Bachelor's thesis

Theoretical Physics

Topological properties of superconducting chains

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Abstract

In this thesis, we study the topological properties of two systems consisting of one-dimensional s-wave superconducting chains, with specific focus on the impact of hopping terms. We derive the energy eigenvalues and topological symmetry class of the dimerized superconducting chain, on the basis that both the simple dimerized SSH model as well as the spinless Kitaev model of superconductivity display topologically interesting properties. Furthermore, we examine the properties of the magnetic helix chain, a system previously proved to be topologically non-trivial, under application of periodic boundary conditions and some variations thereof. The case of the dimerized chain is solved using analytical methods based on quantum many-body theory, particularly BdG formalism and the periodic table of topological insulators. As the infinite magnetic helix chain has already been solved analytically, the research in this thesis will concentrate on finite system PBC solutions which are obtained using numerical methods.

We find that the dimerized chain does not support topologically non-trivial phases. However, the result allows us to make a more general statement regarding potentially topologically interesting systems. In particular, our conclusions are that systems including magnetic field terms are promising candidates for future research. We also find that, as expected, adding periodic boundary conditions to the magnetic helix chain annihilates the pre-existing topological edge modes. Furthermore, connecting two PBC magnetic helix systems by having them share one lattice point creates a topological zero mode at the intersection of the two PBC loops.

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1. Introduction

Materials with new and unusual properties have always been of great interest to physicists. During the last few decades, interest in so-called "topological materials" has been growing rapidly. Topology is the mathematical study of shapes, mainly the aspects of these that remain invariant under continuous transformations (topological invariants). Two shapes are regarded as topologically equivalent if one can be obtained from the other by continuous transformation. This is not a purely mathematical curiosity, and its effects in nature are remarkable. For example, electrical insulators with a non-trivial momentum space topology can have conducting edge states. In addition, the topological properties of materials are robust to perturbations that cannot change the topology of the material. [1]

The effects of topology on the properties of solids have been a subject of research at least since the integer quantum Hall effect (IQHE) was discovered in the 1980s. The IQHE proved the traditional approach of broken symmetry due to Landau inadequate, and in a famous article published in 1982 Thouless *et al.* showed [2] that the system is characterized by topological invariants known as TKNN invariants and later identified as Chern numbers. However, most of the research in the topological aspects of solid state physics has been conducted in the past decade. In 2005, Kane and Mele [3] introduced the concept of topological insulators and the quantum spin Hall (QSH) effect. The term "topological insulator" was coined by Moore and Balents in 2006 [4]. The same year, Bernevig *et al.* [5] proposed that the QSH could occur in HgTe/CdTe semiconductor quantum wells. This was experimentally verified in 2007 [6], making topological insulators one of the few exotic systems predicted theoretically before being discovered in experiment.

Topological insulators are materials which have an energy gap in the bulk, so that a finite energy is required to excite electrons to the conduction band. However, according to definition, two insulators in different topological classes cannot be continuously (adiabatically) deformed to each other without closing the gap [7,8]. Hence, the surface of a 3D TI or the edge of a 2D one is effectively metallic. Being a topological property, this surface effect is robust to perturbations that do not change the fundamental topology of the system. The surface states may also display

some other unusual characteristics, depending on the specifics of the topology. Whereas the original IQHE breaks time-reversal symmetry, in the newly discovered QSHE topological insulators TR remains unbroken [8,9], and from this distinction it follows that the topological edge modes are different in nature. The IQHE edge states are chiral, with the electrons able to move in one direction only [7]. In contrast, the QSHE edge states are helical: they consist of a superposition of chiral and anti-chiral states of opposite spin [3,7] (see figure 1).

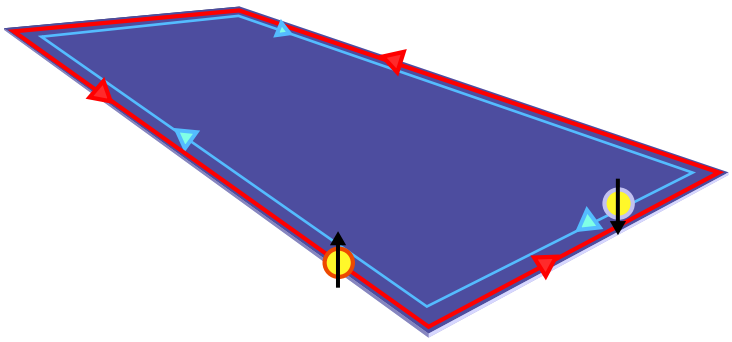

FIGURE 1: *Spin-momentum locking in a 2D TI. The electrons are to be understood as moving along the edge of the insulator.*

The theory developed for TIs has also been generalized to topological superconductors and superfluids, where the mean-field order parameter provides an energy gap. Therefore, the topological properties can be studied analogously to TIs. Topological superconductors, in particular, have been subject to ample research in the past five years. Their particle-hole symmetry allows topologically robust quasiparticle excitations called Majorana fermions. These are composed of a superposition of electrons and holes, and are their own antiparticles; their robustness is mainly due to a delocalization that makes them resistant to local perturbations, which could prove useful in quantum computing [10,11].

In this thesis we study the topological properties of one-dimensional superconducting chains. In particular, we will be looking for systems in which the energy gap closes, as this would indicate the presence of two separate topological phases. The relevance of this thesis is apparent through the increasing number of experiments on similar systems suggested and conducted within recent years [12,13,14]. These systems have been envisioned as promising platforms in quantum information applications.

2. Methods

2.1 Basics of quantum many-body theory

Calculations in many-particle physics are carried out in the Fock space, using the occupation number representation or *second quantization*. The basic principle is as follows. Assuming $\{|s_1\rangle, |s_2\rangle, |s_3\rangle ...\}$, where s is some relevant quantum number, constitute a complete single-particle basis, a many-particle state can be defined simply by listing the occupation number of each state in the basis. If the total number of particles is N, then

$$\psi = |n_{s_1}, n_{s_2}, ns_3, ...\rangle \qquad \sum_i n_{s_i} = N$$

where the ordering of the states is important. The Fock space is then the space spanned by the occupation number basis. For example, the vacuum state is $|0, 0, 0, 0, ...\rangle$, which indicates that none of the states are occupied. The important operators in this formalism are the so-called creation and annihilation operators $a^\dagger_{s_i}$ and a_{s_i}. Their effect is simply to increase or decrease the particle number of state s_i by one. For example,

$$a^\dagger_{s_1} a^\dagger_{s_3} |0, 0, 0, ...\rangle = c|1, 0, 1, 0, 0...\rangle$$

where c is a normalization constant (for fermions $c = 1$). The creation and annihilation operators for bosons satisfy

$$[b^\dagger_{s_i}, b^\dagger_{s_j}] = 0 = [b_i, b_j], \qquad [b_{s_i}, b^\dagger_{s_j}] = \delta_{ij}$$

where $[a, b] = ab - ba$, whereas for fermions,

$$\{c^\dagger_{s_i}, c^\dagger_{s_j}\} = 0 = \{c_{s_i}, c_{s_j}\} \qquad \{c_{s_i}, c^\dagger_{s_j}\} = \delta_{ij}$$

where $\{a, b\} = ab + ba$. In this thesis, we will exclusively consider systems of fermions. In particular, notice that for fermionic operators,

$$c_{s_i} c^\dagger_{s_j} = -c^\dagger_{s_j} c_{s_i} \qquad c_{s_i} c^\dagger_{s_i} = -c^\dagger_{s_i} c_{s_i} + 1 \tag{2.1}$$

Another relevant property which is an immediate effect of the above commutation rules is that fermions obey the Pauli exclusion principle; a creation operator acting on an occupied state will return 0, as will an annihilation operator acting on the vacuum.

