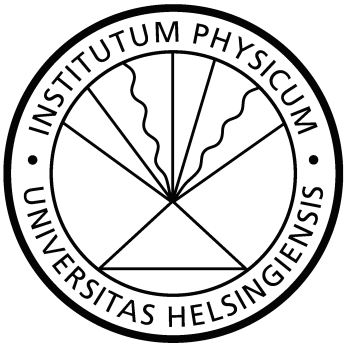

Bachelor's Thesis

Theoretical Physics

Majorana States At Magnetic Domain Walls

Alex Weststrom

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Instructor: Dr. Teemu Ojanen

Supervisor: Dr. Tommy Ahlgren

HELSINGIN YLIOPISTO

FYSIIKAN LAITOS

PL 64 (Gustaf Hällströmin katu 2)

00014 Helsingin yliopisto

Abstract

In this thesis we examined a system in which magnetic atoms are placed on an s-wave superconductor. The goal was to investigate the Majorana fermions forming on the domain walls at the boundary between different topological phases. This was done both analytically and numerically. In the basic setup the magnetic moments were constrained to all be in the same plane and be of the same magnitude. The magnetic moments are oriented such that the angle between adjacent moments is constant throughout the chain. The system was then studied in different parameter regimes.

A change of chirality, i.e. reversing the sign of the angle, halfway through the chain caused the two halves to be in topologically different phases and this in turn created two zero-energy Majorana states on the domain wall between the two halves. This was due to the the continuous move from a positive to a negative angle, effectively forcing the system into a trivial phase at the boundary. The Majorana states were derived both analytically in the continuum limit and through numerical calculations for finite systems.

We then studied the case where the angle between moments was greater in the second half of the chain and argued why an increase of π necessarily formed a domain wall between the two halves. The different angles also introduced a spatial asymmetry that offset the central peaks of the Majorana states to either side. This effect became more prominent with a finite-length transition zone between the two phases. This could in some sense be thought of as an expansion of the trivial phase between the two phases.

Contents

1 Introduction

In 1937, an Italian physicist Ettore Majorana theorized of a new kind of particle [1] with a very interesting property: it is its own antiparticle. For several decades this exotic particle remained more or less unknown and it is only fairly recently that these *"Majorana fermions"* (MFs), as they came to be called, made their grand début in several fields of theoretical physics. In high-energy physics Majorana's idea of neutrinos being MFs remains a possibility even today; in 2008, Avignone, Engel and Elliot [2] showed that the observation of a neutrinoless double beta decay implies that the neutrino is its own antiparticle and consequently a MF . Moreover, in the context of certain versions of supersymmetry the *"superpartners"* to bosonic particles are asserted to be MFs. If true, this would lend more credence to the suggestion that WIMPs are the answer to the mystery of dark matter [3].

Our focus in this thesis, however, will exclusively lie on MFs as they pertain to the field of condensed matter physics (CMP). Here MFs take on an even more exotic role: as opposed to being fundamental particles - which is the case in particle physics - they can only exist as quasiparticles (i.e. excitations) in solid state systems [4] due to the inevitable fact that such systems only consist of regular fermions (electrons for our intents and purposes). The fact that MFs are their own antiparticles implies that they are neutrally charged. For this to be possible with only negatively charged electrons and positively charged holes at our disposal, it must be that MFs are equal superpositions of them both. In fact, the converse is also true: a fermion can be divided into a superposition of MFs. In that regard MFs can be thought of as *"half-fermions"*, meaning that they constitute half of a fermion. However, one does not normally talk about conventional fermions being half MF, since MFs are not, as previously mentioned, fundamental particles in CMP. What makes this splitting of a fermion very interesting from a physicist's perspective is that some systems permit a pair of MFs to be highly delocalized. In other words, they can be spatially separated arbitrarily far apart. This makes the corresponding fermionic state robust against local perturbations caused by the environment [5, 6]. This has obvious applications in quantum computing, where one of the major hurdles is decoherence: qubits interacting with the environment, destroying their current state, thus making the computation unreliable [7].

This, however, is not the whole story; there is an even more exotic property concerning

MFs in CMP: they are *non-Abelian anyons*. This means that contrary to bosonic and fermionic statistics, where the exchange of two identical particles *only* results either in no change of sign (bosons) or a change of sign (fermions) to the wavefunction, non-Abelian exchanges may cause the entire wavefunction to change from one state to another. This is also in contrast to *Abelian* anyons, which only gain a phase factor with an argument between 0 and π. The non-Abelian nature of MFs (bound in vortices) was first discovered by Moore and Read [8] over two decades ago in the context of the fractional quantum Hall effect (FQHE). Read and Green showed in 2000 that some superconducting systems are closely related to the FQHE and are therefore expected to support MF with non-Abelian exchange statistics [9, 10].

This makes superconducting systems a promising platform for finding MFs. Excitations in these systems come in the form of Bogoliubov quasiparticles that are superpositions of electrons and holes [11]. However, if we consider a conventional s-wave superconductor, where the Cooper pairs consist of paired electrons with opposite spins, we are faced with a problem when we try to realize the bogoliubons as MFs. To elucidate, let's consider a lattice of superconducting (s-wave) electrons. Since the electrons combine exclusively into pairs with opposite spin, they only couple locally on each site in the lattice. This effectively prevents the emergence of spatially separated MFs to form. Thus, in a standard s-wave superconductor spin prevents formation of MFs [4]. Let us instead turn our attention to Kitaev's toy model [12] of a spinless p-wave superconducting chain. Kitaev's model is the first simple example of a *topological superconductor* in 1D, which turns out to support two delocalized MF-states, one at each end of the chain. "*Topological*" relates to the fact that the existence of MF states will not be affected by small deformations to the system. In this model, MFs are located at the domain wall between two topologically distinct phases determined by certain parameters of the model.

The research regarding MFs contains lots of new and exciting fundamental physics, while simultaneously being a promising tool to future technological applications. MFs have not yet been experimentally confirmed, but strong indications of their existence have been seen in a number of experiments [13, 14, 15]. The research on MFs is currently one of the most active fields in physics. The theoretical community searches on for new models and systems in which one could realize MFs. In this thesis we will mainly be investigating one-dimensional chains of atoms with magnetic moments placed on a superconducting surface, where we will be looking for the emergence and properties of possible MF states. We introduce different kinks and explore the MF states that arise at the locations of the domain walls. The research in this thesis is motivated by a recent paper by Nadj-Perge *et al.* (2013) [16] who proposed a method to experimentally construct such a system.

