Manipulation Of Quantum States In One-Dimensional Topological Superconductors

THESIS

submitted in partial fulfillment of the
requirements for the degree of

BACHELOR OF SCIENCE
in
MATHEMATICS & PHYSICS

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Leiden, The Netherlands, June 30, 2024

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Abstract

Majorana particles are unique quasiparticles that exhibit a non-abelian exchange statistic, and by exploiting that property one could braid them. In condensed matter systems Majorana quasiparticles occur as zero-energy edge states of topological superconductors, for example in the Kitaev chain. The common protocols proposed to braid these edge states are carried out in real space. In this thesis we investigate the possibility to braid Majorana quasiparticles within a one-dimensional superconductor via their parameter space. We utilise the geometrical phases that particles can obtain from adiabatic changes of the Hamiltonian along closed curves in the parameter space. In the first part, the mathematical background is established that is essential for understanding geometrical phases. In the second part of the study, several extensions of the Kitaev chain are proposed and examined for the presence of loops that give rise to nontrivial geometrical phases. We show how several topological phase transitions occur in those models. Finally, we present a noncontractible loop in the parameter space of a one-dimensional topological superconductor, albeit with a trivial corresponding geometrical phase.

Contents

Chapter 1

Introduction

Ever since Ettore Majorana hypothesised the existence of fermions that are their own antiparticle in 1937 [47] people have been looking for such particle. Although the existence of elementary Majorana particles seems very unlikely nowadays, there is still possibility left. Those particles may exist as quasiparticles in certain condensed matter systems. One model that describes such a system, and that has been of much interest, is the so-called Kitaev chain proposed by Alexei Kitaev in 2001 [33].

It appears, as we will see in Chapter 7, that those Majorana quasiparticles occur as edge states in the Kitaev chain. Furthermore, they are stable under continuous transformations of the Hamiltonian, i.e. they are topologically protected.

One interesting property of Majorana particles is their so-called *non-abelian exchange statistic*, the permutation of those particles do not necessarily commute. This permutation of Majorana particles is called *braiding* and will be further explained in Chapter 7. This property makes them particularly intriguing for quantum computing applications, as information can be stored in the braided particles. However, to be able to utilise these properties we have to find a protocol to perform the braiding. One of the possibilities is so-called braiding in the parameter space. In this thesis we will explore the possibilities of this kind of braiding in different extensions of the Kitaev chain.

First we will establish the relevant mathematical background. This consists, among other things, of Lie groups, Lie algebras, and principal bundles. These notions are used to define *connections* on principal bundles in Chapter 3.

In Chapter 4 we will shift our focus to physical applications and introduce the *adiabatic theorem*. Moreover, we will investigate how the geo-

metrical concepts from the previous chapters combined with the adiabatic theorem give rise to so-called *geometrical phases* of quantum states when moved along closed curves.

To be able to apply this theory to many-body systems we introduce the formalism of second quantisation. This enables us to formulate models is an elegant manner. Subsequently, we will study the symmetries of second quantised Hamiltonians. This symmetries will turn out to be *topologically protected*.

In Chapter 7 we will provide a definition of being topologically protected, and consider topological phases in matter. Afterwards the Kitaev chain will be introduced, and braiding will be further explained.

To perform braiding in the parameter space we have to overcome two problems. The problem of increasing the degeneracy will be discussed in Chapter 8, and the problem of the existence of noncontractible loops in parameter space in Chapter 9 and 10. Here several extension of the Kitaev chain will be proposed and the parameter spaces explored to find not simply connected connected components of the parameter space where Majorana particles exist in the chain and the gaps does not close. Moreover, we will make some remarks about the topological phase transitions that occur.

This thesis is meant to present a topic from theoretical physics that serves as a coat rack for several mathematical concepts. We will encounter numerous topics from mathematics that relate to the physical problem of the manipulation of quantum states in a one-dimensional superconductor. The style of writing of this text is aimed to serve both the physicists and mathematicians, but the main focus remains on the physical systems.

The assumed prior mathematical knowledge for this thesis is basic group theory, topology, analysis, and an advanced undergraduate-level understanding of differential geometry. Moreover, some familiarity with representations and discrete Fourier transforms might be beneficial. Regarding the physics, it is assumed that the reader has an undergraduate-level understanding of quantum mechanics and solid-state physics. Throughout this thesis we will make use of the standard convenient $\hbar = c = 1$.

Chapter 2

Lie groups and Lie algebras

Lie groups bridge the gap between smooth manifolds and groups. This chapter is meant to familiarise the reader with some basic concepts of those Lie groups and their Lie algebras, starting with the definitions of Lie groups and Lie algebras. Subsequently, the action of Lie groups will be discussed. Finally, a relation between differential forms and Lie algebras is established by introducing Lie algebra valued forms. The presented content is mainly based on [39], [15], and [64]. Because the aim of this chapter is to obtain a basic understanding of the mathematical concepts for later use in physical applications, rather than a thorough mathematical comprehension, we will refer to the relevant books for the proofs.

2.1 Lie groups

Let us start with the definition that will play a central role in this section.

Definition 2.1.1. A *Lie group* is a group G that is also a smooth manifold without boundary, such that the multiplication $m : G \times G \to G$ and the inversion $i : G \to G$ are smooth maps.

Notice that our knowledge about Lie groups is already quite extensive, since the results and properties of both groups and smooth manifold apply to Lie groups as well.

Example 2.1.1. The group of invertible $n \times n$ matrices over $\mathbb{R}$ or $\mathbb{C}$ with standard multiplication, $\mathrm{GL}(n, \mathbb{R})$ respectively $\mathrm{GL}(n, \mathbb{C})$, is a Lie group. We know that this is a smooth manifold. The multiplication of matrices is smooth since the entries of the product of two matrices are polynomials in

the entries of the original matrices. Because of Cramer's rule the inversion of a matrix is smooth as well.

The fact that invertible matrices form a Lie group is an interesting result that hints that they are, often as matrix groups, omnipresent in physics since matrices are. We will shortly see many more applications of Lie groups.

2.2 Lie algebras

Via the theory of differential manifolds, Lie groups give rise to another algebraic object that is of great interest to us. We will first consider those objects in such a way that one does not need any knowledge about differential geometry, and later we will see how they relate to Lie groups.

Definition 2.2.1. Let L be a vector space with a bilinear form $[-,-] : L \times L \to L$ satisfying the following properties for all $x, y, z \in L$:

1) $[x, y] = -[y, x]$ (skew-symmetry);

2) $[[x, y], z] + [[z, x], y] + [[y, z], x] = 0$ (Jacobi identity).

Then L is called a *Lie algebra*.

In the context of Lie algebras the corresponding bilinear form is called the *Lie bracket*. For readers with a background in physics these brackets might remind them of the commutator of matrices and that is no coincidence.

Example 2.2.1. Let $\mathrm{Mat}(n, K)$ with $K = \mathbb{R}$ or $K = \mathbb{C}$ be the vector space of all $n \times n$ matrices over K. Then $\mathrm{Mat}(n, K)$ together with the map $[-,-] : \mathrm{Mat}(n, K) \times \mathrm{Mat}(n, K) \to \mathrm{Mat}(n, K)$ defined by $[A, B] = AB - BA$ is a Lie algebra as discussed in [39].

The structure of a Lie algebra can also be given in a coordinate dependent manner. This might be convenient when a natural basis of the vector space is available or when explicit calculation have to be done. Therefore this alternative way of talking about Lie algebras is common in physics literature.

Proposition 2.2.1. *Let $(\mathfrak{h}, [-,-])$ be an n-dimensional Lie algebra and $\{e_i\}_{i=1}^n$ a basis for $\mathfrak{h}$. Then the Lie bracket is uniquely defined by the set of so-called structure constants $\{f_{ij}^k : i, j, k \in \{1, ..., n\}\}$ where $[e_i, e_j] =: f_{ij}^k e_k$.* □

At first glance it is not clear from Def. 2.2.1 how Lie algebras and groups are related. However, we will shortly see how tightly intertwined they are. For this we first consider a Lie group G and an element $g \in G$, and we define the *left-action of* g, $L_g : G \to G$, by $L_g(h) := gh$ and similarly the *right-action* $R_g : G \to G$ by $R_g(h) = hg$.

With this left-action we are able to introduce the following property a vector fields can posses: a smooth vector field $X \in \mathfrak{X}(G)$ is called *left-invariant* if for all $g \in G$ the push-forward of the corresponding left-actions acts trivially on the vector fields, i.e. $(L_g)_* X = X$ and thus for all $h \in G$ $((L_g)_* X)(h) = X(gh)$. This left-invariance provides a way of constructing a Lie algebra from a Lie group.

Proposition 2.2.2. *Let G be a Lie group and $\mathfrak{X}_L(G)$ the set of all left-invariant smooth vector fields over G. Define the Lie bracket $[-,-] : \mathfrak{X}_L(G) \times \mathfrak{X}_L(G) \to \mathfrak{X}_L(G)$ by $[X,Y]f = XYf - YXf$. Then $(\mathfrak{X}_L(G), [-,-])$ is a Lie algebra.* □

The proof of this theorem, however differently formulated, can be found in Chapter 7 of Sontz' book [64].

Although this already enables us to construct a Lie algebra from a Lie group, by a simple observation we can replace the set of left-invariant smooth vector fields by a more intuitive space. The important observation is that any left-invariant smooth vector field is uniquely determined by its value at the unity element of the under lying Lie group.

Corollary 2.2.1. *Let G be a Lie group and $e \in G$ the unit, then $(T_eG, [-,-])$, where for all $a, b \in T_eG$ and $X, Y \in \mathfrak{X}_L(G)$ such that $a = X(e)$ and $b = Y(e)$ the Lie bracket is defined by $[a,b] := [X,Y](e)$, is a Lie algebra.* □

The Lie algebra as constructed in Corollary 2.2.1 corresponding to a Lie group G is called the *Lie algebra of* G and is denoted by $\mathfrak{g}$. This Lie algebra of G is the tangent space along the Lie group at the element of unity, and therefore Lie groups and algebras are indeed closely related. This relation can be made explicit in the following examples discussed in [39]. Firstly, the invertible $n \times n$-matrices and all the $n \times n$-matrices are related in this way.

Example 2.2.2. The Lie algebra of $\mathrm{GL}(n,K)$ is $\mathrm{Mat}(n,K)$, so $\mathfrak{gl}(n,K) = \mathrm{Mat}(n,K)$.

Moreover, there exists an interesting relation between manifolds, diffeomorphisms and vector fields by considering Lie groups and algebras.

Example 2.2.3. Let M be a smooth manifold, then $\mathrm{Diff}(M)$ is a Lie group and $\mathfrak{X}(M)$ is the Lie algebra of $\mathrm{Diff}(M)$.

2.2.1 Actions of Lie groups

Equipped with the basic definitions we can dive deeper into the interplay between Lie groups and general smooth manifolds in the form of an action on the manifold. For the remainder of this chapter M will denote a smooth manifold and G a Lie group.

Definition 2.2.2. Let $\Phi : G \times M \to M$ be a smooth map that is a left group action of G on M. Now define a map $X_{\_} : \mathfrak{g} \to \mathfrak{X}(M)$ by

$$X_\xi(x) := d_t\Phi(g_\xi(t), x)|_{t=0}.$$

Here g_ξ is the integral curve of X_ξ, and X_ξ is a vector field on M called the *infinitesimal generator* of the action Φ corresponding to ξ.

At first sight this definition can be perceived as non-transparent. So to obtain an intuitive idea of this map we make the remark that, as discussed in Chapter 1 of [15], for real matrix groups $\mathrm{GL}(n, \mathbb{R})$ the infinitesimal generator of linear operations corresponding to a matrix $A \in \mathrm{GL}(n, \mathbb{R})$ is A itself. This generator will be use to us in Chapter 3.

Before arriving there we need to elaborate a little bit on the action of Lie groups, where we will make use of the relation between Lie algebras and the tangent space at the unity element in the correspong Lie group.

Combining the left- and right-action of, we obtain a so-called *inner automorphism*, also know as *conjugation*, given by $I_g := L_g \circ R_g^{-1} : G \to G$ for a $g \in G$. This gives rise to a linear operation $T_eI_g : T_eG \to T_eG$, and by identifying the tangent space of a Lie group at the unity with its Lie algebra this is linear operation on $\mathfrak{g}$.

Definition 2.2.3. The *adjoint representation* of G is the map $\mathrm{Ad} : G \to \mathrm{Aut}(\mathfrak{g})$ defined by $\mathrm{Ad}_g := T_eI_g$.

To create an intuitive feeling for what the adjoint representation of an element $g \in G$, i.e. Ad_g, means, it might be fruitful to once again consider the case of matrices.

Example 2.2.4. Let $G = \mathrm{GL}(n, K)$, and $g \in G$. This g is an invertible matrix and the left- and right action are left respectively right multiplication with g respectively g^{-1}. Via the tangent map this conjugation action becomes a conjugation action on the Lie algebra. Since the Lie algebra of $\mathrm{GL}(n, K)$ is a matrix gorup, the adjoint representation is given by $\mathrm{Ad}_g(A) = gAg^{-1}$ for all $A \in \mathfrak{gl}(n, K) = \mathrm{Mat}(n, K)$.

2.3 Lie algebra-valued differential forms

For our eventual use of Lie algebras we have to consider them in a context of differential forms. Let $\Omega^k(M)$ denote the space of k-forms on M where $k \in \mathbb{Z}_{\geq 0}$.

Definition 2.3.1. Let $(\mathfrak{h}, [-,-])$ be a Lie algebra. Define the set of $\mathfrak{h}$-*valued (differential) forms* by $\Omega(M, \mathfrak{h})$. If $\alpha \in \Omega^k(M, \mathfrak{h})$, then $\alpha_x(v_1, ..., v_k) \in \mathfrak{h}$ for all $x \in M$ and $v_1, ..., v_k \in T_x^*M$.

When a basis $\{e_1, ..., e_r\}$ of $\mathfrak{h}$ is given, we can explicitly write every $\alpha \in \Omega(M, \mathfrak{h})$ as $\alpha = \alpha^i \otimes e_i$ where $\alpha^i \in \Omega(M)$, since Lie algebras are a finite-dimensional vector space. Using this representation of the elements we can extend the notion of Lie brackets to the context of Lie algebra-valued differential forms.

Definition 2.3.2. Let $(\mathfrak{h}, [-,-])$ be a Lie algebra, and f_{ij}^k the structure constants of $\mathfrak{h}$ corresponding to a basis $\{e_i\}_{i=1}^r$, then the *(extended) Lie bracket* is a bilinear form $(-,-) : (\Omega(M, \mathfrak{h})) \times (\Omega(M, \mathfrak{h}) \to \Omega(M, \mathfrak{h})$ where $(\alpha, \beta) := (\alpha^i \wedge \beta^i) \otimes [e_i, e_j] = f_{ij}^k(\alpha^i \wedge \beta^j) \otimes e_k$ for all $\alpha \in \Omega^k(M, \mathfrak{h})$, $\beta \in \Omega^l(M, \mathfrak{h})$ and $k, l \in \mathbb{Z}_{\geq 0}$.

As the difference between the Lie brackets and extended Lie brackets is often discarded, we will write $[-,-]$ for an extended Lie brackets as well and we will call it Lie brackets as well. For further use we will list the following properties of the Lie brackets that are just defined.

Proposition 2.3.1. *Let $\mathfrak{h}$ be a Lie algebra, $k, l, m \in \mathbb{Z}_{\geq 0}$, $\alpha \in \Omega^k(M, \mathfrak{h})$, $\beta \in \Omega^l(M, \mathfrak{h})$, and $c \in \Omega^m(M)$ then:*

i) $[\alpha, \beta] = (-1)^{kl+1}[\beta, \alpha]$;

ii) $(-1)^{km}[[\alpha, \beta], c] + (-1)^{ml}[[c, \alpha], \beta] + (-1)^{kl}[[\beta, c], \alpha] = 0$;

iii) $d[\alpha, \beta] = [d\alpha, \beta] + (-1)^k[\alpha, d\beta]$. □

The proof of this follows from the elementary properties of exterior derivatives, wedge products and tensor products.

Now let us look into how the left- and right-action of Lie groups related to Lie algebra valued forms.

Definition 2.3.3. A *left-invariant differential form on* a Lie group G is a differential form, $\alpha \in \Omega(G)$, that is invariant under the pull back of the left-action of g, i.e. $L_g^*\alpha = \alpha$, for all $g \in G$. The set of all left-invariant differential forms on G is denoted by $\Omega_L(G)$.

Since both the exterior derivative as the wedge product commute with the pull-back operation, chapter 14 of [39], we can conclude that $\Omega_L(G)$ is invariant under those operations.

Using the relation between Lie algebras corresponding to Lie groups and tangent spaces to that Lie group at the unit element, we can relate left-invariant differential forms on G to Lie algebras.

Remark. *There exists a bijective map between left-invariant 1-forms, $\Omega^1_L(G)$ and the cotangent space T^*_eG:*

$$\Omega^1_L(G) \ni \alpha \mapsto \alpha(e) \in T^*_e(G). \tag{2.1}$$

Recall that for the Lie algebra $\mathfrak{g}$ of G we have that $\mathfrak{g} \cong T_eG$. Moreover, if $\{e_i\}_{i\in I}$ is a basis of $\mathfrak{g}$, then by Prop. 2.2.1 and Def. 2.3.2 the relations $[e_i, e_j] = f^k_{ij}e_k$ for $i, j \in I$ completely determine the structure of $\mathfrak{g}$.

Proposition 2.3.2. *Let $\{\theta^1, ..., \theta^n\}$ the basis of T^*_eG that is dual to the basis $\{e_1, ..., e_n\}$ of T_eG. Let $\theta^k_L \in \Omega^1_L(G)$ be the unique left-invariant 1-form such that $\theta^k_L(e) = \theta^k$. Then the following holds*

$$d\theta^k_L(e) = -\frac{1}{2} f^k_{ij}\theta^i_L \wedge \theta^j_L \tag{2.2}$$

which is called the Maurer-Cartan equation. □

The proof of Prop.2.3.2 is omitted here, but it immediately follows from the Cartan formula [15].

Let us now consider the following specific example of a left-invariant $\mathfrak{g}$-valued 1-forms on the Lie group G.

Definition 2.3.4. The *Maurer-Cartan* or *canonical form* on G is a left-invariant $\mathfrak{g}$-valued 1-form $\omega_0 : G \to \mathfrak{g}$ defined by

$$[\omega_0(X)](g) := [(L_{g^{-1}})_* X](e) \in \mathfrak{g} \tag{2.3}$$

for all $g \in G$ and $X \in \mathfrak{X}(G)$.

This Maurer-Cartan form just pushes forward a smooth vector field from a point g to the point e. This form has some interesting properties and it will be of great use in Chapter 3. Notice that if $\{e_1, ..., e_n\}$ and $\{\theta^1, ..., \theta^n\}$ are bases as in Prop. 2.3.2, then we can write $\omega_0 = \theta^k_L \otimes e_k$ [15]. Such a expression in basis elements will enable us to do calculations with the Maurer-Cartan form. Furthermore, it introduces a way of working locally, without everything being globally defined, on a manifold G, which will be essential for making the connection between the physical applications and the general theory that is developed here.

Proposition 2.3.3. *The Maurer-Cartan form satisfies*

$$d\omega_0 = -\frac{1}{2}[\omega_0, \omega_0]. \tag{2.4}$$

Proof. Given the bases $\{e_1, ..., e_n\}$ and $\{\theta^1, ..., \theta^n\}$ of G resp. $\mathfrak{g}$ as before we can make use of the observation $\omega_0 = \theta_L^k \otimes e_k$. Then the Maurer-Cartan equation form Prop. 2.3.2 yields

$$d\omega_0 = d(\theta_L^k \otimes e_k) = (d\theta_L^k) \otimes e_k = \left(-\frac{1}{2} f_{ij}^k \theta_L^i \wedge \theta_L^j\right) \otimes e_k = -\frac{1}{2}[\omega_0, \omega_0].$$

□

This result can be seen as a direct consequence of the Maurer-Cartan equation and therefore it is often mentioned in the same breath. Althought following result is a little technical, will be essential to the next chapter.

Proposition 2.3.4. *Under the right action of G the Maurer-Cartan form ω transforms as follows:*

$$R_g^* \omega_0 = \mathrm{Ad}_{g^{-1}} \omega_0 \tag{2.5}$$

for all $g \in G$.

So the pull-back of the Maurer-Cartan form at g is the image of ω_0 under adjoint representation at g^{-1} as defined in Def. 2.2.3. The proof of this is omitted here, and can be found in chapter 10 of Sontz' book [64].

To conclude this chapter we can apply the just developed general theory to one of the most important Lie groups, the invertible matrices $\mathrm{GL}(n, K)$.

Example 2.3.1. Consider $\mathrm{GL}(n, K)$ with $n \in \mathbb{Z}_{\geq 0}$ and $K = \mathbb{R}, \mathbb{C}$. The associated Lie algebra to that group is $\mathfrak{gl}(n, K) = \mathrm{Mat}(n, K)$. The Maurer-Cartan form on $\mathrm{GL}(n, K)$ boils down to $\omega_0 = g^{-1}dg$ with $g \in \mathrm{GL}(n, K)$ [15]. Furthermore, we verify Prop. 2.3.3 and Prop. 2.3.4 for this Lie group. Since $dg^{-1} = -g^{-1}d(g)g^{-1}$ we obtain

$$\begin{aligned} d\omega_0 &= d(g^{-1}dg) = dg^{-1} \wedge dg = -g^{-1}dg \wedge g^{-1}dg \\ &= -\omega_0 \wedge \omega_0 = -\frac{1}{2}[\omega_0, \omega_0]. \end{aligned}$$

For Prop. 2.3.4 we have

$$R_h^* \omega_0 = (gh)^{-1} d(gh) = h^{-1}g^{-1}(dg)h = h^{-1}\omega_0 h = \mathrm{Ad}_{h^{-1}} \omega_0$$

for all $h \in \mathrm{GL}(n, K)$. This shows both Prop. 2.3.3 and Prop. 2.3.4 in the case of matrix Lie groups.

Chapter 3

Bundles and connections

In this chapter we will use the concepts from the study of Lie groups and their algebras to define principal bundles and connections thereon, primarily following [15] and [64]. These connections are an attempt to obtain a notion of parallel transport on a manifold. Afterwards, will introduce the holonomy group, which will be of major importance throughout the rest of this text. Furthermore, over the course of the chapter the perspective is shifted from a purely mathematical viewpoint to one of theoretical physics, and we will conclude with two physical applications. Because our focus still lies on the physical applications of the developed theory, we will refrain from including the proofs of all results.

3.1 Principal bundles

In this section we will enrich the structure of a manifold by attaching another structure, a so-called fibre, to every point in that manifold and combining those pointwise structures. To do that we make use of the action of Lie groups and so both of the previous chapter and the preliminary knowledge come together here.

Definition 3.1.1. Let E, M and F smooth manifolds. E is called the *bundle space*, M the *base space*, and F the *standard fibre*. Let G be a Lie group which acts faithfully on F, i.e. there is a $\Phi : G \times F \to F$ such that if $\Phi(g, f) = f$, then $g = e$. Let $\pi : E \to M$, called the *bundle projection* be a smooth map such that for each $x \in M$ the so-called *fibre* $F_x := \pi^{-1}(x)$ is homeomorfic to F. Furthermore we demand:

i) *local triviality* of the bundle: for every open covering $\{U_j\}$ of M there

exist sets of smooth maps $\{\varphi_j\}$ and $\{\phi_j\}$ with

$$\varphi_j : \pi^{-1}(U_j) \to U_j \times F \tag{3.1}$$
$$\phi_j : \pi^{-1}(U_j) \to F \tag{3.2}$$

such that φ_j is a diffeomorphism and $\varphi_j(p) = (\pi(p), \phi_j(p))$ for all $p \in M$, and the following diagram commutes

$$\begin{array}{ccc} \pi^{-1}(U_j) & \xrightarrow{\varphi_j} & U_j \times F \\ & \searrow^{\pi} & \downarrow \text{Can.Proj.} \\ & & U_j. \end{array} \tag{3.3}$$

The set $\{(U_j, \varphi_j)\}$ is called a *family of local trivialisations*;

ii) The restriction of ϕ_j to the fibre over $x \in U_j$, i.e. $F_x = \pi^{-1}(x)$, defines a diffeomorphism

$$\phi_{j,x} := \phi_j|_{F_x} : F_x \to F. \tag{3.4}$$

For all $x \in U_j \cap U_k$ this yields a diffeomorphism

$$\phi_{k,x} \circ \phi_{j,x}^{-1} : F \to F \tag{3.5}$$

that corresponds to an element of G, i.e. there exist a so-called *transition function* $\gamma_{kj} : M \to G$ such that $\Phi(\gamma_{kj}(x), -) = \phi_{k,x} \circ \phi_{j,x}^{-1}$.

Then the quintuple (E, M, π, G, F) is called a *fibre bundle*.

It is interesting to notice that the whole structure of a fibre bundle is encoded by its transition functions as follows from the next proposition.

Proposition 3.1.1. *Transition functions satisfy the following conditions*

i) $\gamma_{ii}(x) = e,\ x \in U_i$;

ii) $\gamma_{ij}(x) = (\gamma_{ji}(x))^{-1},\ x \in U_i \cap U_j$;

iii) $\gamma_{jk}(x)\gamma_{kl}(x) = \gamma_{jl}(x),\ x \in U_j \cap U_k \cap U_l$ *(cocycle condition).*

Furthermore, a fibre bundle is up to isomorphism determined by the set of transition functions satisfying the conditions above. □

For a neat proof of this proposition on the role of transition functions in determining fibre bundles one could consult chapter 5 of Husemöller's book [25].

Shortly, we will shrink our scope to a specific kind of fibre bundles, but before doing so we will consider a straight forward example of a general fibre bundle.

Definition 3.1.2. A fibre bundle (E, M, π, G, F) is called *trivial* if $E \cong_{\text{Diff}} M \times F$, i.e. there exists a diffeomorphism $h : M \times F \to E$ such that $\pi(h(x, f)) = x$ for all $x \in M$ and $f \in F$.

It is easily checked that a trivial fibre bundle indeed satisfies the conditions of a fibre bundle. The study of trivial fibre bundles, however, is not too interesting. Therefore we will consider another class of fibre bundles which has an intriguing structure which turns out to be strongly related with the action of Lie groups on manifolds.

Definition 3.1.3. A *principal (G-)bundle* is a fibre bundle (E, M, π, G, F) where the standard fibre and the structure group coincide, i.e. $G = F$, and G acts on itself by left-translation L_g.

Such a principle bundle is often referred to as a *(principal) G-bundle* $\pi : E \to M$ over M, and with the quadruple (E, M, π, G). Equipped with Def. 3.1.3, we want to know when such a principle bundle is trivial. This can be decided in the following way.

Definition 3.1.4. A *(smooth) local section* of a fibre bundle (E, M, π, G, F) is a (smooth) map $h : U \to E$, where $U \subset M$ is open, and such that $\pi \circ h = \mathrm{id}|_U$. A local section is called *global* if $U = M$.

With this definition we can formulate condition for a principle bundle to be trivial.

Proposition 3.1.2. *A principle G-bundle is trivial if and only if it admits a global section.*

For a proof of this proposition we refer to chapter 9 of [64]. Although finding a global section can be, and often is, extremely hard and cumbersome this result still reduces the question to finding a right inverse of the bundle projection.

Before stating the most important result of this section, it might be need to consider an example of a principle bundle that is not necessarily trivial.

Example 3.1.1. Let G be a Lie group and $H \subset G$ a closed subgroup. Then $(G, G/H, \pi, H)$ with canonical projection $\pi : G \to G/H$ defines a principle H-bundle. □

Other interesting examples are so-called Hopf-bundles over projective spaces as first studied by Hopf [24]; especially the monopole and instaton bundle are of great importance in physics as discussed in [15]. It goes beyond the scope of this thesis to go further into these bundles.

An interesting and important property of principle G-bundles is that there exists a natural smooth and free right action on the bundle space such that the orbits of that action coincide with the fibres as discussed in chapter 6 of [53]. Moreover, there is an even stronger result is proven in [53], that brings back Lie groups in the discussion of fibre bundles.