The ground state for N fermions at zero temperature is called the *Fermi sea*

$$|FS\rangle \equiv c^\dagger_{k_{N/2}\uparrow} c^\dagger_{k_{N/2}\downarrow} \dots c^\dagger_{k_2\uparrow} c^\dagger_{k_2\downarrow} c^\dagger_{k_1\uparrow} c^\dagger_{k_1\downarrow} |0,0,0,....\rangle$$

where all possible states for the fermions is filled from lowest energy up to the Fermi energy ϵ_F. Because ϵ_F generally corresponds to temperatures of the order of $10^5\,K$, the Fermi sea remains an accurate approximation of the ground state of fermions at low temperatures. The Fermi sea is formed as a direct consequence of the Pauli exclusion principle. Contrast with bosons, which at low temperatures form a Bose-Einstein condensate where all particles are in the state with the lowest energy.

While it is immediately evident that the creation and annihilation operators are not Hermitian, one notices that $a^\dagger_{s_i} a_{s_i}$ is a Hermitian operator. This combination acts as the particle number operator; operating on a many-body state, it returns the same state multiplied by the number of particles in the single-particle state s_i. In fact, any operator in many-particle physics can be expressed as a combination of creation and annihilation operators multiplied by some function,

$$U = \sum_{s_i, s_j} U_{s_i s_j} a^\dagger_{s_i} a_{s_j}, \qquad V = \sum_{s_i, s_j, s_k, s_l} V_{s_i s_j s_k s_l} a^\dagger_{s_i} a^\dagger_{s_j} a_{s_k} a_{s_l}$$

for single-particle and two-particle operators, respectively. Despite the fact that the creation and annihilation operators are not Hermitian, a given many-body Hamiltonian will only contain them in combinations that are.

2.2 Discrete Fourier transforms

In this text we will be considering one-dimensional chains of atoms, which are effectively 1D lattices; hence, operators will fulfil the normal periodic boundary conditions. Because of this, they can be written as a Fourier series

$$A_n = \frac{1}{\sqrt{N}} \sum_k e^{i a_0 n k} A_k \tag{2.2}$$

where a_0 is the lattice constant, and the sum goes over all k. It is important to notice here that n is the site position of the operator. We can normalize $a_0 \equiv 1$ with no loss of generality, and will do so henceforth. Because the electrons are confined on a lattice with periodic boundary conditions, the FT will be discrete in both directions:

$$A_k = \frac{1}{\sqrt{N}} \sum_n e^{-ink} A_n$$

Where the sum goes over all n in the lattice. A property of the sums that will be useful later is

$$\frac{1}{N} \sum_k e^{ink} = \delta_{n0}, \qquad \frac{1}{N} \sum_n e^{-ink} = \delta_{k0} \tag{2.3}$$

which is used to FT products of operators:

$$\sum_n a_n^\dagger b_n = \frac{1}{N}\sum_{nkk'} e^{in(k-k')} a_k^\dagger a_{k'} = \frac{1}{N}\sum_{kk'} a_k^\dagger a_{k'} \sum_n e^{in(k-k')} = \sum_{kk'} a_k^\dagger a_{k'} \delta_{kk'} = \sum_k a_k^\dagger a_k$$

2.3 BCS theory of superconductivity

In the BCS (Bardeen-Cooper-Schrieffer) theory, superconductivity is a natural consequence of any weakly attractive interaction between electrons in a solid at low temperatures. In conventional superconductors, this effect is caused by electrons interacting with each other indirectly through positive phonon trails. If two electrons are in time-reversed states, this interaction lowers their energy below the Fermi level and they enter a loosely bound pair state.

The BCS Hamiltonian describing this superconducting system is

$$H_{BCS} = \sum_{k\alpha} \xi_k c_{k\alpha}^\dagger c_{k\alpha} + \sum_{k,k'} V_{kk'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}$$

where α represents spin. In order to simplify this, we make the assumption that the values of the operators only deviate a little from their average values. This allows the use of a Hartree-Fock mean field approximation to convert the interaction term into a non-interacting one. The resultant mean-field BCS Hamiltonian is

$$H_{MF} = \sum_{k\alpha} \xi_k c_{k\alpha}^\dagger c_{k\alpha} + \sum_k (\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta_k^* c_{-k\downarrow} c_{k\uparrow})$$

where $\Delta_k = \sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$. For systems without spin, the Hamiltonian will take on a different appearance. That is the case in the Kitaev model treated in the next section.

2.4 The Bogoliubov-de-Gennes (BdG) formalism

Assuming the system being considered is a mean-field BCS superconductor, the problem can often be simplified by defining the vector

$$\Psi_k \equiv \begin{pmatrix} a_{k\uparrow} & a_{k\downarrow} & a_{-k\downarrow}^\dagger & -a_{k\uparrow}^\dagger \end{pmatrix}^T$$

This can be used to express sums over the creation and annihilation operators as vector products. Using the FT formula for operators and then applying the vector defined above, one can express the original Hamiltonian as

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

where H_{BdG} is a 4×4 matrix. This formalism contains a redundancy, as the BdG Hamiltonian appears to have twice as many bands as the original Hamiltonian. This will have the effect of

doubling the number of eigenstates and eigenvalues, but the number of independent solutions will remain constant. Since it is still an equivalent formulation of the Hamiltonian, if the eigenvalues of H_{BdG} can be found then the eigenvalues of H follow from those. In this thesis we will use the notation H_k for the BdG matrix to emphasize its dependence on k.

When writing down the Hamiltonians in the BdG formalism, H_k can be expressed as a sum of tensor products of 2×2 matrices, namely the Pauli matrices σ_i and the 2×2 identity matrix.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad I_{2\times 2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.4}$$

Unless otherwise stated, we will use the notation

$$\tau_i\sigma_i \equiv \tau_i \otimes \sigma_i \qquad \tau_i \equiv \tau_i \otimes I_{2\times 2} \qquad \sigma_i \equiv I_{2\times 2} \otimes \sigma_i$$

so that, for example, if A, B and C are complex numbers,

$$A\sigma_x + B\tau_z\sigma_z + C = AI_{2\times 2} \otimes \sigma_x + B\tau_z \otimes \sigma_z + CI_{2\times 2} \otimes I_{2\times 2}$$

Note that if the number of bands in the original Hamiltonian is N, then H_k will be a $2N \times 2N$ matrix.