2 Theory

2.1 A short introduction to quantum many-body theory

We begin with a brief review of some of the basics concepts in quantum many-body theory. At the heart of this theory, we have what is known as the occupation number representation. In this representation, N-particle states are expressed in terms of how many particles occupy each single-particle state. In order to construct these states, we must first choose a complete set of single-particle states $\{|\nu_i\rangle\}$. When constructing the many-body states great care must be taken in order to properly symmetrize the products of single-particle states according to their many-body behaviour. Bosons require symmetry upon particle exchanges while fermion states need antisymmetry. We can then express the N-particle system with

$$|\Psi\rangle_{\{n_{\nu_i}\}} = |n_{\nu_1}, n_{\nu_2}, n_{\nu_3}, ...\rangle, \qquad N = \sum_i n_{\nu_i}. \tag{2.1}$$

The set of occupation number state vectors span what is known as the *Fock space*. By construction, states with different values of N are automatically orthogonal. The manipulation of these states is done via creation and annihilation operators that act on the states. In fact, the creation and annihilation operators are universal in the sense that we can express any other operator as combinations of them. A creation operator, $a^\dagger_{\nu_i}$, when acting on a state, introduces a particle in the single-particle state $|\nu_i\rangle$, and conversely, the annihilation operator a_{ν_i}, which is the Hermitian conjugate of the creation operator, destroys a particle in this state. The equations

$$a^\dagger_{\nu_i}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}, ...\rangle = \sqrt{n_{\nu_i}+1}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}+1, ...\rangle \tag{2.2}$$

$$a_{\nu_i}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}, ...\rangle = \sqrt{n_{\nu_i}}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}-1, ...\rangle \tag{2.3}$$

encapsulate their action on a state. If we now combine them and apply this new operator on a state, we get

$$a^\dagger_{\nu_i}a_{\nu_i}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}, ...\rangle = n_{\nu_i}|n_{\nu_1}, n_{\nu_2}, ..., n_{\nu_i}, ...\rangle \tag{2.4}$$

As we can see, this gives us the occupation number of the state $|\nu_i\rangle$ and we can therefore define an operator $\hat{n}_{\nu_i} \equiv a^\dagger_{\nu_i}a_{\nu_i}$ called the occupation number operator. Note, however, that we must be careful in choosing the order of $a^\dagger_{\nu_i}$ and a_{ν_i}, otherwise we run into an inconsistency when we

apply them to the vacuum state. We get $aa^\dagger|0\rangle = |0\rangle$ instead of $a^\dagger a|0\rangle = 0|0\rangle$, which is the desirable answer. In fact, this raises a question about the relation between the two orderings of the operators. As it turns out, the commutation relations of the two operators depend on what kind of particle they represent. For bosons, we have

$$[b_i^\dagger, b_j^\dagger] = 0, \qquad [b_i, b_j] = 0, \qquad [b_i, b_j^\dagger] = \delta_{ij}, \tag{2.5}$$

where [A,B]=AB-BA is the usual commutator. We will not make use of bosons in this thesis; the bosonic relations (2.5) are only mentioned for the sake of completeness. Our discussion will hereinafter only concern fermions. The fermionic commutation relations make use of the anti-commutator, defined by $\{A,B\} \equiv AB+BA$

$$\{f_i^\dagger, f_j^\dagger\} = 0, \qquad \{f_i, f_j\} = 0, \qquad \{f_i, f_j^\dagger\} = \delta_{ij}. \tag{2.6}$$

The advantage of eqs. (2.6) lies in the fact that they completely encode the fermionic many-body behaviour into the operators themselves. As the notation suggests $f \neq f^\dagger$, which means that f is not Hermitian. For fermions created by $f^\dagger$ this is because they are not in general their own antiparticles. This gives us a new way of looking at f. The act of removing one fermion from an occupied state can also be thought of as creating one corresponding antifermion or a hole. Therefore f can also be viewed as the antifermion/hole creation operator.

An important concept in CMP is the *Fermi sea*

$$|FS\rangle = \prod_i^{N/2} f_{\nu_i\downarrow}^\dagger f_{\nu_i\uparrow}^\dagger |0\rangle,$$

where the single-particle states are in ascending order of energy. This is the ground state at zero temperature, where the electrons are packed from the lowest energy single-particle state up to some higher energy state. The energy of the highest occupied state in $|FS\rangle$ is called the Fermi energy or Fermi surface.

2.2 The Fourier transforms

Many problems in CMP involve lattices or spaces with some form of periodic structure. In such systems, it is often natural to map the problem into momentum space through a Fourier transform (FT). We will therefore briefly discuss the theory of FTs

A FT of a function, $f(x_j) \equiv f_j$, on a finite discrete space is defined as

$$f_j = \frac{1}{\sqrt{N}} \sum_k e^{ix_j k} \hat{f}_k \tag{2.7}$$

where

$$\hat{f}_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ix_j k} f_j. \tag{2.8}$$

We refer to both of these as the discrete Fourier transforms (DFT). The latter, eq. (2.8), is often called the inverse DFT. Combining (2.7) and (2.8) yield the following two identities

$$\frac{1}{N}\sum_{k} e^{i(x_k - x_l)k} = \delta_{kl}, \text{ and } \frac{1}{N}\sum_{j=1}^{N} e^{ix_j(k-k')} = \delta_{kk'} \tag{2.9}$$

which will used extensively when we analyze different models later on.

2.3 Majorana fermions

In CMP, MFs are equal superpositions of electrons and holes. This is because MFs are their own antiparticles and must therefore have zero charge. Formally, we say that the Majorana creation operator, γ, is of the form $\gamma_1 = uc + u^* c^\dagger$ or $\gamma_2 = i(vc - v^* c^\dagger)$, where $u, v \in \mathbb{C}$. This ensures charge neutrality and self-adjointness. In the more general case of N electrons, we have

$$\gamma_{2i-1} = uc_i + u^* c_i^\dagger, \quad \gamma_{2i} = i(vc_i - v^* c_i^\dagger), \quad i = 1, 2, ..., N. \tag{2.10}$$

The two flavours of MFs in (2.10) are needed to make up one fermion, $c_i^\dagger$. The commutation relation for Majorana operators is easily derived with the use of eqs. (2.6)

$$\{\gamma_k, \gamma_l\} = 2\delta_{kl}, \quad \text{which implies } \gamma_k^2 = 1. \tag{2.11}$$

The equation γ_k^2 $(= \gamma_k^\dagger \gamma_k) = 1$ (2.11) tells us that it is not sensible to define an occupation number operator for MFs, because so defined the occupation number is always 1. Another way to think of this problem is that since the creation and annihilation operators are the same operator, removing a MF is equal to introducing a MF and hence it does not make sense to talk about whether the state is occupied or not. The only well-defined occupation number is that of the fermionic state consisting of a pair of MFs.

Our main interest will lie on MFs forming at the domain wall between two topologically different phases of a system, but why do we expect MFs to form there at all? When two different topological phases are brought in contact we cannot continuously move from one phase to the other, without closing the band gap somewhere between them. This suggests that there will exist zero energy modes on the boundary. Because the two MFs have no energy, we have a degeneracy in the ground state. Removing the MF pair or introducing them comes at no energy cost. This degeneracy thus means that we can choose to have an even or an odd number of electrons without affecting the total energy of the system.