Theorem 3.1.1. *Every principle G-bundle is obtained from the right action of a Lie group G on a manifold E.* □

This fact will be thoroughly used in the next section, where we will explore the structure of G-bundles even further to define a notion of parallel transportation on manifolds.

3.2 Ehresmann connections

The concept that we want to make rigorous in this section is the idea of parallel transportation. In a plane it is unambiguous what is meant by moving parallel to a line, but already on a familiar manifold as a sphere this is no longer clear what moving parallel to a curve means. We will do this for principal bundles, but the concepts can be generalised to fibre bundels. For the remainder of the chapter, let (P, M, π, G) denote a principal G-bundle, such a bundle is endowed with a canonical right action, $\tilde{R} : P \times G \to P$, according to Thm. 3.1.1.

Let us first specify the conditions that we want for parallel transport. Consider a (piecewise) smoot curve $\gamma : [0,1] \to M$. Then a *connection* provides a rule for parallel transporting the fibre F along the curve γ. This rule defines a smooth map $T_\gamma : F_{\gamma(0)} \to F_{\gamma(1)}$ satisfying the following conditions:

i) T_γ depends smoothly on γ;

ii) $T_{\gamma_1 * \gamma_2} = T_{\gamma_1} \circ T_{\gamma_2}$, where γ_1, γ_2 are two curves as defined above and $*$ is the concatenation operation;

iii) $T_{\gamma^{-1}} = (T_\gamma)^{-1}$, where $\gamma^{-1}(t) = \gamma(1-t)$.

This map T_γ is called the *operator of parallel transport* determined by the connection, but how to find such a map - or if it even exists - is not yet clear.

So we have an idea of what a connection should encode for. With this idea we will now work towards the formulation of a connection, but we need some other definitions before we are able to do so.

Definition 3.2.1. Let $v \in T_pP$ and $p \in M$. We call v a *vertical vector* if $v \in T_p\pi^{-1}(p)$, i.e. v is *vertical* at p if it is tangent to the fibre passing through p. The space of all vertical vectors at p is called the *vertical subspace* of T_pP, i.e. $V_p := \{v \in T_pP : v \in T_p\pi^{-1}(p)\}$.

We can also write $V_p = \{v \in T_pE : (T_p\pi)(v) = 0\}$ where $T_p\pi$ is the tangent map, or derivative, at p corresponding to π. We can also define the space of vertical vector fields on E: $\mathfrak{X}_{\text{ver}} = \{X \in \Gamma(TE) : X(p) \in V_p\}$. Provided with a vertical subspaces it is a natural next step to define a horizontal counterpart.

Definition 3.2.2. Let V_p a vertical subspace of T_pP, the a *horizontal subspace* of T_pP denoted by H_p is a complementary subspace to V_p. An element of H_p is called a *horizontal vector*.

Notice that for all $v \in T_pP$ we can write $v = \text{hor}(v) + \text{ver}(v)$ where $\text{hor} : T_pP \to H_p$ and $\text{ver} : T_pP \to V_p$ a projection on the subspace H_p respectively V_p. Now we are equipped with all of the vocabulary to define a connection.

Definition 3.2.3. An *Ehresmann connection* on the principal G-bundle (P, M, π, G), is a smooth map

$$E \ni p \mapsto H_p \subset T_pP \tag{3.6}$$

where H_p is a horizontal subspace at p that satisfies the following conditions:

i) the derivative map $T_p\pi : H_p \to T_{\pi(p)}M$ is an isomorphism for all $p \in P$;

ii) the assignment of horizontal subspace is compatible with the right action of G, i.e. $(T_p\tilde{R}_g)(H_p) = H_{p\cdot g}$ for all $p \in P$ and $g \in G$.

Let us investigate how this definition corresponds to parallel transport. We need the following definition to connect those two concepts.

Definition 3.2.4. Let $\zeta : [0,1] \to E$ be a smooth curve. ζ is called *horizontal* if $d_t\zeta(t)$ is horizontal for all $t \in [0,1]$. Furthermore, Let $\gamma : [0,1] \to M$ be a smooth curve, a smooth curve $\tilde{\gamma} : [0,1] \to E$ is called a *lift* of γ if $\pi \circ \tilde{\gamma} = \gamma$. If $\tilde{\gamma}$ is a horizontal curve, then it is called a *horizontal lift*.

An Ehresmann connection on a manifold defines what the horizontal subspaces are, and therefore what horizontal curves are. Now let $\gamma(t)$ be a curve in M with $\gamma(0) = x_0$ and $\gamma(1) = x_1$. Let $p_0 \in F_{x_0}$ and assume that there exist a unique horizontal lift $\tilde{\gamma}$ of γ such that $\tilde{\gamma}(0) = p_0$. Then we can define the operator of parallel transport as the map that sends the point p_0 to the end point of the horizontal lift of γ, i.e. $T_\gamma(p_0) := \tilde{\gamma}(1) \in F_{x_1}$. This map being well-defined heavily depends on the uniqueness and existence of horizontal lifts. However, the question remains how to find those lifts. In chapter 10 of [64] a differential equation is obtained which solution is the lift we are looking for. This smooth differential equation in combination with the uniqueness and existence theorem for solution of systems of smooth ordinary differential equations with given initial values yields both the existence and the uniqueness of these lifts. Everything that remains is to check if this map indeed satisfies the conditions of an operator of parallel transportation. The last two are easily checked with the definition of lifts, and the third one follows from the construction of the lift given in [64]

Now we have seen the definition of an Ehresmann connection, this is a description of a connection in terms of vectors in TP. However, it we can define connection in terms of differential forms. That definition turns out to be equivalent to the Ehresmann connection [64].

Before we are able to define this form, we have to notice that for all $p \in M$ the fibre passing through p is isomorphic to G, i.e. $F_{\pi(p)} \cong G$, and so the tangent space to the fibre at p, i.e. the vertical subspace at p, is tangent to the structure group. Therefore the vertical subspace is isomorphic to the Lie algebra of the structure group, i.e. $V_p \cong \mathfrak{g}$.

Let us study that isomorphism in more depth. Let $\xi \in \mathfrak{g}$ and $\mathbf{X}_\xi$ the corresponding infinitesimal generator of the right action of G on P corresponding to ξ as defined in Def. 2.2.2. The fibres being the orbits of the right action leads to the infinitesimal generator being tangent to the fibre. Therefore $\mathbf{X}_\xi(p) \in V_p$ for all $p \in P$, and the map $\varphi_p : \mathfrak{g} \to V_p$ defined by $\varphi_p(\xi) = \mathbf{X}_\xi(p)$ defines an isomorphism. This map effectively is the infinitesimal generator of the right action for a fixed point $p \in P$, for a fixed $\xi \in \mathfrak{g}$ the infinitesimal generator gives rise to a so-called *fundamental vector field* $p \mapsto \mathbf{X}_\xi(p)$.

This isomorphism is of interest to us, since now for all $v \in V_p$ there

exists a unique element $\overline{v} \in \mathfrak{g}$ such that $\mathbf{X}_{\overline{v}}(p) = v$. This enables us to define the following map that is an equivalent of Def. 3.2.3 for connection on a principal bundle.

Definition 3.2.5. Let (P, M, π, G) be a principal bundle and let $\mathcal{A} : P \times \mathfrak{X}(P) \to \mathfrak{g}$ be a $\mathfrak{g}$-valued 1-form on P defined by $\mathcal{A}_p(u) := \overline{\text{ver}(u(p))}$. The 1-form $\mathcal{A}$ is called a *connection (1-)form* on the principal bundle.

So the connection form on a principal bundle sends a vector field at a point p in the base space to the unique element of $\mathfrak{g}$ such that the infinitesimal generator at p evaluated at that element yields the vertical component of the vector field at p.

This $\mathfrak{g}$-valued 1-form on P can be restricted to a fibre, and since the fibres are diffeomorphic to the structure group G the restricted connection form $\mathcal{A}$ can be considered as a $\mathfrak{g}$-valued 1-form on G. This map satisfies $\mathcal{A}|_G(g) = \overline{g}$ for all $g \in G$. Using Def. 2.2.2 and Def. 2.3.4 one finds that $\mathcal{A}|_G$ is indeed the Maurer-Cartan form on G. Then Prop. 2.3.4 immediately yields the following result.

Theorem 3.2.1. *Let $\mathcal{A}$ be a connection form on a principal bundle. The canonical right action of G on P induces the transformation rule*

$$\tilde{R}_g^* \mathcal{A} = \text{Ad}_{g^{-1}} \mathcal{A} \tag{3.7}$$

for all $g \in G$. □

This transformation rule provides us how the connection form changes under the pull-back of the right action. In specific cases of G being a matrix Lie group this enables us to write down an explicit transformation law for the connection form.

Example 3.2.1. Let G be a matrix Lie group and $\mathcal{A}$ a connection form on a principal bundle, then $\tilde{R}_g^* \mathcal{A} = g^{-1} \mathcal{A} g$ for all $g \in G$. □

To be able to apply a version of Stokes' theorem in the end of this section we need to define a map that behaves similar as an exterior derivative. Before doing so we need the definition of yet another kind of derivation.

Definition 3.2.6. Let V a vector space and let $\mathcal{D} : \Omega^k(E, V) \to \Omega^{k+1}(E, V)$ be a map from V-valued k-forms to V-valued $(k+1)$-forms defined by

$$\mathcal{D}\alpha(u_1, ..., u_{k+1}) := d\alpha(\text{hor}(u_1), ..., \text{hor}(u_{k+1})) \tag{3.8}$$

for all $\alpha \in \Omega^k(E)$ and all $u_1, ..., u_{k+1} \in \mathfrak{X}(E)$. The map $\mathcal{D}$ is called the *covariant exterior derivative*.

This means that the covariant exterior derivative evaluated at $(u_1, ..., u_{k+1}) \in \mathfrak{X}(E)^{k+1}$ consists of evaluating the exterior derivative at the horizontal projection of each term of that vector. Since we can write down the exterior derivative using the Cartan formula as described in [15], the exterior covariant derivative can be written as

$$\mathcal{D}\alpha(u_1, ..., u_{k+1}) = \sum_{i=1}^{k+1}(-1)^i \mathrm{ver}[\mathrm{hor}u_i, \alpha(\mathrm{hor}u_1, ..., \widehat{\mathrm{hor}u_i}, ..., \mathrm{hor}u_{k+1})]$$
$$+ \sum_{i=1}^{k}\sum_{j=i+1}^{k+1}(-1)^{i+j}\alpha([\mathrm{hor}u_i, \mathrm{hor}u_j], \mathrm{hor}u_1, ..., \widehat{\mathrm{hor}u_i}, ..., \widehat{\mathrm{hor}u_j}, ..., \mathrm{hor}u_{k+1}). \tag{3.9}$$

This covariant derivative enables us to define the following map.

Definition 3.2.7. Let $\mathcal{A}$ be a connection form on a principal bundle. Then the $\mathfrak{g}$-valued 2-form $\mathcal{F} := \mathcal{D}\mathcal{A}$ is the *curvature form* on a principle bundle corresponding to $\mathcal{A}$.

Since the exterior covariant derivative is often impractical to work with, an alternative expression for the curvature form in terms of the connection form would be more than welcome. Fortunately, the Cartan formula, Eq. 3.2, yields the following result.

Proposition 3.2.1. *Let $\mathcal{A}$ a connection form and $\mathcal{F} := \mathcal{D}\mathcal{A}$ the corresponding curvature form. Then $\mathcal{F}$ satisfies the following* Cartan structure equation

$$\mathcal{F} = d\mathcal{A} + \frac{1}{2}[\mathcal{A}, \mathcal{A}] \tag{3.10}$$

with d the exterior derivative and $[-,-]$ the extended Lie bracket, Def. 2.3.2.

For a proof of this theorem one should consult chapter 11 of [64]. The exterior derivative and the Lie bracket are much more intuitive. Especially for the example of matrices groups this yields the following rule immediately.

Example 3.2.2. Let G be a matrix group and $\mathcal{A}$ a connection form, then $\mathcal{A} = d\mathcal{A} + \mathcal{A} \wedge \mathcal{A}$. Furthermore

$$\tilde{R}_g^* \mathcal{F} = d(g^{-1}\mathcal{A}g) + (g^{-1}\mathcal{A}g) \wedge (g^{-1}\mathcal{A}g) = g^{-1}(d\mathcal{A} + \mathcal{A} \wedge \mathcal{A})g = \mathrm{Ad}_{g^{-1}}\mathcal{F}. \tag{3.11}$$

Furthermore, let us state the following version of the *Bianchi identity*, which is an covariant analogue of the Bianchi identity for exterior derivatives.

Theorem 3.2.2 (Bianchi Identity)**.** *Let $\mathcal{F}$ be a curvature 2-form on E. The curvature satisfies the following Bianchi identity*

$$\mathcal{D}\mathcal{F} = 0. \tag{3.12}$$

A proof for this theorem is provided by Sontz in chapter 11 of [64]. This identity has important applications as we will see in Section 3.3.

For the remainder of this chapter, let $\pi : P \to M$ denote a principal G-bundle endowed with a connection form $\mathcal{A}$, and denote the corresponding curvature by $\mathcal{F}$.

3.2.1 Holonomies

Here we will revisit the interpretation of connection in terms of parallel transport. Let $\gamma : [0,1] \to M$ be a smooth curve, and define the operator of parallel transport $T_\gamma : \pi^{-1}(\gamma(0)) \to \pi^{-1}(\gamma(1))$ along γ by $p \mapsto \tilde{\gamma}(1)$. Here $\tilde{\gamma}$ is the unique horizontal lift of γ with $\tilde{\gamma}(0) = p$. This parallel transportation commutes with the right action of G on P, i.e. $p' = p \cdot g$ implies $T_\gamma(p') = T_\gamma(p) \cdot g$. For a proof of this statement one could consult chapter 10 of Sontz' book [64].

When we consider closed curves or loops, the lift also returns to the same fibre. Because the right action on the fibres is transitive and free this means there exist a unique element of G that sends the starting point of the horizontal lift to its end point.

Definition 3.2.8. Let $\gamma : [0,1] \to M$ be a closed curve, i.e. $\gamma(0) = \gamma(1)$, and consider the operator of parallel transport $T_\gamma : F_{\gamma(0)} \to F_{\gamma(1)} = F_{\gamma(0)}$. Then there exists a unique $\Phi(\tilde{\gamma}) \in G$ such that

$$T_\gamma(\tilde{\gamma}(0)) =: \tilde{\gamma}(0) \cdot \Phi[\tilde{\gamma}]. \tag{3.13}$$

The element $\Phi[\tilde{\gamma}]$ is called the *holonomy* of a loop γ with respect to the connection $\mathcal{A}$. The *holonomy group* of the connection with reference point $p_0 \in P$ is defined by

$$\mathrm{Hol}(p_0) := \{\Phi[\tilde{\gamma}] | \gamma \text{ closed }, \ \gamma(0) = \gamma(1) = \pi(p_0), \ \tilde{\gamma}(0) = p_0\} \tag{3.14}$$

The holonomy group of a connection with reference point $p_0 \in P$ is a subgroup of the structure group G. This group consists of all the elements

of G that by the canonical right action on a fibre send p_0 to the end point of a possible horizontal lift of a possible loop in M starting at $\pi(p_0)$.

By Def. 3.2.8 it seems like the holonomy group depends on the reference point in the fibre above $\gamma(0)$. Since we will consider loops in the base space and we want to study their holonomy groups, we want to find some relation between holonomy groups with reference points in the same fibre.

Proposition 3.2.2. *Let γ be a loop in M, $p_0, p_0' \in F_{\gamma(0)}$ two reference points. Then there exists a $g \in G$ such that* $\mathrm{Hol}(p_0') = g^{-1}\mathrm{Hol}(p_0)g$.

Proof. Because the canonical right action of G on the fibre, $F_{\pi(p_0)} = F_{\pi(p_0')}$, is transitive there exists a $g \in G$ such that $p_0' = p_0 \cdot g$. Let T_γ be the operator of parallel transportation along a curve γ with $\gamma(0) = \gamma(1) = \pi(p_0)$. On the one hand, this yields

$$T_\gamma(p_0') = p_0'\Phi[\tilde{\gamma}'] = p_0 \cdot g \cdot \Phi[\tilde{\gamma}'],$$

and on the other hand the compatibility of the operator of parallel transport and the canonical right action yields

$$T_\gamma(p_0') = T_\gamma(p_0) \cdot g = p_0 \cdot \Phi[\tilde{\gamma}] \cdot g.$$

Since the right action is free this means that $\Phi[\tilde{\gamma}'] = g^{-1} \cdot \Phi[\tilde{\gamma}] \cdot g$. □

Prop. 3.2.2 says that the holonomy groups of two reference points in the same fibre are conjugated subspaces of G and therefore isomorphic. This means that all holonomy groups with reference points in the same fibre are isomorphic. Hence we can omit writing the reference point and just refer to a holonomy group corresponding to a point in the base space.

3.3 Local connections and gauge transformations

In this section we will pave the way towards physics. This mostly consist of moving away from a global description of connections and towards a description in terms of local trivialisations. This shift in formalism is motivated by the fact that the base space often has some physical value, and therefore we would like to define local connections and curvatures there.

Let us now consider $f : U \to P$ with $U \subset M$ a local section of the principal bundle, and let α be a $\mathfrak{g}$-valued form on P, i.e. $\alpha \in \Omega(P, \mathfrak{g})$. This form can be pulled back via f, $f^*\alpha \in \Omega(U, \mathfrak{g})$. This same procedure can be carried out for connection and curvature forms.

Definition 3.3.1. Let $\{(U_i, \varphi_i)\}$ be a family of trivialisations. For every $x \in U_i$ define $f_i(x) := \phi_{i,x}(e)$, $\phi_{i,x}$ as defined in Def. 3.1.1. Then $A_{(i)} := f_i^* \mathcal{A}$ is the *connection form in the local trivialisation* φ_i, and $F_{(i)} := f_i^* \mathcal{F}$ the *curvature form in the local trivialisation* φ_i.

This enables us to express the connection and curvature on the base space, albeit only on in a local trivialisation. We want to know what happens when we change from local trivialisation. When it is known how the local connection changes between different local trivialisations we can go from one to the other, and through this consider the connection on the complete base space.

Theorem 3.3.1. *Let (U_i, φ_i) and (U_j, φ_j) be two local trivialisations. Consider the transition function γ_{ji}, and ω_0 the canonical Maurer-Cartan form on G. Then the local connections $A_{(i)}$ and $A_{(j)}$ are related as follows:*

$$A_{(i)}(x) = \mathrm{Ad}_{\gamma_{ji}^{-1}(x)} A_{(j)}(x) + (\gamma_{ji}^* \omega_0)(x), \tag{3.15}$$

and the local curvatures $F_{(i)}$ and $F_{(j)}$ as follows:

$$F_{(i)}(x) = \mathrm{Ad}_{\gamma_{ji}^{-1}(x)} F_{(j)}(x) \tag{3.16}$$

for all $x \in U_i \cap U_j$.

These transformation laws, of which the proof can be found in chapter 10 of Nakahara's book [54], do not look too friendly. This changes however when we consider the example of G a matrix Lie group, because the adjoint representation with matrix Lie groups is a well-behaved map.

Example 3.3.1. Consider the situation of Thm. 3.3.1 with G a matrix Lie group. Then Eq. 3.15 and Eq. 3.16 become

$$A_{(i)}(x)(u) = \gamma_{ji}^{-1}(x) \cdot A_{(j)}(x)(u) \cdot \gamma_{ji}(x) + \gamma_{ji}^{-1}(x) \cdot d\gamma_{ji}(x)(u),$$

respectively

$$F_{(i)}(x)(u, v) = \gamma_{ji}^{-1}(x) \cdot F_{(j)}(x)(u, v) \cdot \gamma_{ji}(x)$$

for all $x \in U_i \cap U_j$ and all $u, v \in T_x M$.

From this example we see that, although the local connection obtains an extra factor when transformed, the local curvature is transformed by

just conjugating. The physicists would say that the local curvature transforms in a tensorial way. This property hints on the curvature being a nice object to work with.

Now we will make a transition from the vocabulary and formalism of mathematics to that of physicists. First of all, a local section $f : U \to P$ is called a *local gauge*. Just as with local section a local gauge gives rise to a local connection and curvature form. A local connection form becomes a *(local) gauge potential*, and a local curvature form becomes a *(local) gauge field*. Also the use trivialisation moves to the background.

Definition 3.3.2. Let (U_i, φ_i) and (U_j, φ_j) be two local trivialisations, and denote the transition function from (U_i, φ_i) to (U_j, φ_j) by $\gamma_{ji} : U_i \cap U_j \to G$. This transition is called a *(local) gauge transformation*.

Let $f, f' : U \to P$ be two local gauges, then they differ by a gauge transformation, i.e. there exists a $g : U \to G$ such that $f'(x) = g(x) \cdot f(x)$ for all $x \in U$, because the transition function between the two corresponding local trivialisation always exists.

In the case of finite-dimensional manifolds and $G = \mathrm{Diff}(M)$, every diffeomorphism can be represented as a matrix and therefore G is a matrix group. From Ex. 3.3.1 it then follows that a local gauge transformation induces the following transformation

$$A' = g^{-1} \cdot A \cdot g + g^{-1} \cdot dg \tag{3.17}$$

of gauge potentials for $A' = f'^{*}\mathcal{A}$, $A = f^{*}\mathcal{A}$, and $f' = g \cdot f$, and

$$F' = g^{-1} \cdot F \cdot g \tag{3.18}$$

of the corresponding gauge fields. Two gauge potentials are said to be *gauge equivalent* if there exist a gauge transformation g such that Eq. 3.17 holds.

Now we have "translated" local trivialisations of connections and curvatures to gauges potentials and fields. We want to do the same for the notion of holonomies, since it will turn out that those will play a big role in the physical theory of geometrical phases.

Let γ be a closed curve in U, and let $f : U \to P$ be a local gauge. This gives rise to a closed curve $f \circ \gamma$ with starting and end point $p_0 = f(\gamma(0))$. Now let $\tilde{\gamma}$ be the horizontal lift of γ, and let $\Phi[\tilde{\gamma}]$ be its holonomy. It turns out [15] that

$$\Phi[\tilde{\gamma}] = P \exp\left(\int_{f(\gamma)} \mathcal{A}\right) = P \exp\left(\int_{\gamma} A\right) =: \Phi_f[\gamma] \tag{3.19}$$

where P denotes a path ordering operator, $A = f^*\mathcal{A}$ the local gauge potential in the gauge f, and $\Phi_f[\gamma]$ is called the *Wilson loop* in the local gauge f. For the Wilson loop changing from local gauge, i.e. $f'(x) = g(x) \cdot f(x)$ for all $x \in U$, induces the transformation law

$$\Phi_{f'}[\gamma] = g(\gamma(0))^{-1} \cdot \Phi_f[\gamma] \cdot g(\gamma) \tag{3.20}$$

similarly to Prop. 3.2.2. This gives rise to a value that is the same for all equivalent gauges, since the trace of the Wilson loop is invariant under gauge transformation according to Eq. 3.20.

Equipped with some theory about gauge transformations, gauge potentials, and gauge fields, is a perfect moment to introduce some examples of physical theories that can be formulated in terms of gauge potentials and gauge fields.

3.3.1 Electrodynamics

Electrodynamics, and especially Maxwell's laws, is arguably the biggest accomplishment of physics in the nineteenth century. Later it turned out that the theory of electrodynamics was already a relativistic theory in itself, and that fact comes forward in the gauge potential formulation of the theory. Although we will not dive deep into the whole description of electrodynamics as a gauge theory, shortly we see two of Maxwell's laws occur from a purely mathematical reasoning.

Let the base space M be a four dimensional pseudo-Riemannian manifold. This is our physical Minkowski space-time. Consider $U \subset M$ an open subset, and let $A_\mu : \mathbb{R} \to \mathbb{R}$ a component function of the $U(1)$-valued 1-form $A := iA_\mu dx^\mu$. We can define a local gauge $g : U \to U(1)$ be $g(x) = e^{i\lambda(x)}$ with $\lambda : U \to \mathbb{R}$ smooth. So at every point in our space-time we can smoothly assign a phase. Then we can write down the transformation law for our gauge potential:

$$\begin{aligned} A' &= g^{-1}Ag + g^{-1}dg = e^{-i\lambda(x)}(iA_\mu dx^\mu)e^{i\lambda(x)} + e^{-i\lambda(x)}e^{i\lambda(x)}id\lambda \\ &= iA_\mu dx^\mu + id\lambda = i(A_\mu + \partial_\mu\lambda)dx^\mu = A + id\lambda. \end{aligned}$$

This yields the know rule from undergraduate electrodynamics that you may add the derivative of a continuous differentiable function to your potential without changing the physics. That exactly corresponds to the gauge transformations of assigning a different phase to a point in your space-time.

Let us now consider the curvature, using the Cartan structure equation Eq. 3.10. We make use of the fact that $U(1)$ is abelian, and therefore it holds that $[A, A] = 0$, this yields

$$\begin{aligned} F = \mathcal{D}A = dA + \frac{1}{2}[A, A] = dA = d(iA_\mu dx^\mu) \\ = i\partial_\nu A_\mu dx^\nu \wedge dx^\mu = \frac{i}{2}(\partial_\nu A_\mu - \partial_\mu A_\nu)dx^\nu \wedge dx^\mu =: \frac{i}{2}F_{\mu\nu}dx^\mu \wedge dx^\nu, \end{aligned}$$

which leaves us with the following relation between the component functions of the gauge field and potential

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \tag{3.21}$$

Furthermore, in this abelian case the gauge field is invariant under gauge transformation. This is what you would expect from a physical point of view, since the components of the gauge field consist of physical information which should not be affected by a change in gauge.

Given the gauge field, or the local curvature, we can work a version of the Bianchi identity:

$$\begin{aligned} 0 = d^2A = dF = \frac{i}{2}(F_{\mu\nu}dx^\mu \wedge dx^\nu) = \frac{i}{2}\partial_\lambda F_{\mu\nu}dx^\lambda \wedge dx^\mu \wedge dx^\nu \\ = \frac{i}{6}(\partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} + \partial_\lambda F_{\mu\nu})dx^\mu \wedge dx^\nu \wedge dx^\lambda. \end{aligned}$$

Therefore $\partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} + \partial_\lambda F_{\mu\nu} = 0$, and it turns out that this expression that simply followed from a mathematical identity, corresponds with both Faraday's law of induction and Gauss' law of magnetism. How this formalism works in more detail, how it is related to Lorentz transformation, and how the other Maxwell's laws are obtain from these gauge potentials, goes beyond the scope of this example. A more elaborate consideration of Maxwell's laws in the formalism of connections on principal bundles is found in chapter 12 of [64].

3.3.2 Yang-Mills

Yang-Mills theory is a widely studied physical theory investigated not only because of its physical applicability, but also because of the geometrical beauty. Here we will only slightly touch upon this topic from a geometrical point of view and try to point out the similarities between Yang-Mills' and Maxwell's theory.

Consider a structure group $\mathrm{SU}(N)$ with $N > 1$. Let $\{L_1, ..., L_{N^2-1}\}$ be a basis of the Lie algebra $\mathfrak{su}(N)$. For this vectors we define the structure constants

$$[L_a, L_b] =: f_{ab}^c L_c. \tag{3.22}$$

Consider the following local connection

$$A = A_\mu dx^\mu$$

and local curvature

$$F = \frac{1}{2} F_{\mu\nu} dx^\mu \wedge dx^\nu.$$

With our knowledge about $\mathfrak{su}(N)$ we now that we can represent the generators $L_1, ..., L_{N^2-1}$ by anti hermitian matrices. Then we can express the gauge potential and gauge field as follows

$$A_\mu = A_\mu^a L_a, \quad F_{\mu\nu} = F_{\mu\nu}^a L_a. \tag{3.23}$$

To compare the geometry underlying Yang-Mills theory with the geometry of electrodynamics we will consider the relation between the gauge potential and gauge field.