The general method of solving the models analytically will be Fourier transforming the Hamiltonian, converting it to BdG form and then finding its eigenvalues. To simplify the eigenvalue calculations, we utilize some properties of the Pauli matrices and the Kronecker product:

$$\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij} \qquad \sigma_i^2 = I_{2\times 2} \qquad [\tau_i, \sigma_j] = 0$$

Using these one can square the Hamiltonian to attempt to find the square of the eigenvalues.

2.5 Topological classification of 1D single-particle Hamiltonians

Topological effects in materials are in general connected to breaking or preserving generic discrete symmetries. Knowing this, it is possible to classify Hamiltonians by their symmetries, and to determine whether they support could non-trivial topological phases. The periodic table of topological insulators introduced by Schnyder *et al.* [15] classifies both insulators and superconductors by three discrete symmetries: time-reversal symmetry, particle-hole symmetry and sublattice symmetry (TRS, PHS and SLS respectively). For a Hamiltonian to preserve one of the given symmetries, it has to fulfil the following conditions

$$\begin{aligned} TRS: &\quad C_T H^T C_T^{-1} = H, \qquad C_T C_T^\dagger = 1 \qquad C_T^T = \pm C_T \\ PHS: &\quad C_P H^T C_P^{-1} = -H, \qquad C_P C_P^\dagger = 1 \qquad C_P^T = \pm C_P \\ SLS: &\quad C_S H C_S^{-1} = -H, \qquad C_S C_S^\dagger = 1 \qquad C_S^2 = 1 \end{aligned}$$

where C_i are unitary matrices of the same dimension as the Hamiltonian. Note that as a consequence of these, a Hamiltonian satisfying two symmetries will automatically satisfy all three.

Table 1: Classification of one-dimensional single-particle Hamiltonians based on their symmetries. The sign of ± 1 depends on the square of the operator implementing the symmetry. In the topological sectors column, $\mathbb{Z}$ indicates that the space of possible quantum ground states of the system can be divided into topological sectors labelled by an integer, whereas $\mathbb{Z}_2$ indicates division into two separate topological sectors.

	Class	TRS	PHS	SLS	Topological sectors
Standard	A (unitary)	0	0	0	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-
	AII (symplectic)	–1	0	0	-
Chiral	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$
(sublattice)	BDI (chiral orthogonal)	+1	+1	1	$\mathbb{Z}$
	CII (chiral symplectic)	–1	–1	1	$\mathbb{Z}$
					-
BdG	D	0	+1	0	$\mathbb{Z}_2$
	C	0	–1	0	-
	DIII	–1	+1	1	$\mathbb{Z}_2$
	CI	+1	–1	1	-

From table 1, it is evident that there are five different symmetry classes that can give rise to topological effects in non-interacting one-dimensional systems. If the system being considered displays topological effects, it will generally be characterized by a $\mathbb{Z}_2$ or $\mathbb{Z}$-valued invariant. As a consequence, the system supports zero modes localized at the interface between two topological phases, or alternately between a non-trivial phase and the vacuum.

3. Models

3.1 Su-Schrieffer-Heeger model

Historically one of the first models exhibiting interesting topological properties, the SSH model is a basic model of a non-superconducting chain of atoms [16]. It describes a dimerized system where the strength of the hopping amplitude alternates from site to site, as seen in figure 2 below. The model was originally developed to describe the behaviour of electrons in conjugated polymers, where the alternating single and double bonds give rise to a modulated hopping amplitude[17].

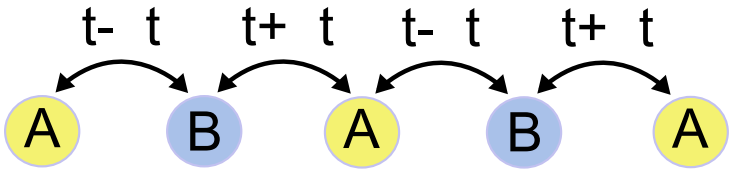

Figure 2: *Schematic picture of dimerized hopping, relevant to the SSH system*

A simplified SSH Hamiltonian for a system without spin can be written as

$$H = \sum_n \Big[(t-\delta t)(a_n^\dagger b_n + b_n^\dagger a_n) + (t+\delta t)(b_n^\dagger a_{n+1} + a_{n+1}^\dagger b_n)\Big] - \mu \sum_n (a_n^\dagger a_n + b_n^\dagger b_n) \tag{3.1}$$

where t is the hopping amplitude, δt is its modulation due to dimerization, and μ is the chemical potential. The Hamiltonian describes a lattice with two atoms in the unit cell, and the operators a and b are to be understood as fermion operators corresponding each to one of the atoms.

Due to dimerization the Fourier transform for the b operators can be written as

$$b_n = \frac{1}{\sqrt{N}} \sum_n e^{ia_0 k(n+\frac{1}{2})} \ .$$

Note the shifted exponent compared to the standard transform in Eqn. (2.2). As we will be normalizing a_0 this only has the effect that any terms containing both a and b operators will gain an extra e^{ik} in the Fourier transform. Performing the sum over n as in Eqn. (2.3), and defining the vector

$$\Psi_k = (a_k \quad b_k)^T$$

we get

$$H = \sum_k \Psi_k^\dagger H_k \Psi_k$$

$$H_k \equiv 2t\cos(k)\sigma_x + 2\delta t \sin(k)\sigma_y - \mu I_{2\times 2}$$

where all terms are 2×2 matrices. Since there is no superconductivity, the BdG redundancy is not present in this case. The energy bands are given by

$$E = -\mu \pm 2\sqrt{t^2\cos^2(k) + \delta t^2 \sin^2(k)}$$

If we assume the system has half-filled energy bands, the μ term can be dropped. The resultant Hamiltonian is

$$2t\cos(k)\sigma_x + 2\delta t \sin(k)\sigma_y$$

which satisfies both TRS and PHS and hence also SLS. The system is thus part of the BDI symmetry group, but has only two topological phases due to the low number of parameters involved. The two phases are $\delta t > 0$ and $\delta t < 0$, and it is evident that δt cannot attain both values in a system without the energy gap closing. The zero modes emerging from the interface are possible to calculate explicitly by making a continuum approximation. Assuming the dimerization is allowed to vary so that δt is negative at $-\infty$ and positive at $+\infty$, we get zero modes of the form

$$|\Psi\rangle = Ae^{-\frac{1}{at}\int_0^x \delta t dx}|\uparrow\rangle$$

where A is a constant in x. This does not depend on the precise form of $\delta t(x)$, as it is a topological effect. The wavefunction is sharply peaked around the topological domain wall, which in turn can move around as a topological soliton [17].