2.4 Superconductivity

The Bardeen-Cooper-Schrieffer (BCS) theory is one of the great achievements of modern theoretical physics, and is the standard description of superconductivity at the microscopic level. In

the simplest version of this theory, electrons or holes combine with their time-reversed counterparts, forming a *Cooper pair* with a net spin and momentum of zero. Other pairings are also possible but this s-wave pairing turns out to be energetically favored in conventional superconducting materials. The electron-pairs interact through phonons in the system, leading us to the effective Hamiltonian

$$H_{BCS} = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}\sigma} f_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} f^\dagger_{\boldsymbol{k}\uparrow} f^\dagger_{-\boldsymbol{k}\downarrow} f_{-\boldsymbol{k}'\downarrow} f_{\boldsymbol{k}'\uparrow} \tag{2.12}$$

where $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ and $V_{\boldsymbol{k}\boldsymbol{k}'}$ is the phonon-mediated coupling strength. If we apply a Hartree-Fock type mean-field approximation to this Hamiltonian (2.12) and define $\Delta_{\boldsymbol{k}} \equiv \sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} \langle f_{-\boldsymbol{k}'\downarrow} f_{\boldsymbol{k}'\uparrow} \rangle$, where $\langle\ \rangle$ denotes the mean-field expectation value, we end up with

$$H^{MF}_{BCS} = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}\sigma} f_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} (\Delta_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}\uparrow} f^\dagger_{-\boldsymbol{k}\downarrow} + h.c.) + const. \tag{2.13}$$

This Hamiltonian can be solved using Bogoliubov transformations

$$\gamma_{\boldsymbol{k}\uparrow} = u^*_{\boldsymbol{k}} f_{\boldsymbol{k}\uparrow} + v_{\boldsymbol{k}} f^\dagger_{-\boldsymbol{k}\downarrow} \tag{2.14}$$

$$\gamma^\dagger_{-\boldsymbol{k}\downarrow} = -v^*_{\boldsymbol{k}} f_{\boldsymbol{k}\uparrow} + u_{\boldsymbol{k}} f^\dagger_{-\boldsymbol{k}\downarrow}, \quad u_{\boldsymbol{k}}, v_{\boldsymbol{k}} \in \mathbb{C}. \tag{2.15}$$

The bogoliubons diagonalize the Hamiltonian, transforming (2.13) into

$$H^{MF}_{BCS} = \sum_{\boldsymbol{k}\sigma} \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2} \gamma^\dagger_{\boldsymbol{k}\sigma} \gamma_{\boldsymbol{k}\sigma} + const. \tag{2.16}$$

where the constants satisfy

$$\begin{aligned} |u_{\boldsymbol{k}}|^2 &= \frac{1}{2}\left(1 + \frac{\xi_{\boldsymbol{k}}}{\sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}}\right) \\ |v_{\boldsymbol{k}}|^2 &= \frac{1}{2}\left(1 - \frac{\xi_{\boldsymbol{k}}}{\sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}}\right) \end{aligned} \tag{2.17}$$

As we can immediately see from (2.16), the energy-spectrum for this system is given by

$$E = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}. \tag{2.18}$$

This short analysis should make the similarity between bogoliubons and MFs apparent. However, bogoliubons are not generally their own antiparticles. The relations (2.17) tells us that the bogoliubons are not Hermitian, and therefore cannot be MFs. This is the technical reason why no MF states are present in the standard s-wave superconductor.

2.5 The Bogoliubov-de-Gennes formalism

In the previous section we derived the energy spectrum for an s-wave superconductor using bogoliubons. This was done to illustrate that quasiparticles naturally emerging in superconducting

systems resemble MFs. In this section we present the Bogoliubov-de-Gennes (BdG) formalism, which will be convenient for our purposes.

The main goal is to rewrite the Hamiltonian of the system in the form

$$H = \sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}} H_{\boldsymbol{k}} \Psi_{\boldsymbol{k}} + const.$$

where $\Psi_{\boldsymbol{k}}$ is a spinor

$$\Psi_{\boldsymbol{k}} = \begin{pmatrix} f_{\boldsymbol{k}\uparrow} & f_{\boldsymbol{k}\downarrow} & f^\dagger_{-\boldsymbol{k}\downarrow} & -f^\dagger_{-\boldsymbol{k}\uparrow} \end{pmatrix}^T \tag{2.19}$$

Note that this definition is only appropriate for single band spin-1/2 systems. In the general case with n degrees of freedom, the spinor has length $2n$ and consequently the dimensions of $H_{\boldsymbol{k}}$ is $2n \times 2n$. This implies that the BdG-formalism comes with a built-in degeneracy. For every eigenvalue $E_{\boldsymbol{k}}$ to $H_{\boldsymbol{k}}$, $-E_{-\boldsymbol{k}}$ is also an eigenvalue.

The BdG-Hamiltonian $H_{\boldsymbol{k}}$ is often written with the use of Pauli spinors

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Here we have used their symbol conventionally associated with spin space, but we will also need a similar set in the electron-hole space, where we denote them by τ_i. The 2×2-identity matrix is also needed in order to completely span the spaces of 2×2 Hermitian matrices. If we index the matrices by numbers, the identity matrix is often written as σ_0 and τ_0 respectively. Now the BdG-Hamiltonian can be re-expressed as

$$H_{\boldsymbol{k}} = \sum_{ij} a_{ij}(\boldsymbol{k})(\tau_i \otimes \sigma_j), \quad i,j = 0,1,2,3. \tag{2.20}$$

3 Models

In this chapter we will present the different models that we will employ to study MFs. We begin by reviewing perhaps the simplest 1D model of a topological superconductor that supports MF states. Then we will move on to the magnetic chain model which is the main focus of this thesis.

3.1 Kitaev's spinless p-wave superconductor in 1D

We start off by the simplest supeconducting system that supports MFs [12, 17]

$$H = -t\sum_{j=1}^{N-1}(f_{j+1}^{\dagger}f_j + h.c.) - \mu\sum_{j=1}^{N} f_j^{\dagger}f_j + \sum_{j=1}^{N-1}(\Delta f_j f_{j+1} + h.c.) \tag{3.1}$$

where t is the hopping amplitude between nearest neighbours, μ is the chemical potential and $\Delta = |\Delta|e^{i\phi}$ is the superconducting gap. In order to write (3.1) in its BdG-form, we must first do a FT. This results in

$$H = \sum_k(-t(e^{-ik}f_k^{\dagger}f_k + e^{ik}f_k^{\dagger}f_k) - \mu f_k^{\dagger}f_k + \Delta e^{-ik}f_k f_{-k} + \Delta^* e^{ik}f_{-k}^{\dagger}f_k^{\dagger})$$