From the structure formula in Eq. 3.10, which easily generalises to local curvature, the follow relation is obtained

$$\frac{1}{2} F_{\mu\nu} dx^\mu \wedge dx^\nu = \frac{1}{2} (\partial_\mu A_\nu - \partial_\nu A_\mu) dx^\mu \wedge dx^\nu + \frac{1}{2} [A, A]. \tag{3.24}$$

In component functions Eq. 3.24 reads

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]. \tag{3.25}$$

Be careful that in this step we have used two different Lie-brackets denoted by the same symbols, one for differential forms, Def. 2.3.2 and one for elements of a Lie algebra, Def. 2.2.1. Moreover, making use of Eq. 3.22 and Eq. 3.23 this yield the following relation for every generator

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + f_{bc}^a A_\mu^b A_\nu^c. \tag{3.26}$$

By comparing the gauge field in classical electrodynamics, Eq. 3.21, and Yang-Mills theory, Eq. 3.26, one could say that for every generator L^a a the Lie algebra $\mathfrak{su}(N)$ A_μ^a is a gauge potential analogue to the electromagnetic gauge potential. The same could be say about the field, albeit with an additional factor due to the group $\mathrm{SU}(N)$ not being commutative.

Furthermore, if we define a covariant derivative $D_\mu := \mathbb{1}\partial_\mu - A_\mu$, then we obtain

$$D_\mu F_{\nu\lambda} + D_\nu F_{\lambda\mu} + D_\lambda F_{\mu\nu} = 0, \tag{3.27}$$

which is similar to the identity in electrodynamics that encapsulates both Faraday's and Gauss' law. Therefore Yang-Mills theory can be interpreted as a noncommutative version of Maxwell's theory of electrodynamics.

Chapter 4

Geometrical phases

This chapter delves into an important approximation in quantum mechanics, the *adiabatic approximation*. This approximation is applicable when the Hamiltonian is "slowly" perturbed. Firstly, the adiabatic theorem is introduced as an asymptotic property of unitary operators. Subsequently, the results of the adiabatic theorem is utilised to define connections, the *Berry-Simon* and the *Wilczek-Zee connection*. Eventually, we will observe that the adiabatic approximation can lead to a non-trivial transformation of quantum states.

4.1 Adiabatic theorem

Let us consider a Hamiltonian $H(t)$ that continuously changes over a time T from an initial state $H(t_0)$ to a final state $H(t_1)$, with $T := t_1 - t_0$. Rewrite the Hamiltonian as $H(s)$ where $s := (t - t_0)/T$. The main idea of the adiabatic approximation is that in the infinitely slow limit, i.e. $T \to \infty$, a system that is initially in an eigenstate of $H(0)$ will pass into an eigenstate of $H(1)$. This idea originated from Ehrenfest's work on classical mechanics and the old quantum theory [17], and was later extended to quantum mechanics by Born and Fock [13]. Shortly we will see what the exact conditions are for the adiabatic approximation, and how it can be rigorously formulated mainly following the work of Kato and the textbook of Messiah [30], [51].

Theorem 4.1.1 (Adiabatic theorem)**.** *Let $H(s)$ be a continuous Hamiltonian, with $s \in [0, T]$. Assume that $H(s)$ has a discrete spectrum with eigenvalues $\{E_j(s)\}_j$ for all $s \in [0, T]$. Define $\{P_j(s)\}_j$ as the set of projections onto the*

eigenspaces, i.e. $P_j(s)$ projects a vector on the eigenspace corresponding to $E_j(s)$. Suppose that the following conditions hold:

i) E_j and P_j depend continuous on s for all $s \in [0, T]$;

ii) the eigenvalues remain distinct, i.e. $E_i(s) \neq E_k(s)$ for all $E_i, E_k \in \{E_j\}_j$ and $s \in [0, T]$;

iii) the derivatives $d_s E_j(s)$, $d_s P_j(s)$, and $d_s^2 P_j(s)$ are piece-wise continuous for all $s \in [0, T]$.

Furthermore, denote the evolution operator satisfying the Schrödinger equation by $U_T(s)$, i.e.

$$id_s U_T(s) = TH(s)U_T(s), \tag{4.1}$$

where $H(s)$ is the diagonalised Hamiltonian, i.e. $H(s) = \sum_j E_j(s)P_j(s)$. Then $U_T(s)$ has the asymptotic property

$$\lim_{T\to\infty} U_T(s)P_j(0) = P_j(s) \lim_{T\to\infty} U_T(s) \tag{4.2}$$

for all $P_j \in \{P_j\}_j$.

Before this theorem can be proven a couple of remarks should be made. First of all, it is important to note that the spectrum does not have to be continuous [30]. However, to simplify the proof a bit this is assumed. Secondly, the theorem boils done to Eq. 4.2 which says that it does not matter whether you first project onto an eigenspace, and subsequently let that state evolve through time, or if you first let a state evolve through time and then project it onto an eigenspace. Therefore Thm. 4.1.1 is indeed inline with the main idea of the adiabatic approximation that the eigenstates of the initial Hamiltonian are deformed into eigenstates of the final Hamiltonian, provided infinitely slow and continuous changes of the Hamiltonian.

Furthermore, some preparations should be done for the proof of Thm. 4.1.1, because exactly solving the Schrödinger equation, Eq. 4.1, using integration is no longer possible since the eigenvectors of $H(s)$ - despite being in the same Hilbert space - under go some kind rotation. We want to transform the Hamiltonian in such a way that exactly solving the Schödinger equation becomes feasible again.

Introduce a unitary operator $A(s)$ satisfying

$$P_j(s) = A(s)P_j(0)A^\dagger(s). \tag{4.3}$$

This operator sends the eigenvectors of $H(0)$ to the corresponding eigenvectors of $H(s)$ that follow from continuity. It is not yet completely evident how this $A(s)$ is defined. The existence of such a $A(s)$ becomes clear by defining it as the solution to the following differential equation

$$id_sA(s) = K(s)A(s), \;\; A(0) = 1 \tag{4.4}$$

where $K(s)$ is a Hermitian operator that obeys the commutation relations

$$[K(s), P_j(s)] = id_sP_j \tag{4.5}$$

for all projections on eigenspaces. This is a necessary requirement of $K(s)$ since it is immediately yielded by differentiating Eq. 4.3 and Eq. 4.4. Furthermore, $A(s)$ and $P_j(s)$ satisfying Eq. 4.4 and Eq. 4.5 respectively implies that

$$d_s(A^\dagger(s)P_j(s)A(s)) = 0$$

for all $s \in [0, 1]$, and hence

$$A^\dagger(s)P_j(s)A(s) = A^\dagger(0)P_j(0)A(0) = P_j(0).$$

Therefore Eq. 4.5 is restrictive enough on $K(s)$. However, there is still some ambiguity in the definition of $K(s)$. This can be resolved by the imposing the condition

$$P_j(s)K(s)P_j(s) = 0. \tag{4.6}$$

Combining this yields an expression for $K(s)$ [51]

$$K(s) = i\sum_j (d_sP_j(s))P_j(s). \tag{4.7}$$

Now $K(s)$ has been found and it is continuous. Since this means that Eq. 4.4 has a solution, by Peano's existence theorem, and therefore the existence of a $A(s)$ is proven. Using Eq. 4.3 we can write our Hamiltonian is the so-called *rotating axis representation*

$$H^{(A)}(s) := A^\dagger(s)H(s)A(s). \tag{4.8}$$

Similarly we can rewrite other operators is the rotating axis representation,

$$U^{(A)}(s) := A^\dagger(s)U_T(s) \tag{4.9}$$

and

$$K^{(A)}(s) := A^\dagger(s)K(s)A(s). \tag{4.10}$$

Combining Eq. 4.1, 4.4, 4.8, 4.9, and 4.10 we obtain an alternative formulation of the Schrödinger equation

$$id_s U^{(A)}(s) = [TH^{(A)}(s) - K^{(A)}(s)]U^{(A)}(s), \;\; U^{(A)}(0) = 1. \tag{4.11}$$

In the proof of the adiabatic theorem that we will give shortly, we will see that in the limit $T \to \infty$ the effect of $K^{(A)}$ on the solution of Eq. 4.11 is negligible, yielding an straight forward solvable differential equation.

Proof. Let $\Phi_T(s)$ be the solution of the following Schrödinger equation

$$id_s \Phi_T(s) = TH^{(A)}(s)\Phi_T(s), \;\; \Phi_T(0) = 1. \tag{4.12}$$

One can find Φ_T by integrating the equation

$$\Phi_T(s) = \sum_j e^{-iT\varphi_j(s)} P_j(0), \tag{4.13}$$

where

$$\varphi_j(s) := \int_0^s E_j(t)dt. \tag{4.14}$$

Now define a new unitary transformation using this solution

$$W := \Phi_T^\dagger U_T^{(A)} = \Phi_T^\dagger A^\dagger U_T. \tag{4.15}$$

Because Φ_T satisfies Eq. 4.12 and $U^{(A)}$ Eq. 4.11, we obtain a Volterra equation of the second kind for W

$$W(s) = 1 + i\int_0^s \overline{K}(t)W(t)dt, \tag{4.16}$$

where

$$\overline{K} := \Phi_T^\dagger K^{(A)} \Phi_T. \tag{4.17}$$

We want to show that the integral part of Eq. 4.16 vanishes when $T \to \infty$. Therefore we will look into the components of $\overline{K}$.

Before doing so, notice that any Hermitian operator L can be written in a spectral decomposition form, which reads

$$L = \sum_{j,k} P_j(0) L P_k(0) =: \sum_{j,k} L_{jk}. \tag{4.18}$$

From Eq. 4.3, 4.13, and 4.17 we obtain the spectral decomposition of $\overline{K}$ with components

$$\overline{K}_{jk} = e^{iT(\varphi_j - \varphi_k)} K_{jk}^{(A)} := e^{iT(\varphi_j - \varphi_k)} A^\dagger P_j K(s) P_k A. \tag{4.19}$$

From this expression it becomes clear why Eq. 4.6 is imposed, since this yields $\overline{K}_{jj} = 0$.

Let us again define an auxiliary operator

$$F(s) := \int_0^s \overline{K}(t)dt, \tag{4.20}$$

for which the components are immediately clear by Eq. 4.19

$$F_{jk} = \int_0^s e^{iT(\varphi_j - \varphi_k)} K_{jk}^{(A)} dt. \tag{4.21}$$

By partially integrating these components we obtain

$$\begin{aligned} F_{jk} = \frac{1}{iT}\Bigg(&\left[e^{iT(\varphi_j(t)-\varphi_k(t))} \frac{K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right]_0^s \\ &- \int_0^s e^{iT(\varphi_j(t)-\varphi_k(t))} \frac{d}{dt}\left(\frac{K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right) dt \Bigg). \end{aligned} \tag{4.22}$$

We want to show that these components all converge to 0. For the diagonal components we already have $F_{jj} = 0$. Therefore we will only consider the off-diagonal components, where we use our assumption that $E_j(s) \neq E_k(s)$ for all $s \in [0,1]$ and $j \neq k$. Using the triangle inequality we obtain

$$\begin{aligned} ||F_{jk}|| \leq \frac{1}{T}\Bigg(&\left|\left| e^{iT(\varphi_j(t)-\varphi_k(t))} \frac{K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right|\right| \\ &+ \left|\left| e^{iT(\varphi_j(t)-\varphi_k(t))} \frac{K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right|\right| \\ &+ \int_0^s \left|\left| e^{iT(\varphi_j(t)-\varphi_k(t))} \frac{d}{dt}\left(\frac{K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right) \right|\right| dt \Bigg) \\ = \frac{1}{T}\Bigg(&\left|\left| \frac{K_{jk}^{(A)}(s)}{E_j(s) - E_k(s)} \right|\right| + \left|\left| \frac{K_{jk}^{(A)}(0)}{E_j(0) - E_k(0)} \right|\right| + \int_0^s \left|\left| \frac{d_t K_{jk}^{(A)}(t)}{E_j(t) - E_k(t)} \right|\right| dt \\ &+ \int_0^s \left|\left| \frac{K_{jk}^{(A)}(t)}{(E_j(t) - E_k(t))^2} (d_t E_j(t) - d_t(E_k(t)) \right|\right| \Bigg). \end{aligned} \tag{4.23}$$

Since $E_j(s)$, $E_k(s)$, and $K_{jk}^{(A)}(s)$ and their derivatives are least piecewise continuous on $[0,1]$, they are bounded. Therefore, it follows that

$$F(s) = O(T^{-1}) \tag{4.24}$$

for $T \to \infty$.

Returning to the integral of Eq. 4.16, we can write it as

$$\int_0^s \overline{K}(t)W(t)dt = F(s)W(s) - \int_0^s F(t)d_tW(t)dt \tag{4.25}$$

and by substituting $d_tW = i^{-1}\overline{K}(t)W(t)$ this becomes

$$\int_0^s \overline{K}(t)W(t)dt = F(s)W(s) - i^{-1}\int_0^s F(t)\overline{K}(t)W(t)dt \tag{4.26}$$

Now let $\varepsilon(T) \in \mathbb{R}$ be an upper bound of $||F||$ for a given T with $\varepsilon(T) = O(T^{-1})$, and let $\delta \in \mathbb{R}$ be an upper bound of $||K||$. Notice that W is a unitary operator, this yields:

$$\begin{aligned}\left|\left|\int_0^s \overline{K}(t)W(t)dt\right|\right| &\leq ||F(s)W(s)|| + s\sup(||F(t)\overline{K}(t)W(t)||) \\ &\leq ||FW|| + s||F(t)\overline{K}(t)W(t)|| = (1 +^{-1} \delta s)\varepsilon(T).\end{aligned} \tag{4.27}$$

Hence Eq. 4.16 can be written as

$$W = 1 + O(T^{-1}). \tag{4.28}$$

Substituting Eq. 4.28 in the definition of our auxiliary operator W, Eq. 4.15, yields

$$U_T(s) = A(s)\Phi_T(s)(1 + O(T^{-1})), \tag{4.29}$$

thus

$$\lim_{T\to\infty} U_T(s) = A(s)\Phi_T(s). \tag{4.30}$$

For both $A(s)$ and $\Phi_T(s)$ we know how they commute with the projections $P_j(s)$ and $P_j(0)$, Eq. 4.3 and Eq. 4.13. Therefore we conclude

$$A(s)\Phi_T(s)P_j(0) = P_j(s)A(s)\Phi_T(s). \tag{4.31}$$

Eq. 4.31 together with Eq. 4.30 verifies the asymptotic property

$$\lim_{T\to\infty} U_T(s)P_j(0) = P_j(s)\lim_{T\to\infty} U_T(s).$$

□

The adiabatic theorem is a beautiful piece of mathematics, but unfortunately in physics the limit of $T \to \infty$ can never be fulfilled. Although the value of T can be enormous, and the Hamiltonian can vary extremely "slow", the change of the Hamiltonian still happens in finite time. Therefore in physics the adiabatic theorem is never directly applicable, one would always make use of the *adiabatic approximation*. In the adiabatic approximation on replaces the evolution operator with its asymptotic one that occurs in the adiabatic theorem.

When one follows the derivation of the adiabatic approximation in Sakurai's [61] or Messiah's [51] book on quantum mechanics the following constraint on the energies is obtained for the adiabatic approximation to hold for a state starting in the eigenspace corresponding to $E_i(0)$

$$\frac{|\langle E_j(s)|d_s|E_i(s)\rangle|}{|E_j(s) - E_i(s)|} << 1 \tag{4.32}$$

for all energies E_j with $j \neq i$, and all $s \in [0,1]$ [61]. This criterion can be equivalently formulated as

$$\frac{\max_{s\in[0,1]} \left\{ \sqrt{\sum_{j\neq i} |\langle E_j(s)|d_s|E_i(s)\rangle|^2} \right\}}{\min_{s\in[0,1], j\neq i}\{|E_j(s) - E_i(s)|\}} << 1 \tag{4.33}$$

which can be physically interpreted as the ratio between the maximum angular velocity of $|E_i(s)\rangle$ in the numerator and the minimum Bohr frequency in the denominator being much smaller than one [51].

At first sight these criteria do not look easily verifiable. However, in certain cases this the ratio can be estimated in a straight forward way. Consider a system with a state starting in the ground state with corresponding energy $E_1(s) = 0$, and an energy gap of E between the ground state and the other states. In this system the denominator is just the energy gap in the spectrum, i.e. E. The numerator can be bounded from above by 1, because of the normalisation of the states. Therefore the criterion for applying the adiabatic approximation to states in the zero-energy ground state and a gapped spectrum becomes

$$\frac{1}{E} << 1. \tag{4.34}$$

Yet one more step is required is to obtain an indication for the "slowness" of the variation of the Hamiltonian, namely the criterion in terms of energy has to be translated to a criterion in terms of time. To do that we

make use of the uncertainty relation of time and energy

$$\delta t \delta E \geq \frac{1}{2} \tag{4.35}$$

which says that the uncertainty in time multiplied by the uncertainty in energy is bounded from below. By considering the equality in Eq. 4.35 a relation between the energy and time can be obtained. Let δE be the energy gap and δt the time scale of the adiabatic variation of the Hamiltonian, then the criterion for applying the adiabatic approximation becomes

$$2\delta t = \frac{1}{E} << 1. \tag{4.36}$$

The criteria in Eq. 4.32 and Eq. 4.33 are generally used as the conditions a system has to satisfy for being suitable for applying the adiabatic approximation. However, it is shown by Marzlin and Sanders that those equivalent criteria may not be enough, when the change in the eigenstates is significant [50]. Fortunately, there exist some additional conditions which ensures that the approximation is still widely applicable [72]. Going in to the details of these conditions would go beyond the scope of this thesis. However, it is important to notice that the problems with the original criterion, Eq. 4.32, occur when the changes in the Hamiltonian are small instead of taking place "slowly" [46]. Therefore we assume that when slow variations of the Hamiltonian are considered - a naive notion of adiabatic movement - the criterion of Eq. 4.33 is sufficient, and corollaries such as Eq. 4.36 hold.

4.1.1 Ehrenfest's intermezzo

Let us take a moment to step back from the mathematical formulation of the adiabatic theorem and take a moment to reflect on the physical meaning. In the spirit of Paul Ehrenfest, one of the founders of the adiabatic principle [17] and a physicist of huge importance for the physics community in Leiden, we should try to develop some understanding of the theorem without any of the mathematics. Ehrenfest once said in a letter to Oppenheimer: *"If you intend to mount heavy mathematical artillery again during your coming year in Europe, I would ask you not only not to come to Leyden, but if possible not even to Holland..."* [34]. In line with his metaphor of dogs and fleas to explain irreversible processes, we will come up with a metaphor for the adiabatic theorem.

Image the old town of Leiden, surrounded by the canals, "de singels". A student needs to clear his head after an excruciatingly difficult exam,

and decides to go for a run. We can think of the student running at his own constant pace as a system in an eigenstate. The eigenstate is characterised by the movement of his legs and his heart beat. Then, with a change of the reference frame, we take the student to be fixed and the canals and the whole of Leiden to move around him, these form the changing potential. The running pace translate to the relevant time scale, and since the average running speed is not too high we call this adiabatic movement. Because the turns in the road and road crossing only come towards the runner slowly the runner can keep its pace with only minor changes in direction and speed. Hence the runner stays in the same eigenstate despite the changing potential around him.

Now imaging a different system, a cyclist, riding by the old canals around Leiden. His pace is much faster, and so the potential landscape, i.e. his surroundings, change much faster. The result is that the cyclist has to use his breaks constantly, and slow down and accelerate several times during his round trip. This means that the cyclist does not stay in his eigenstate, which can be understood from the point of view of the adiabatic theorem, since the student does not cycle slow enough and the adiabatic approximation does not apply.

4.2 Berry phase

In 1984 M. Berry theoretically discovered that periodic adiabatic changes in the Hamiltonian could lead to an additional phase of a state that was *non-trivial*, i.e. that had a physical consequences and could not be brushed away with a gauge transform [12]. This additional phase can be explained using the result of the adiabatic theorem and the geometric formalism of connections and gauges.

Let M be a smooth manifold, $\mathcal{H}$ a finite-dimensional Hilbert space, and consider a smooth Hamiltonian $H : M \to \mathcal{C}^\infty(\mathcal{H})$ with $H(x)$ being Hermitian for all $x \in M$. Furthermore, we make the same assumptions for the eigenvalues and projections on the corresponding eigenspaces as in the adiabatic theorem, Thm. 4.1.1, and on top of that we assume that those projections and energies are smooth. For every $x \in M$ we denote the nth eigenspace of $H(x)$ by $\mathcal{H}_n(x)$, and we attach the fibre $F_x := \mathbb{P}\mathcal{H}_n(x)$. Therefore we obtain the bundle space

$$P := \bigsqcup_{x\in M} F_x = \bigsqcup_{x\in M} \mathbb{P}\mathcal{H}_n(x), \tag{4.37}$$

which we will refer to as the nth spectral bundle of H.

For the remainder of this section we will assume that the nth eigenspace is non-degenerate. This simplifies the fibres defined above drastically. Let $|\psi(x)\rangle$ be a nth ground state of $H(x)$, then $\mathbb{P}\mathcal{H}_n(x) = \{e^{i\theta}|\psi(x)\rangle : \theta \in \mathbb{R}\} \cong U(1)$, since the space is non-degenerate. This gives rise to a principal $U(1)$-bundle.

We want to endow this principal $U(1)$-bundle with a connection which captures the adiabatic theorem. A natural way of assigning a horizontal subspace to the fibres, is to call a vector $|h(x)\rangle \in T_xP$ horizontal if it is orthogonal to $|n(x)\rangle$, i.e. $P_n(x)|h\rangle = 0$. That this is smooth should follow from the smoothness of P_n. A connection defined in this way is called a *Berry-Simon connection* [15], [62]. In this assignment it is crucial that a state that started in the nth eigenspace, remains there. Therefore this connection heavily depends on the adiabatic theorem, Thm. 4.1.1.

Let us study how we can interpret this in terms of horizontal lifts. Let $\gamma : [0,1] \to M$ be a smooth curve in M, then $\tilde{\gamma} : [0,1] \to P$ is a horizontal lift with respect to the Berry-Simon connection if $\tilde{\gamma}$ satisfies

$$P_n(\gamma(s))\partial_s\tilde{\gamma}(s) = 0 \tag{4.38}$$

Therefore a horizontal lift in this case would lift a point x from a curve in the parameter space M to an nth eigenstate of $H(x)$ which is in the so-called *Born-Fock gauge*, i.e. $P_n(\gamma(s))\partial_s|n(\gamma(s))\rangle = 0$. This can physically be seen that adiabatic evolution corresponds to parallel transport, since one can find that for adiabatic evolution one automatically fulfils the Born-Fock gauge [15].

From now on we might discard writing the projection operators explicitly as above and write them in the so-called *bra-ket notation*, where a projection is written as $P_n(x) = |n(x)\rangle\langle n(x)|$. When one is not familiar with this convention, an comprehensive introduction can be found in undergraduate quantum mechanics textbooks [19].

The local section $x \mapsto |n(x)\rangle$ of the nth spectral bundle gives rise to a $\mathfrak{u}(1)$-valued 1 form. This (local) *Berry-Simon connection 1-form* is given by

$$A^{(n)}(x) := i\langle n(x)|\partial_s n(x)\rangle ds = i\langle n(x)|dn(x)\rangle. \tag{4.39}$$

Expressing Eq.4.39 in local coordinates (x^μ) defines the component functions of the local connection

$$A^{(n)}(x) = i\langle n(x)|dn(x)\rangle = i\langle n(x)|\partial_\mu n(x)\rangle dx^\mu =: A^{(n)}_\mu(x)dx^\mu. \tag{4.40}$$

Equipped with the connection 1-form it is reasonable to consider the holonomy of a curve $C \subset M$ with respect to the Berry-Simon connection. With

this holonomy we define the *Berry phase* $\gamma_(C)$ of a state in the nth eigenspace corresponding to the curve C with respect to given connection

$$e^{i\gamma_n(C)} := \exp\left(\oint_C A^{(n)}\right) = \exp\left(i\oint_C \langle n|dn\rangle\right). \tag{4.41}$$

From Eq. 4.41 and $U(1)$ being Abelian it is immediately clear that the Berry phase is gauge invariant. This phase does not depend on a gauge is solely dependent on the geometry of the curve in the base space, the structure of the principal bundle and the connection on the fibres. Hence the Berry phase is an example of a *geometrical phase*.

This integral over the curve C can be transformed to a integral over a surface by introducing the (local) *Berry-Simon curvature*

$$F^{(n)} = dA^{(n)} = -\frac{1}{2}\mathrm{Im}(\langle\partial_\mu n|\partial_\nu n\rangle - \langle\partial_\nu n|\partial_\mu n\rangle)dx^\mu \wedge dx^\nu \tag{4.42}$$

where the components are defined by

$$F^{(n)}_{ij} := \mathrm{Im}(\langle\partial_\mu n|\partial_\nu n\rangle - \langle\partial_\nu n|\partial_\mu n\rangle). \tag{4.43}$$

Let Σ be a submanifold M such that $\partial\Sigma = C$, then applying Stokes' theorem [39] to Eq. 4.41 yields

$$e^{i\gamma_n(C)} = \exp\left(\oint_C A^{(n)}\right) = \exp\left(\int_\Sigma F^{(n)}\right). \tag{4.44}$$

In physics the Berry-Simon connection is derived from the assumption that after a adiabatic loop the gained phase can be divide in a dynamical part and a geometrical part

$$\varphi(t) = -\int_0^t E_n(\tau)d\tau + \gamma_n(t) \tag{4.45}$$

where $\gamma_n(t)$ is the geometrical phase. Eventually, manipulating the state $\psi(t) = e^{i\varphi(t)}\psi(0)$ and the Schrödinger equation yields the same integral expression as Eq. 4.41. For a long time it was thought that this phase could be cancelled by an appropriate gauge transformation, which turned out to be not the case [12]. From this alternative derivation it becomes clear that there is a one-to-one correspondence between the holonomies of a principle $\mathfrak{u}(1)$-bundle in mathematics and the Berry phase in physics.

The Berry phase and geometrical phases in general are essential to explain certain phenomena in classical optics [56], molecular physics [43],

electrodynamics [1], and condensed matter [77]. Some of these phenomena, such as the Aharonov-Bohm effect [1], were known well before the theoretical discovery of the Berry phase.

Let us quickly discuss a methods to measure a Berry phase. In this method one state should be prepare and divided in two subsystems. One of them is cycled adiabatically, while the other is not. When brought back together the phase difference results into a certain interference which differs from the initial state. One of the hardships of finding the Berry phase is taking into account the dynamical phase that should be subtracted, which can difficult because phases are defined up to 2π. With a protocol such as described above Zhang *et. al.* succeed in measuring a Berry phase in optical fibres in 1986 [77].

4.3 Wilzcek-Zee phase

In last section we defined a connection on a bundle space P with the fibres being the projective non-degenerate nth eigenspaces. However, degenerate eigenstate are omnipresent in physics, and the adiabatic theorem is applicable to systems with degenerate eigenstates as well. Therefore it is interesting and possible to generalise the notion of a Berry phase to a non-degenerate setting as shown by Wilzcek and Zee [75].

Let $M, \mathcal{H}$, and H be as in last section, and this gives rise to the bundle space from Eq. 4.37. Now say that $\mathcal{H}_n(x)$ is m-fold degenerate, with $m > 1$. Let $\{|\psi_i\rangle\}_{i=1}^m$ be an orthonormal basis of of $\mathcal{H}_n(x)$, then the fibres can be expressed as

$$F_x := \mathbb{P}\mathcal{H}_n(x) = \left\{ |\varphi(x)\rangle = \sum_{i=1}^{m} U_i^j |\psi_j(x)\rangle : U \in U(m) \right\} \cong U(1), \quad (4.46)$$

where the fibres are identified with the *unitary group of degree n*. Eq. 4.46 enables us to consider a principal $U(m)$-bundle over M.

Equipped the setting is similar to that of the Berry phase and hence it is natural to try generalising the Berry-Simon connection. Here we call a vector $|h(x)\rangle \in T_x P$ is horizontal if it is orthogonal to the basis $\{|\psi_i\rangle\}_{i=1}^m$, i.e. $\langle\psi_i(x)|h\rangle = 0$ for all $i \in \{1, ..., m\}$. The connection defined in this way is called a *Wilczek-Zee connection* [75].