3.2 The Kitaev model of a 1D p-wave superconductor

Since the models treated in this thesis will be of superconducting systems, it is prudent to introduce the basics through the Kitaev model [18], which is a simple example of a one-dimensional superconducting system with interesting topological characteristics. Historically, this was the first example of a one-dimensional model displaying topological superconductivity. The Hamiltonian of the Kitaev model is

$$H = \sum_n t(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n) - \mu \sum_n a_n^\dagger a_n + \Delta_0 \sum_n (a_n^\dagger a_{n+1}^\dagger + a_{n+1} a_n)$$

where t is the hopping amplitude, μ is the chemical potential and Δ_0 is the superconducting gap, which we have here assumed to be real. The superconducting term creates Cooper pairs in

adjacent lattice points. Note the absence of spin in this system. Because of the superconducting term in the Hamiltonian, it is convenient to work in Nambu space

$$\Psi_k \equiv \begin{pmatrix} a_k & a_{-k}^\dagger \end{pmatrix}^T$$

in order to express the Hamiltonian in the BdG form:

$$\begin{aligned} H &= \frac{1}{2}\sum_k \Psi_k^\dagger H_k \Psi_k \\ H_k &\equiv (2t\cos(k) - \mu)\sigma_z - 2\Delta_0 \sin(k)\sigma_y \end{aligned} \tag{3.2}$$

where, again, σ_i are simply the 2×2 Pauli matrices due to the absence of spin. Constants created through anticommutation have been suppressed as they have no effect on the behaviour of the system. The eigenvalues are now

$$E = \pm\sqrt{(2t\cos(k) - \mu)^2 + 4\Delta_0^2 \sin^2(k)} \tag{3.3}$$

It is clear that the for the energy gap to close, both terms inside the square root must vanish. The term proportional to $\sin(k)$ does so for $k = 0$. The border between two topological phases is thus at $|2t| = |\mu|$, with lower t being the case of non-trivial topology. At the interface between two topological phases, the Kitaev model displays zero modes called Majorana fermions, which can be derived in the same way as the zero modes for the SSH model.

3.3 Dimerized s-wave superconducting chain

As the SSH and Kitaev models both exhibit topological properties, we are motivated to examine a more realistic model which incorporates both dimerization, superconductivity and spin. The system we will examine is an s-wave superconductor, with the Cooper pairs being created at each site with opposite spin. The system is of some interest as it may be possible to construct with current technology by using a sweep-tunnel microscope. The required modulation of the hopping amplitude should be possible to realize by individually placing the atoms in the lattice. The Hamiltonian for this model is

$$\begin{aligned} H =& \sum_{n,\alpha}(t-\delta t)a_{n\alpha}^\dagger b_{n\alpha} + (t+\delta t)b_n^\dagger a_{n+1,\alpha} + h.c. - \mu\sum_{n,\alpha} a_{n\alpha}^\dagger a_{n\alpha} + b_{n\alpha}^\dagger b_{n\alpha} \\ &+\Delta_0 \sum_n a_{n\uparrow}^\dagger a_{n\downarrow}^\dagger + b_{n\uparrow}^\dagger b_{n\downarrow}^\dagger + h.c. \end{aligned} \tag{3.4}$$

where h.c. stands for the Hermitian conjugate. Note that the Hamiltonian incorporates dimerization, superconductivity and spin. Because of this, H_k will be an 8×8 matrix, the full BdG formalism with an added doubling due to the dimerization. Define

$$\Psi_k \equiv \begin{pmatrix} a_{k\uparrow} & a_{k\downarrow} & b_{k\uparrow} & b_{k\downarrow} & a_{-k\downarrow}^\dagger & -a_{-k\uparrow}^\dagger & b_{-k\downarrow}^\dagger & -b_{-k\uparrow}^\dagger \end{pmatrix}^T$$

To express the 8×8 Hamiltonian matrix in terms of Kronecker products of Pauli matrices, we will introduce three sets of matrices, τ_i, σ_i, s_i in order. Hence, terms will be of the type $\tau_i \otimes \sigma_i \otimes s_i$. Using these, the Hamiltonian can be written

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

$$H_k = 2t\cos(k)\tau_z\sigma_x + 2\delta t\sin(k)\tau_z\sigma_y - \mu\tau_z + \Delta_0\tau_x \tag{3.5}$$

Notice that H_k does not contain s_i matrices. The eigenvalues are

$$E^2 = \left(\mu \pm \sqrt{t^2\cos^2(k) + \delta t^2\sin^2(k)}\right)^2 + \Delta_0^2$$

We see that this system will always be gapped as long as $\Delta_0 \neq 0$. The dimerized s-wave superconductor is, in its basic form, a topologically trivial material. The Hamiltonian satisfies all three symmetries introduced in section 2.5 and is of symmetry class CI. As seen in table 1, CI-class systems in one dimension do not support non-trivial topological phases.

3.4 Magnetic helix chain with periodic boundary hopping

It may also be possible to alter the topology of a system by changing hopping amplitudes other than the standard next-nearest neighbour hopping. To test this, we examine a magnetic helix chain model. This model was examined first as a random-moment model by T.-P Choy *et al.* [19] and later studied in a helix chain by S. Nadj-Perge *et al.* [20]. The model we will be studying is a one-dimensional chain where the magnetic moment of the lattice atoms rotates, with the change in angle between each lattice site constant.

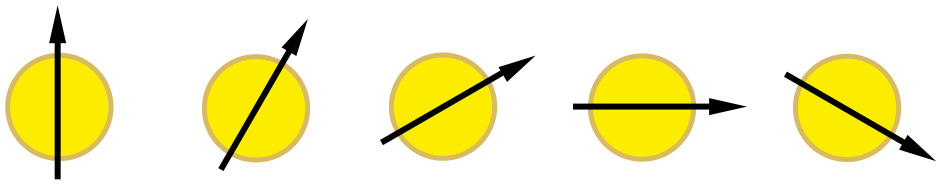

FIGURE 3: *The magnetic helix chain. The arrows represent the direction of the magnetic moment.*

The Hamiltonian of the model is

$$\sum_{n\alpha} t_n c_{n\alpha}^\dagger c_{n+1\alpha} + h.c. - \mu\sum_{n\alpha} c_{n\alpha}^\dagger c_{n\alpha} + \sum_{n\alpha\beta}(\vec{B}_n\cdot\vec{\sigma})_{\alpha\beta}c_{n\alpha}^\dagger c_{n\beta} + \sum_n \Delta_0 c_{n\uparrow}^\dagger c_{n\downarrow}^\dagger + h.c.$$