Where we have for simplicity set the lattice constant to unit length. Now, through some change of indices, we can rewrite it as

$$H = \frac{1}{2}\sum_k -(2t\cos(k) + \mu)(f_k^{\dagger}f_k + f_{-k}^{\dagger}f_{-k}) + 2i\Delta\sin(k)f_{-k}f_k + 2i\Delta^*\sin(k)f_{-k}^{\dagger}f_k^{\dagger}. \tag{3.2}$$

This system only has one band, making it sufficient to have a 2-spinor

$$\Psi_k = \begin{pmatrix} f_k & f_{-k}^{\dagger} \end{pmatrix}^T.$$

Now (3.2) expressed in the BdG-formalism becomes

$$H = \frac{1}{2}\sum_k \Psi_k^{\dagger}H_k\Psi_k$$

where

$$H_k = (-2t\cos(k) - \mu)\tau_z + 2\sin(k)\mathrm{Re}(\Delta)\tau_y - 2\sin(k)\mathrm{Im}(\Delta)\tau_x. \tag{3.3}$$

From (3.3) we see that the energy spectrum is given by

$$E_k = \pm\sqrt{(2t\cos(k) + \mu)^2 + 4\sin^2(k)|\Delta|^2}.$$

This band gap closes when $|2t| = |\mu|$, hinting at the existence of different topological phases in the regions $|2t| < |\mu|$ and $|2t| > |\mu|$ of the parameter space.

If we rewrite our Hamiltonian using (2.10) with $u = -v = e^{i\frac{\phi}{2}}$ we get

$$H = \frac{i}{2}\sum_{j=1}^{N-1}\{(|\Delta| + t)\gamma_{2j}\gamma_{2j+1} + (|\Delta| - t)\gamma_{2j-1}\gamma_{2j+2}\} - \mu\frac{i}{2}\sum_{j=1}^{N}\gamma_{2j-1}\gamma_{2j} + const. \tag{3.4}$$

Setting μ to zero and assuming $|t| = |\Delta| \neq 0$ reduces our Hamiltonian to either the first or the second term in the first sum. If we for example take $t = |\Delta|$ we are left with

$$H = \frac{i}{2}\sum_{j=1}^{N-1} 2t\gamma_{2j}\gamma_{2j+1}. \tag{3.5}$$

This sum lacks both γ_1 and γ_{2N}, meaning that the fermionic state $f_0 = \frac{1}{2}(\gamma_1 + i\gamma_{2N})$ does not contribute to the energy of the system. This is precisely the kind of MF states with zero energy located at the domain walls between two topological phases that we have been talking about. Kitaev, in his seminal paper from 2001 [12], further goes on to show that these really are the same MF states that emerge in the more general case $|2t| > |\mu|,\ |\Delta| \neq 0$ while they are not present in the trivial phase $|2t| < |\mu|,\ |\Delta| \neq 0$.

S-wave systems are generally easier to realize and it is therefore desirable to be able to somehow map an s-wave system to Kitaev's p-wave model, where we know MF states are possible. One of the most common examples of such an s-wave system is a nanowire with strong spin-orbit coupling placed on an s-wave superconductor

$$H = \int_{wire} \mathrm{d}x\psi^\dagger_\sigma(x)(\frac{-\partial_x^2}{2m} - \mu + i\alpha\sigma_y\partial_x + V\sigma_x)_{\sigma\sigma'}\psi_{\sigma'}(x) + \int_{wire}\mathrm{d}x(\Delta\psi_\uparrow(x)\psi_\downarrow(x) + h.c.)$$

where m is the effective mass of the electron, μ is the chemical potential and α is the Rashba coupling. There is also Zeeman splitting due to a magnetic field $V = -g\mu_B B_x/2$ in the x-direction and a superconducting gap Δ. If we assume that only the lower energy band of the non-superconducting part of the Hamiltonian

$$E(k)_\pm = \pm(\xi_k \pm \sqrt{(k\alpha)^2 + V^2})^2, \quad \xi_k = \frac{k^2}{2m} - \mu$$

is occupied, we can project the complete Hamiltonian to the lower band

$$H = \sum_k E(k)_- f^\dagger_-(k)f_-(k) + \{\hat{\Delta}kf^\dagger_-(k)f^\dagger_-(-k) + h.c.\}$$

where $f_-(k)$ is the annihilation operator for the lower band and $\hat{\Delta} = i\alpha\Delta/\sqrt{V^2 + \alpha^2k^2}$ [18, 19]. This has the same form as a continuous p-wave superconductor in k-space, thus showing us that the low-energy limit is isomorphic to Kitaev's model.

3.2 Magnetic chain with s-wave pairing

We will study a system in which magnetic atoms are placed on a superconducting substrate with s-wave pairing. The magnetic moments of the atoms are oriented in such a way that the angle between adjacent moments is constant (see Fig. 3.1). We will also assume that the moments all lie in the x-z plane parallel to the chain.

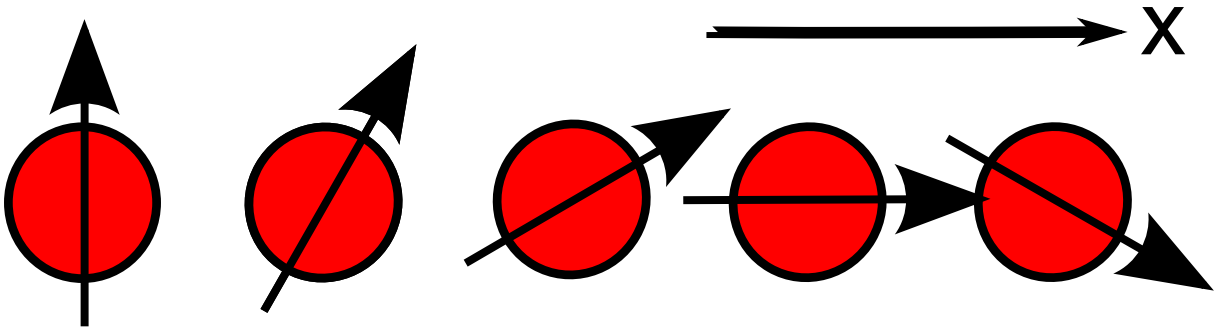


Figure 3.1: *The direction of the magnetic moments in the chain are configured in a helix-like fashion.*

This system is described by the Hamiltonian

$$H = t\sum_{n\sigma}(f^\dagger_{n\sigma}f_{n+1\sigma} + h.c.) - \mu\sum_{n\sigma} f^\dagger_{n\sigma}f_{n\sigma} + \sum_{n\alpha\beta}(\vec{B}_n\cdot\vec{\sigma})_{\alpha\beta}f^\dagger_{n\alpha}f_{n\beta} + \Delta\sum_n(f^\dagger_{n\uparrow}f^\dagger_{n\downarrow} + h.c.) \quad (3.6)$$

where t, μ and Δ are the usual hopping amplitude, chemical potential and superconducting gap respectively and they are all taken to be real. The term $\vec{B}_n\cdot\vec{\sigma}$ describes the local coupling between the magnetic moment of the atom and the electron's spin. As we previously mentioned, the magnetic moments are constrained to the x-z plane. In addition we will assume the magnitude of the moments to be constant: $\vec{B}_n = B_0\{\sin(n\theta)\hat{\boldsymbol{x}} + \cos(n\theta)\hat{\boldsymbol{z}}\}$.