If $C : [0,1] \to M$ a smooth curve with a lift $\tilde{C} : [0,1] \to P$ given by $\tilde{C}(s) = (\varphi_1(t), ..., \varphi_m(t))$, then this lift is horizontal if for all $i, j \in \{1, ..., m\}$ it holds that $\langle\psi_i|\partial_s\varphi_j\rangle = 0$. This means that having a state in the generalised Born-Fock gauge the physical analogue of being parallel transported with respect to the Wilczek-Zee connection.

Similarly to the non-degenerate case the local section $x \mapsto |\varphi\rangle$ gives rise to a $\mathfrak{u}(m)$-valued 1-form, the so-called *Wilczek-Zee connection 1-form*, where every element of the matrix is defined in the following way

$$\left(A^{(m)}\right)_{ij}(x) := i\langle\psi_j(x)|\partial_s\psi_i(x)\rangle = i\langle\psi_j(x)|d\psi_i(x)\rangle. \tag{4.47}$$

Notice that these are not the component function expressed in local coordinates, but the entries of the matrix $A^{(m)}(x)$ since $A^{(m)}$ is $\mathfrak{u}(m)$-valued. In local coordinates (x^μ) the component functions (per entry) read

$$\left(A^{(m)}_\mu\right)_{ij} := i\langle\psi_j(x)|\partial_\mu\psi_i(x)\rangle. \tag{4.48}$$

This connection is very similar to the Berry phase. However, there are some essential differences, mainly because $U(m)$, in contrast to $U(1)$, is non-abelian. This has some important implication for the transformation of the connection. Let $\{|\psi_i'\rangle\}_{i=1}^m$ be a new basis orthonormal basis of $\mathcal{H}_n(x)$ obtained from $\{|\psi_i\rangle\}_{i=1}^m$ by applying the unitary transformation U. One can check that this results in the transformation rule

$$\left(A'^{(n)}\right)_{ij} = \left(U\cdot A^{(n)}\cdot U^\dagger + i(dU)\cdot U^\dagger\right)_{ij} \tag{4.49}$$

which is exactly what you would expect for a gauge potential.

Similar to the Berry-Simon curvature in the non-degenrate case, we can define a $\mathfrak{u}(m)$-valued 2-form called the (local) *Wilczek-Zee curvature*

$$F^{(n)} = dA^{(n)} - iA^{(n)}\wedge A^{(n)}, \tag{4.50}$$

the entry functions of which can be expressed as

$$\left(F^{(n)}\right)_{ij} = \frac{1}{2}\left(\partial_\mu\left(A^{(n)}_\nu\right)_{ij} - \partial_\nu\left(A^{(n)}_\mu\right) - i\left([A^{(n)}_\mu, A^{(n)}_\nu]\right)_{ij}\right)dx^\mu\wedge dx^\nu, \tag{4.51}$$

and therefore the component functions can be defined by

$$\left(F^{(n)}_{\mu\nu}\right)_{ij} := \partial_\mu\left(A^{(n)}_\nu\right)_{ij} - \partial_\nu\left(A^{(n)}_\mu\right) - i\left([A^{(n)}_\mu, A^{(n)}_\nu]\right)_{ij}. \tag{4.52}$$

The components look way more complicate than the non-degenerate case. Fortunately, Eq. 4.49 and Eq. 4.50 provide a transformation rule for the curvature that is quite neat and in line with what you would expect from a gauge field

$$F'^{(n)} = U\cdot F^{(n)}\cdot U^\dagger, \tag{4.53}$$

i.e. the curvature transforms in a tensorial way.

A non-degenerate counterpart of the Berry phase, the *geometric Wilczek-Zee factor* can be defined as the holonomy of a curve $C \subset M$ with respect to the Wilczek-Zee connection as the *path ordered integral*

$$V(C) := \mathcal{P} \exp\left(\oint_C A^{(n)} \right), \tag{4.54}$$

where $\mathcal{P}$ is the *path ordering operator* that takes care of the order of operations. This is necessary because the connection is $\mathfrak{u}(m)$-valued and two elements of $\mathfrak{u}(m)$ do not necessarily commute.

Making use of Stokes' theorem Eq. 4.54 can be rewritten in terms of the curvature

$$V(C) = \mathcal{P} \exp\left(\int_\Sigma F^{(n)} \right), \tag{4.55}$$

where $\Sigma \subset M$ is a submanifold such that $\partial\Sigma = C$. From Eq. 4.55 and the transformation rule of the Wilczek-Zee factor, Eq. 4.53, it is immediately clear that the geometrical Wilczek-Zee factor is gauge invariant.

An actually measurement of the geometric Wilczek-Zee factor can be done in a way that is similar to measuring the Berry phase. Although there has been a lot of theoretical and experimental interest in the non-degenerate counterpart of the Berry phase, synthesised systems that exhibit these factors are rare. A lot of contemporary research goes into designing cold-atom systems that give rise to non-trivial Wilson loops [66].

Chapter 5

Second quantisation

The main aim of many-body quantum mechanics is to describe the properties of systems with many particles. In this chapter a formalism will be introduced that is extremely suitable for this purpose, *second quantisation*. Following [5] and [49], we will build up a description of fermionic many-body systems from first principles that encapsulates both the indistinguishability of quantum particles and the anti-symmetry of fermionic wave functions. The *fermionic Fock space* and *creation* and *annihilation operators* will be introduced. It turns out that an algebra of these operators unique determine our formalism. We will conclude the discussion of second quantisation with several elementary applications and a by highlighting the similarities between the creation and annihilation operators and the familiar ladder operators. By the end of the chapter we are fully equipped to describe many-body systems in a concise manner.

5.1 First and second quantisation

The name second quantisation of course implies that there exist a formalism called first first quantisation. This is indeed true, such a formalism exists. Let us start with a classical system that is described by a phase space with p_i a momentum vector and x_j a position vector. Now we want to quantise our phase space. Although quantising a space is an active field of research in mathematical physics, using *canonical quantisation* is most common in physics. This means that we impose the following condition on the momentum and position vector p_i and x_i:

$$[p_i, x_j] = -i\delta_{ij}, \tag{5.1}$$

where $[-,-]$ is the commutator and δ_{ij} the Kronecker delta. This is a very intuitive way of quantising a space. However, the problems occur when one wants to describe interactions in a system that is quantised using canonical first quantisation. To include interactions in the Hamiltonian of a system all configurations of the particles in the system have to be added by hand.

Fortunately, there is away around this. Let $\pi(x)$ be a vector field corresponding to the momentum in phase space, and let $\psi(x)$ be a vector field corresponding to the positions. Then the idea of second quantisation is imposing the condition

$$[\pi(x), \psi(y)] = -i\delta^3(x_i - y_i), \tag{5.2}$$

where $\delta^3(x_i - y_i)$ is the three dimensional Dirac delta function. As a consequence of this formalism the interactions are embedded in the description [52].

The conclusions drawn in this section are hand-wavy, since no actual quantisation is performed, no system is specified, and no interaction is described explicitly. However, the second quantisation has enough advantages to make it the most popular description in contemporary physics. In the following section we will not perform an explicit quantisation. We will construct a formalism for many body systems from first principles, without explicitly referring to the quantisation of a phase space. Nevertheless, it should be ensured that the formalism arising from Eq. 5.2 and the formalism that will be constructed in the following sections are two sides of the same coin as one can see in chapter 1 of Kaku's book [52].

5.2 Number representation and Fock space

Let us consider a system of N particles. When such a system is first encountered, it is natural to write down the state of each of these particles separately. This sounds most reasonable to do, because the system consists of N particles, and from a classical point of view this would mean that we have to deal with N different or distinct particles. In quantum mechanics however, we know that fermions and bosons are indistinguishable particles. This enables us to represent the total state of our system by just describing the number of particles in a specific state. Moreover, in this new formalism we want to let go of the fixed particle number, since there are systems, e.g. systems displaying superconductivity, where particle number is not conserved. This *occupation number representation* will be formalised further in this chapter.

Before we go any further with formalising this number representation, it is important to be aware of another problem we have in many-body systems. Namely that the total wave function of a system should be anti-symmetric for fermions and symmetric for bosons. Which means that switching two (indistinguishable) particles must lead to a minus sign in front of the wave function in the case of fermions and to no changes in the case of bosons. Taking care of that requirement is very cumbersome if the states of all particles are represented separately.

Because of the different nature of bosonic and fermionic wave functions, both types of particles behave very differently. Therefore the formalism of systems of bosons and systems of fermions is quite different. Here we will only study fermionic systems.

We will start with a *single particle Hilbert space* H, and assume that it is finite-dimensional, $\dim H =: m$. H is a Hilbert space over $\mathbb{C}$ that consists of all (not necessarily normalised) states of a single particle. The space being finite-dimensional is not necessary for the construction of the theory, but since it makes some definitions clearer and only finite-dimensional spaces are considered, it is still assumed. Now we need to construct a space for a many-body system of fermions, that has both the indistinguishability and the anti-symmetric properties internalised.

Definition 5.2.1. Let H be a finite-dimensional Hilbert space, then we define the *fermionic Fock space* over H by

$$\mathcal{F} := \Lambda(H) := \bigoplus_{n\in\mathbb{Z}_{\geq 0}} \Lambda^n(H), \tag{5.3}$$

where

$$\Lambda^n(H) = \text{Span}\{v_1 \wedge ... \wedge v_n : v_j \in H, j \in \{1, ..., n\}\}. \tag{5.4}$$

When an orthonormal basis $B := \{h_i\}_i$ of H is provided, then $\Lambda^n(H) = \{h_{i_1} \wedge ... \wedge h_{i_n} : i_1 < ... < i_n \leq m,\ h_{i_j} \in B, j \in \{1, ..., n\}\}$. Therefore we can write every element of the fermionic Fock space as a (formal) linear combination of wedge products.

One peculiar subspace in this direct sum is the one-dimensional Hilbert space $\Lambda^0(H)$, the space generated by linear combination of the wedge product of zero vectors. We call this space the *vacuum space* with *vacuum states* as elements. We denote the generator of that vacuum space by $|0\rangle$, to which we often refer as the vacuum state even though nor the choice of a generator nor the choice of a vacuum state is unambiguous, and although the notation can be confussion it is important to keep in mind that

$|0\rangle$ as vacuum state and the 0 as zero element of the vector space are different elements. The vacuum state is fundamental to our occupation number representation as we will shortly see.

To obtain the occupation number representation of a state from elements of the Fock space, we look at an element of $\Lambda^n(H)$ for a specific n, and we choose an (ordered) orthonormal basis of H, i.e. $\{h_1, ..., h_m\}$ where $m = \dim(H)$. Let $|\psi\rangle := v^{i_1 ... i_n} h_{i_1} \wedge ... \wedge h_{i_n} \in \Lambda^n(H)$ where the states in the wedge products are ordered and no state occurs more than once. Then every term $h_{i_1} \wedge ... \wedge h_{i_n}$ can be written as $|n_1, n_2, ..., n_m\rangle$ where $n_j = 1$ if $j \in \{i_1, ..., i_n\}$ and $n_j = 0$ otherwise. Hence the state $|\psi\rangle$ can be written as a linear combination of those *number states*.

At first sight it may seem that information is lost when a step is made from a wedge product to a number state representation, since we only register if a state is in the wedge product instead of the specific position in the expression. Fortunately that is not the case. Firstly because we can order the states in a wedge product by changing only the sign of the prefactor. Secondly because the wedge product can be reconstructed from the number representation state, namely we include h_i in the wedge product if and only if $n_i = 1$.

Now we are able to write a general fermionic many-body state in the occupation number representation. Let $|\psi\rangle \in \mathcal{F}$ and let the single particle Hilbert space be of dimension m, then $|\psi\rangle = c^{n_1, n_2, ..., n_m} |n_1, n_2, ..., n_m\rangle$. This notation includes the anti-symmetry of the wave function and the indistinguishability of the particles implicitly. It is important to notice that such a state above can, and often will, consist of terms with different total number of particles.

5.3 Creation and annihilation operators

Last section provided us with a space that describes the possible state of a fermionic many-body system. However, a thorough and useful study of these spaces, i.e. physical fermionic many-body systems, is only possible when we there are maps available that act on the states in the Fock space. These operators should create or annihilate particles in a certain state.

Definition 5.3.1. Let H be a finite-dimensional Hilbert space and $\{h_i\}_i$ an orthonormal basis of H. A linear operator $a_i^\dagger : \mathcal{F} \to \mathcal{F}$ defined by $h_{i_1} \wedge ... \wedge h_{i_n} \mapsto h_i \wedge h_{i_1} \wedge ... \wedge h_{i_n}$, exterior multiplication with h_i, is called a *creation operator* for a particle in state h_i. A linear operator $a_i : \mathcal{F} \to \mathcal{F}$ defined by $h_{i_1} \wedge ... \wedge h_{i_n} \mapsto h_i' \lrcorner h_{i_1} \wedge ... \wedge h_{i_n}$, interior multiplication by h_i', is called an *annihilation operator* for a particle in state h_i with dual h_i'.

In Def. 5.3.1 there is some slight abuse of notation in the definition of a annihilation operator. Normally we would have a vector space V, and a map $\Lambda^n(V^*) \to \Lambda^{n-1}(V^*)$ that is defined by

$$\omega^1 \wedge ... \wedge \omega^n \mapsto v \lrcorner \omega^1 \wedge ... \wedge \omega^n := \sum_{j=1}^{n} (-1)^{j-1} \omega^j(v) \omega^1 \wedge ... \wedge \widehat{\omega^i} \wedge ... \wedge \omega^n$$

where $\widehat{\omega^j}$ is omitted from the wedge product. For the annihilation operator the role of the vectors and covectors are switched. This is possible however, because of the fact that Hilber spaces are reflexive, and hence the evaluation maps provides a canonical isometry between the Hilbert space and its bidual [60]. Therefore the vectors h_{i_j} can be identified with the evaluation map in h_{i_j} which yields the expression:

$$\begin{aligned} h_i' \lrcorner h_{i_1} \wedge ... \wedge h_{i_n} :&= \sum_{j=1}^{n} (-1)^{j-1} \mathrm{ev}_{h_{i_j}}(h_i') h_{i_1} \wedge ... \wedge \widehat{h_{i_j}} \wedge ... \wedge h_{i_n} \\ &= \sum_{j=1}^{n} (-1)^{j-1} \delta_{i i_j} h_{i_1} \wedge ... \wedge \widehat{h_{i_j}} \wedge ... \wedge h_{i_n}, \end{aligned} \tag{5.5}$$

where we have made use of the basis $\{h_j\}_j$ of H being orthonormal. From this it becomes clear that despite the abuse of notation an annihilation operator for a particle in state h_i is indeed interior multiplication by its dual h_i'.

Before studying the mathematical properties of these operators any further it is important to stress the physical interpretation using the occupation number representation of states. Be aware that we will use the same notation for operators working on elements of the Fock space as above and operators working on number states.

Consider $|\psi\rangle = |n_1, ..., n_i, ...\rangle \in \mathcal{F}$ and the creation operator $a_i^\dagger$. The state $|\psi\rangle$ corresponds to a wedge product where h_j is included if and only if $n_j \neq 0$. The operator $a_i^\dagger$ adds the state h_i to the wedge product, and when the product is ordered again according to the ordered basis, a factor $(-1)^{s_i}$ with $s_i = \sum_{j=1}^{i-1} n_j$ is added. Note that if $|\psi\rangle$ already contained a h_i term this ordering is not well defined, but the wedge product will become zero. Transforming back to the number representation yields $a_i^\dagger |\psi\rangle = (-1)^{s_i} |n_1, ..., n_i + 1, ...\rangle$ if $n_i = 0$, i.e. a particle in state i is created if it was not yet occupied, and $a_i^\dagger |\psi\rangle = 0$ if $n_i = 1$.

Similarly we are able to study the action of the annihilation operator a_i on a state $|\psi\rangle$. The operator a_i effectively removes a term h_i from

the wedge product representation of $|\psi\rangle$ and it adds a factor $(-1)^{s_i}$, as described in Eq. 5.5, if it contains such a term, and it maps the product to zero otherwise. In the number representation this yields $a_i|\psi\rangle = (-1)^{s_i}|n_1, ..., n_i, ...\rangle$ if $n_i = 1$, and $a_i|\psi\rangle = 0$ if $n_i = 0$.

Provided with the knowledge about the action of the creation and annihilation operators on the number states, we are able to build up certain states from the vacuum. Starting from the vacuum state $|0\rangle$ we can obtain a arbitrary state by repeated application of creation operators, this yields:

$$|n_1, n_2, ...\rangle = \prod_i (a_i^\dagger)^{n_i}|0\rangle. \tag{5.6}$$

Here we see the essential role of the vacuum state. Equipped solely with $|0\rangle$ and the annihilation and creation operators we are able to construct every element of the fermionic Fock space just by taking linear combinations of expression of the form of Eq. 5.6. The observation that we just need the operators $a_i^\dagger$ and a_i, and a vacuum state to describe every state in our formalism will be made more rigorous in the remainder of this section. To do so we need to study the mutual relations between the operators.

Returning to the definition it becomes clear that the annihilation operator is the Hermitian conjugate of the creation operator and vice versa [49]. Furthermore, there exist some simple anti-commutation relations which will turn out to be essential in the use and description of these operators.

Proposition 5.3.1. *Let H be a finite-dimensional Hilbert space with $dim(H) = m$, $\{h_i\}_i$ an orthonormal basis of H, and $a_i^\dagger, a_i$ the corresponding creation resp. annihilation operator. Then the following anti-commutation relations hold:*

$$\{a_i^\dagger, a_j^\dagger\} := a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0; \tag{5.7}$$

$$\{a_i, a_j\} := a_i a_j + a_j a_i = 0; \tag{5.8}$$

$$\{a_i^\dagger, a_j\} := a_i^\dagger a_j + a_j a_i^\dagger = \delta_{ij}. \tag{5.9}$$

Proof. It is sufficient to consider basis elements of the Fock space. Let $n \in \mathbb{Z}_{\geq 0}$ and $h_{i_1} \wedge ... \wedge h_{i_n} \in \Lambda^n(H)$. Then we find:

$$\begin{aligned}
\{a_i^\dagger, a_j^\dagger\}(h_{i_1} \wedge ... \wedge h_{i_n}) &= (a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger)(h_{i_1} \wedge ... \wedge h_{i_n}) \\
&= a_i^\dagger(h_j \wedge h_{i_1} \wedge ... \wedge h_{i_n}) + a_j^\dagger(h_i \wedge h_{i_1} \wedge ... \wedge h_{i_n}) \\
&= h_i \wedge h_j \wedge h_{i_1} \wedge ... \wedge h_{i_n} + h_j \wedge h_i \wedge h_{i_1} \wedge ... \wedge h_{i_n} \\
&= h_i \wedge h_j \wedge h_{i_1} \wedge ... \wedge h_{i_n} - h_i \wedge h_j \wedge h_{i_1} \wedge ... \wedge h_{i_n} = 0.
\end{aligned}$$

Therefore $\{a_i^\dagger, a_j^\dagger\} = 0$, and by taking the Hermitian conjugate this implies $\{a_i, a_j\} = 0$. For the last relation we will use Eq. 5.5:

$$\begin{aligned}
\{a_i^\dagger, a_j\}(h_{i_1} \wedge ... \wedge h_{i_n}) &= (a_i^\dagger a_j(h_{i_1} \wedge ... \wedge h_{i_n}) + a_j a_i^\dagger(h_{i_1} \wedge ... \wedge h_{i_n}) \\
&= a_i^\dagger \left(\sum_{k=1}^{n} (-1)^{k-1} \delta_{ji_k} h_{i_1} \wedge ... \wedge \widehat{h_{i_k}} \wedge ... \wedge h_{i_n} \right) \\
&\quad + a_j \left(h_i \wedge h_{i_1} \wedge ... \wedge h_{i_n} \right) \\
&= \sum_{k=1}^{n} ((-1)^{k-1} - (-1)^{k-1}) \delta_{ji_k} h_{i_1} \wedge ... \wedge \widehat{h_{i_k}} \wedge ... \wedge h_{i_n} \\
&\quad + \delta_{ij} \widehat{h_i} \wedge h_{i_1} \wedge ... \wedge h_{i_n} \\
&= \delta_{ij} h_{i_1} \wedge ... \wedge h_{i_n}.
\end{aligned}$$

Therefore we indeed obtained $\{a_i^\dagger, a_j\} = \delta_{ij}$. □

From Prop. 5.3.1 it is immediately clear that operators are nilpotent. This is a property of fermionic creation and annihilation operators, and it implicitly encodes for the Pauli exclusion principle. When a particle is added to an already occupied state, this yields a zero, i.e. multiple particles in one state is not allowed. Therefore there can be at most one particle in a certain state, and hence annihilating the same state twice yields a zero.

The remainder of this section will consist of a more rigorous explanation of the observation made earlier that we just need the annihilation and creation operators, and a vacuum state to establish the formalism. For this it is necessary to define a mathematical object that adds a structure of multiplication of vectors to a vector space, or modules in general.

Definition 5.3.2. Let R a commutative ring. A(n) *(associative) R-algebra* $\mathcal{A}$ is a ring with an operation $\_ \cdot \_ : \mathcal{A} \times \mathcal{A} \to \mathcal{A}$ such that for all $r, s \in R$ and $a, b \in \mathcal{A}$ it satisfies

$$\begin{aligned}
r \cdot (ab) &= (r \cdot a)b = a(r \cdot b; \\
r \cdot (a + b) &= r \cdot a + r \cdot b; \\
(r + s) \cdot a &= r \cdot a + s \cdot a; \\
(rs) \cdot a &= r \cdot (s \cdot a); \\
1 \cdot a &= a.
\end{aligned}$$

This operation is called *scalar multiplication*.

Here the multiplication sign of the scalar multiplication is often omitted. A careful reader with a mathematical background might recognise

relations that are very similar to that of a R-module, and indeed it is possible to define an associative R-algebra $\mathcal{A}$ as a ring $\mathcal{A}$ that is also a R-module such that the ring addition and the module addition are the same operation and scalar multiplication satisfies

$$r \cdot (xy) = (r \cdot x)y = x(r \cdot y)$$

for all $r \in R$ and $x, y \in \mathcal{A}$.

Familiarity with R-modules is not necessary, but this observation becomes useful when we recall that for the case that R is a field, a R-module is just a R-vector space. That means that for a field K a K-algebra defines a notion of multiplication of vectors in a vector space.

Let us now consider a $\mathbb{C}$-vector space $\mathcal{A}$ generated by a_i, b_i for $i \in I$ where I is an index set. We can endow a structure of a $\mathbb{C}$-algebra on $\mathcal{A}$ by imposing the following anti-commutation relations:

$$\{a_i, b_j\} = \delta_{ij}, \quad \{a_i, a_j\} = 0, \quad \{b_i, b_j\} = 0. \tag{5.10}$$

These relations are motivated by Eq. 5.7, 5.8 and 5.9 for creation and annihilation operators. Let $\mathcal{F}$ be a vector space. We will assign to every a_i and b_i a linear map $T_{a_i}, T_{b_i} : \mathcal{F} \to \mathcal{F}$ sucht that T respects the commutations relations, i.e. $T_{\{a_i, b_j\}} = \{T_{a_i}, T_{b_j}\}$, and $T_{b_i} = T_{a_i}^\dagger$. We say that the algebra $\mathcal{A}$ is *unitarily represented* in the vector space $\mathcal{F}$. To stress the connection to creation and annihilation operators we will denote T_{a_i} by a_i, and T_{b_i} by $a_i^\dagger$.

Remark. *While for physical applications the relevant representation theory can be formulated specifically for operators on a Fock space as above, the mathematical theory underlying these principles can be generalised. This uses the notion of $*$-rings, $*$-algebras, and $*$-algebra representations. Although a detailed discussion of this would go beyond the scope of this thesis, the main idea is to assign a involution map to a ring, and from there develop the theory of algebra representations. In physics this whole generalisation would be redundant, since the only $*$-ring that is considered is* $\mathbb{C}$.

The *Stone-Von Neumann theorem*, originally proven by Jordan and Wigner in 1928 [28], and discussed in chapter 2 of Altland and Simons book on condensed matter [5], states that the representation above is unique up to unitary transformations of the basis. For a proof of this statement an explicit construction for a basis of $\mathcal{F}$ is given. In this proof the vacuum state is defined as the state that has eigenvalue 0 for all operators of the form $a_i^\dagger a_i$ with $i \in I$, and the elements of that form the basis are constructed as in Eq. 5.6. Therefore the vector space $\mathcal{F}$ of the representation

coincides with the fermionic Fock space in the text, and we can indeed capture the formalism of second quantisation and the occupation number representation solely with creation and annihilation operators and their anti-commutation relations.

Equipped with this result we can, and will, from now on omit referring to the fermionic Fock space and number states, and speak about operators and sporadically about states of a single particle.

5.4 Elementary applications

To study physical system and to describe for instance changes of basis, one-body interaction, and two-body interaction we need to know how to apply creation and annihilation operators in those situation.

First of all, we want to transform the creation and annihilation operators along with a basis.

Proposition 5.4.1. *Let $\{|\lambda\rangle\}$ and $\{|\tilde{\lambda}\rangle\}$ be two orthonormal bases of the single particle Hilbert space. Then the creation operators transform as follows*

$$a^\dagger_{\tilde{\lambda}} = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda \tag{5.11}$$

and the annihilation operators transform similarly

$$a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda. \tag{5.12}$$

Proof. We have $\mathrm{Id} = \sum_\lambda |\lambda\rangle\langle\lambda|$, $|\lambda\rangle =: a^\dagger_\lambda|0\rangle$, and $|\tilde{\lambda}\rangle =: a^\dagger_{\tilde{\lambda}}|0\rangle$. From this it follows

$$a^\dagger_{\tilde{\lambda}}|0\rangle = |\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda|0\rangle.$$

Therefore $a^\dagger_{\tilde{\lambda}} = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda$. The annihilation operators follow immediately by taking the hermitian conjugate. □

An important application of this change of basis would be the Fourier transformation as we will see in Chapter 7.

Let us make a small side note. Although we assume a finite-dimensional single particle Hilbert space, evertything that we will define in this section can be generalised to an infinite case just by replacing the sums with integrals.

Secondly, one-body operators represent the kinetic part of the Hamiltonian. This is an essential part of the description of physical systems. Consider a one-body operator $\mathcal{O}_1$ and a basis $\{|\lambda\rangle\}$ of eigenvectors of that operator. This means that $\mathcal{O}_1 = \sum_\lambda o_\lambda |\lambda\rangle\langle\lambda|$ with $o_\lambda := \langle\lambda|\mathcal{O}_1|\lambda\rangle$ from which it follows

$$\mathcal{O}_1 = \sum_\lambda o_\lambda a_\lambda^\dagger a_\lambda. \tag{5.13}$$

From Eq. 5.13 it is clear that a one body operator just engages with all particles separately. A special kind of one-body operator is the so-called *occupation number operator*

$$\hat{n}_\lambda = a_\lambda^\dagger a_\lambda \tag{5.14}$$

which has the property $\hat{n}_\lambda (a_\lambda^\dagger)^n|0\rangle = n(a_\lambda^\dagger)^n|0\rangle$. One can easily check this using the anticommutation relations

$$\begin{aligned}\hat{n}_\lambda (a_\lambda^\dagger)^n|0\rangle &= (a_\lambda^\dagger a_\lambda a_\lambda^\dagger)(a_\lambda^\dagger)^{n-1}|0\rangle = a_\lambda^\dagger(1 + a_\lambda^\dagger a_\lambda)(a_\lambda^\dagger)^{n-1}|0\rangle \\ &= \cdots = (a_\lambda^\dagger)^n(n + a_\lambda)|0\rangle = n(a_\lambda^\dagger)^n|0\rangle.\end{aligned}$$

On top of that $\hat{n}_\lambda$ commutes with all creation operators of different states. Therefore we conclude that $\hat{n}_\lambda$ just counts the number of particles in state $|\lambda\rangle$. In the fermionic case this means that it yield a 1 if the state is occupied and a 0 otherwise. Using the occupation number operator we can rewrite Eq. 5.13 as

$$\mathcal{O}_1 = \sum_\lambda o_\lambda \hat{n}_\lambda. \tag{5.15}$$

In general, for an arbitrary orthonormal basis B of the single particle Hilbert space, Eq. 5.13 can be rewritten by applying a basis transformation

$$\mathcal{O}_1 = \sum_{\mu,\nu \in B} \langle\mu|\mathcal{O}_1|\nu\rangle a_\mu^\dagger a_\nu. \tag{5.16}$$

The two-body operators are used to describe pairwise interactions between particles. Embedding those interactions in a quantum many-body system might be cumbersome because of the indistinguishability of particles. Fortunately, this is where second quantisation comes into its own. A two-body operator $\mathcal{O}_2$ can be expressed as

$$\mathcal{O}_2 = \sum_{\mu\mu'\nu\nu'} \langle\mu,\mu'|\mathcal{O}_2|\nu,\nu'\rangle a_\mu^\dagger a_{\mu'}^\dagger a_\nu a_{\nu'} \tag{5.17}$$

where μ, μ', ν, and ν' are elements of an orthonormal basis of the single particle Hilbert space [5].