For the system to enter the non-trivial topological phase, B must be confined by

$$\sqrt{\Delta_0^2 + (|\mu| + 2|\cos(\frac{\theta}{2})t|)^2} > |B_0| > \sqrt{\Delta_0^2 + (|\mu| - 2|\cos(\frac{\theta}{2})t|)^2} \tag{3.6}$$

as shown in [20]. We will now study a case where the Hamiltonian gains an extra term

$$\sum_{\alpha} r c_{1\alpha}^{\dagger} c_{N\alpha} + r c_{N\alpha}^{\dagger} c_{1\alpha}$$

which corresponds to periodic boundary conditions in a circular chain, as seen in fig. 4. The hopping amplitude between the ends of the chain is r. Initially, the system will be in its topological phase with $r = 0$. This should be evident from the zero modes emerging at the edges of the chain. In the non-trivial case, the magnetic helix chain displays Majorana fermions at the edges of the chain, similarly to the Kitaev model. In the next section we will study the evolution of the system on increasing r gradually from 0 to t. The central focus is the existence of zero modes and the shape of the edge wavefunctions. This will be done numerically. The expectation is that the zero modes will vanish, as in the PBC case there are essentially no edges for topological effects to emerge on.

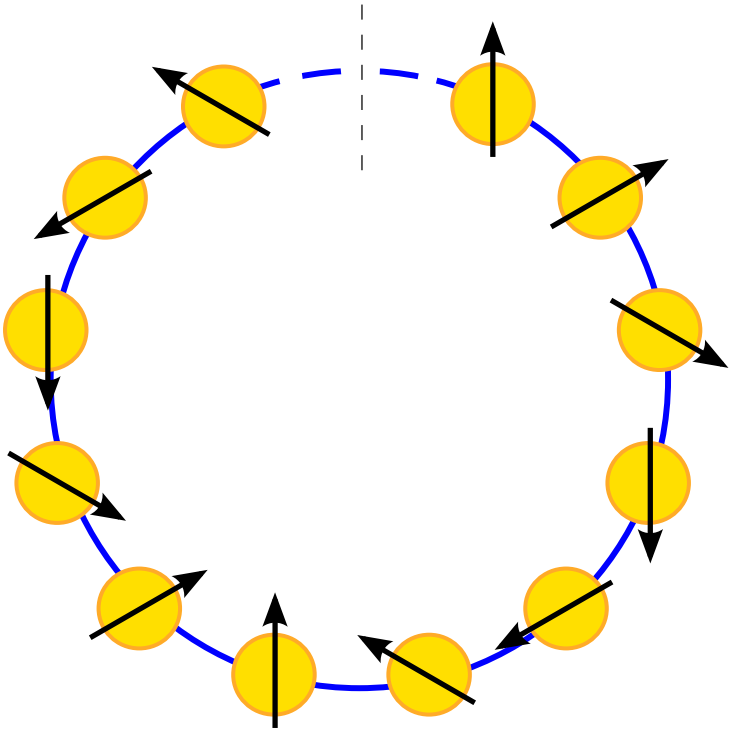

FIGURE 4: *PBC for the magnetic helix chain, pictorial representation. The amplitude of the hopping represented by the dashed line will be modulated in the simulation as explained in the text. Amplitude 0 is equivalent to a non-circular open chain, wheras amplitude t corresponds to a closed circle.*

Should the PBC case prove interesting from a topological point of view, we will also examine cases where the system includes two closed loops that can be joined together. While the topology relevant to condensed-matter physics is usually that of momentum space, in real space, shapes with different numbers of holes are topologically distinct, and so the case may be worth investigating.

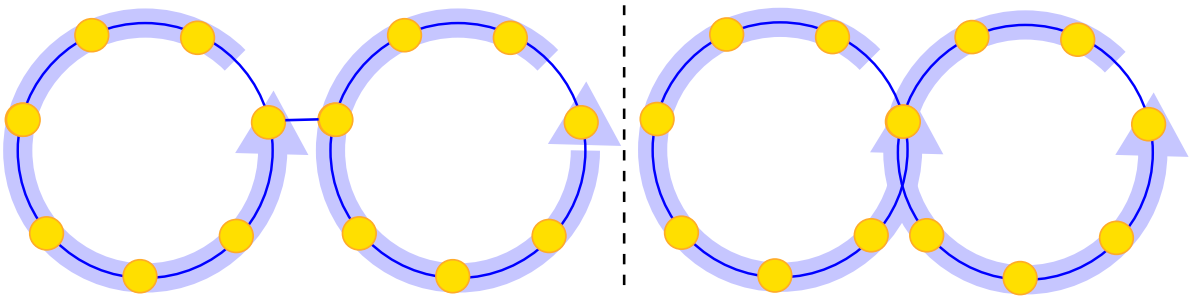

FIGURE 5: *Systems made of two closed loops. On the left, the loops are separated but are near each other in a spot which allows hopping. On the right, the loops are joined, as one lattice point is shared between the loops. The arrows represent the direction in which θ increases; simulations will be made for different rotation configurations.*

While there may still be no clear edges in the system so created, unlike the single-loop case the translational symmetry is broken, which allows localization of the wavefunction in nontrivial cases. We will study the energy spectrum and wavefunction amplitudes attained through the simulation in order to detect any topological effects. This will be done for both cases shown in fig. 5. The left-hand case will be designated the connected loops system, whereas we will use the term joined loops system for the right-hand case. We will also examine the impact which varying the parameters of one of the loops has on the combined system.

4. Results

4.1 Dimerized s-wave chain

The energy spectrum of the dimerized 1D s-wave chain does not support non-trivial topological phases. This despite the fact that both a non-superconducting dimerized chain and a simple spinless p-wave superconductor exhibit energy gap closings. It may hence be relevant to examine the universal properties of Hamiltonian matrices in order to find a method that would allow one to detect topologically trivial systems. With that as the goal, the following two statements were obtained:

1. If a Hamiltonian is of the form $a_1 A_1 + \sum_{i=2}^{n} a_i A_i$, with a_i real and A_i unitary Hermitian matrices, and $\{A_1, A_i\} = 0 \quad \forall i \neq 1$, the energy gap cannot close unless a_1 vanishes.

2. If $H = \sum_i a_i A_i$, with a_i real and A_i unitary Hermitian matrices, and all pairs of matrices A_i, A_j fulfil $[Ai, Aj] \neq 0 \Leftrightarrow \{A_i, A_j\} = 0 \Leftrightarrow \exists k : [A_i, A_k] = [A_j, A_k] = 0$,[1] then there exists a configuration of the system parameters which allows $E = 0,\ a_i \neq 0\ \forall i$.

This can be understood easily as

1)

$$H = a_1 A_1 + \sum_{i=2}^{n} a_i A_i = a_1 A_1 + H_0, \quad \{A_1, H_0\} = 0$$

$$H^2 = a_1^2 + H_0^2$$

Hence, the square of the eigenvalue must be at least $a_1^2 > 0$, preventing gap closing.

