting islands. Here I define three distinct regimes of the barrier potentials. I find novel, coupled Majorana modes in the intermediate barrier regime. These modes are responsible for an increase in zero bias pinning observed in the differential conductance measured at the end of the system. Furthermore, I discuss how to decompose these coupled Majorana modes into weakly-overlapping, low-energy modes located at the ends of each island.

These results act to further the characterization of one dimensional spinless superconductors. Although, this work is an important step towards better understanding Majorana wires, there is still a lot of exciting research to be done in the field.

An important effect that has not been considered in this thesis is the charging energy of these Majorana devices. When the parent superconductor is thin, the Coulomb repulsion between electrons becomes appreciable. Among other things, this provides a pathway for the so-called teleportation effect predicted to occur when the parent superconductor is thin[46][29]. If the superconductor is not grounded, when an electron hits the end of the wire containing well separated Majorana modes it occupies the modes and then can either bounce back or emerge from the other end of the device. If it emerges from the other end, it picks up a phase that is independent of the length of the wire. Because the electron does not pick up the normal phase change ($e^{ikL}$) that comes from traveling a length $L$, we say that it has teleported.

This type of teleportation has been utilized in proposals for realistic computational devices [47]. Figure 9.1 shows one such device. The Majorana wires are all parallel so that a single magnetic field can be used to put them all into the topological phase. Quantum dots are created between the Majorana states and coupling between the dots and the Majorana’s can be switched on and off.
Figure 9.1: An example of a scalable hexon architecture. The minimal building block defining a qubit and an ancilla are one sided hexons, which are topological Cooper pair boxes containing six MZMs (magnified in the left panel). Note: the illustration is not drawn to scale; in practice, the length $L$ of 1DTS wires is much larger than the correlation length $\zeta$ and vertical separation distances between wires are much smaller than $\zeta$. The measurement of joint parities of MZMs becomes possible by selective coupling to quantum dots. The latter are defined and controlled by gates as depicted in the magnification in the right panel. Two-MZM measurements within a hexon and four-MZM measurements involving two hexons (with two MZMs from a given hexon) enable Clifford complete operations on the array of qubits[47].

In section VII, we saw an example of how to braid Majorana bound states and how braiding can be used to build quantum gates. However, reading out the state was not discussed. The design in figure 9.1 has the advantage that the energy levels of the quantum dots depend on whether the associated Majorana modes host an even or odd number of electrons (i.e. on the parity of the Majorana modes). In other words, the state of the q-bit can be measured by measuring the energy level of the associated quantum dot.

Figure 9.2 shows the energy dependence of induced charges in a two quantum dot system for both parities ($p_{i,j} = i\gamma_i\gamma_j = \pm 1$) of four different states. The symbols $\epsilon_{0}^{\text{tot}}$, $\epsilon_{1}^{\text{tot}}$, $\epsilon_{2}^{\text{tot}}$, $\epsilon_{3}^{\text{tot}}$ represent the states of the quantum dot with fermion occupation (0,0), (0,1), (1,0) , (1,1) respectively. One sees that the odd number occupation states are parity dependent. Thus, by measuring the energy level of a quantum dot one measures the parity of the associated Majoranas. Furthermore, by continuing to measure the energy level until you
Figure 9.2: Energy as a function of dimensionless induced charges on the quantum dots. The four lowest energies $\epsilon_{\beta}^{\text{tot}}/E_C$ as a function of $n_{g,1}$ for $n_{g,2} = (1 + \hbar/\epsilon_C)/2$ with tunneling amplitudes $t_1 = 0.1E_C$ and $t_{j \neq 1} = 0.2E_C$. They use the parameter values $N_{g,a} = 0, \epsilon_C = 10E_C, \hbar = E_C/2, \text{and} \epsilon_M = E_C/2$. For non-vanishing tunneling amplitudes, the quantum dot states $(1,0)$ and $(0,1)$ hybridize. The symmetric combination of the $(1,0)$ and $(0,1)$ states has energy $\epsilon_2^{\text{tot}}$ (shown in red) and the antisymmetric combination has energy $\epsilon_1^{\text{tot}}$ (shown in black). These energies depend on the joint parity $p$ of the four MZMs; the solid curves correspond to even parity $p=1$ and dashed curves to odd parity $p=-1$. As their model only considers two quantum dot levels, the states $(0,0)$ and $(1,1)$ do not hybridize. These states have corresponding parity independent energies $\epsilon_0^{\text{tot}}$ (shown as the blue dot-dashed curve) and $\epsilon_3^{\text{tot}}$ (shown as the purple dot-dashed curve), respectively.