We would like to conclude this chapter with making a connection between our creation and annihilation operators, and ladder operators. Let us consider a Hamiltonian $\hat{H}$, which is a complex polynomial of creation and annihilation operators, and a creation operator $a_i^\dagger$. Assume that the commutation relation between $\hat{H}$ and $a_i^\dagger$ is given by

$$[\hat{H}, a_i^\dagger] = E_i a_i^\dagger, \tag{5.18}$$

where $E \in \mathbb{R}_{\geq 0}$ a positive constant. This seems quite a strong assumption, but we will see that Hamiltonians that you encounter fulfil this property.

From Eq. 5.18 and the fact that the H is an observable - and thus Hermitian - the commutation relation of $\hat{H}$ with the annihilation operator a_i immediately follows

$$-[\hat{H}, a_i^\dagger]^\dagger = -\left(\hat{H}a_i^\dagger - a_i^\dagger \hat{H}\right)^\dagger = -\left(a_i \hat{H} - \hat{H}a_i\right) = [\hat{H}, a_i], \tag{5.19}$$

and thus

$$[\hat{H}, a_i] = -E_i a_i^\dagger. \tag{5.20}$$

Consider an eigenstate of $\hat{H}$, $|\psi\rangle$, corresponding to an eigenvalue E_ψ. Applying $a_i^\dagger$ to that eigenstate yields the state $a_i^\dagger|\psi\rangle$, and by letting $\hat{H}$ act on this state we obtain

$$\hat{H}a_i^\dagger|\psi\rangle = \left([\hat{H}, a_i^\dagger] + a_i^\dagger \hat{H}\right)|\psi\rangle = (E_\psi + E_i)a_i^\dagger|\psi\rangle. \tag{5.21}$$

Hence $a_i^\dagger|\psi\rangle$ is a new eigenstate of $\hat{H}$ with energy $E_\psi + E_i$. Similarly, we find that $a_i|\psi\rangle$ is and eigenstate with energy $E_\psi - E_i$. Starting with just one eigenstate this enables us to find several just by applying creation or annihilation operators. A careful reader with a physical background might recognise this construction from the harmonic oscillator, where this is especially powerful since it generates all the excited states from the ground state [19].

Chapter 6

Symmetries of second-quantised Hamiltonians

Symmetries are essential in theoretical physics. They not only enable us to analyse physical systems in a comprehensive manner, but often they correspond to certain properties. Here we will investigate the symmetries of second-quantised Hamiltonians, starting with unitary transformations. Afterwards, important non-unitary symmetries are introduced, the *time-reversal*, *particle-hole*, and *chiral symmetry*. It appears that the second-quantised Hamiltonians which contain operators up to quadratic order can be classified by these symmetries. In this chapter we shift entirely from a mathematical viewpoint to one rooted in theoretical physics, which has its influence on the style of writing. This might be a little awkward for a reader with a mathematical background, but it will fit the expectations of a physicist better.

6.1 Second-quantised Hamiltonians

In the formalism of second quantisation one-body operators are given by Eq. 5.16, and hence a Hamiltonian of a non-interacting system can be written as

$$\hat{H} = \sum_{ij} \hat{\Psi}_i^\dagger h_{ij} \hat{\Psi}_j, \tag{6.1}$$

where $\hat{\Psi}_i^\dagger$ and $\hat{\Psi}_j$ satisfy the canonical anticommutations relations as given by Eq. 5.10, and $h_{ij} \in R$ and so $\hat{H}$ is Hermitian [20]. Here h is also called the *first quantised* or *singel particle Hamiltonian*.

The Hamiltonian of Eq. 6.1 is strikingly elegant, but quite restrictive since there are no interactions. To introduce pairwise interactions two-body operators should be added to the Hamiltonian. However, this new terms cannot be expressed as the non-interacting Hamiltonian, making the analysis much harder. Fortunately, there exists an approximation that enables us to write particle number conserving interaction with one-body operators, a *mean field approximation*. The main idea of this mean field approximation reduces the pairwise interaction to an interaction with an average field. Therefore the Hamiltonian of a mean field approximated system with particle conserving pairwise interaction can be written as Eq. 6.1. In the next Chapter 7 we will see an explicit example of such a mean field approximation.

Besides particle number conserving interaction there exist interaction that do not conserve the number of particles. The most most famous example is the formation of Cooper pairs in superconductivity. The details of superconductivity will be discussed in Chapter **??** in more depth, but for now it is important to notice that this interaction can be approximated by a mean field theory as well. This results in a Hamiltonian of the form

$$\hat{H} = \sum_{ij} \hat{\Psi}_i^\dagger h_{ij} \hat{\Psi}_j + \frac{1}{2} \sum_{ij} \hat{\Psi}_i^\dagger \Delta_{ij} \hat{\Psi}_j^\dagger + \frac{1}{2} \sum_{ij} \hat{\Psi}_i \Delta_{ij}^* \hat{\Psi}_j, \tag{6.2}$$

where $\Delta_{ij} \in \mathbb{C}$.

To overcome the problems of the violation of particle number conservation that make it impossible to study the Hamiltonian in similar ways to the non-interacting or mean field one from Eq. 6.1, a transformation can be performed. A so-called *Bogoliubov transformation* introduces operators that are a linear combination of creation and annihilation operators [5]. Those operators preserve the number of *Bogoliubons*, a *quasiparticle* that partially consists of a *particle*, something created by a creation operator, and partially consists of a *hole*, something created by an annihilation operator.

The Bogoliubov transformation might be preformed by introducing a *Nambu spinor*

$$\hat{\chi}^\dagger := (\hat{\Psi}_1^\dagger, ..., \hat{\Psi}_N^\dagger, \hat{\Psi}_1, ..., \hat{\Psi}_N). \tag{6.3}$$

Using Eq. 6.3 we can write the Hamiltonian in Eq. 6.2 in a similar way as Eq. 6.1

$$\hat{H} = \frac{1}{2} \hat{\chi}^\dagger \mathcal{H}_{BdG} \hat{\chi} = \frac{1}{2} \sum_{ij} \hat{\chi}_i^\dagger (\mathcal{H}_{BdG})_{ij} \hat{\chi}_j, \tag{6.4}$$

where $\mathcal{H}_{BdG}$ is called the *(first quantised) Bogoliubov-de-Gennes (BdG) Hamil-*

tonian which is given by

$$\mathcal{H}_{BdG} := \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \tag{6.5}$$

Notice that here the assumption that h is real can be dropped. One can easily check that the same anticommutation relations hold for $\hat{\chi}_i^\dagger$ and $\hat{\chi}_j$ as for $\hat{\Psi}_i^\dagger$ and $\hat{\Psi}_j$. Therefore it is perfectly fine to only consider Hamiltonians of the form of Eq. 6.1, with the small adaption that $h_{ij} \in \mathbb{C}$, for the remainder of this chapter.

6.2 Unitary symmetries

In general a symmetry is a transformation of a system that preserve certain properties. This is a extremely vague statement, and therefore we will look into a specific kind of symmetry. Consider a fermionic system that is described by a second-quantised Hamiltonian $\hat{H}$, Eq. 6.1, and the canonical anticommutation relations. A system is symmetric under the action of a unitary symmetry, if there exists a unitary matrix "representing" that symmetry, U, that commutes with the Hamiltonian, i.e. $\hat{U}\hat{H}\hat{U}^{-1} = \hat{H}$. For the single particle Hamiltonian h this imposes the condition $U^\dagger h U = h$.

Since $\hat{U}$ commutes with the Hamiltonian $\hat{H}$, there exists a basis of our Hilbert space such that both $\hat{H}$ and $\hat{U}$ are block diagonal. Such a block is called an *irreducible representation of the symmetry* [20].

One of the crucial roles of symmetries in quantum mechanics is that they give rise to degeneracies. Let $|\psi\rangle$ be an eigenstate of $\hat{H}$ with corresponding energy E, and let $\hat{U}$ be a symmetry of the Hamiltonian. Then we obtain

$$\hat{H}\hat{U}|\psi\rangle = \hat{U}\hat{H}|\psi\rangle = E\hat{U}|\psi\rangle. \tag{6.6}$$

So $\hat{U}|\psi\rangle$ is an eigenstate of $\hat{H}$ with the same energy as $|\psi\rangle$, which means that E is a degenerate energy level, assuming that $\hat{U}|\psi\rangle \neq |\psi\rangle$. This implies that degeneracies can be lifted by breaking a symmetry in a system [61]. A famous example of this is the Zeeman splitting, where a magnetic field breaks the rotational symmetry of the orbit of an atomic electron.

It is important to notice that, although we are not going in more depth on how to find the corresponding matrix, there are differences in how to obtain the unitary matrix between different symmetries. In some cases one uses an infinitesimal generator, these are called *continuous symmetries*. How these exactly relate to Lie algebras goes beyond the scope of this thesis. Symmetries where the matrix is not obtained in that way are called *discrete symmetries* [61].

6.3 Non-unitary symmetries

For thus far we have considered unitary transformations to block-diagonalise the Hamiltonian. When all the unitary transformation that correspond to symmetries of the Hamiltonian are performed we are left with irreducible blocks. However, a natural question that arises is if this is all we can say about the structure of the Hamiltonian. It turns out that there are three particular, non-unitary, symmetries which are essential to answer that question: the time-reversal, the particle-hole/charge-conjugation, and the chiral/sublattice symmetry.

6.3.1 Time-reversal symmetry

An important symmetry a system can posses in the so-called *time-reversal symmetry*. This means that the system is invariant under the direction of time, i.e. it does not matter if time goes backwards or forwards. Let us try to understand the relation between the second-quantised Hamiltonian $\hat{H}$ and this symmetry.

Define the time-reversal operator as

$$\hat{T} : t \mapsto -t. \tag{6.7}$$

This operator is the identity on the position operator and minus the identity on the momentum operator. Therefore the uncertainty principle implies

$$\hat{T}i\hat{T}^{-1} = \hat{T}[\hat{x}, \hat{p}]\hat{T}^{-1} = -[\hat{x}, \hat{p}] = -i. \tag{6.8}$$

Eq. 6.8 determines that the time-reversal operator should be expressed as the combination of a unitary matrix, $\hat{U}_T$, and complex conjugation, $\mathcal{K}$, i.e.

$$\hat{T} = \hat{U}_T\mathcal{K}. \tag{6.9}$$

Since $\hat{T}$ is a symmetry of the second-quantised Hamiltonian $\hat{H}$ they should commute. This imposes the following requirement on the single particle Hamiltonian:

$$U_T^\dagger h^* U_T = h. \tag{6.10}$$

Furthermore, it might be interesting how the single particle Hamiltonian transforms in k-space. For a system without spin it is derived in [20] that $h(k)$ transforms as

$$U_T h(k)^* U_T^\dagger = h(-k). \tag{6.11}$$

Let us conclude the discussion of the time-reversal symmetry with one more observation. When $\hat{T}$ is applied twice, there are two possibilities:

either $T^2 = \mathrm{id} = 1$ or $T^2 = -\mathrm{id} = -1$. These two possible squares of the time-reversal operator lead to significant physical differences. It can be shown that in systems that exhibit time-reversal symmetry *Kramers' degeneracy theorem* applies if $T^2 = -1$ and not if $T^2 = 1$ [9], which states that there exist pairs of time-reversed states that have the same energy.

6.3.2 Particle-hole symmetry

Another symmetry a system can exhibut is the *particle-hole (PHS)* or *charge-conjugation symmetry*. For a system to posses this symmetry it means that it is invariant under the change of particles and holes, i.e. the change of creation and annihilation of particles.

The particle-hole operator is defined by

$$\hat{C}\Psi_i\hat{C}^{-1} := (U_C)^*_{ij}\Psi^\dagger_j. \tag{6.12}$$

Where the invariance of the canonical anticommutation relations imply that U_P is unitary. Since $\hat{C}$ is a symmetry, it commutes with $\hat{H}$, and from that it is clear that the single particle Hamiltonian transforms as

$$U_C^\dagger h^* U_C = -h. \tag{6.13}$$

Therefore $\hat{C}$ is a antiunitary operator, and we can write $\hat{C} = \hat{U}_C\mathcal{K}$. This form looks like the the time-reversal operator, and similarly $C^2 = \pm 1$.

Moreover, the transformation of h in momentum space is similar, but not the same, as in the case of time-reversal symmetry

$$U_C h(k)^* U_C^\dagger = -h(-k). \tag{6.14}$$

Physically this transformation makes sense, since with the creation of a particle-hole pair one would expect two particles that are travelling in opposite directions, i.e. having momentum of opposite sign, and are counterparts in terms of energy.

Finally, let us consider an important example of a Hamiltonian that exhibits particle-hole symmetry, the (second quantised) Bogoliubov-de-Gennes Hamiltonian, Eq. 6.4. The relation between $\hat{\chi}^\dagger$ and $\hat{\chi}$ is given by

$$\hat{\chi}^\dagger = \hat{\chi}^T\tau_x, \tag{6.15}$$

where τ_x is the Kronecker product of the σ_x, a Pauli spin matrix, and the identity of dimension N:

$$\tau_x = \sigma_x \otimes 1_N = \begin{pmatrix} 0_N & 1_N \\ 1_N & 0_N \end{pmatrix}. \tag{6.16}$$

Using Eq. 6.15 to change $\hat{\chi}^\dagger$ to $\hat{\chi}$ in Eq. 6.4, and vice versa, yields that

$$\tau_x \mathcal{H}_{BdG} \tau_x = -\mathcal{H}_{BdG}. \tag{6.17}$$

Hence a Bogoliubov-de-Gennes Hamiltonian possesses the particle-hole symmetry, with operator $\hat{C} = \tau_x \mathcal{K}$.

Be careful that this symmetry is not a property of the system an sich, but a symmetry imposed on the Hamiltonian by the Bogoliubov transformation. In Eq. 6.4 it seems that we double the degrees of freedom in the system, which makes no physical sense. Fortunately, the imposed symmetry takes care of that apparent doubling of the degrees of freedom by relating pairs of particles and holes, making half of the degrees of freedom redundant.

Before considering the next symmetry, let us become aware of the fact that the operation corresponding to the time-reversal and particle-hole symmetry are unique up to unitary transformation, a proof of which can be found in [44].

6.3.3 Chiral symmetry

Combining both time-reversal and particle-hole symmetry give rise to the *chiral symmetry*, with corresponding operator

$$\hat{S} := \hat{T} \cdot \hat{C}. \tag{6.18}$$

The alternative combination of those operators, i.e. $\hat{S} := \hat{C} \cdot \hat{T}$, amounts to a change of basis [20].

From our study of $\hat{C}$ and $\hat{T}$ it follows that $\hat{S}$ commutes with the Hamiltonian $\hat{H}$, and is antiunitary. However, with respect to the single particle Hamiltonian the matrix that corresponding to the symmetry is $S = U_S = U_T (U_C)^*$, and thus it is unitary. On top of that it anticommutes with h

$$U_S h U_S^\dagger = U_S h U_S^{-1} = -h \tag{6.19}$$

both in real and momentum space. Because of that the eigenstates of h come in positive-negative energy pairs [44].

The chiral symmetry is also know as the sublattice symmetry. When a system can be divided into two sublattices that only interact with each other, then such a system possesses the chiral symmetry, hence its alternative name. This immediately provides us with several examples of systems where the chiral symmetry is present.

Since S is unitary we solely have $S^2 = 1$. With this piece of information we can make a complete table of all the combinations of non-unitary

symmetries. The classes in this Table 6.1 have seemingly arbitrary names. These classes refer to so-called Cartan classes from the first classification of simple Lie algebras [14]. Going into the details here would go beyond the scope of this thesis, and a reader interested in a mathematical treatment of the classification of Lie algebras should turn to [23]. However, the main idea is that one can study and classify Hamiltonians by considering the non-unitary symmetries that are present. How the symmetries correspond to those classifying space is based on the early work of Wigner [74] and Dyson [16] on random matrices, and the later work of Altland and Zirnbauer [6], and Kitaev [32]. In the last two papers they discuss how certain *topological properties* of systems are the same in each class, and how this can be explained by methods from K-theory. In the next chapter we will discuss what those topological properties are in a little bit more depth, but for a more comprehensive treatment one should consult Bernevig's book on topological insulators and superconductors [10].

Class	Time-reversal	Particle-hole	Chiral
A	0	0	0
AI	1	0	0
AII	-1	0	0
AIII	0	0	1
BDI	1	1	1
CII	-1	-1	1
D	0	1	0
C	0	-1	0
DIII	-1	1	1
CI	1	-1	1

Table 6.1: *The classification of Hamiltonians of the form of Eq. 6.1 based on the presence of time-reversal, particle-hole, and chiral symmetries. The names of the classes refer back to the classification of simple Lie groups by Cartan [14]. A 0 indicates the absence of a symmetry, a -1 indicates the presence of that symmetry with a corresponding operator squaring to -1, and a so does a 1 with a corresponding operator squaring to 1.*

Study the presence of these non-unitary symmetries in specific models allows one to assign a symmetry class to those models. This relates them to the broader physical context and provides insight about the behaviour of the model.

Chapter 7

The homogeneous Kitaev Chain

In this chapter we will explain what is meant by the topological properties of last chapter. This is done by defining *topologically protected* properties and *topological phase transitions*. It turns out that the topological phase of a system can be determined by properties of the bulk according to the *bulk-boundary correspondence*. Subsequently, we formulate an one-dimensional superconducting chain that exhibits certain topologically protected properties, the *Kitaev chain*. To understand why this model is particularly interesting, *Majorana quasiparticles* and the concept of *braiding* is introduced. Here we propose braiding in the parameter space as an alternative for braiding in real space. Eventually, we will investigate the topological properties of the chain by considering the bulk spectrum

7.1 Topological phases

Let us consider a Hamiltonian H in which certain non-unitary symmetries are present and which is *gapped*, i.e. the infimum of the set of positive eigenvalues is larger than zero. In physics literature it is often said certain properties, such as the symmetries, of such a Hamiltonian are topologically protected when small deformation of H do not effect those properties. We formalise that idea in the following definition.

Definition 7.1.1. Let $H, H' : X \to Y$ be continuous Hamiltonians with X, Y subspaces of $\mathbb{R}^n$, and assume that H is gapped. Let P be a property of H that is not a property of H'. Then P is said to be *topologically protected* if for every homotopy $K : X \times [0,1] \to Y$ with $K(0) = H$ and $K(1) = H'$ there exists a $t \in (0,1]$ such that $K(t)$ is not gapped.

Put differently, a property of a gapped Hamiltonian is topologically protected if property cannot be altered by continuously transforming the Hamiltonian without closing the gap. It turns out that the non-unitary symmetries from Chapter 6 are topologically protected properties [32].

When there is a change in topologically protected properties in a system we call this a *topological phase transition*. We would like to describe such phase transitions in a similar way as "classical" phase transition where a symmetry changes. Before we can introduce "topology" in the world of phase transitions in this way, we need to discuss the classical theory of phase transitions developed by Landau [37]. We will assume previous knowledge on this topic as far as discussed in David Tong's lecture notes [71] or Landau's and Lifshitz' course on theoretical physics [36]. In Landau theory a second order (continuous) or first order phase transition is characterised by a so-called *order parameter*, i.e. a parameter that is zero in the one phase and non-zero in the other phase. The order parameter often, but not necessarily, indicates some sort of order in a material such as magnetic susceptibility in a Ising model for ferromagnetism.

The simple concept of Landau theory, and its generalisations, e.g. Ginzburg-Landau theory [38], and its enormous successes in understanding and classifying phase transitions, make it a widely applicable method to describe phase transitions. Unfortunately, it turns out it is not always possible to define an order parameter in the conventional manner that continuously changes from a zero to a non-zero value at the transition. It turned out that there are phase transitions, those where topologically protected properties change, where the corresponding order parameter is a so-called *topological quantum number*, e.g. in the case of the quantum Hall effect [69]. Shortly, we will see some examples of such topological order parameters. By use of those examples it will be made clear what is "topological" about those quantum numbers, this hopefully clears the skies of the mathematicians that watch the physicist's use of the word "topological" with Argus' eyes.

7.1.1 Topological quantum numbers

We will consider three of the most important topological order parameters, how they relate to the Hamiltonian of the system and the mathematical notion of topology.

Chern numbers

Let us consider a principal G-bundle $\pi : P \to M$ where $G = \mathrm{GL}(n, \mathbb{C})$, that is endowed with a connection $\mathcal{A}$ and a curvature $\mathcal{F} = \mathcal{D}\mathcal{A}$. Together with a local section s this will give rise to a local curvature $F = s^*\mathcal{F}$. For $k \in \{0, ..., n\}$ we define the kth *Chern form* as

$$\det\left(\mathbb{1} - \frac{i}{2\pi}F\right) =: \sum_{k=0}^{n} c_k(F). \tag{7.1}$$

It turns out that these forms give rise to a well-defined integral valued integral for certain bundles [15]. Let our base space M be an oriented compact manifold of dimension $2n$, then we can define the *Chern number* of the bundle as

$$\mathrm{Ch}(M) = \int_M c_n(F). \tag{7.2}$$

In a physical case we can, given a suitable Hamiltonian, construct a principal G-bundle with a spectral bundle as its bundle space, and endow it with the Berry-Simon connection. In a certain gauge this naturally gives rise to a local curvature and therefore a Chern number, assuming that the base space is appropriate to define a Chern number.

One of the most famous examples of a phenomenon where the Chern number plays a role as quantum order parameter is the quantum Hall effect. Here the topological invariant corresponds to the Hall conductance in units of e^2/h [69].

Winding number

The idea behind the winding number is that it assign a number to a smooth function on a smooth manifold. This can be defined in the language of differential geometry.

Definition 7.1.2. Let $F : X \to Y$ be a smooth map between compact, connected, and orientable n-dimensional manifolds and a volume form $\omega \in \Omega^n(Y)$. The *Brouwer degree* of F is defined by

$$\int_X F^*\omega =: \deg(F) \int_Y \omega. \tag{7.3}$$

For $X = Y = S^n$ this Brouwer degree is known as the *winding number* of F.

It happens that $\deg(f) \in \mathbb{Z}$, and that it is independent of the choice of the volume form ω.

This topological quantum number is often encountered in the study of systems with chiral symmetry [32]. In such systems the winding number often indicate the number of edge states.

Sign of the Pfaffian

The definition of the following topological quantum number is based in differential geometry, but depends solely on our finite-dimensional Hamiltonian matrix. Let $\tilde{H} = (h_{ij})_{i,j=1}^{2n}$ be an antisymmetric $2n \times 2n$-matrix. Then the *Pfaffian* of $\tilde{H}$ is defined by

$$\mathrm{pf}(\tilde{H}) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \mathrm{sgn}(\sigma) \prod h_{\sigma(2i-1)\sigma(2i)}, \tag{7.4}$$

where S_{2n} is the symmetric group of degree n, and sgn is the sign map. Shortly we will see what properties of the Pfaffian are such that is an excellent candidate for a topological order parameter. The property of the Pfaffian that we want to isolate is its sign. Therefore we define the following topological quantum number

$$Q(\tilde{H}) := \mathrm{sign}(\mathrm{pf}(i\tilde{H})). \tag{7.5}$$

A curious reader might carefully ask if this is well-defined, since we take the sign of a possibly complex number. To explain this we have to shine some light on the kind of matrices that we will encounter when we want to calculate its Pfaffian. It turns out that this will often be Bogoliubov-de-Gennes Hamiltonians. Although it goes beyond the scope of this thesis, this can be explained by considering at the classes described by the symmetries in Table 6.1. One can assign a certain topological order parameters to symmetry class, and the sign of the Pfaffian suits classes in which the particle hole symmetry is present.

Starting from the general formulation of the BdG Hamiltonian in Eq. 6.5 we can apply a unitary transformation to obtain an anti-symmetric matrix that contains the same physical information. The transformation yields the following expression

$$\begin{aligned}
\tilde{\mathcal{H}}_{BdG} &= \frac{1}{2}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ i\mathbb{1} & -i\mathbb{1} \end{pmatrix} \mathcal{H}_{BdG} \begin{pmatrix} \mathbb{1} & -i\mathbb{1} \\ \mathbb{1} & i\mathbb{1} \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ i\mathbb{1} & -i\mathbb{1} \end{pmatrix} \begin{pmatrix} C & S \\ -S^* & -C^* \end{pmatrix} \begin{pmatrix} \mathbb{1} & -i\mathbb{1} \\ \mathbb{1} & i\mathbb{1} \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} C - C^* + S - S^* & -i(C + C^*) + i(S + S^*) \\ i(C + C^*) + i(S + S^*) & C - C^* - (S - S^*) \end{pmatrix}.
\end{aligned} \tag{7.6}$$

The Hamiltonian $\tilde{\mathcal{H}}_{BdG}$ is antisymmetric, because Δ is antisymmetric, $H - H^*$ is antisymmetric, and $H + H*$ is symmetric. The latter two statements follow from the fact that H is Hermitian. It is possible, but cumbersome,

to check that the Pfaffian of $i\tilde{\mathcal{H}}_{BdG}$ is indeed real.

The work of Kitaev [32], among others, showed how the topological quantum numbers are related to the symmetry classes in Table 6.1. Since one can prove that each the topological quantum numbers is homotopy invariant, it is not possible to continuously deform the Hamiltonian to change the topological quantum numbers, while preserving the symmetries present in the Hamiltonian. Otherwise that deformation of the Hamiltonian would be a suitable homotopy, which contradicts the homotopy invariance of the values.

One may wonder what the physical quantities or properties are that correspond to these order parameters. In the case of the Chern number an example is already given. The other two parameters often occur in system called *topological insulators*, insulators in which topological phase transitions are present, or *topological superconductors*, superconductors in which topological phase transitions are present. In this systems the winding number or the sign of the Pfaffian indicate the number of or the existence of so called edge states. Such edge states do not occur in the bulk spectrum, i.e. the spectrum that is obtained when considering an infinite size system without defects, but there existence is suggested by the topological order parameter. This is called the *bulk-boundary correspondence*, which is thoroughly discussed from a mathematical perspective for topological insulators in [57].

For reasons that will become clear in the remainder of this chapter, we are interested in studying superconducting toy models that do exhibit such edge states. Therefore we will shift our focus to superconducting models with topological phase transitions.

7.2 Formulation of the model

Although the role of topology in the quantum Hall effect was know since the last decades of 20th century, it took until this millennium before superconductors where predicted that were topological non-trivial, i.e. in which topological phase transitions were present. The first prediction of such a system was by Read and Green [58], and that involved a two-dimensional system. Within a year Kitaev proposed a one-dimensional system. That system was a tight-binding and mean field approximation of a homogeneous chain of spinless fermions with p-wave superconductivity [33], the so-called *Kitaev chain*. Let us consider the second quantised Hamiltonian

of chain of length N with open boundary condition

$$\hat{H}(\mu, t, \Delta) = -\sum_{j=1}^{N} \mu c_j^\dagger c_j - \sum_{j=1}^{N-1} t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \sum_{j=1}^{N-1} (\Delta c_j^\dagger c_{j+1}^\dagger + \Delta^* c_{j+1} c_j), \tag{7.7}$$

where $\mu \in \mathbb{R}$ is the *chemical*, or on-site, *potential*, $t \in \mathbb{R}$ the *hopping amplitude*, and $\Delta \in \mathbb{C}$ the *superconducting gap*. Be aware of the fact that we can take Δ to be real, since the complex phase can be absorbed by a transformation of the operators.