2)

$$H^2 = \sum_i a_i^2 + 2a_{i_1} a_{i_2} A_{i_1} A_{i_2} + 2a_{i_2} a_{i_3} A_{i_2} A_{i_3} + 2a_{i_3} a_{i_4} A_{i_3} A_{i_4} + ...$$

where the terms on the right only include products between commuting matrices. The square of H is a sum of an identity matrix and another matrix, so the eigenvalues must be $\sum_i a_i^2$ plus the

[1] That is, if the two matrices do not commute, they anticommute and there is a third matrix that commutes with them both, and if they do commute, there is no matrix that commutes with both of them

eigenvalue of the cross-term matrix. We can get that eigenvalue by squaring the matrix. Note that since $[A_{i_1}, A_{i_2}] = 0$ and $[A_{i_2}, A_{i_3}] = 0$, then according to our assumption $\{A_{i_1}, A_{i_3}\} = 0$. Thus $[A_{i_1}A_{i_2}, A_{i_1}A_{i_3}] = 0$. That leaves terms of the sort $A_{i_1}A_{i_4}A_{i_2}A_{i_3}$ (since, according to our assumption, A_{i_1} must commute with A_{i_4}). However, $A_{i_1}A_{i_4}A_{i_2}A_{i_3} = -A_{i_1}A_{i_2}A_{i_3}A_{i_4}$, leaving no cross terms at all. Hence

$$H^2 = \sum_i a_i^2 \pm \sqrt{a_{i_1}^2 a_{i_2}^2 + a_{i_2}^2 a_{i_3}^2 + ...}$$

$$H^2 = \sum_i a_i^2 \pm \sqrt{(a_{i_1}^2 + a_{i_3}^2 + ..)(a_{i_2}^2 + a_{i_4}^2 + ...)}$$

$$H^2 = (\sqrt{a_{i_1}^2 + a_{i_3}^2 + ..} \pm \sqrt{a_{i_2}^2 + a_{i_3}^2 + ...})^2$$

where all the matrices corresponding to the constants in the left square root anticommute and likewise for the right square root. If the square roots are equal in magnitude, the gap can be closed. This concludes the sketched proof. Note that $a_1 = 0$ in 1) is a necessary requirement whereas 2) is sufficient; the gap can close in systems that do not satisfy 2). In addition, there are systems in which the gap closes but the topological phase does not change.

In the case of a dimerized s-wave superconductor, the superconducting term anticommutes with the remainder of H_k. It is clear that only effects giving rise to terms proportional to τ_x or to the τ-space identity matrix will be able to close the gap. Excluding effects that break translation invariance, there are three ways of doing this:

- Terms that contain only creation or annihilation operators
- Terms that have opposite sign for spin up and spin down, or mix spins
- Terms containing $a_k^\dagger a_k$ and $a_{-k}a_{-k}^\dagger$ with the same sign

In practice, this means superconducting effects, magnetic fields, or anisotropic effects. Unfortunately, this excludes isotropic modulations of the hopping term such as dimerization. Models with several modes of superconductivity could hypothetically have topologically non-trivial states. However, transitioning between those states would likely require adjusting the mean-field order parameter and hence other systems may be more viable.

4.2 Magnetic helix chain with periodic boundary hopping

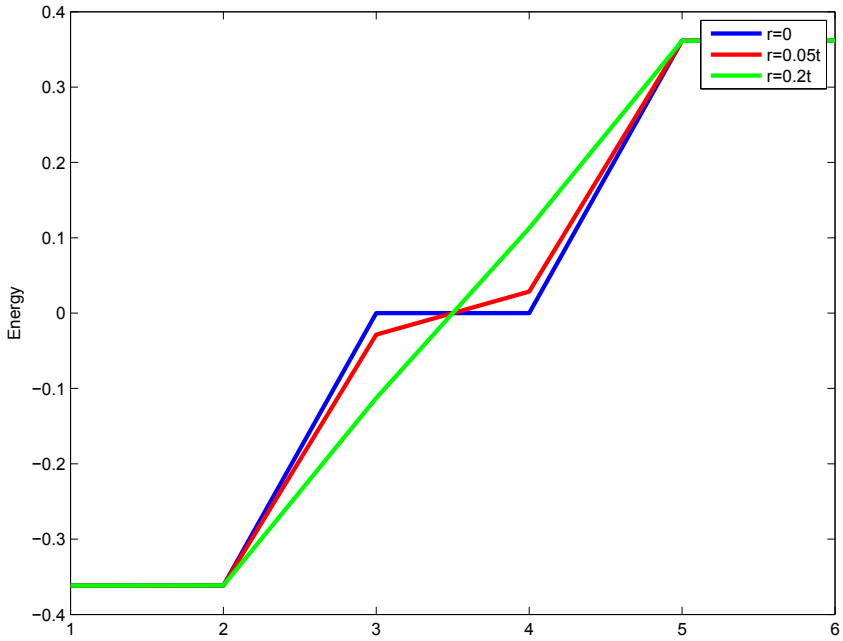

FIGURE 6: *System energy as r increases, normalized to* Δ_0. *Only the energy levels near zero energy are shown; the energy spectra as a whole remains nearly unchanged, and can be seen in fig. 8 at the end of this section. The simulation was for 300 lattice points, with* $|B| = 2t = 2\mu = 4\Delta_0$ *and* $\theta = \frac{\pi}{3}$. *The blue curve shows the existence of zero modes, with parameters consistent with Eqn. (3.6) The* x *axis is an ordering of eigenstates by eigenvalue in ascending order for viewing clarity.*

We studied the dependence of the energy spectrum and the wavefunction amplitude as a function of r. As seen in fig. 6, there is a definite change in the topology as r increases. This is because the energy gap closes at the interface between two topological phases. By increasing the hopping between the end points of the chain, we are effectively creating a one-dimensional loop with no edge states. At $r = 0$, there are two zero modes signifying a change in topological phase; increasing r to only 5% of t already shifted the edges away from the origin. The energy spectrum as a whole remains nearly unchanged during the entire transition, and the appearance of the wavefunction amplitude changes slowly. Interestingly, around $r = t$, we have two clearly distinct cases. In fig. 7, it is seen that if the magnetic moments of the atoms make an integer number of rotations around the loop, the energy is clearly gapped and the groundstate wavefunction is evenly distributed around the loop. However, if the number of rotations is not an integer, the groundstate wavefunction has distinct peaks at the end points of the chain. The effect can also be detected as a narrowing of the band gap in the energy graph. This is apparent only when r approaches t, and the two cases are practically indistinguishable even at $r = 0.5t$.