To get the result you want, you can effectively project onto a particular parity state. One can then use this parity operation to braid two Majorana bound states $\gamma_i$ and $\gamma_j$ with the relation $B_{i,j} = 2^{-1/2}(1 + p_{ij})$ where $B_{i,j}$ is the braiding operator for the $i^{th}$ and $j^{th}$ Majoranas.

Beyond quantum computation, Majorana bound states may also be useful in studying quantum gravity. In the early nineties, Sachdev and Ye studied a fermionic model of spin fluids [48]. Recently, Kitaev pointed out that a Majorana version of that model has properties similar to a black hole [49]. The model is of quadratic order in interaction. The Hamiltonian is

$$H = \frac{1}{4!} \sum_{i,j,k,l=1}^{N} J_{ijkl} \gamma_i \gamma_j \gamma_k \gamma_l$$

(9.1)
where the coupling constants $J_{ijkl}$ are randomly Gaussian distributed. The connection between the model and black holes is through out-of-time correlation functions:

$$\langle \gamma_i(t)\gamma_j(0)\gamma_i(t)\gamma_j(0) \rangle$$

(9.2)

which can be shown to be proportional to $e^{kt}$ the rate of separation between infinitesimally close points. In other words $k$ can be identified with the Lyapunov exponent. Kitaev showed that the exponent for the Majorana system of equation 9.1 is $(k = T)$ equal to the temperature [49]. This is the maximum possible value for $k$ and is the same value that is associated with black holes.

Figure 9.3: Depiction of a nanowire partitioned by two back gates of length L creating two Kitaev chains. Each back gate can be turned on or off changing the effective distance between the MBS.

The Shachdev-Ye-Kitaev (SYK) model is quite beautiful but it has some disadvantages. For one the out-of-time correlation functions are simply obscure which makes the connection to gravity challenging to consider. They are also difficult to measure in a real system since they involve going backwards in time. One way they can be measured is to time reverse the Hamiltonian so that although time goes forward in reality, the system behaves as if time was going backwards. The other major disadvantage is that it is not at all clear what type of real system would behave according to equation 9.1. I am fairly confident that these troubles could be overcome with time. However, I would like to propose a more straightforward Majorana model that makes an analogy to gravity. To the best of
my knowledge, this is the first time such a model has been proposed.

The idea is to utilize Majorana teleportation to effectively curve space. Let us first consider four Majorana bound states in a line.

If there are two gates of length $L$ along the nanowire as in figure 9.3 that can be turned on to take that section of the nanowire out of the topological phase then the phase difference between one side of the wire to the other can be changed from $1$ to $e^{ikL}$ to $e^{2ikL}$. Thus, in the reference frame of an electron traveling through the wire, the length of the wire is changed from 0 to $L$ to $2L$.

Now let us build a two dimensional lattice of these wires. Such a lattice is difficult to build if one needs to apply an external magnetic field to induce the topological phase. However, it has been pointed out that semiconductors with internal magnetic structure.
would not require external magnetic fields \([50]\). When all the gates are turned on the phase at any quantum dot is independent of the path taken by an electron. In this case geodesics are straight lines. If, on the other hand, some of the gates are turned off then the phase becomes path dependent and the favored paths are curved. One could calculate the Riemann tensor for any given set of gate configurations and consequently the effective gravity.

All of these applications make Majorana bound states a fascinating field of study. With recent experiments and ever increasing theoretic understanding it seems only a matter of time before such devices become a reality. Who knows what other extraordinary devices will be dreamed up that utilize the strong quantum properties of the Majorana. Baring some unforeseen problem, the Majorana fermion is on course to change the world.
Appendix A

A.1 Deriving The Matrix Equation in the BTK Formalism

\[0 = -t_m^x (1 + r_N^\uparrow) + (\epsilon_m - \omega)(e^{ik_e} + r_N^\uparrow e^{-ik_e}) - t_m^x \Psi_{e,2}^x\]
\[0 = -t_m^x (1 + r_N^\uparrow) + (\epsilon_m - \omega)(e^{ik_e} + r_N^\uparrow e^{-ik_e}) - t_m^x \Psi_{e,2}^x\]
\[0 = -t_m^x (e^{ik_e} + r_N^\uparrow e^{-ik_e}) + (\epsilon_m - \omega)\Psi_{e,2}^x - t_m^x \Psi_{e,3}^x\]
\[0 = -t_m^x (e^{ik_e} + r_N^\uparrow e^{-ik_e}) + (\epsilon_m - \omega)\Psi_{e,2}^x - t_m^x \Psi_{e,3}^x\]