Before we are being carried away by the beautiful properties that this system has and by attempts to enrich it even further, we will stand still with the physical meaning of each of the terms and how this toy model came to be.

In a superconducting chain of fermions we have to consider three terms. The first is an on-site or chemical potential that accounts for the energy that is needed to add a particle to your system. In the formalism of second quantisation this can be written down as the occupation number operator that subtracts a certain chemical potential from the Hamiltonian for every particle.

Secondly, interactions have to be considered. To obtain a Hamiltonian which only has pairs of creation and annihilation operators, such as Eq. 6.1, a mean field theory is needed. In a chain of fermions in the tight-binding approximation where there are a distinct number of sites the Coulomb interaction, that is physically present, can be described by a *hopping term*. This assign an energy to a particle jumping from one site to another. In the tight-binding approximation it is reasonable to assume that only nearest-neighbour interactions occur, since the electron are bound tightly to their atoms or, more general, sites.

Thirdly, we have to include superconductivity. It goes beyond the scope of this thesis to discuss the theory of superconductors in much depth, but we need to point out some of the key-features. The mainstream description of superconductors is the BCS-theory, which is comprehensively introduced in chapter 3 of Tinkham's book [70]. The relevant mechanism is the formation of pairs, so-called *Cooper pairs*, by conducting electrons in a superconductor. There are different ways the electron can form pairs, these depend on the orbitals which give the names *s*-, *d*-, *p*-, and f-wave superconductivity. In the first two mechanisms the Cooper pairs are singlet states, i.e. pairs of electrons with opposite spin, and in the latter two they are triplet states, i.e. pairs of electrons with aligned spin. The details are not too relevant here, but let us notice that in a chain of spinless fermions only fermions with the same spin, or aligned spin for that matter,

can exist.

Although it might not be immediately clear, this results in problems in experimental implementing this chain, since the existence of p-wave superconductivity has not yet been experimentally discovered. In theory there is nothing that prohibits this kind of superconductivity from occurring, but in comparison to the mainstream s-wave superconductivity it is rare and not dominant. Only recently strong evidence for p-wave superconductivity was found in two-dimensional systems [2], [21], [27].

Hopefully careful physics reader have survived until here reading about "spinless fermions", which is a contradictio in terminis, since fermions have half-integer spin. This leaves us with the problem that the Kitaev cannot be simply implemented in experiments. An idea to overcome this problem is isolate one spin, for example by applying a magnetic field such that the energy splitting of the different spin states due to the Zeeman-effect is sufficiently large. This is indeed part of the solution, but more adjustments need to be done. In this thesis we are not too much interested in implementing theoretical models in experiments, and therefore we will not go into much depth here. However, it is indeed possible to construct a Hamiltonian that mimics the Kitaev chain, and that is physical feasible by a semi-conducting wire in contact with a s-wave superconductor, this so-called one-dimensional Rashiba nanowire is discussed in more depth here [45]. This concludes the discussion of the terms in the Hamiltonian of the Kitaev chain. Let us now introduce a phenomenon, which makes the this chain especially interesting.

7.2.1 Majorana (quasi)particles

In 1937 Ettore Majorana predicts that uncharged fermions can be described by a real wave function, and therefore there are their own antiparticles [47]. A particle that is described by such a wave function, i.e. a particle that is its own antiparticle, is called a *Majorana particle*. Since we consider quasiparticles as states described with one wave function that are a linear combination of elementary particles, but not elementary particles themselves, we call quasiparticles that are their own antiparticles *Majorana quasiparticles*.

Until now we have worked with a formulation of the second quantisation that uses the creation and annihilation operators, $c_i^\dagger$ resp. c_i, as a basis of the operator algebra that is present on the background. Of course this is not the only useful choice of a basis. We can define a basis of operators

such that every element in the basis is self-adjoint, namely

$$\gamma_{i,1} := c_i^\dagger + c_i; \tag{7.8}$$
$$\gamma_{i,2} := i(c_i^\dagger - c_i). \tag{7.9}$$

Since self-adjoint operators describe particles that are their own antiparticle, we call these *Majorana operators*. It is immediately clear that these operators are indeed self-adjoint

$$\gamma_{i,1}^\dagger = c_i^{\dagger\dagger} + c_i^\dagger = c_i + c_i^\dagger = \gamma_{i,1};$$
$$\gamma_{i,2}^\dagger = -i(c_i^{\dagger\dagger} - c_i^\dagger) = i(-c_i + c_i^\dagger) = \gamma_{i,2}.$$

Using the anti-commutation relations of the creation and the annihilation operators, Eq. 5.7, 5.8, and 5.9, we obtain the following anti-commutation relations for fermions:

$$\{\gamma_{i,1}, \gamma_{j,1}\} = 2\delta_{ij}; \tag{7.10}$$
$$\{\gamma_{i,2}, \gamma_{j,2}\} = 2\delta_{ij}; \tag{7.11}$$
$$\{\gamma_{i,1}, \gamma_{j,2}\} = 0. \tag{7.12}$$

It immediately follows that $\gamma_{i,1}^2 = \gamma_{i,2}^2 = 1$. We will see that these relations make it possible to represent another kind of algebra with Majorana operators than with the original creation and annihilation operators. Before diving into this mathematical interpretation of Majorana operators, we will consider a unique property of those operators which has to do with changing the order of the corresponding quasiparticles in a chain.

7.2.2 Physical braiding

Here we will explore the so-called *non-abelian exchange statistic* of Majorana quasiparticles. It turns out that order of exchanging Majorana quasiparticles matters, both one-dimensional systems [4] and two-dimensional systems [26].

Let us first consider the exchange of Majorana quasiparticles, also called *braiding*, in a 2D-system. Although 2D-systems are of minimal relevance to the Kitaev chain, the concept of braiding works similar, and an explanation in 2 dimensions is more intuitive. Therefore we follow the discussion about two-dimensional braiding in the review paper of Leijnse [40]. In a 2D $p + x \pm ip_y$ superconductors, a specific case of p-wave superconductivity in 2 dimensions, Majorana quasiparticles are present at vortices where

the superconducting gap vanishes [58]. Around such a vortex the superconducting gap is unambiguously defined, except at a branch cut where the gap changes by 2π. Although the exact position of the branch cut can be chosen freely, when two Majorana quasiparticles are exchanged, as schematically shown in Fig. 7.1, one of them certainly crosses the branch cut of the other, acquiring a phase of -1.

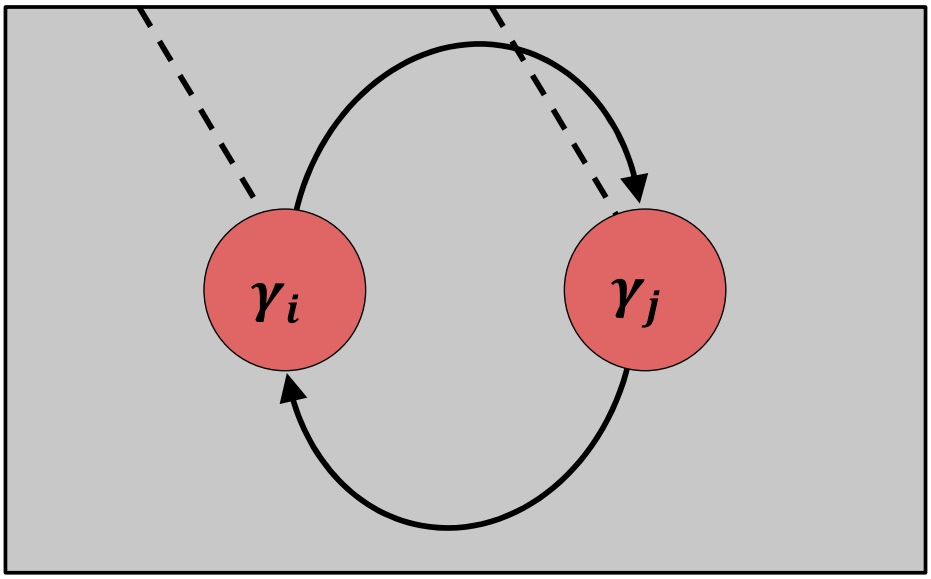


Figure 7.1: *When two Majorana particles γ_i and γ_j centred at vortices in a two-dimensional superconductor, depicted by red dots, are interchanged, one of them crosses the branch cut at the dashed line.*

Because of the fact that the particles are indistinguishable, the exchange operation can be summarised by

$$\gamma_i \mapsto -\gamma_j \tag{7.13}$$

$$\gamma_j \mapsto +\gamma_i. \tag{7.14}$$

When one takes into account that other vortices are not related to this exchange, we can define an operator that is unique up to choice of the branch cut and the choice of the exchange being (anti)clockwise. The transformation can be described by

$$\gamma_k \mapsto B_{ij}\gamma_k B_{ij}^\dagger, \tag{7.15}$$

where the *braiding operator* is given by

$$B_{ij} = \frac{1}{\sqrt{2}}(1 + \gamma_i\gamma_j). \tag{7.16}$$

In the case of two vortices, and hence two Majorana quasiparticles, there is just one braiding operator. For a $2n$-fold degenerate ground state where $n > 1$ there exist more braiding operators, and this is where the interesting effect occurs. For exchanges where at least one quasiparticle is shared we obtain the commutation relation

$$[B_{i-1,i}, B_{i,i+1}] = \gamma_{i-1}\gamma_{i+1}, \tag{7.17}$$

and exchanges that take place on different Majoranas do commute.

It turns out that this braiding works similar in 1D systems. Even in a 1D nanowire that is used to experimentally implement the Kitaev chain braiding is possible [4]. Of course there are differences in the intuition and practicalities of this 1D braiding. Moving particles "around" each other is not possible in a chain. Therefore we have to find alternatives.

In real space the main idea is to braid different chains that are close together. This protocol is thoroughly studied, but yet there exists no experimental realisation. A neat discussion of braiding in real space can be found in review papers of Beenakker [7, 8].

For an alternative way of braiding one has to make the observation that braiding eventually boils down to the addition of a phase or a unitary transformation. In this way braiding can be obtained via the parameter space. When a system is in a topological non-trivial phase, there exists a gap and edge states, we can perform an adiabatic loop and define a Wilczek-Zee connection. When the relevant subspace of parameter space is not simply connected these loops result in a non-trivial Wilczek-Zee factor. In the remainder of this thesis we will aim to perform such *braiding in the parameter space*.

Finally, with this braiding it is possible to store information in a set of Majorana quasiparticles. In this way Majorana quasiparticles are proposed as building blocks for quantum computations [8].

7.2.3 Mathematical braiding

In section 7.2.2 we have discussed the concept of braiding from a physical point of view. To obtain a broader understanding of braiding we will roughly follow the discussion by Kauffman [31] to study the same concept from a mathematical point of view.

Definition 7.2.1. Let B_n be a group generated by $\sigma_1, ..., \sigma_{n-1}$ called *elementary braids* satisfying the following relations:

$$\sigma_i\sigma_j = \sigma_j\sigma_i, \text{ for } |i-j| > 1; \tag{7.18}$$

$$\sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1}, \text{ for } i = 1, ..., n-2. \tag{7.19}$$

This group is called the *Artin braid group (for n strands)*.

In trying to understand this group we might see B_n as a group of actions on n strands that are held on one side, where the elementary braid σ_i corresponds to crossing the ith under the $(i+1)$th strand.

In this interpretation the relation of Eq. 7.18 is perfectly in line with our naive idea of braiding, since the order of braiding strands that do not overlap should not matter. The relation is a little harder to see visualise directly.

From this intuition behind braiding it is reasonable to ask if it is also possible to braid the first and the last strand, physicist would ask if we could "apply periodic boundary conditions". This gives rise to the *circular Artin braid group*.

Definition 7.2.2. Let B_n^c be an Artin braid group for n strands, and impose the extra relation on the elementary braids

$$\sigma_n\sigma_1\sigma_n = \sigma_1\sigma_n\sigma_1. \tag{7.20}$$

The group B_n^c is called the *Artin braid group (for n strands)*.

A natural step in studying this groups is studying its relation with certain vector spaces or algebras, i.e. studying representations of the group. We have already seen the definition of an associative algebra when studying the properties of creation and annihilation operators. For this group however we will first define a specific kind of algebras that will turn out to bridge the gap from braiding groups to Majorana fermions.

Definition 7.2.3. Let $m, n \in \mathbb{Z}_{\geq 0}$ and consider the vector space $\mathbb{R}^{m+n}$ together with a degenerated quadratic form $\_ \cdot \_ : \mathbb{R}^{m+n} \times \mathbb{R}^{m+n} \to \mathbb{R}^{m+n}$. A *(real) Clifford algebra* is the associative algebra over $\mathbb{R}$ by $m+n$ orthonormal basis elements $\{e_i\}_{i=1}^{m+n}$ such that the following relations are satisfied

$$e_i \cdot e_i = 1, \text{ for } 1 \leq i \leq m; \tag{7.21}$$

$$e_i \cdot e_i = -1, \text{ for } m < i \leq m+n; \tag{7.22}$$

$$e_i \cdot e_j = -e_j e_i, \text{for } i \neq j. \tag{7.23}$$

The Clifford algebra as defined above is denoted by $\mathrm{Cl}(m, n)$. From Eq. 7.23 it follows that it is only necessary to look at unordered combinations of generators e_i to construct basis vectors for the Clifford algebra as vector space, and for that it is clear that $\mathrm{Cl}(m, n)$ is a vector space over $\mathbb{R}$ of dimension 2^{m+n}. Furthermore, we say that an element $v \in \mathrm{Cl}(m, n)$ that can be constructed as a linear combination of unordered pairs of k unique generators e_i has *grade k*, and this is well-defined because of the remark above.

This enables us to write the real Clifford algebra $\mathrm{Cl}(m, n)$ as a direct sum of subspaces of the same grade. When the subspace of $\mathrm{Cl}(m, n)$ of elements of grade k is denoted by M_k, then it holds that

$$\mathrm{Cl}(m, n) = M_0 \oplus M_1 \oplus \cdots \oplus M_{p+q}. \tag{7.24}$$

This decomposition shows a lot of structure that might be hidden in other formulation of the Clifford algebra.

A subspace of the Clifford algebra that plays an important role in the remainder of this section is the *second Clifford algebra* defined as the subspace of linear combinations of elements of even grade, i.e.

$$\mathrm{Cl}^+(m, n) := M_0 \oplus M_2 \oplus \cdots . \tag{7.25}$$

Equipped with the basis definition of real Clifford algebras we can again involve Majorana operators in our discussion.

Let us consider n pairs of Majorana operators $\gamma_{i,1}, \gamma_{i,2}$, and consider the real Clifford algebra $\mathrm{Cl}(2n, 0)$. Now we can do a similar observation as with the creation and annihilation operators. Because $\gamma_{i,1}^2 = \gamma_{i,2}^2 = 1$ and different operators anticommute, we can send generators of $\mathrm{Cl}(2n, 0)$ to Majorana operators. Just as we could represent the abstract algebra defined by the relations in Eq. 5.10 with creation and annihilation operators, we can represent $\mathrm{Cl}(2n, 0)$ with Majorana operators. The algebra defined by the anticommutation relations in Eq. 5.10 is often called a *fermionic algebra*, in the same spirit we could (unconventionally) say that $\mathrm{Cl}(2n, 0)$ is a *Majorana algebra*.

Finally we will return to braiding and to bridge the gap between Majoranas and braiding with Clifford algebras. Before stating the main theorem define $L_v : \mathrm{Cl}(k,0) \to \mathrm{Cl}(k,0)$ left multiplication by $v \in \mathrm{Cl}(k,0)$ as the map defined by $L_v(w) = v \cdot w$, where $\cdot$ is the quadratic form associated to the Clifford algebra. It is easy to see that this map is linear and well-defined.

Theorem 7.2.1 (Clifford Braiding Theorem)**.** *Let $k \in \mathbb{Z}_{\geq 0}$, B_k^c the circular Artin braid group of n strands and $Cl(k,0)$ a real Clifford algebra. Then B_k^c can be represented by a linear map $\varphi : B_k^c \to Aut(Cl(k,0))$ defined by*

$$\sigma_i \mapsto L_{\frac{1}{\sqrt{2}}(1+e_{i+1}e_i)}, \text{ for } 1 \leq i < k; \tag{7.26}$$

$$\sigma_k \mapsto L_{\frac{1}{\sqrt{2}}(1+e_1e_k)}. \tag{7.27}$$

Proof. Using the relations Eq. 7.21 and 7.23 the defining properties of elementary braids can be checked. □

It is important to keep in mind that in the theorem above the Clifford algebra $\mathrm{Cl}(k,0)$ is consider as a 2^k dimensional vector space, and therefore the representation is a group representation.

Notice that we only use elements of the second Clifford algebra $\mathrm{Cl}^+(k,0)$, so we could even conclude that B_k^c can be represented in $\mathrm{Cl}^+(k,0)$. Moreover, it is important to stress that this is not the only possible representation of B_k^c, since it can be shown that the elementary braids here are of order 8 [31], and in the definition of a (circular) Artin braid group that is not required for those braids. That is a property of this representation that is a little counter intuitive, since in our naive idea of braiding the operation of crossing two strands has infinite order.

Nevertheless, we can braid Majoranas by identifying them with the generators of a real Clifford algebra $\mathrm{Cl}(2n,0)$, and then identify elementary braids with those (multi)vectors of Majorana operators according to Eq. 7.26, and 7.27. This construction ultimaterly connects the notion of Majorana operators with braiding.

Although this is a great result it, such braiding of Majoranas is not enough to obtain a complete set of operators to carry out all unitary operations to some precision. Hence Majoranas and braiding are not a suitable candidate for quantum calcultions, especially the possibilities with Majoranas in 1D systems are limited [31]. On the contrary, the option to use Majoranas and braiding for quantum memory is still on the table.

Furthermore, remember that they seldom mention the Artin braid group, when they discuss braiding. Often they would just refer to some nontrivial holonomy group as treated in section 7.2.2.

7.2.4 Majorana (quasi)particles in a Kitaev chain

Provided with the homogeneous Kitaev chain, Eq. 7.7, we start our search for the occurrence of Majorana quasiparticles. Firstly, we look into a specific set of parameters, $t = |\Delta| = 0$. Using Eq. 7.8 and Eq. 7.9 the expression from Eq. 7.7 can be rewritten as

$$\hat{H}(\mu) = \frac{i}{2}\mu \sum_{j=1}^{N} \gamma_{j,1}\gamma_{j,2}, \tag{7.28}$$

where we have omitted a constant depending on μ. It is discussed in the book of Altland and Simons [5] that this constant does not change the properties of the operator as those are essentially fixed by there commutation relations. Immediately we observe that the *excitations* in this system, i.e. the eigenvectors of this Hamiltonian, are paired Majorana operators, and they have energy $\pm|\mu|/2$. All these state are *local* instead of edge states.

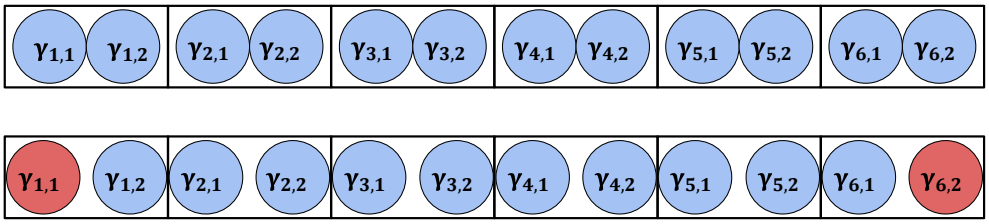


Figure 7.2: *The upper chain depicts a Kitaev chain of 6 sites where all the Majorana operators are paired locally at the same site. This system is in a topological trivial phase. The lower chain depicts the same system where non-local pairing of Majorana operators is present, the red dots form one physical edge state. This system is in topological non-trivial phase.*

Let us now consider another set of parameters, namely $t = |\Delta|$ and $\mu = 0$. If Δ is assumed to be real the homogeneous Kitaev Chain, Eq. 7.7, can be rewritten as

$$\hat{H}(t) = it \sum_{j=1}^{N-1} \gamma_{j+1,1}\gamma_{j,2}. \tag{7.29}$$

A careful reader directly notices that $\gamma_{1,1}$ and $\gamma_{N,2}$ do not occur in this Hamiltonian. This leaves us with a zero-energy state $\gamma_{1,1}\gamma_{N,2}$ called a *Majorana Zero Mode* or *MZM*. A schematic depiction of this state can be found in Fig. 7.2.

It is obvious that this state is an edge state, because both the Majorana operators are located at the different ends of the chain, and the this eigenstate is an effect of the open boundary conditions as periodic boundary conditions would include $\gamma_{1,1}\gamma_{N,2}$ in Eq. 7.29.

One should be aware about the fact that in a finite-sized system with different t and Δ or non-zero chemical potential there are no states that exists exactly at the edge. The topologically protected edge states with zero-energy that will occur will decay rapidly over the chain. So in a way MZMs are ill-defined in that sense. Nevertheless, we will refer to those edge states satisfying Eq. 7.8 and Eq. 7.9 as MZMs.

Now we have seen the first occurrence of MZMs in the homogeneous Kitaev chain, but only for a specific parameter regime. Shortly we will study the existence of these states for more general combinations of parameters, combinations where both the chemical potential and the hopping are nonzero.

7.3 Analytically solving the bulk spectrum

Before we are able to study the general existence of MZMs as mentioned above, we need to study the Hamiltonian of the chain in more depth and rewrite Eq. 7.7 is such a way that we can investigate the bulk and subsequently the bulk-boundary correspondence.

The first step is to obtain a Hamiltonian of the form of Eq. 6.1 from Eq. 7.7. We will consider this as a special case of an even more general Hamiltonian, an example of an *inhomogeneous Kitaev chain* which is described by the Hamiltonian

$$\hat{H}(\mu_j, t_j, \Delta_j) := -\sum_{j=1}^{N} \mu_j c_j^\dagger c_j - \sum_{j=1}^{N-1} t_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \sum_{j=1}^{N-1} (\Delta_j c_j^\dagger c_{j+1}^\dagger + \Delta_j^* c_{j+1} c_j), \tag{7.30}$$

where $\mu_j \in \mathbb{R}$ the chemical potential on site $j \in \{1, ..., N\}$, and $t_j \in \mathbb{R}$ and $\Delta_j \in \mathbb{C}$ the hopping potential respectively the superconducting gap between site j and $j+1$ for all $j \in \{1, ..., N-1\}$.

This Hamiltonian can be transformed by a Bogoliubov transformation transformation. Let us use a Nambu spinor

$$\hat{\chi}^\dagger = (c_1^\dagger, ..., c_N^\dagger, c_1, ..., c_N), \tag{7.31}$$

which can be used to obtain the Bogoliubov-de-Gennes Hamiltonian ac-

cording to Eq. 6.4. The BdG Hamiltonian reads

$$\mathcal{H}_{KC} = \begin{pmatrix} C & S \\ -S^* & -C^* \end{pmatrix}, \tag{7.32}$$

where

$$C' = \begin{pmatrix} -\mu_1 & -t_1 & 0 & 0 & \cdots & 0 & 0 \\ -t_1 & -\mu_2 & -t_2 & 0 & \cdots & 0 & 0 \\ 0 & -t_2 & -\mu_3 & -t_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -\mu_{N-1} & -t_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & -t_{N-1} & -\mu_N \end{pmatrix} \tag{7.33}$$

and

$$S = \begin{pmatrix} 0 & -\Delta_1 & \cdots & 0 & 0 \\ \Delta_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & -\Delta_{N-1} \\ 0 & 0 & \cdots & \Delta_{N-1} & 0 \end{pmatrix} \tag{7.34}$$

the matrices that capture the model dependent parameters. This enables use to rewrite Eq. 7.30 in the following way

$$\hat{H}(\mu_j, t_i, \Delta_j) = \frac{1}{2}\hat{\chi}^\dagger \mathcal{H}_{KC}\hat{\chi}, \tag{7.35}$$

and notice once again that this equality is only true up to a constant. However, as we have seen above, and as discussed in [5], this does not change the physical properties of the Hamiltonian.

Although the formulation of the Kitaev chain in Eq. 7.32, 7.33, 7.34, and 7.35 is not too insightful, it enables us to numerically calculate the spectrum and the eigenstates including the edge states. We will make elaborate use of that through this thesis and the investigation of this model and similar ones in Chapter 8, 9, and 10. For certain parameter regimes the explicit solutions of the homogeneous variant of this matrix are known [41].

To obtain more insight in this model we will calculate the energy spectrum of the bulk. Let us assume periodic boundary conditions, and introduce the Fourier transform of the creation and annihilation operators

$$c_j^\dagger := \frac{1}{\sqrt{N}} \sum_k e^{-ijkd} c_k^\dagger; \tag{7.36}$$

$$c_j := \frac{1}{\sqrt{N}} \sum_k e^{ijkd} c_k, \tag{7.37}$$

where d is the lattic constant, $d_k^\dagger$ the creation operator in k-space, d_k the annihilation operator in k-space, and the summation is over $k \in [-\pi/d, \pi/d]$ where the values of k are equally spaced. Transforming the term with the chemical potential leaves us with

$$-\frac{\mu}{N}\sum_j\sum_k\sum_{k'} e^{idk(k'-k)} d_k^\dagger d_{k'} = -\frac{\mu}{N}\sum_k\sum_{k'}\delta_{kk'} d_k^\dagger d_{k'} = -\mu\sum_k d_k^\dagger d_k, \quad (7.38)$$

and the term with hopping amplitude with

$$\begin{aligned} &-\frac{t}{N}\sum_j\left(\sum_k\sum_{k'} e^{ijd(k'-k)}e^{-idk} d_k^\dagger d_{k'} + \sum_k\sum_{k'} e^{ijd(k'-k)}e^{idk'} d_k^\dagger d_{k'}\right) \\ &= -\frac{t}{N}\sum_k\sum_{k'}\delta_{kk'}\left(e^{idk'} + e^{-idk}\right) d_k^\dagger d_{k'} = -2t\sum_k \cos(kd) d_k^\dagger d_k. \end{aligned} \quad (7.39)$$

For the superconducting term we initially apply the same transformation yielding

$$\begin{aligned} &\frac{1}{N}\sum_j\sum_k\sum_{k'}\left(\Delta e^{-idk(j+1)} d_k^\dagger e^{-idk'j} d_{k'}^\dagger + \Delta^* e^{idkj} d_k e^{idk'(j+1)} d_{k'}\right) \\ =&\frac{1}{N}\sum_j\sum_k\sum_{k'}\left(\Delta e^{-idk} e^{-idk(k+k')} d_k^\dagger d_{k'}^\dagger + \Delta^* e^{idk'} e^{idk(k+k')} d_k d_{k'}\right) = (*). \end{aligned} \quad (7.40)$$

Unfortunately, we do not immediately recognise the Kronecker delta. However, the ks and k's are summed over equally spaced values. Making use

of that fact and replacing k' by $-k'$ in Eq. 7.40 we obtain

$$\begin{aligned}
(*) &= \frac{1}{N}\sum_j\sum_k\sum_{k'}\left(\Delta e^{idk}e^{ijd(k-k')}d^\dagger_{-k}d^\dagger_{k'} + \Delta^* e^{-idk'}e^{ijd(k-k')}d_k d_{-k'}\right)\\
&= \frac{1}{N}\sum_k\sum_{k'}\left(\Delta\delta_{k'k}e^{idk'}d^\dagger_{-k}d^\dagger_{k'} + \Delta^*\delta_{k'k}e^{-idk}d_k d_{-k'}\right)\\
&= \sum_k\left(-\Delta e^{idk}d^\dagger_k d^\dagger_{-k} + \Delta^* e^{-idk}d_k d_{-k}\right)\\
&= \frac{\Delta}{2}\left(\sum_k\left(e^{ikd}d^\dagger_{-k}d^\dagger_k - e^{-ikd}d_{-k}d_k\right) + \sum_k\left(-e^{ikd}d^\dagger_k d^\dagger_{-k} + e^{-ikd}d_k d_{-k}\right)\right)\\
&= \frac{1}{2}\left(\sum_k\left(\Delta e^{-ikd}d^\dagger_k d^\dagger_{-k} - \Delta^* e^{ikd}d_k d_{-k}\right) + \sum_k\left(-\Delta e^{ikd}d^\dagger_k d^\dagger_{-k} + \Delta^* e^{-ikd}d_k d_{-k}\right)\right)\\
&= \frac{1}{2}\sum_k\left(-\Delta(e^{ikd}-e^{-ikd})d^\dagger_k d^\dagger_{-k} + \Delta^*(e^{ikd}-e^{-ikd})d_{-k}d_k\right)\\
&= \frac{1}{2}\sum_k\left(-2i\Delta\sin(kd)d^\dagger_k d^\dagger_{-k} + 2i\Delta^*\sin(kd)d_{-k}d_k\right). \qquad (7.41)
\end{aligned}$$

Combining Eq. 7.38, 7.39, and 7.41 we obtain the following Fourier transform of the Kitaev chain

$$\hat{H}_{KC}(k) = \frac{1}{2}\sum_k \hat{\psi}^\dagger_k\begin{pmatrix}-\mu-2t\cos(kd) & -2i\Delta\sin(kd)\\ 2i\Delta^*\sin(kd) & \mu+2t\cos(kd)\end{pmatrix}\hat{\psi}_k, \qquad (7.42)$$

where $\hat{\psi}^\dagger_k := (c^\dagger_k, c_{-k})$ is a Nambu spinor. Notice that this is the Fourier transform of Eq. 7.7, up to an unimportant constant.