This system can also be shown to be isomorphic to Kitaev's model under some circumstances [20]. We can see this if we rotate our operators alongside $\vec{B}_n$:

$$\begin{pmatrix} f_{n\uparrow} \\ f_{n\downarrow}\end{pmatrix} = U_n\begin{pmatrix} g_{n\uparrow} \\ g_{n\downarrow}\end{pmatrix}, \quad U_n = \begin{pmatrix} \cos(n\theta/2) & -\sin(n\theta/2) \\ \sin(n\theta/2) & \cos(n\theta/2)\end{pmatrix}.$$

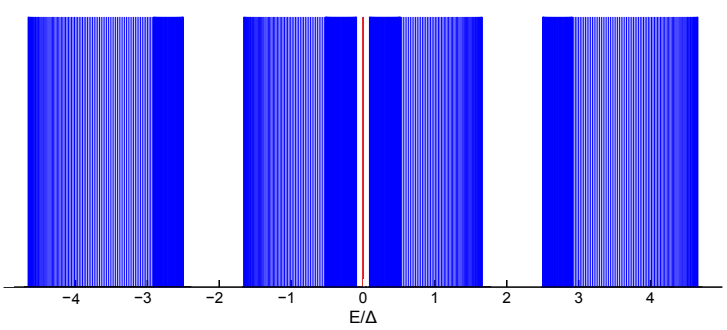
Then our Hamiltonian becomes

$$H = \sum_{n\alpha\beta}(t\Omega_{n\alpha\beta}g^\dagger_{n\alpha}g_{n+1\beta} + h.c.) + \sum_{n\alpha\beta}B_0\sigma_{z\alpha\beta}g^\dagger_{n\alpha}g_{n\beta} - \mu\sum_{n\alpha}g^\dagger_{n\alpha}g_{n\alpha} + \sum_n\Delta(g^\dagger_{n\uparrow}g^\dagger_{n\downarrow} + h.c.) \quad (3.7)$$

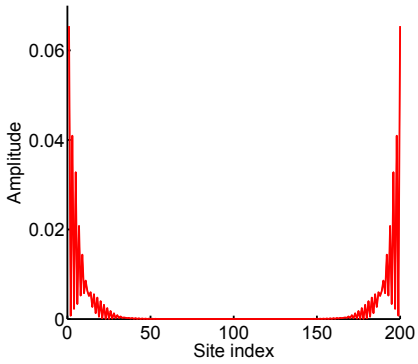
where

$$\Omega_n = U_nU_{n+1} = \cos(\frac{\theta}{2})\mathbb{I}_{2\times2} - i\sin(\frac{\theta}{2})\sigma_y.$$

The diagonal terms in Ω_n give us regular hopping terms, while the off-diagonal terms introduce an effective spin-orbit coupling. We previously argued that the s-wave model with Rashba spin-orbit coupling under some conditions give rise to an effective p-wave symmetry and is therefore



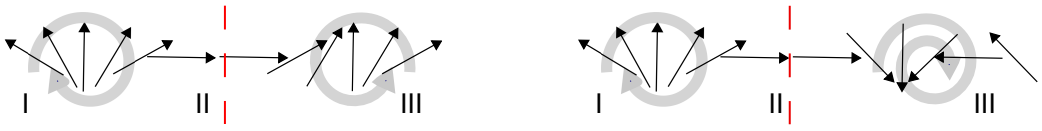
(a)



(b)

Figure 3.2: (a) *The energy spectrum of a spin-helix system with* 200 *atoms and parameters* $t = \mu = \Delta$ *and* $B_0 = 1.5\Delta$. *The angle between adjacent moments is set to* $\theta = \pi/20$. *As we can see, this system supports zero energy states.* (b) *Wavefunctions of MFs at the edges of the same chain as in* (a).

isomorphic to Kitaev's model. Although we then only considered the continuum version, the same arguments can be used to reach the same conclusion in the discrete case. Indeed, a simple numerical computation shows that MF states at the edges of the chain are possible in this system (see Fig. 3.2). We will study the effects of a system where the chirality of the rotation changes in the middle. Thus having one half rotating in one direction while the other rotates in the opposite direction. A pictorial representation of this system can be seen in Fig. 3.3a.



(a) (b)

Figure 3.3: (a) *Illustration of a model with rotation reversal. In region* I *the magnetic moments have clockwise orientation, and in region* III *anti-clockwise. Region* II *denotes the transition point between* I *and* III. (b) *A representation of a model where the angle of rotation increases from region* I *to* III *with the transition happening in region* II.

We will also be looking at the consequences of having the two halves rotating at different rates, while preserving the rotational direction and see how possible MF states are affected by transitions with different levels of smoothness between the phases (see Fig. 3.3b).

4 Results

4.1 Rotation reversal in spin-helix chain

In this section we study the effects of changing the rotational chirality halfway through the chain in the spin-helix model. The Majorana bound state solutions can be derived in the continuum limit. This is done by transforming the Hamiltonian (3.7) to Fourier space, re-expressing it in the BdG form with spinors similar to (2.19) and solving for zero energy modes $H_k|\Psi_M\rangle = 0$ around some k, where the band gap closes. We have

$$H = \frac{1}{2}\sum_k \Psi_k^\dagger H_k \Psi_k$$

where

$$H_k = (2t\cos(\theta/2)\cos(k) - \mu - 2t\sin(\theta/2)\sin(k)\sigma_y)\tau_z + B_0\sigma_z + \Delta\tau_x.$$

The four energy bands, E_k, for our system can then be summarized in the equation

$$\begin{aligned} E_k^2 = B_0^2 + 4\beta^2 t^2\sin^2(k) + (\mu - 2t\alpha\cos(k))^2 + \Delta^2 \\ \pm 2\sqrt{B_0^2\Delta^2 + (\mu - 2\alpha t\cos(k))^2(B_0^2 + 4\beta^2 t^2\sin^2(k))} \end{aligned} \tag{4.1}$$

where $\alpha = \cos(\theta/2)$ and $\beta = \sin(\theta/2)$. We wish to study the situation where $\theta = \theta(x)$ jumps from a positive angle $\theta_0 \in (0, \pi)$ to $-\theta_0$ when we go from $x < 0$ to $x > 0$. We can see from (4.1) that $k = 0$ allows the gap to close. When k is small, it suffices to approximate k-dependent functions up to linear order. By writing the momentum operator in real space $k \to -i\partial_x$ the zero-energy condition $H_k|\Psi_M\rangle = 0$ becomes a differential equation which reads

$$\partial_x|\Psi_M\rangle = \mathbf{A}|\Psi_M\rangle$$

where

$$\mathbf{A} = \frac{1}{\beta}(i\xi_\theta\sigma_y - B_0\tau_z\sigma_x - \Delta\tau_y\sigma_y), \quad \xi_\theta = 2\alpha t - \mu.$$