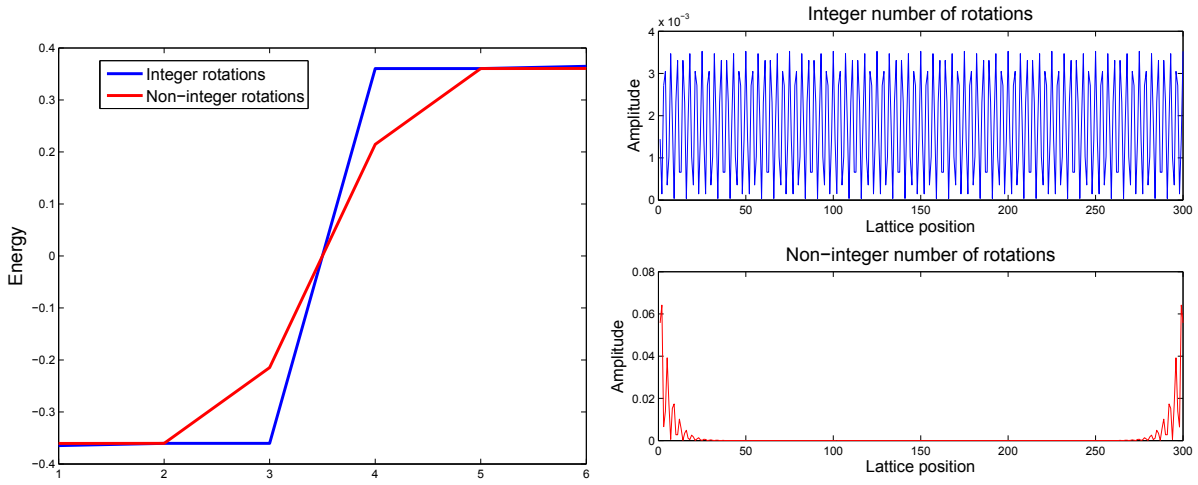

FIGURE 7: *A comparison between the cases* $N\theta = 2n\pi$ *and* $N\theta \neq 2n\pi$*, where* $n \in \mathbb{N}$*. The left figure is a close-up of the energy spectrum, while the right figure shows the wavefunction amplitudes. The red graph lines represent a reduction in* θ *by about* 0.7%

As the topological phase has a θ dependency, one might suppose the changes seen are due to a topological phase shift. However, while the change in the near-zero energy spectrum is noticeable, the lack of zero states suggests that any topological effects due to the local θ change are cancelled out by wavefunction overlap. The reason for the peaks seen in the lower right of fig. 7 is likely the breaking of translational symmetry which allows for the wavefunction to localize. The resultant amplitude profile is functionally identical to that of a true topological zero mode, but carries no topological significance.

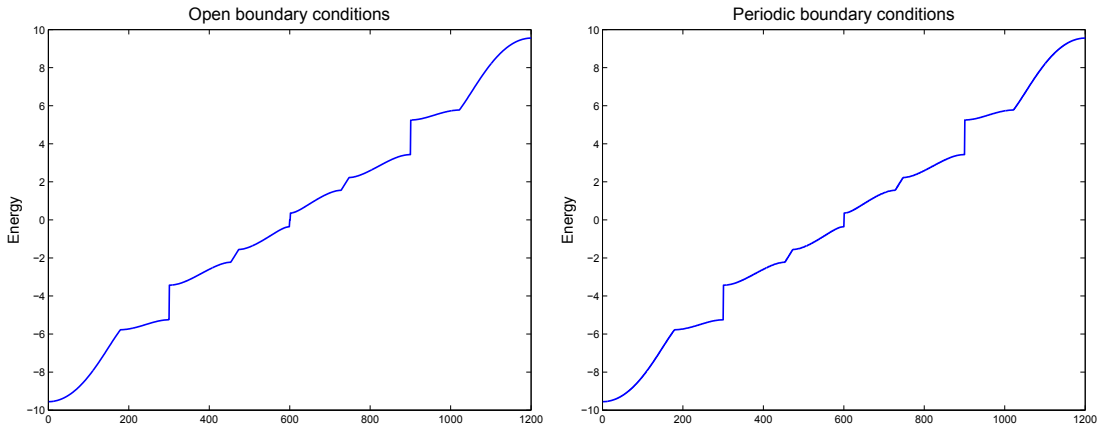

FIGURE 8: *A comparison of energy spectra. The left-hand figure is a plot of the energy for the* $r = 0$ *case, whereas the right-hand figure shows the energy spectrum for the* $r = t$ *case. The left-hand and right-hand figures correspond to the blue lines in figures* 6 *and* 7*, respectively.*

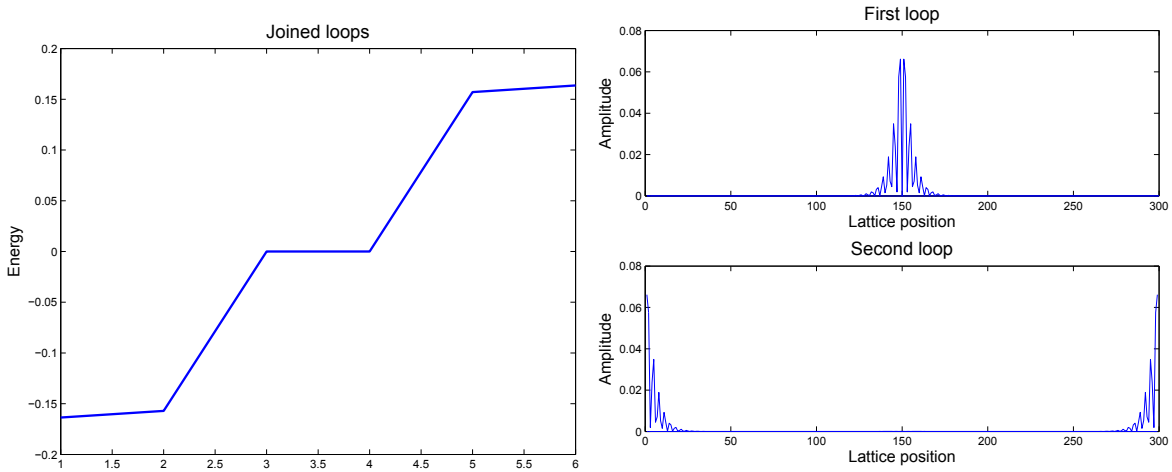

FIGURE 9: *Near-zero energy levels and wavefunctions for the joined loops case. Both loops have 300 lattice points, with the total number of lattice points being 599 due to one being shared. Other parameters are equal to those in fig. 6. The shared lattice point is indexed 150 in the first loop and lies between lattice points 1 and 299 in the second.*

As seen in fig. 9 above, the joined loops system (right-hand picture in fig. 5) does support zero-modes at the point where the circles intersect. This is not affected by whether the magnetic moments in the respective loops rotate in the same direction or not. The existence of zero modes is also unaffected by the number of atoms in the chain. although for non-integer rotations there is a non-topological excitation similar to that seen in fig. 7. If we allow a phase difference in Δ between loops, dropping the assumption that it is real, we find that if the phase difference $\phi = \pi$ the zero modes vanish. This is a generic property of Majorana systems, which appears in systems with connected topologically nontrivial superconducting chains [18]. Thus, we see that by connecting two systems that alone display no topological effects, it is possible to construct one which does. Joining a third loop to the second (or first) creates another zero mode at whichever lattice point is shared with the new loop, assuming it is distant from the existing one to minimize overlap.