The matrix in Eq. 7.42 is the Bogoliubov-de-Gennes Hamiltonian corresponding to the chain in k-space, and its (non-negative) eigenvalues give the energies of the elementary excitations of the system. be aware of the fact that it seems that this Hamiltonian allows excitations of negative energy. Those correspond to the excitations of holes, and therefore the particle-hole symmetry instruct that they always come in pairs.

To obtain these energies we consider the characteristic polynomial of the BdG Hamiltonian, where we again used our assumption that $\Delta \in \mathbb{R}$:

$$(\varepsilon+\mu+2t\cos(kd))(\varepsilon-(\mu+2t\cos(kd)) - 4\Delta^2\sin^2(kd) = 0 \qquad (7.43)$$

$$\varepsilon^2 - (\mu+2t\cos(kd))^2 - 4\Delta^2\sin^2(kd) = 0. \qquad (7.44)$$

This yields the excitation energies

$$\varepsilon(k) = \pm\sqrt{(\mu+2t\cos(kd))^2 + 4\Delta^2\sin^2(kd)}. \qquad (7.45)$$

We observe that for $\mu = 0$ there is a gap in the energy spectrum of $2|t|$ between the lowest energy bulk state and zero-energy if $|t| \leq |\Delta|$ and $2|\Delta|$ if $|\Delta| < |t|$. Furthermore, it is clear that in the case of $|\mu| = 2|t|$ the gap closes, while for all $|\mu| \in [0, 2|t|)$ and $\Delta \neq 0$ there is a gap present.

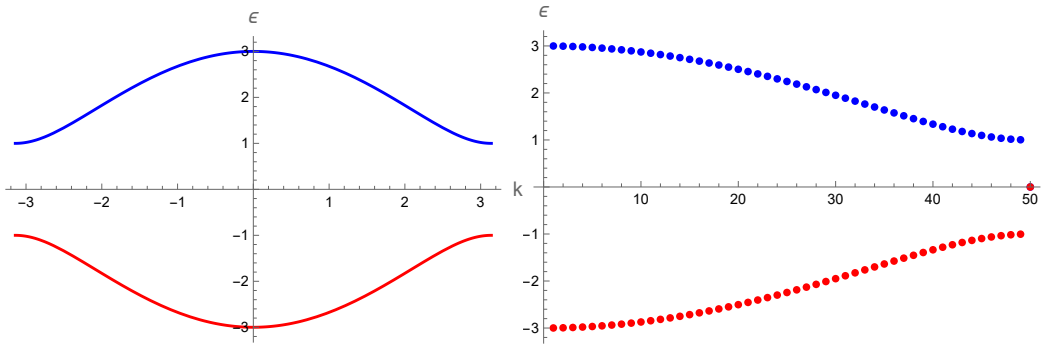
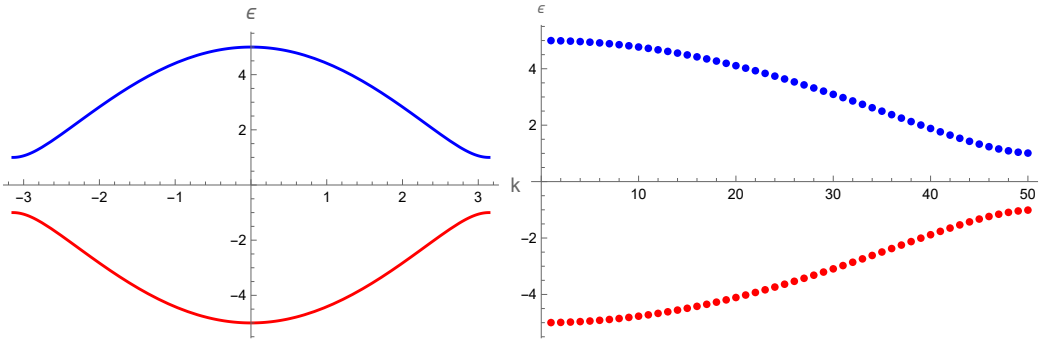


Figure 7.3: *(a) The analytic energy spectrum of the infinite homogeneous Kitaev chain with periodic boundary conditions in k-space for the parameters $\mu = 1$, $t = 1$, and $\Delta = 1$. (b) The numerical energy spectrum of the homogeneous Kitaev chain with 50 sites and open boundary conditions for the parameters $\mu = 1$, $t = 1$, and $\Delta = 1$. These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32. This spectrum exhibits two energies of order 10^{-15} corresponding to edge states.*

Let us compare the bulk spectrum with the spectrum that is obtained by numerically diagonalising Eq. 7.32. The calculated spectra are shown in Fig. 7.3 and Fig. 7.4 for different sets of parameters. Although both analytical and numerical spectra look quite similar, we notice that Fig. 7.3b exhibits energies which correspond to edge states, and which are approximately zero, while Fig. 7.4b does not. In the bulk this can be observed by the fact that the parity of the the electrons in the bulk changed. The first one is in the topological non-trivial phase with a sign of the Pfaffian which is 1, while the second one is in a topological trivial phase where the a sign of the Pfaffian is valued -1. The topological phase transition happened at the closing of the gap, $|\mu| = 2|t|$.

We will conclude this chapter with some remarks on the symmetries of the homogeneous Kitaev chain. We have already seen that the particle-hole symmetry is present after the Bogoliubov transformation, with the corresponding operator $\hat{C} = \tau_x \mathcal{K}$. Hence the Kitaev chain exhibits PHS with $C^2 = 1$. Moreover, the model described a chain of spinless fermions, and therefore we see that for a time-reversal operator we can take the conjugation operator, i.e. $\mathcal{T} = \mathcal{K}$, which commutes with the real Hamiltonian $\hat{H}$. So the Kitaev chain is time-reversal symmetric with $T^2 = 1$. Since we



(a) **(b)**

Figure 7.4: *(a) The analytic energy spectrum of the infinite homogeneous Kitaev chain with periodic boundary conditions in k-space for the parameters $\mu = 3$, $t = 1$, and $\Delta = 1$. (b) The numerical energy spectrum of the homogeneous Kitaev chain with 50 sites and open boundary conditions for the parameters $\mu = 3$, $t = 1$, and $\Delta = 1$. These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32. This spectrum does not exhibit energies that are not already present in the bulk spectrum.*

obtain a operator corresponding to the chiral symmetry by $\hat{S} = \hat{C} \cdot \hat{T}$, the chiral symmetry is also present in the Kitaev chain. Therefore it belongs to the BDI-class, Table 6.1. When we would allow for complex pairing, i.e. complex parameters in the Hamiltonian, the TRS is broken and the Kitaev chain belongs to the D-class. According to Kitaev [32] these classes have corresponding topological quantum numbers that take values in $\mathbb{Z}$ and $\mathbb{Z}_2$ respectively, being the number of MZMs at the edges and the existence of MZMs respectively.

Equipped with the elementary knowledge of the homogeneous Kitaev chain we will need to look into extensions of the model to facilitate braiding of Majorana modes via the parameter space.

Chapter 8

The inhomogeneous Kitaev chain

One of the problems we need to overcome before braiding in the parameter space would be possible is: how to obtain a ground state that is $2n$-fold degenerate with $n > 1$? However, when the degeneracy of Majorana states is increased at the edges, for example by introducing spin to double the degeneracy, the Majorana operators would most probably couple to each other instead of forming non-local edge states. Therefore we will discuss how *topological defects* and corresponding *domain walls* can be introduced in the system, and how MZMs will form not only at the edges of the chain, but also at those domain walls. In this chapter this behaviour is numerically studied in finite-sized chains by consideration of spectra and zero-energy edge states.

8.1 Topological defects

A well-informed reader might be familiar to so-called *topological defects* in the context of field theories, solitons, and kink solutions as discussed in for example [48] by Manton and Sutcliffe. However, let us develop a natural idea of the concept of such defects.

Let us return to the main idea of a topological material. Recall we call a material a topological material if there are certain edge states of the system that cannot be destroyed by continuous deformations of the Hamiltonian that respect the present symmetries. A mathematician would formulate this as: there does not exist a homotopy between two Hamiltonian, one with property of edge states and one without. Naturally the same vocabulary can be used for defects. Then a topological defect would be a inhomogeneity in a material, or in a Hamiltonian, that cannot be made up

for by continuous deformations of that Hamiltonian.

An example of such a defect in gapped systems is a change in parameters in the material in such a way that locally the parameters would close the gap if they would extend to the entire system. The locality of this defect implies that the edge states of the original homogeneous material are unaffected. These regions in the system where the local parameters would close the gap are called *domain walls*, and a common property of those domain walls is that give rise to edge states besides not destroying the already present edge states at the boundaries of the whole system [68, 73]. Therefore we propose to introduce topological defects in the Kitaev chain to increase the degeneracy.

8.2 Majorana zero modes at defects

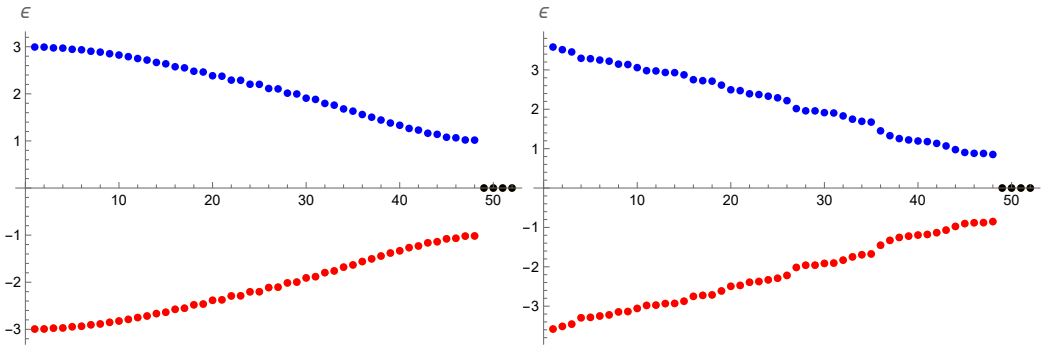
For the homogeneous Kitaev chain, with a spectrum given by Eq. 7.45, we can distinguish two ways the gap could close. The first way is by vanishing of the superconducting gap, i.e. $\Delta = 0$, and the second way by vanishing of the combined chemical potential and hopping amplitude term, i.e. $|\mu| = 2|t|$. We will consider chains where domain walls occur because of parameters fulfilling these conditions locally.

8.2.1 Vanishing superconducting gap

Let us first assume that the hopping amplitude is non-zero. This is reasonable, because for $t = 0$ we encounter a topological trivial situation independent of Δ. This enables us to normalise all terms by t. Furthermore, we will leave μ constant over the whole chain. The defect will consist of a change of the parameter Δ_i in the matrix of Eq. 7.34 from Δ to $-\Delta$ by means of a strictly decreasing sinusoid is evaluated at $l + 1$ sites centred around some site $n \in \{0, N\}$ where N is the length of the chain. Be aware of the fact that for it to be a topological defect, hence not influencing the existence of edge states, the defect should not be centred near the edges.

Let us consider a finite-sized homogeneous Kitaev chain, length N, with a defect centred in the middle, $n = \lfloor N/2 \rfloor$, with $\Delta = t$. Fig. 8.1a exhibits both the gap and zero-energy states corresponding to MZMs that you would expect for the homogeneous chain, and an additional pair of zero-energy states.

Despite the fact that the spectrum shows the existence of zero-energy states it is not at all clear from the spectrum that these new zero-energy states are edge states. To ensure that the topological defect gives rise to a



(a) *Unperturbed spectrum with defect* ***(b)*** *Perturbed spectrum with defect*

Figure 8.1: *(a) The numerical energy spectrum of the homogeneous Kitaev chain with* 50 *sites and open boundary conditions for the parameters* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32 and four zero-energy states with energies of the order of* 10^{-7}. *(b) The spectrum of the same system with a white noise perturbation of the parameters in Eq. 7.32 with noise level* $t/2$. *The zero-energy states have energies in the order of* 10^{-6}.

edge state centred around the domain wall on should calculate the eigenstates of the BdG Hamiltonian with the defect. Fig. **??** unambiguously shows that the zero-energy states are positioned at the domain walls and the edges of the chain. Be aware that the zero-energy states are mixed states between states at the edges and at the domain walls. However, it is clear that by suitable linear combination pure edge and defect states can be obtained.

We already expected MZMs to form at those defects, but it is still crucial to perform some cross-checks. On of the test to see if such a edge state is indeed a MZM, is to include noise into the chain. An effective way of doing this is to add white noise with a standard deviation of a fraction of t, since t is the parameter used to normalise, to every parameter. In the perturbed spectrum shown in Fig. 8.1b the gap and the zero-energy states are still present.

Besides the fact that noise does not influence the existence of defect states there is another strong indication that we are dealing with MZMs. When one carefully inspects Fig. 8.2 and Fig. 8.3 it is noticed that there is some relation between the ψ_i of the creation and annihilation operators. It can be checked that these relations are obeying the basis transformation form creation and annihilation operators to Majorana operators, i.e. Eq. 7.8 and Eq. 7.9. This implies that the founded eigenstates are self-adjoint, i.e.

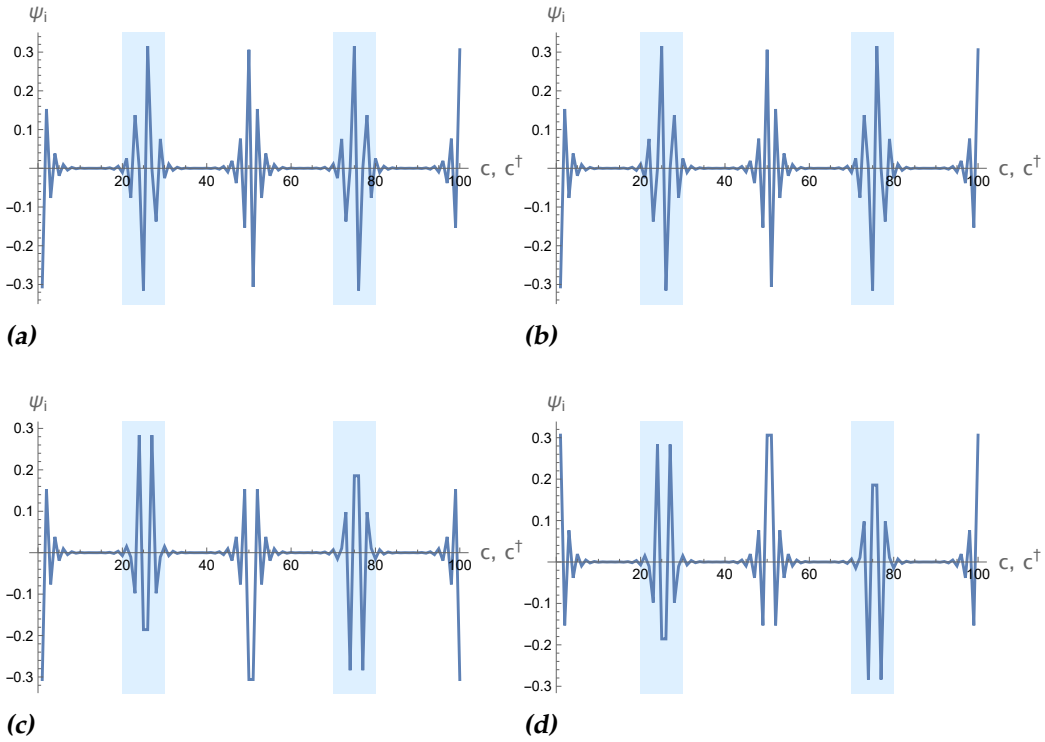


Figure 8.2: *(a),(b),(c),(d) The eigenstates corresponding to the zero-energy modes of a Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state. The shaded areas mark the position of the defect.*

their own antiparticle.

Based on these examples it is premature to draw general conclusion. However, in the Appendix A the results are shown for different parity of the chain and different positions of the defect, and all these results show similar properties as the examples in this section. Therefore it is safe to say that Majorana quasiparticles do indeed occur at the domain walls imposed by topological defects in the superconducting gap.

8.2.2 Chemical potential outside of the bandwidth

From Eq. 7.45 it is easily deduced that $|\mu| = 2|t|$ leaves us with a closing of the gap independent of the superconducting gap. The interval $(-2|t|, 2|t|) \subset \mathbb{R}$ is called the *bandwidth*. For μ in that interval and $\Delta \neq 0$ it is observed that MZMs are present in the homogeneous Kitaev chain.

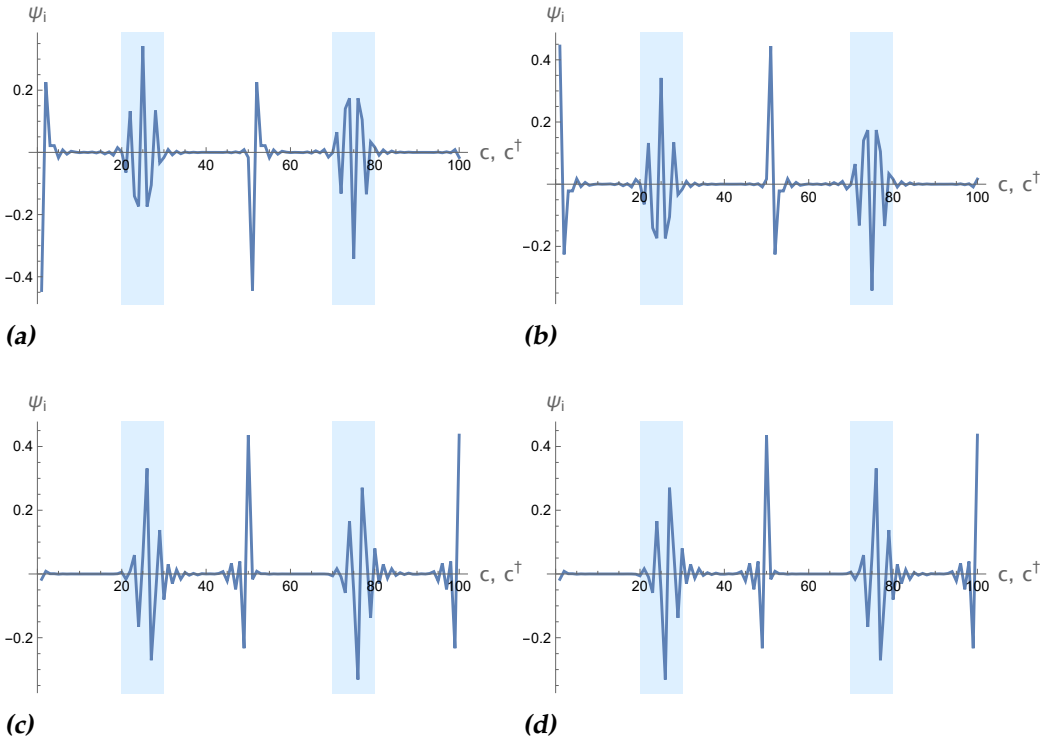
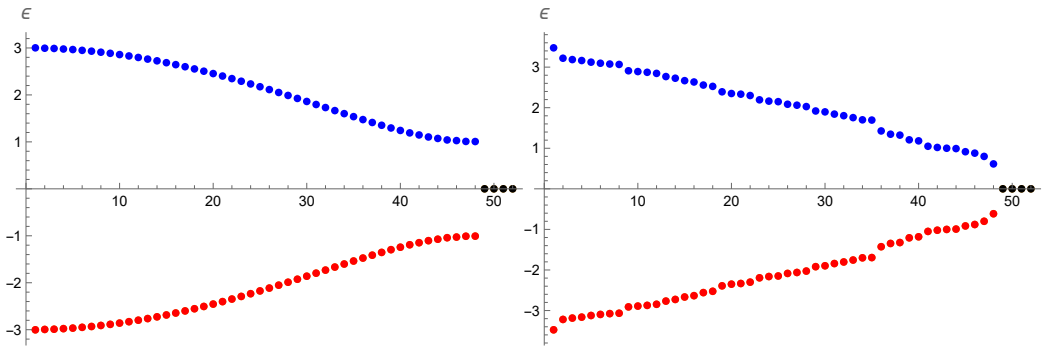


Figure 8.3: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32. The* x*-axis depicts the Nambu spinor, Eq. 7.31, and the* y*-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state. The shaded areas mark the position of the defect.*

With this knowledge we want to create a domain wall, and attached to that MZMs.

Consider a homogeneous chain with $\Delta \neq 0$, otherwise there are gap closings independent of t, and vanishing chemical potential. We introduce a defect in the same way as above with the necessary change that now the defect consists of a chain in the hopping amplitude t that will cross 0. Fig. 8.4a shows the spectrum of such a chain. Again the energies present in the homogeneous system are present here, and there is a new pair of zero-energy states. It is interesting to directly notice that, despite the different nature of the defect, the spectrum of the system with a defect in the superconducting gap and the spectrum of the system with a defect in the hopping amplitude are the same up to minimal differences,

in Fig. 8.1a the energies in the bulk seem a little bit more paired. This is a consequence of the topological defects not influencing the bulk, and the disagreements are most probably due to the finite size of the system.



(a) *Unperturbed spectrum with defect.* ***(b)*** *Perturbed spectrum with defect.*

Figure 8.4: *(a) The energy spectrum of the homogeneous Kitaev chain with* 50 *sites and open boundary conditions for the parameters* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32 and four zero-energy states with energies of the order of* 10^{-7}. *(b) The spectrum of the same system with a white noise perturbation of the parameters in Eq. 7.32 with noise level* $t/2$. *The zero-energy states have energies in the order of* 10^{-6}.

When noise is introduced the observed zero-energy modes persist. This is a strong indication for MZMs. In contrast with the unperturbed state the perturbed bulk spectrum in Fig 8.4b differs from Fig. 8.1b, but we cannot conclude anything about that since it is very well possible that this is due to the noise that is different for both spectra.

We have still to verify that the new zero modes are indeed attached to the domain walls, and Fig. 8.5 shows that this is indeed the case. Moreover, even in the noisy chain this presence of the edge states at the defects is clear, Fig. 8.6.

By comparing the eigenstates in Fig. 8.2 and Fig. 8.5 for a system with a defect in the superconducting gap and hopping amplitude respectively a significant differences presents itself. While there seems to be some sort of oscillation in all zero-energy eigenstates of the system with a superconducting defect, in the case of a hopping defect there is a state which is much "smoother". Although the state as a whole still fulfils the relations of Eq. 7.8 and Eq. 7.9, which implies that it is a MZM, it seems not possible to separate the edge and defect states by taking a linear superposition of the shown states. This dissimilarity persists when noise is added to the

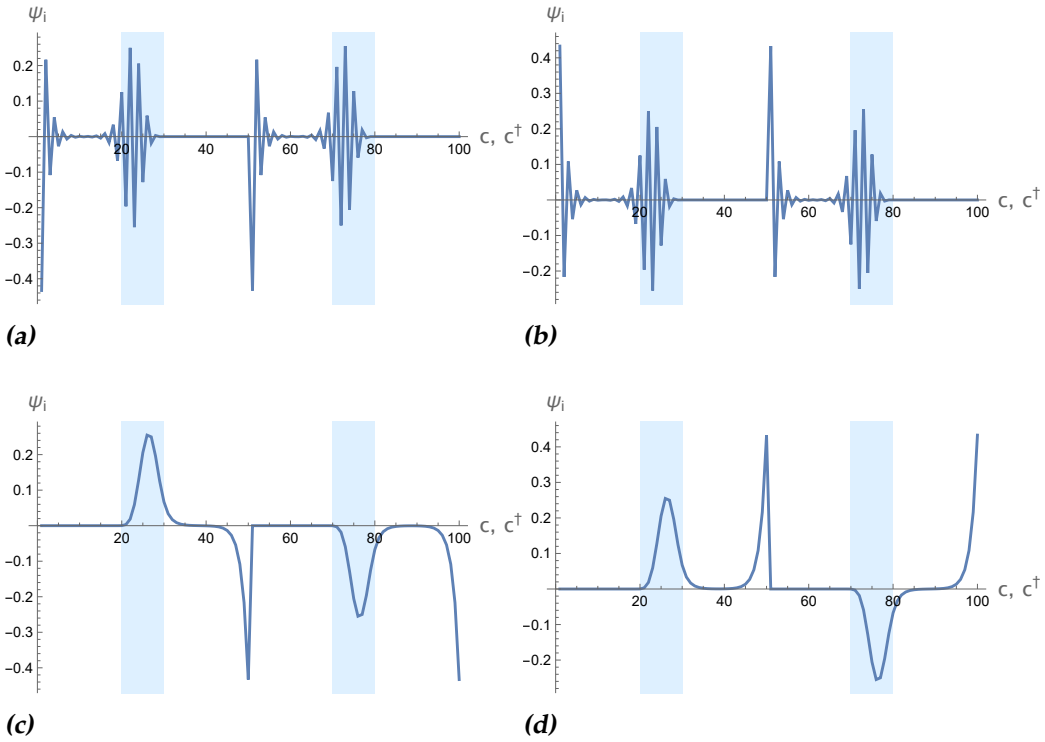


Figure 8.5: *(a),(b),(c),(d) The eigenstates corresponding to the zero-energy modes of a Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the hopping amplitude centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state. The shaded areas mark the position of the defect.*

system, Eq. 8.6. We are unaware of a possible explanation of this observation. However, it seems to indicate an important difference between the two kinds of topological defects that does appear in the bulk. Nevertheless, we should take this into account when introducing defects for practical purposes in later analysis, since it drastically effects the possibility of splitting the edge and defect states.

With the same degree of certainty as before for the superconducting gap we can confidently conclude that MZMs occur at domain walls imposed by topological defects in the hopping amplitude.