The general solution to this equation is

$$|\Psi_M\rangle = \frac{1}{\sqrt{N}}\exp(\int_0^x \mathbf{A}(x')\mathrm{d}x')|\phi\rangle$$

where $|\phi\rangle$ is some constant vector and N is a normalization constant. If we consider the case where $\xi_\theta = 0$ one solution can be written as

$$|\Psi_M\rangle = \frac{1}{\sqrt{N}} \exp(-\frac{|x|(\Delta + |B_0|)}{\sin(\theta_0/2)})(|z^+\rangle_\tau |x^-\rangle_\sigma + |z^-\rangle_\tau |x^+\rangle_\sigma) \tag{4.2}$$

from which it is clear that we have a bound zero energy state at the domain wall between the two phases. The field operator corresponding to this state can be obtained by $\gamma = \Psi_M \cdot \Psi_x$ where Ψ_x is the real space spinor corresponding to (2.19):

$$\gamma = \frac{1}{\sqrt{N}} \exp(-\frac{|x|(\Delta + |B_0|)}{\sin(\theta_0/2)})(g_{x\uparrow} - g_{x\downarrow} + g^\dagger_{x\downarrow} - g^\dagger_{x\uparrow}).$$

A U(1) gauge transformation makes this field operator self-adjoint

$$e^{i\frac{\pi}{2}}\gamma \equiv \underline{\gamma} = \underline{\gamma}^\dagger = \frac{i}{\sqrt{N}} \exp(-\frac{|x|(\Delta + |B_0|)}{\sin(\theta_0/2)})(g_{x\uparrow} - g_{x\downarrow} + g^\dagger_{x\downarrow} - g^\dagger_{x\uparrow})$$

and hence $\underline{\gamma}$ is a MF operator. It is important to note that this is not the only solution since MFs always come in pairs. The matrix $\mathbf{A}$ has four eigenvalues with corresponding eigenvectors. Two of these support normalizable bound states.

Theoretically we therefore expect to see two MF states at the domain wall. The numerical solution for a system with 200 atoms and parameters $\Delta = \mu = t = 1, \theta = 3\pi/2$ and $B_0 = 2$, the eigenenergies and -states can be seen in Fig. 4.1. We have four possible zero energy MF states which give us a fourfold groundstate degeneracy. This means that there are two fermion states which can be either occupied or empty without affecting the total energy of the system. The lower graph in Fig. 4.1 shows the existence of MF zero modes precisely where we anticipated them to form.

S. Nadj-Perge *et al.* (2013) [16] showed that the topologically non-trivial phase is present when

$$\sqrt{\Delta^2 + (|\mu| - 2|\cos(\theta/2)t|)^2} < |B_0| < \sqrt{\Delta^2 + (|\mu| + 2|\cos(\theta/2)t|)^2} \tag{4.3}$$

which means that changing θ moves the boundaries for the topological phase. This is most easily seen if we first assume $\mu = 2\cos(\theta/2)t$ making Δ the lower bound. If we now change θ, the lower bound will be pushed forward since $(|\mu| - 2|\cos(\theta/2)t|)^2 > 0$. If B_0 is sufficiently close to the initial lower boundary, the system will go into a trivial phase.

4.2 Varying θ in spin-helix chain

Now we will look at how domain walls where the rate of rotation changes affect the system. From (4.3) we can see that the range for B_0 depends on the angle of rotation θ. For example, if we had an antiferromagnetic material ($\theta = \pi$) the lower bound would equal the higher bound resulting in a trivial phase. Since the absolute value of cosine has a period of π, we expect the

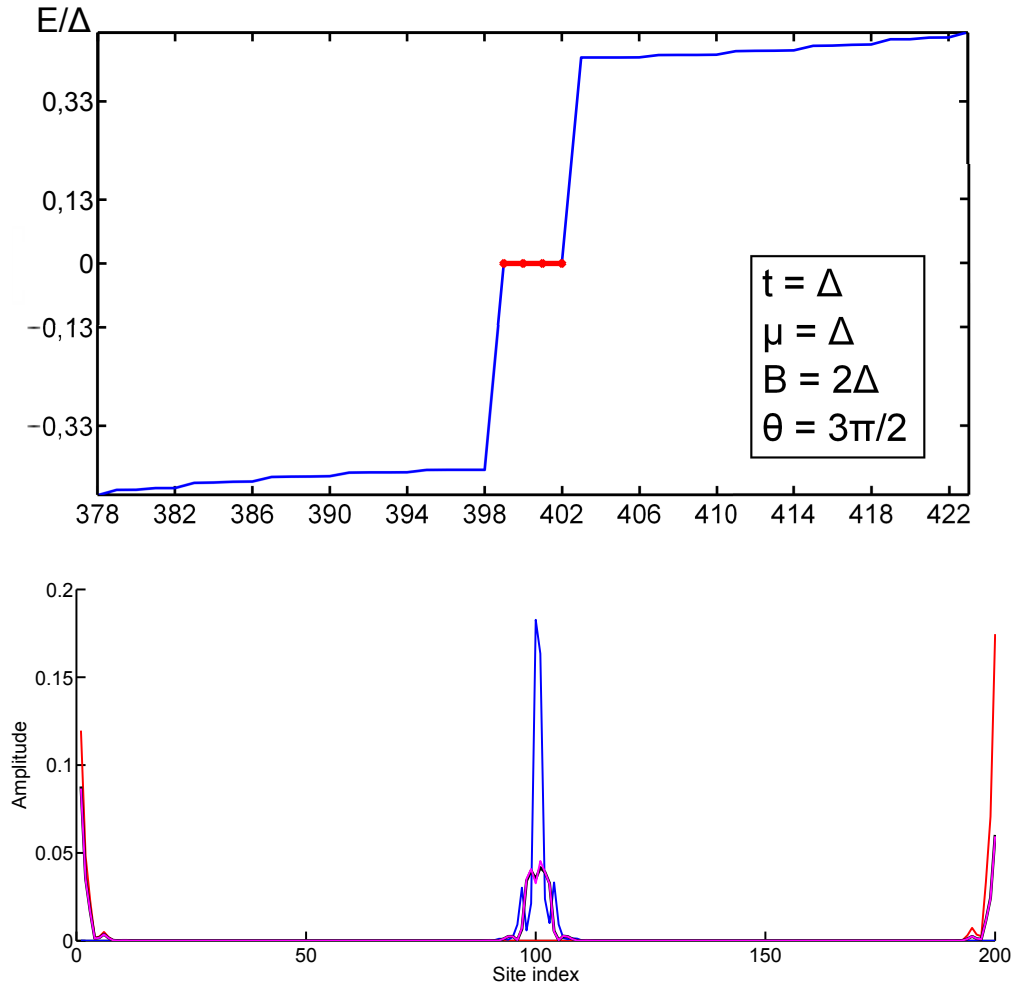


Figure 4.1: (Upper) *A plot of the energy spectrum around E=0, showing the existence of four zero energy eigenvalues (marked in red). The x-axis only numbers the eigenenergies in ascending order.* (Lower) *The four zero energy states from the upper graph. The MF states can be seen to emerge at either the edges of the chain and/or at the domain wall between the two topological phases. Two of the states are nearly identical and align with the magenta line.*