...
The sum of equations in [6.10] are written out fully above for a given incoming spin and mode and a given reflected and transmitted mode. The notation for these indices have been dropped. In these equations, \( \epsilon_{m,sc} = -\mu_{m,sc} - 2t_y \cos(n\pi/N_y + 1) \)

If we write a new wave vector that is two elements shorter than the original, we can turn this system of equations into a square matrix equation.

\[
\psi_{\sigma,n,n'} = \begin{pmatrix}
    r_{N(\sigma,n',\uparrow,n)}e^{-ikc,a} \\
r_{N(\sigma,n',\downarrow,n)}e^{-ikc,a} \\
\psi_e(\sigma,n',\uparrow,n,2) \\
\psi_e(\sigma,n',\uparrow,n,3) \\
\vdots \\
\psi_e(\sigma,n',\uparrow,n,N-3) \\
\psi_e(\sigma,n',\uparrow,n,N-2) \\
u_0t_{N(\sigma,n',\uparrow,n)}e^{-iqc,a'} + v_0t_{A(\sigma,n',\downarrow,n)}e^{iqc,a'} \\
u_0t_{N(\sigma,n',\downarrow,n)}e^{-iqc,a'} - v_0t_{A(\sigma,n',\downarrow,n)}e^{iqc,a'} \\
r_{A(\sigma,n',\uparrow,n)}e^{ikc,a} \\
r_{A(\sigma,n',\downarrow,n)}e^{ikc,a} \\
\psi_e(\sigma,n',\uparrow,n,N+2) \\
\psi_e(\sigma,n',\uparrow,n,N+3) \\
\vdots \\
\psi_e(\sigma,n',\uparrow,n,2N-3) \\
\psi_e(\sigma,n',\uparrow,n,2N-2) \\
u_0t_{A(\sigma,n',\uparrow,n)}e^{iqc,a'} - v_0t_{N(\sigma,n',\downarrow,n)}e^{-iqc,a'} \\
u_0t_{A(\sigma,n',\downarrow,n)}e^{iqc,a'} + v_0t_{N(\sigma,n',\downarrow,n)}e^{-iqc,a'}
\end{pmatrix}
\]

\[
J = \begin{pmatrix}
t_{sc} + (\omega - \epsilon_{m})e^{ikc,a} \\
t_{sc} + (\omega - \epsilon_{m})e^{ikc,a} \\
t_{sc}e^{ikc,a} \\
t_{sc}e^{ikc,a} \\
0 \\
0 \\
0 \\
\vdots
\end{pmatrix}
\] (A.2)
A.1. DERIVING THE MATRIX EQUATION IN THE BTK FORMALISM

Now the set of equations can be written as a single square matrix equation

\[
\bar{\Psi}_{\sigma,n',n} = (\bar{H}_n + Q_n - \omega) J_{\sigma,n'}
\]  

(A.3)

where \( \bar{H} \) is just the full Hamiltonian with the first and last columns and rows removed.

The boundary condition matrix \( Q \) is given below. All elements not written explicitly are zero. In the equations below the mode index and \( \omega \) dependence are not explicitly written on \((k_e, k_l, q_e, q_l) = (k_{n_e}^e(\omega), k_{n_l}^h(\omega), q_{n_e}^e(\omega), q_{n_l}^h(\omega))\)

\[
Q_n = \begin{pmatrix}
Q_{n,1} & 0 & \cdots & 0 & 0 \\
& Q_{n,2} & \cdots & 0 & 0 \\
& & Q_{n,3} & \cdots & 0 \\
& & & Q_{n,4} & 0 \\
& & & & Q_{n,5}
\end{pmatrix}
\]  

(A.4)
A.2. THE LANGRETH THEOREM

In section 6.2.2 I motivate the Keldysh matrix.

\begin{equation}
G = \begin{pmatrix}
G^+ & G^K \\
0 & G^-
\end{pmatrix}
\end{equation}

(A.6)

The real point of this matrix is to correctly calculate products of greens functions like \( G_L G_D \) where \( G_L \) and \( G_D \) might be the greens functions for the source and the drain, for example. Thus far, however, I have not proven that the Keldysh matrix guarantees the correct bookkeeping. Let us now turn to that endeavor.