However, the connected loops system (left-hand picture in fig. 5) does not show any topological effects, although the wavefunction is localized at the lattice points connecting the loops. The relative rotation of magnetic momenta in the loops does not affect this, nor does the precise number of lattice points. In this case, the existence of zero modes is not dependent on the superconducting phase. It appears that the connected loops have no edges for the zero modes to localize on, as is the case for a single loop. One can compare this with two-dimensional systems with PBC in one direction, which are also likely to have no edges, and are essentially equal to several connected loops, with several connected lattice points per loop instead of one.

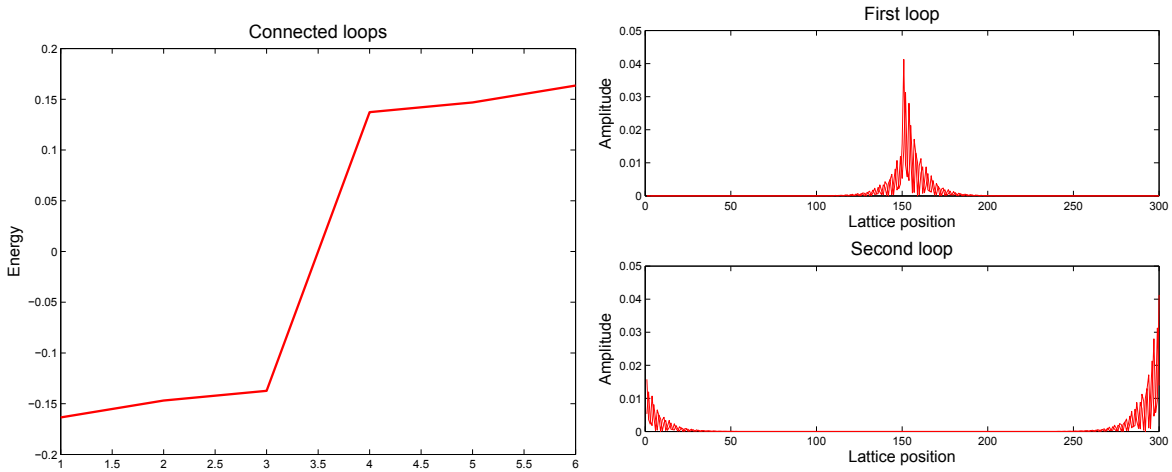

FIGURE 10: *Near-zero energy levels and wavefunctions for the connected loops case. Both loops have 300 lattice points. Other parameters are equal to those in fig.* 6. *Lattice point 150 in the first loop is connected to lattice point 1 in the second.*

The joined loop system, on the other hand, contains a shared lattice point from which hopping to four separate lattice points is allowed, which is the main difference between the systems. This explains the existence of zero modes, and as can be seen in fig. 11, the impact on the energy spectrum as a whole is minor. Essentially, the topological effects caused by PBC are only visible in the area around zero energy, making no impact on the rest of the system.

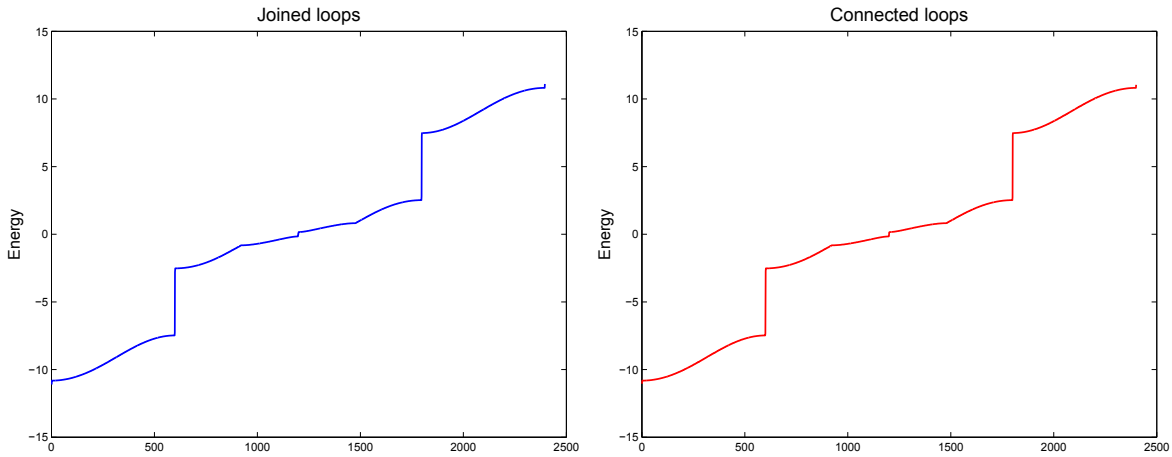

FIGURE 11: *A comparison of energy spectra. Note that the connected loops system contains one more lattice point in total than the joined loops system, which shifts its energy spectrum one step to the right.*

5. Conclusions

We have examined the topological properties of a few variations on the 1D s-wave superconducting chain. We saw that dimerization cannot cause a shift in topology in an s-wave superconductor in otherwise topologically trivial systems, contrasting the result attained for the non-superconducting case. In general, modifying the hopping terms will not make a simple s-wave superconductor topological. Examining the mathematical properties of the system makes it clear that there are significant limits on the s-wave systems that could be expected to support topologically nontrivial phases. Of these, it is likely that systems containing magnetic terms are the easiest to produce, implying that these are the most promising candidates for future research.

We have also seen that specific, spatially asymmetric modifications of the hopping amplitudes can have a significant impact on the topology of a system. The case treated in this thesis was periodic boundary conditions, where we saw that increasing the hopping between the end points of a magnetic helix chain immediately annihilates the existing edge modes, without significantly changing the energy spectrum. This could potentially be useful if one needs a system where topological zero modes can be annihilated and created anew at will. As the PBC hopping approaches the hopping term in the rest of the chain, the behaviour of the system shows a dependence on $N\theta$; for $N\theta \neq 2n\pi$ the groundstate wavefunction was clearly localized at the lattice point where the the magnetic field rotation was locally aberrant. However, the energy gap did not close at this point, leading one to the conclusion that this is not a topological effect.

From examining the systems with joined PBC chains, it is clear that combining two systems displaying no topological effects can create a system in which there are zero modes. The method used in this thesis is based on position-space topology, although it is possible that similar results could be achieved by other means. It is certainly interesting that two systems which in contact with vacuum appear seemingly trivial can support zero modes when joined together.

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