system to remain either trivial or non-trivial if we decrease/increase the rotation by π. However, continuously translating from θ to $\theta + \pi$ requires us to go through a region of parameter space supporting trivial topology. This is perhaps best illustrated in the following way: both sine and cosine have a period of 2π. Physically this means that placing two magnetic moments at an angle is equivalent to placing them at the angle plus some arbitrary amount of full revolutions. Our rotational angle θ is hence defined only mod 2π. Therefore we can restrict θ to be in the interval $(0, \pi)$ and our translated angle to be in $(\pi, 2\pi)$. To go from θ to $\theta + \pi$, we must necessarily cross the anti-ferromagnetic point. This means that the system has to move through a trivial region to smoothly rotate the angle by half a revolution. This transition corresponds to moving to the right in Fig. 4.2. One could think that it is possible to smoothly go between θ and $\theta + \pi$ mod 2π by instead going to the left, but $\theta = 0$ is in fact also trivial since the system turns

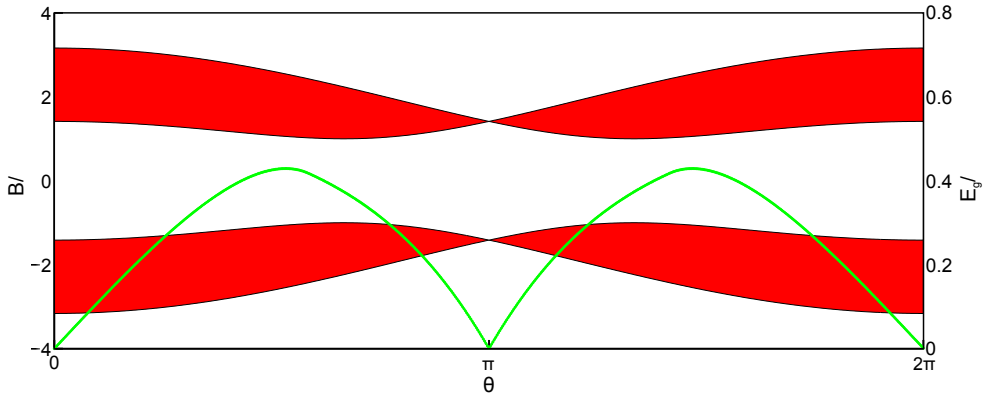


Figure 4.2: *The $B_0 - \theta$ plane in parameter space when $\mu = t = \Delta$. The non-trivial regions are marked in red. Also included in this graph is the smallest energy gap E_g (green line) of all possible values of B_0 that satisfy (4.3) for each θ.*

out to be gapless for all values of B_0 satisfying (4.3). This suggests the existence of a domain wall with bound MFs if the rate of rotation is increased by π. In the case of a system with 200 atoms, $\Delta = \mu = t = 1$, $\theta = 5\pi/17$ and $B_0 = 2$ numerical results seen in Fig. (4.3) tell us that we indeed get zero energy MFs at the domain wall and the edges. The difference in rotation

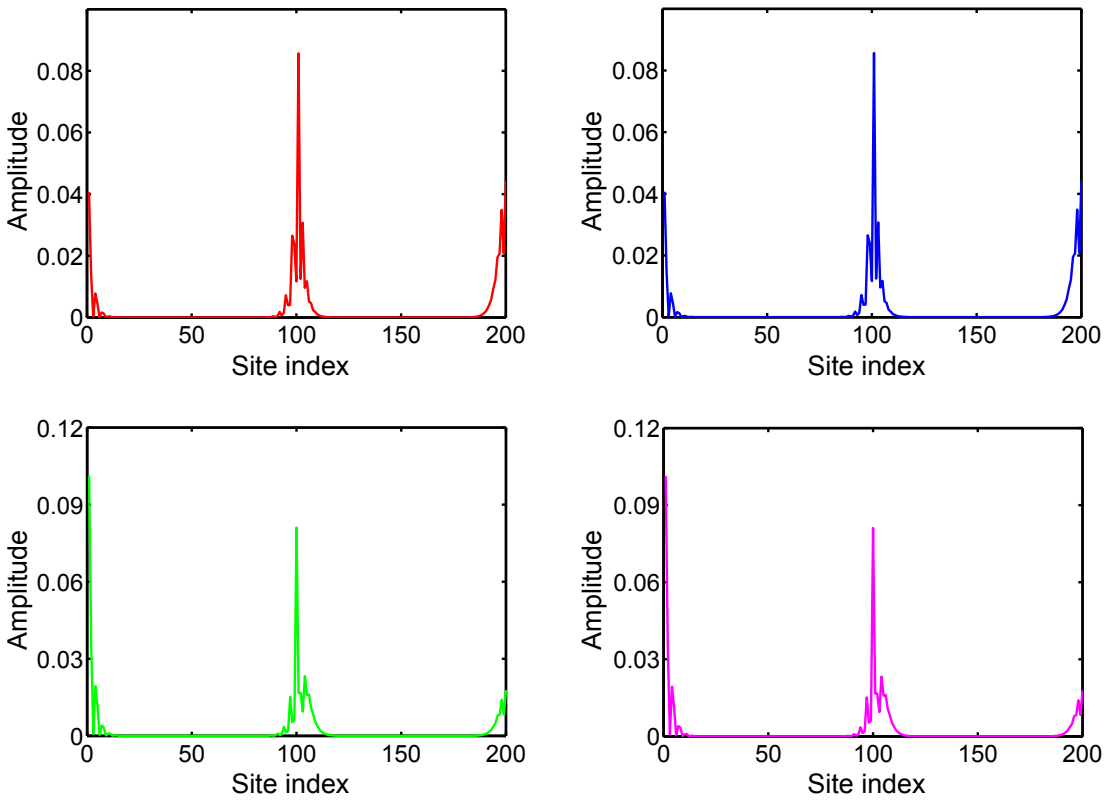


Figure 4.3: *The four zero energy MF states in a system with $N = 200$, $\Delta = \mu = t = 1$, $B_0 = 2$, and $\theta = 5\pi/17$ for site indices ≤ 100 and $\theta = 22\pi/17$ for the rest.*

on both sides introduces a spatial asymmetry that manifests itself in the MF states by giving

the central peaks a tail going to the side of greater rotation and - compared to the rotational reversal scenario - to some extent making the right edge states less prominent than the left. The special case $\theta = \pi/2$, gives us symmetric MF states superficially similar to the lower graph in Fig. 4.1. This is because increasing $\pi/2$ by π is a full revolution away from reversing the sign to $-\pi/2$. Generally, if we increase the angle of rotation by $2(\pi - \theta)$ it is the same as reversing the sign of θ. We can thus see that the act of reversing and the act of translating are in some special cases equivalent.