Let us begin by writing these three Green functions in terms of the lesser and greater...
Green functions. From Eqns. 6.28 and 6.24 we have,

\[
G^k(t_1, t_2) = G^>(t_1, t_2) + G^<(t_1, t_2)
\]

\[
G^+(t_1, t_2) = \Theta(t_1 - t_2)(G^>(t_1, t_2) - G^<(t_1, t_2))
\]

\[
G^+(t_1, t_2) = \Theta(t_2 - t_1)(G^<(t_1, t_2) - G^>(t_1, t_2))
\]

We are interested in terms like \(G_L G_D\) which is shorthand for \(\int_C d\tau G_L(t_1, \tau)G_D(\tau, t_2)\) the contour integral. Let us start by assuming that \(t_1\) is on the first branch and \(t_2\) is on the second. In other words we start by examining the lesser Green functions.

\[
G^< = \int_C d\tau G_L(t_1, \tau)G_D(\tau, t_2)
\]

The strategy will be to deform the contour back to negative infinity in between \(t_1\) and \(t_2\) like in Fig. A.1 below. To form this contour we took advantage of properties of the time evolution operator: \(S(t_2, \infty)S(\infty, t_1) = S(t_2, \infty)S(\infty, -\infty)S(-\infty, \infty)S(\infty, t_1) = S(t_2, -\infty)S(-\infty, t_1)\). Doing this will allow us to write \(G_L\) and \(G_R\) in terms of lesser and greater Green functions.

In the first contour \((C_a)\), \(t_2 > \tau\) and in the second contour \((C_b)\), \(\tau > t_1\).

![Figure A.1: Deformation of the time contour](image-url)
A.2. THE LANGRETH THEOREM

\[ G^< (t_1, t_2) = \int_{C_a} d\tau G_L(t_1, \tau) G_D^< (\tau, t_2) + \int_{C_b} d\tau G_L^< (t_1, \tau) G_D (\tau, t_2) \]
\[ = \int_{-\infty}^{t_1} dt G_L^< (t_1, t) G_D^< (t, t_2) + \int_{t_1}^{\infty} dt G_L^< (t_1, t) G_D^< (t, t_2) \]
\[ + \int_{-\infty}^{t_2} dt G_L^< (t_1, t) G_D^< (t, t_2) + \int_{t_2}^{\infty} dt G_L^< (t_1, t) G_D^< (t, t_2) \]
\[ = \int_{-\infty}^{\infty} dt [G_L^+ (t_1, t) G_D^< (t, t_2) + G_L^< (t_1, t) G_D^- (t, t_2)] \]

(A.9)

So in our condensed notation we have that \( G^< = G_L^+ G_D^< + G_L^< G_D^- \). For the greater Green function the derivation is the same except that \( t_2 \) is before \( t_1 \) everywhere. We can take this clear through to the end of the derivation and see that \( G^> = G_L^+ G_D^> + G_L^< G_D^- \).

Now we can find the rule for the other Green functions. The Keldysh Green function is easy.


The other two are just slightly more involved.

\[ G^\pm (t_1, t_2) = \Theta (\mp t_1 \pm t_2) (\mp G^> (t_1, t_2) \pm G^< (t_1, t_2)) \]
\[ = \Theta (\mp t_1 \pm t_2) \int_{-\infty}^{\infty} dt [G_L^+ (t_1, t) (\mp G_D^> (t, t_2) \pm G_D^< (t, t_2)) \]
\[ + (\mp G_L^< (t_1, t) \pm G_D^< (t_1, t)) G_D^- (t, t_2)] \]
\[ = \Theta (\mp t_1 \pm t_2) \left[ \int_{-\infty}^{t_1} dt (G_L^< (t_1, t) - G_L^> (t_1, t) G_D^> (t, t_2) \pm G_D^< (t, t_2)) \]
\[ + \int_{-\infty}^{t_2} dt (\mp G_L^> (t_1, t) \pm G_L^< (t_1, t)) (G_D^< (t, t_2) - G_D^> (t, t_2)) \]
\[ = \int_{-\infty}^{\infty} dt G_L^\pm (t_1, t) G_D^\pm (t, t_2) \]

(A.11)

In the last step I added the two integrals together which either cancels the integral to \( t_1 \) or
A.3. EXPANDING $G$ IN TERMS OF $G_m$ AND $G_{sm}$

that to $t_2$ depending if we are examining the retarded or advanced Green function.