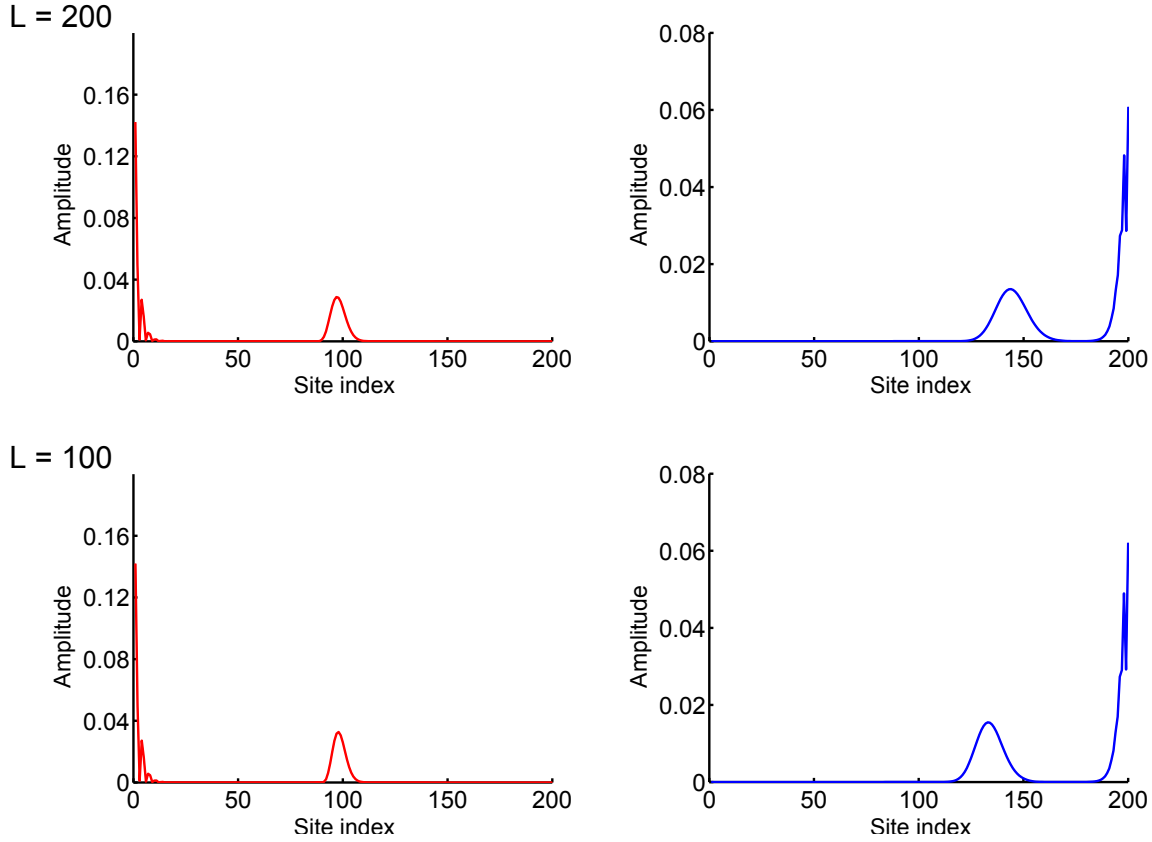


Figure 4.4: (Upper) *MF zero modes of a system with* $N = 200$ *atoms,* $\Delta = \mu = t = 1$, $B_0 = 2$ *and a transition zone with length* $L = 200$. (Lower) *Same system with* $L = 100$ *instead. The transition is done with a function of the form* $\beta \tanh(\alpha x) + \gamma$ *fitted to go through the points* $(0, (\theta_1 + \theta_2)/2)$ *and* $((N + L)/2, (1 - 10^{-6})\theta_2)$ *in the* (x, θ) *coordinate system. In both the upper and the lower figures there are really four MF states, but they are too similar to the two states shown to add anything new.*

If we let θ vary smoothly from the first to the second value in a transition zone of a given length, the central peaks of the MF states are drawn to one side of the chain or another. However, they never disappear even as the transition zone is taken to be the whole chain. The central peaks almost never get close enough to the edges to significantly overlap with the edge modes. The length of our chain may go down to as little as 30 atoms and still exhibit MF zero modes with the same system parameters as before and $\theta : \pi/2 \to 3\pi/2$. For other angles the sensitivity

can be somewhat greater. For example $\theta : 5\pi/17 \to 22\pi/17$ needs a chain length of the order of one hundred atoms to accommodate zero modes when the transition happens over the whole chain. In Fig. 4.4 we see the similarities between having a transition zone of 100 versus 200 atoms on a chain of 200. The central peaks are slowly moving towards the edges but generally will not come close enough to combine into finite energy fermionic states. This can also be further compared to Fig. 4.3 where the transition zone has zero length.

5 Conclusions

In this thesis we studied MFs in a magnetic chain. We saw that this system is isomorphic to the Kitaev model in the low energy limit and hence was expected to support MFs. We then focused on mainly two different features of this system, where we in the first case had the magnetic moments rotating in one direction in one half and the opposite direction in the second to create a phase boundary supporting two Majorana states. The existence of zero energy bound states was then shown analytically in the continuum limit. Numerically we confirmed that MF states form at the domain walls between topological phases in this system.

Our second model was one in which we instead of reversing the chirality of rotation increased the rate of rotation in the second half of the chain. We argued why an increase of π to the rate necessarily caused the two halves of the system to have a domain wall with bound MF states if the first half was topologically non-trivial. We also saw that the second model had some special cases that were identical to the first model because of the periodicity of the angle of rotation. Contrary to the first model, however, the second had a spatial asymmetry that often forced the MF states at the boundary to move to one side or the other with a more noticeable effect on the states offset to the side with greater rotation. This asymmetry got more prominent with the introduction of a transition zone, where the angle of rotation varied smoothly from the first angle to the next using an s-curve. In sufficiently long systems the central MF states generally never had enough overlap with the edge states to form finite energy fermions. It should be noted that this type of domain wall is one of many. Other kinds of domain walls would possibly have different effects - especially if they were asymmetric in some way - but these were not considered in this thesis.

We chose to study the spin-helix chain as it is a fairly simple system to theoretically analyze while still holding promise to be able to be experimentally realized. The ultimate goal is to be able to not only prove the existence of these MF quasiparticles in nature, but also to be able to manipulate them. In addition to potentially being the first ever observed non-Abelian anyons, these discoveries could provide a long-sought breakthrough in the field of quantum computing providing robust qubits topologically protected from decoherence.

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