All three rules together are,

\[
\begin{align*}
G^+ &= G_L G_D^+ \\
G^- &= G_L G_D^- \\
G^K &= G_L G_D^K + G_L^K G_D^-
\end{align*}
\]  

(A.12)

which contains the exact same information as the matrix equation A.6.

A.3 Expanding $G$ in terms of $G_m$ and $G_{sm}$

From appendix A.2 we had that,

\[
\begin{pmatrix}
G^+ & G^K \\
0 & G^-
\end{pmatrix} = G = G_{sm} T_m G_m + G_{sm} T_m G_m G_{sm} T_m G_m + \ldots 
\]  

(A.13)

which is simply a sum over all possible propagation that start in the metal and end in the semiconductor. We can factor out the last semiconductor $G_{sm} T_m G_m$ term and we are left with a geometric series.

\[
G = G_{sm} T_m G_m \sum_{p=0}^{\infty} (T_m G_{sm} T_m G_m)^p = G_{sm} T_m G_m (1 - T_m G_{sm} T_m G_m)^{-1} 
\]  

(A.14)

Now its a matter of taking the inverse. Let us proceed one step at a time. First,

\[
G_{sm} T_m G_m = \begin{pmatrix}
G_{sm}^+ & G_{sm}^k \\
0 & G_{sm}^-
\end{pmatrix} \begin{pmatrix}
T_m & 0 \\
0 & T_m
\end{pmatrix} \begin{pmatrix}
G_m^+ & G_m^k \\
0 & G_m^-
\end{pmatrix} 
\]  

(A.15)
which, with simple matrix multiplication is,

\[
G_{sm} T_m G_m = \begin{pmatrix} G_{sm}^+ T_m G_m & G_{sm}^+ T_m G_k^+ + G_{sm}^+ T_m G_m^- G_{sm}^+ T_m G_m^- \end{pmatrix}
\]  

(A.16)

Now one can check that for the following inverse \((1 - TG_{sm} T_m G_m)(1 - TG_{sm} T_m G_m)\)^{-1} = 1. The matrix with that property is,

\[
(1 - T_m G_{sm} T_m G_m)^{-1} = \begin{pmatrix} (1 - T_m G_{sm}^+ T_m G_m)^{-1} & (1 - T_m G_{sm}^+ T_m G_m)^{-1}(G_{sm}^+ T_m G_k^+ + G_{sm}^+ T_m G_m^-)(1 - T_m G_{sm}^+ T_m G_m)^{-1} \\ 0 & (1 - T_m G_{sm}^+ T_m G_m)^{-1} \end{pmatrix}
\]

(A.17)

At this point we are all set up to find \(G = G_{sm} T_m G_m(1 - T_m G_{sm} T_m G_m)^{-1}\). For the current, equation 6.29, we need \(TG^k\) the Keldysh quadrant of the full Green function.

\[
TG^k = T_m G_{sm}^+ T_m G_m^+ (1 - T_m G_{sm}^+ T_m G_m^+)^{-1}(T_m G_{sm}^+ T_m G_m^+ + T_m G_{sm}^+ T_m G_m^-)(1 - T_m G_{sm}^+ T_m G_m^-)^{-1} \\
+ (T_m G_{sm}^+ T_m G_m^+ + T_m G_{sm}^+ T_m G_m^-)(1 - T_m G_{sm}^+ T_m G_m^-)^{-1}
\]

(A.18)

By multiplying the last term by the identity, \(1 = (1 - T_m G_{sm}^+ T_m G_m^+)(1 - T_m G_{sm}^+ T_m G_m^+)^{-1}\), we can add the terms together to get,

\[
TG^k = (1 - T_m G_{sm}^+ T_m G_m^+)^{-1}(T_m G_{sm}^+ T_m G_m^+ + T_m G_{sm}^+ T_m G_m^-)(1 - T_m G_{sm}^+ T_m G_m^-)^{-1}
\]

(A.19)

This is what is used in section 6.2.2.
A.4 Superconductor Self Energy Below the Bulk Gap

For energies below the bulk gap of the parent superconductor the exact form of the superconductor Green function can be calculated. From section 6.3 we had,

\[ \Sigma(\omega) = T_{sc} G_{sc}(\omega) T_{sc} \] \hspace{1cm} (A.20)

If we write this in mode space, we can integrate out the \( k_z \) degrees of freedom since the coupling is restricted to the bottom of the superconductor.

\[ \Sigma(k_{\parallel}, \omega) = \tilde{t}_{sc}^2 \int \frac{dk_z}{2\pi} G_{sc}(k, \omega) \] \hspace{1cm} (A.21)

So we need the Green function,

\[ G_{sc}(k, \omega) = (\omega - H_{sc}(k))^{-1} \] \hspace{1cm} (A.22)

where the BCS Hamiltonian is,

\[ H_{sc}(k) = \begin{pmatrix} -\epsilon(k) & -\Delta \\ -\Delta & \epsilon(k) \end{pmatrix} \] \hspace{1cm} (A.23)

where \( \epsilon(k) = \mu + 2t_{sc}^{x} \cos[k_{x}a] + 2t_{sc}^{y} \cos[k_{y}a] + 2t_{sc}^{z} \cos[k_{z}a] \). From the form of \( H_{sc} \), we can find the Green function.

\[ G_{sc}(k, \omega) = \frac{1}{\omega^2 - \epsilon(k)^2 - \Delta^2} \begin{pmatrix} \omega + \epsilon(k) & \Delta \\ \Delta & \omega - \epsilon(k) \end{pmatrix} \] \hspace{1cm} (A.24)
A.4. SUPERCONDUCTOR SELF ENERGY BELOW THE BULK GAP

Since the Green function is a simpler function of $\epsilon$ than of $k$ we take

$$\Sigma(k\parallel, \omega) = t^2_{sc} \int_{-\Lambda+\mu}^{\Lambda+\mu} d\epsilon \int \frac{dk_z}{2\pi} \delta(\epsilon - \epsilon(k)) G_{sc}(\epsilon, \omega)$$  \hspace{1cm} (A.25)$$

where $\Lambda = 2t^z_{sc}$ is the half bandwidth. The delta function can be evaluated in terms of $k_z$

$$\delta(\epsilon - \epsilon(k)) = \frac{\delta(k - k_0)}{\epsilon(k_0)} = \frac{\delta(k - k_0)}{2t_{sc} \sqrt{1 - \left(\frac{\epsilon - \mu}{2t_{sc}}\right)^2}}$$  \hspace{1cm} (A.26)$$

where $k_0 = (1/a) \cos^{-1}(1/2t^z_{sc}(\epsilon - \mu))$ is the pole. The density of states $\int \frac{dk_z}{2\pi} \delta(\epsilon - \epsilon(k))$ is weakly dependent on energy so we set it to its value at the fermi energy, which is zero in this model, and take it out of the integral.

$$\Sigma(k\parallel, \omega) = \frac{t^2_{sc}}{2\pi} \frac{1}{\sqrt{4(t^z_{sc})^2 - (\mu)^2}} \int_{-\Lambda+\mu}^{\Lambda+\mu} d\epsilon G_{sc}(\epsilon, \omega)$$  \hspace{1cm} (A.27)$$

Now we must evaluate the integral

$$I = \int_{-\Lambda+\mu}^{\Lambda+\mu} d\epsilon \frac{\omega\tau_0 + \epsilon\tau_z + \Delta\tau_x}{\omega^2 - \epsilon^2 - \Delta^2}$$  \hspace{1cm} (A.28)$$

where $\tau_i$ is a Pauli matrix. This integral can be solved by trig substitution.

$$\epsilon \rightarrow \sin(x)\sqrt{\omega^2 - \Delta^2}$$  \hspace{1cm} (A.29)$$

then we have,

$$I = \int_a^b dx \sqrt{\omega^2 - \Delta^2} \cos(x) \frac{\omega\tau_0 + \sin(x)\sqrt{\omega^2 - \Delta^2}\tau_z + \Delta\tau_x}{(\omega^2 - \Delta^2)(1 - \sin^2(x))}$$  \hspace{1cm} (A.30)$$
### A.5 Normalization of the ZBP

Within this thesis I have referred to the fact that the zero bias peak is normalized but I have not motivated why that must be. Here I present a simple scattering calculation. What we will find is that, for states with an equal number of particles and holes, the conductance is normalized independent of the barrier strength.

$$I = \int_a^b dx \left[ \frac{\omega \tau_0 + \Delta \tau_x}{\sqrt{\omega^2 - \Delta^2}} Sec(x) + Tan(x) \tau_z \right]$$  \hspace{1cm} (A.31)

$$I = \frac{\omega \tau_0 + \Delta \tau_x}{\sqrt{\omega^2 - \Delta^2}} ln[Sec(x) + Tan(x)]_a^b - ln[Sec(x)]_b^a \tau_z$$  \hspace{1cm} (A.32)

$$I = \frac{\omega \tau_0 + \Delta \tau_x}{\sqrt{\omega^2 - \Delta^2}} ln \left[ \frac{\omega^2 - \Delta^2 + \Lambda + \mu}{\omega^2 - \Delta^2 - \Lambda + \mu} \right] - ln \left[ \frac{\sqrt{\omega^2 - \Delta^2 - (\Lambda + \mu)^2}}{\sqrt{\omega^2 - \Delta^2 - (\Lambda + \mu)^2}} \right] \tau_z$$  \hspace{1cm} (A.33)

Assuming \( \Lambda >> \omega, \Delta, \mu \) we get the result in section 6.3.

$$\Sigma(\omega) = \frac{\tau^2_{sc}}{2\pi \Lambda^2 - \mu^2} \left( \frac{\omega \tau_0 + \Delta \tau_x}{\sqrt{\omega^2 - \Delta^2}} \right) + 2 \frac{\mu \Lambda}{\Lambda^2 - \mu^2} \tau_z$$  \hspace{1cm} (A.34)

### A.5 Normalization of the ZBP

Within this thesis I have referred to the fact that the zero bias peak is normalized but I have not motivated why that must be. Here I present a simple scattering calculation. What we will find is that, for states with an equal number of particles and holes, the conductance is normalized independent of the barrier strength.

![Figure A.2: The normal wire-superconductor configuration. Z is defined as pure imaginary. The BCS coherence factors \(u\) and \(v\) are implicitly functions of \(k\). I use the Andreev approximation where \(k = k_F\) on both sides of the barrier and for particles and holes.](image)
A.5. NORMALIZATION OF THE ZBP

I make the approximation that \( k = k_f \) on either side of the barrier and that particles and holes have the same wave vector. This is reasonable as long as we recognize that below the superconductor’s gap we need to redefine the wave vector in the superconductor as imaginary so that normal current does not propagate. The phase of the wave vector is not really important for the intuition I want to convey in this section. Since the only spin mixing in the problem is due to cooper pairing, we can consider only particles with spin up and holes with spin down. The boundary equations that characterize the system are:

\[
1 + r_N = u t_N + v t_A \\
r_A = v t_N + u t_A \\
1 - r_N = u t_N - v t_A + Z + Z r_N \\
r_A = v t_N - u t_A + Z r_A
\]

(A.35)

These have the general solution:

\[
\begin{align*}
r_N &= -\frac{(u^2 - v^2)(Z - 2) Z}{Z^2(u^2 - v^2) - 4u^2} \\
r_A &= -\frac{4uv}{Z^2(u^2 - v^2) - 4u^2} \\
t_N &= \frac{2u(Z - 2)}{Z^2(u^2 - v^2) - 4u^2} \\
t_A &= -\frac{2vZ}{Z^2(u^2 - v^2) - 4u^2}
\end{align*}
\]

(A.36)

These solutions have the special property that when \( u = v \) the barrier dependence goes away and \( r_N = 0 \) while \( r_A = 1 \). Therefore, when \( u = v \) the conductance is quantized. However, for any \( u \neq v \) the \( r_N \) goes to one as the barrier strength goes to infinity. Thus, the barrier strength controls the width of the normalized peak. Note that the transmission coefficients should not be taken to seriously in the \( u = v \) limit since in this limit the
superconducting wave vector is zero.

The normalized conductance result should be interpreted as the case when there are an equal number of particle states as hole states at the barrier, which is exactly the situation for Majorana bound states. In this case, the weight of the incoming electron has to be perfectly balanced by the weight of the reflected hole. Thus, there is no probability left over for normal reflection. This property can be seen, right away, from the scattering equations if we set $u = v$. In this case we have:

\begin{align}
1 + r_N &= t_N + t_A = r_A \\
1 - r_N &= t_N - t_A + Z(t_N + t_A) = r_A
\end{align}

(A.37)

clearly these equations tell us that $r_N = 0$ and that $r_A = 1$ meaning conduction is quantized. Note that this property does not require the wave vectors in the superconductor and the normal wire to be the same.
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