A critical reader might not be convinced by the examples given in this section, and they have every right to do so. However, besides the theoretical background and the examples provided above the claims and discussion in section are supported by much more evidence in Appendix A. This

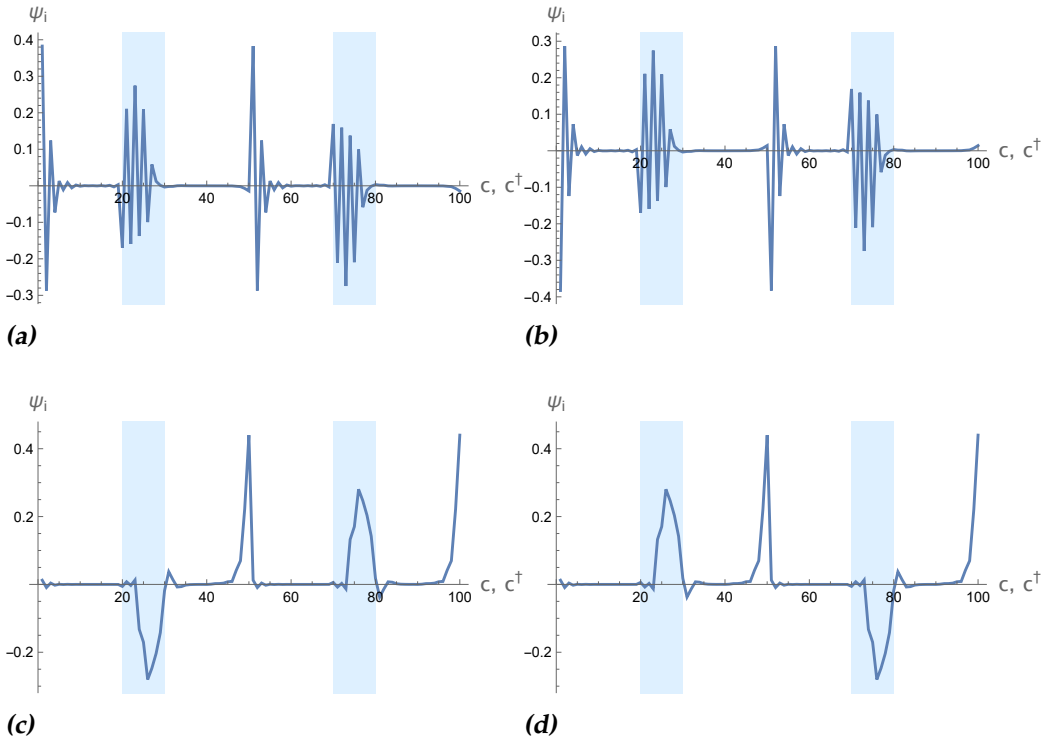


Figure 8.6: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32. The x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state. The shaded areas mark the position of the defect.*

puts us in the position to comfortably conclude that topological defects in the the Kitaev chain that introduce domain walls increase the degeneracy of the ground state by introducing MZMs at those defects without influencing the overall properties of the bulk spectrum, such as the closing of the gap.

Although we have successfully increased the degeneracy of the ground state by introducing MZMs at domain walls, we are not yet able to perform braiding in the parameter space. This is due to the fact that the subspace of the parameter space of the (homogeneous) Kitaev chain where MZMs are present is simply connected. Since the holonomy corresponding to a point is 1, i.e. the identity of the holonomy group, this contractibility of every loop immediately implies that the Wilczek-Zee phase is always trivial.

Chapter 9

Extensions of the Kitaev chain

In Chapter 7 we have seen that braiding of MZMs in the parameter space should be possible by utilising geometrical phases. However, to obtain a non-trivial geometrical phase, noncontractible loops have to exists. Because the connected components of the parameter space of the homogeneous Kitaev chain where the gap does not close are all simply connected, such loops do not exist.

In this chapter we will propose three extension of the Kitaev chain by introducing a periodic perturbation on the chemical potential or the hopping amplitude. These models are inspired by *topological insulators* [22], and can be viewed as superconducting generalisations of those systems. We will study the simply connectedness of the connected components of the parameter space, and investigate some topological phase transitions.

9.1 Superconducting SSH-model

Let us first introduce a Kitaev chain with periodic perturbation on the hopping amplitude, where the hopping alternates between two values. This perturbation introduces a Peierls distortion which usually opens a gap in the spectrum. Without superconducting term this models is now as the SSH-model. In 1979 Su, Schrieffer and Heeger studied the existence so-called *soliton* solutions in polyacetylene [65]. The alternating hopping was due to the single and double bonds in the molecule, and the soliton solution existed at a defect created by two single or double bonds. Much later the SSH-model turned out to be a *topological insulator*. Topological insulators are a class of materials predicted in 2005 [29] and experimentally confirmed in 2006 [11], which have topologically protected properties an

behave somewhat similar to insulators. Because of that interesting behaviour as a topological insulator we are interested in generalising it by adding p-wave superconductivity.

The Hamiltonian of the SSH-model is

$$\hat{H}(\mu, t, \delta) = -\sum_{j=1}^{N} \mu c_j^\dagger c_j - \sum_{j=1}^{N-1} (t + (-1)^j \delta)(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j), \tag{9.1}$$

where $\mu \in \mathbb{R}$ the chemical potential, $t \in \mathbb{R}$ the hopping amplitude, and $\delta \in \mathbb{R}$ a periodic perturbation of the hopping amplitude. Combining this with the Kitaev chain leaves us with the Hamiltonian for the *superconducting SSH-model*

$$\begin{aligned}\hat{H}(\mu, t, \delta, \Delta) = &-\sum_{j=1}^{N} \mu c_j^\dagger c_j - \sum_{j=1}^{N-1} (t + (-1)^j \delta)(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \\ &+ \sum_{j=1}^{N-1} (\Delta c_j^\dagger c_{j+1}^\dagger + \Delta^* c_{j+1} c_j),\end{aligned} \tag{9.2}$$

where $\Delta \in \mathbb{C}$ is the superconducting gap. Notice that this model has a sublattice structure, i.e. we can enlarge the unit cell and define the following operators

$$b_j := c_{2j-1}; \tag{9.3}$$

$$a_j := c_{2j}. \tag{9.4}$$

To obtain an analytical expression for the spectrum of the bulk of this model we will assume $N = 0 \mod 2$, which should not be a very restricting property when $N \to \infty$, and we will apply periodic boundary conditions Substituting the sublattice operators in Eq. 9.2 adjusted for periodic boundary conditions yields

$$\begin{aligned}\hat{H}(\mu, t, \delta, \Delta) = \sum_{m=1}^{M=N/2} \Big[&-\mu(b_m^\dagger b_m + a_m^\dagger a_m) \\ &- (t - \delta)(a_m^\dagger b_m + b_m^\dagger a_m) - (t + \delta)(b_{m+1}^\dagger a_m + a_m^\dagger b_{m+1}) \\ &+ (\Delta a_m^\dagger b_m^\dagger + \Delta^* b_m a_m + \Delta b_{m+1}^\dagger a_m^\dagger + \Delta^* a_m b_{m+1})\Big].\end{aligned} \tag{9.5}$$

The spectrum of the bulk should ideally be studied in k-space. The Fourier

transforms of a_m and b_m,

$$a_j^\dagger := \frac{1}{\sqrt{N}} \sum_k e^{-2ijkd} a_k^\dagger,\ b_j^\dagger := \frac{1}{\sqrt{N}} \sum_k e^{-2ijkd} e^{ikd} b_k^\dagger, \tag{9.6}$$

$$a_j := \frac{1}{\sqrt{N}} \sum_k e^{ijkd} a_k,\ b_j := \frac{1}{\sqrt{N}} \sum_k e^{2ijkd} e^{-ikd} b_k, \tag{9.7}$$

are obtained by small adjustments to Eq. 7.36 and Eq. 7.37. Be aware of the fact that here k is summed over M equally spaced values in $[-\pi/2d, \pi/2d]$. Following a similar method as in section 7.3 we obtain

$$\begin{aligned}\hat{H}(k) = \sum_k \Big[& -\mu(b_k^\dagger b_k + a_k^\dagger a_k) - (t-\delta)\left(e^{-ikd} a_k^\dagger b_k + e^{ikd} b_k^\dagger a_k\right) \\ & - (t+\delta)\left(e^{-ikd} b_k^\dagger a_k + e^{ikd} a_k^\dagger b_k\right) \\ & + \left(\Delta e^{ikd} a_{-k}^\dagger b_k^\dagger + \Delta^* e^{-ikd} b_k a_{-k} + \Delta e^{-ikd} b_k^\dagger a_{-k}^\dagger + \Delta^* e^{ikd} a_{-k} b_k\right) \Big].\end{aligned} \tag{9.8}$$

Making elaborate use of the symmetric distribution of k in $[-\pi/2d, \pi/2d]$ we can simplify this even further to

$$\begin{aligned}\hat{H}(k) = \sum_k \Big[& -\mu(b_k^\dagger b_k + a_k^\dagger a_k) + 2\left[t_0 \cos(kd) - i\delta \sin(kd)\right] b_{-k} a_{-k}^\dagger \\ & + 2\left[t \cos(kd) + i\delta \sin(kd)\right] a_{-k} b_{-k}^\dagger \\ & - i\Delta \sin(kd) b_k^\dagger a_{-k}^\dagger - i\Delta \sin(kd) a_k^\dagger b_{-k}^\dagger \\ & + i\Delta^* \sin(kd) b_{-k} a_k + i\Delta^* \sin(kd) a_{-k} b_k \Big].\end{aligned} \tag{9.9}$$

Introduce a Nambu spinor

$$\hat{\psi}_k^\dagger = (b_k^\dagger, a_k^\dagger, b_{-k}, a_{-k}) \tag{9.10}$$

to perform a Bogoliubov transformation to. Up to an insignificant constant [5] we obtain

$$\hat{H}(k) = \frac{1}{2} \sum_k \hat{\psi}_k^\dagger \mathcal{H}_{SSH+sc} \hat{\psi}_k, \tag{9.11}$$

here the BdG Hamiltonian is given by

$$\mathcal{H}_{SSH+sc} = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{9.12}$$

where

$$C = \begin{pmatrix} -\mu & -2\left[t\cos(kd) - i\delta\sin(kd)\right] \\ -2\left[t\cos(kd) + i\delta\sin(kd)\right] & -\mu \end{pmatrix}, \quad (9.13)$$

and

$$S = \begin{pmatrix} 0 & -2i\Delta\sin(kd) \\ -2i\Delta\sin(kd) & 0 \end{pmatrix}. \quad (9.14)$$

Assuming Δ is real, the BdG Hamiltonian can be written in a more concise way using Pauli spin matrices

$$\begin{aligned} \mathcal{H}_{SSH+sc} = &-2\delta\sin(kd)\sigma_z \otimes \sigma_y + \mu\sigma_z \otimes \mathbb{1}_2 + 2t\cos(kd)\sigma_z \otimes \sigma_x \\ &+ 2\Delta\sin(kd)\sigma_y \otimes \sigma_x. \end{aligned} \quad (9.15)$$

The assumption that Δ is real is not of much influence on the closing of the gap as we will later see that only $|\Delta|^2$ occurs in important expressions.

As made clear earlier the topological phase transitions occur when the topological order parameter changes sign, and this can only happen when the gap in the bulk closes. Therefore it is essential to know when zero-energy states are present in the bulk. To investigate for which sets of parameters the gap closes we construct the *critical manifold*. This manifold is a submanifold, perhaps with boundaries and corners, of the parameter space where the determinant of the BdG Hamiltonian is zero, i.e. the submanifold of the parameter space where zero-energy states are present in the bulk. In the limit of an infinite chain the critical manifold can be defined by

$$\mathcal{M} := \{x \in M : \det(\mathcal{H}(k, x)) = 0 \text{ for a } k \in [-\pi/2d, \pi/2d]\}, \quad (9.16)$$

where M is the considered parameter space, in this case $\mathbb{R}^3 \times \mathbb{C}$. The determinant of the BdG-Hamiltonian is easily obtained

$$\begin{aligned} \det(\mathcal{H}_{SSH+sc}(k)) = &-\mu^4 + (\mu^2 - 4t^2\cos^2(kd))^2 \\ &+ (\mu^2 + 4(\Delta^2 - \delta^2)\sin^2(kd))^2 \\ &+ 8t^2\sin^2(2kd)(\Delta^2 + \delta^2). \end{aligned} \quad (9.17)$$

This enables us to study the closings of the gap.

For a more comprehensive understanding of the bulk spectrum we calculate the energies

$$\begin{aligned} \varepsilon(k) = \pm\Big[&\mu^2 + 2\Delta^2 + 2t^2 + 2\delta^2 + 2(t^2 - \delta^2 - \Delta^2)\cos(2kd) \\ &\pm 2\sqrt{2}\left[-2\mu^2\delta^2\cos^2(kd) + \mu^2t^2(1 + \cos(2kd)) + 8\Delta^2\delta^2\cos(kd)^2\right]^{1/2}\Big]^{1/2}. \end{aligned} \quad (9.18)$$

When $\delta = 0$ one can easily check that Eq. 9.18 reduces to Eq. 7.45. As one notices, the expression for the energies becomes much more complicated for this extended SSH-model than for the homogeneous Kitaev chain. Therefore we stick to the critical manifold for the investigation of the topology of the parameter space.

Unfortunately studying the critical manifold is not too straightforward because of the several parameters that play a role. To obtain a general starting point for the study of the parameter space we consider several specific values of the momentum kd.

Firstly, we investigate the middle of the Brillouin zone, i.e. $kd = 0$. With $kd = 0$ Eq. 9.17 reduces to

$$(\mu^2 - 4t^2)^2 = 0. \tag{9.19}$$

Hence the gap closes if $|\mu| = 2|t|$ independent of every other parameter of the system, exactly as we would have expected from the homogeneous Kitaev chain.

For the edges of the Brillouin zone, $kd = \pm\pi/2$, the gap closes when

$$(\mu^2 + 4\Delta^2 - 4\delta^2)^2 = 0. \tag{9.20}$$

So we identify the cone described by $\delta = \pm\sqrt{\mu^2/4 + \Delta^2}$ that is part of the critical manifold. We can decide that $t \neq 0$, since otherwise the gap closes independent of Δ as seen above, then we can normalise all the parameters by dividing them by t. The cone of the critical manifold that is embedded in the parameter space, that is 3 dimensional after remormalisation, is depicted in Fig. 9.1.

The not simply connected subspace of Fig. 9.1 draws our attention. Let us study the occurrence of gap closings in that space. Setting Eq. 9.17 to zero and solving for the chemical potential μ yields

$$\mu = \pm 2\Big[t^2\cos^2(kd) - \sin^2(kd)(\Delta^2 - \delta^2) \pm i[4t^2\Delta^2\cos^2(kd)\sin^2(kd)]^{1/2}\Big]^{1/2}. \tag{9.21}$$

For μ being a real number it is required that

$$4t^2\Delta^2\cos^2(kd)\sin^2(kd) = 0, \tag{9.22}$$

which enables us to study four distinct cases. The first one, $t = 0$, can be discarded, since we have assumed that $t \neq 0$. The restrictions on kd, being $kd = 0$ or $kd = \pm\pi/2$, reduce the problem to the already studied cases before. The remain condition of interest is $\Delta = 0$, this can be regarded as

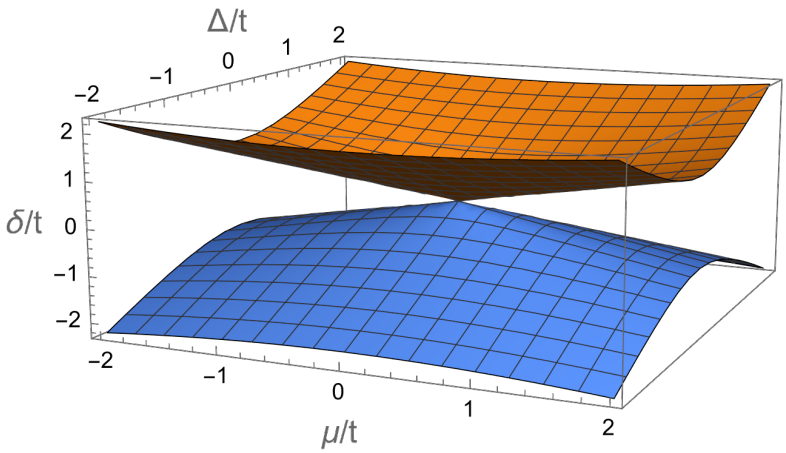


Figure 9.1: *The level set of* $\det(\mathcal{H}_{SSH+sc}(\pm\pi/2) = 0$ *normalised by* t *by substituting* $t = 1$ *in Eq. 9.17. This is a part of the critical manifold of the superconducting SSH-model.*

a trivial situation since the model just reduces to an ordinary SSH-model. However, for our understanding of the topological phase transitions of this model it is crucial.

The gap closings in the shaded areas of Fig. 9.2 in combination with the fact that for $|\mu| > 2|t|$ the gap is always closed tells us that the subspace that seemed not simply connected is actually divided into two simply connected subspaces. Therefore noncontractible loops cannot exist in this parameter space. Nevertheless, we have found different topological phases in the parameter space. Further (numerical) analysis could point out which part of the parameter space is exhibiting edge states.

We could study another specific case of Eq. 9.17, namely the situation of $\mu = 0$. Substituting $\mu = 0$ and normalising by t leaves us with

$$\cos^4(kd) + 2(\Delta^2 + \delta^2)\sin^2(kd)\cos^2(kd) + (\Delta^2 - \delta^2)^2\sin^4(kd) = 0. \quad (9.23)$$

We immediately notice that every term of this expression is non-negative, and it is easy to check that the only solution is $kd = \pm\pi/2$ and $\Delta = \delta$.

Despite the fact that a noncontractible loop is not possible, we are still interested in the topological phase transitions that might occur. Therefore we will perform a loop in the $\mu = 0$ plane. Let $\gamma : [0,1] \to \mathbb{R}^4$ be defined by $\gamma(T) = (\mu(T), t(T), \delta(T), \Delta(T))$ with

$$\mu(T) = 0, \quad t(T) = 1, \quad \delta(T) = 0.5\sin(2\pi T), \quad \Delta = 0.5\cos(2\pi T). \quad (9.24)$$

For this loop we expect the gap to close at $T = 1/4 + l/2$ with $l \in \{0,1,2,3\}$. So let us study the edge states of a finite-sized chain between

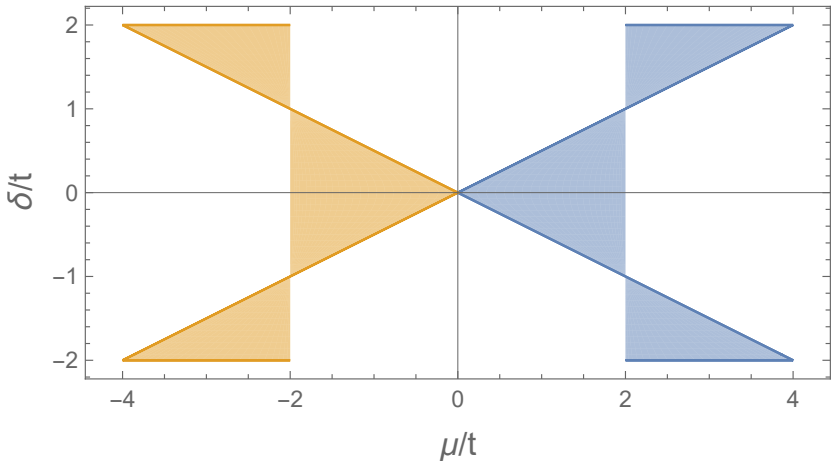


Figure 9.2: *The shaded areas are the parameter regimes in $(\mu/t, \delta/t)$-space where the gap in the analytic bulk spectrum of the superconducting SSH-model closes for a vanishing superconducting gap, $\Delta = 0$. These are the solutions of Eq. 9.22 for some $kd \in [-\pi/2, \pi/2]$.*

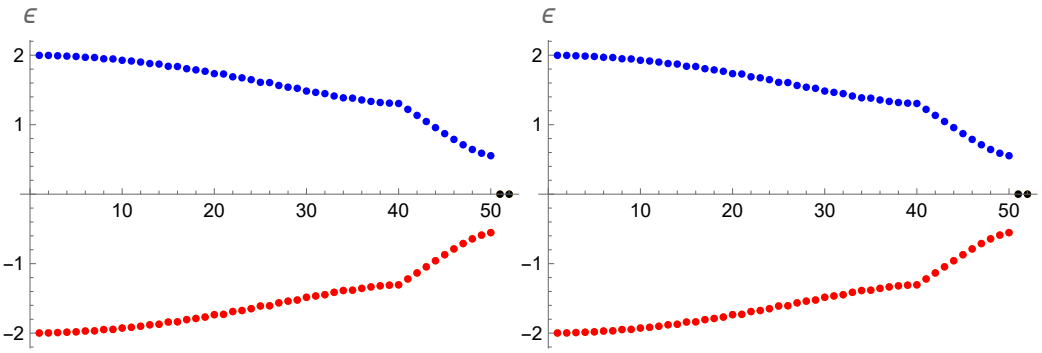
those closings. It is important to be careful with the parity of the number of sites here as we will see shortly.

From the spectra in Fig. 9.6 it seems that no topological phase transition occurs, since there are zero-energy modes on both sides of the critical manifold. However, the edge states themselves indicate a phase transition. In Fig. 9.4 the edge states and all there linear combinations satisfy both Eq. 7.8 and Eq. 7.9, so those are MZMs. On the contrary, there are linear combination of the states in Fig. 9.5 that do not satisfy those relation. Hence there are always edge modes present along the loop, but the nature of these edge modes changes.

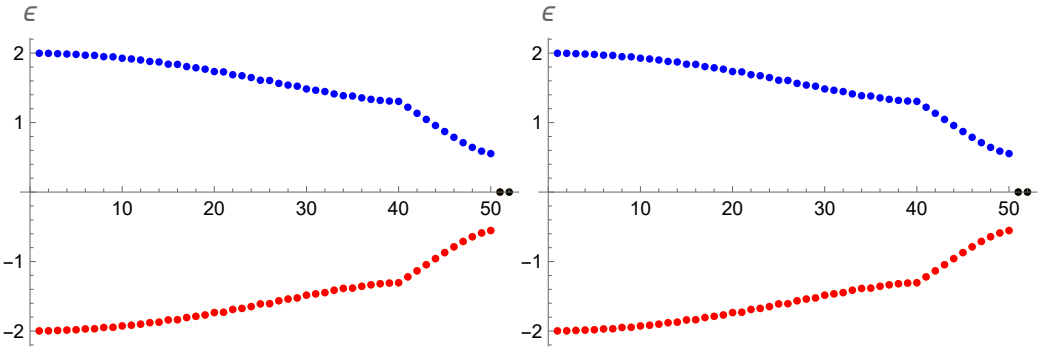
In the case of a chain with an even number of sites the topological phase transitions can be recognised by the spectrum. In the parameter regime where the chain with an odd number of sites exhibits MZMs the chain with an even number exhibits two edge states, Fig. 9.6a and Fig. 9.6c, which turn out to be MZMs, and in where the first exhibit different edge states the there are four, Fig. 9.6b, or zero, Fig. 9.6d, edges modes present in the chain with an even number of sites.

The different nature of the edge states in those finite system can also be made clear by turning on the chemical potential. This leads to a splitting of ground state energies, Fig. 9.7. This is not expected for Majorana modes and hence it makes clear that the nature of the edge states differs tremendously.

All in all it turned out that a noncontractible loop in a topological non-



(a) $T = \pi/8$ ***(b)*** $T = 5\pi/8$



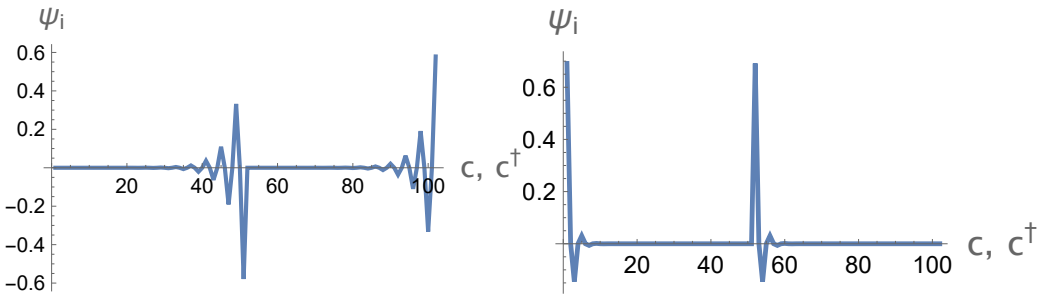
(c) $T = 9\pi/8$ ***(d)*** $T = 13\pi/8$

Figure 9.3: *(a),(b),(c),(d) The spectra of a superconducting SSH-model with* 51 *sites along a loop described by Eq. 9.24 at* $T = \pi/8$, $T = 5\pi/8$, $T = 9\pi/8$, *and* $T = 13\pi/8$ *respectively. The spectra are identical.*

trival parameter regime was not possible. However, this superconducting generalisation of the SSH-model exhibits interesting topological phase transitions.

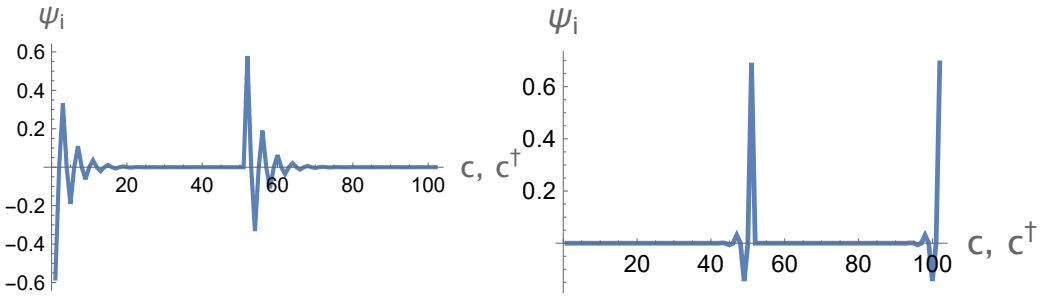
9.2 Staggering chemical potential

A next step in our search for a suitable not simply connected parameter space is to consider related models with the idea that the Peierls distortion, that is due to the perturbation of the 1D lattice, might open a gap there via a different physical mechanism. A periodic perturbation of the Kitaev chain that is very similar to the superconducting SSH-model is a Kitaev chain with a periodic perturbation of the chemical potential. This staggering chemical potential can be interpret as a the simplest version of



(a) $T = \pi/8$

(b) $T = \pi/8$



(c) $T = 9\pi/8$

(d) $T = 9\pi/8$

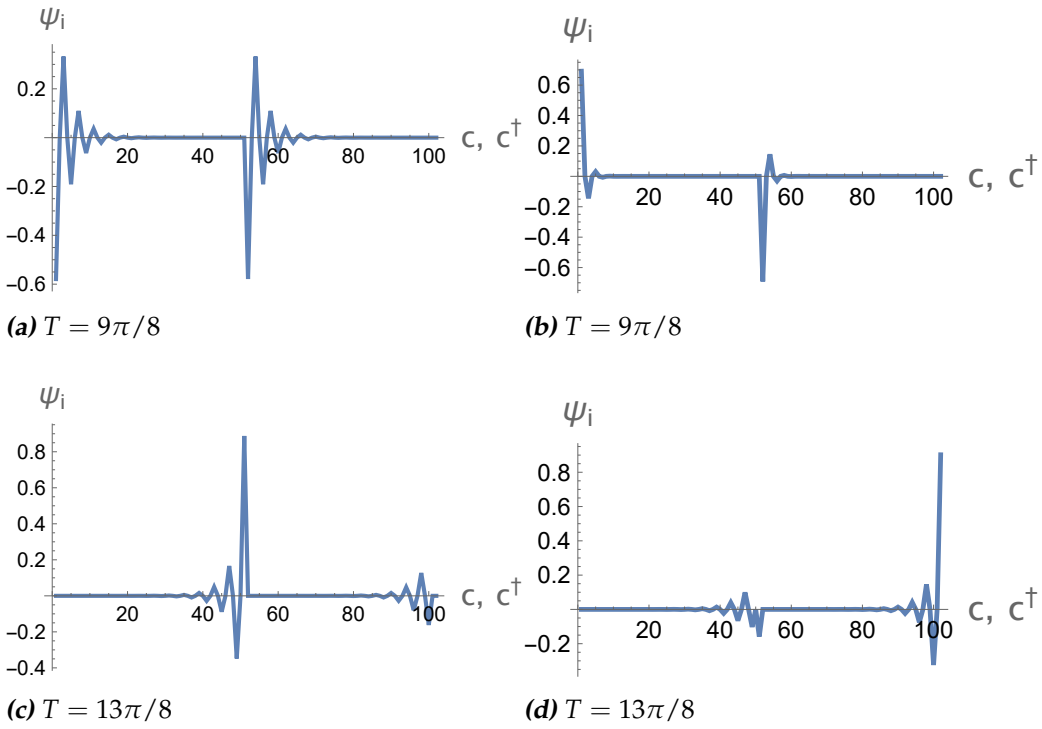
Figure 9.4: *(a),(b) The edge states corresponding to the point of the loop described by Eq. 9.24 at $T = \pi/8$. (c),(d) The edge states corresponding to the point at $T = 9\pi/8$ on that loop. These states are MZMs. The x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ is a normalised state.*

a superconducting generalisation of the *diagonal Harper model*. This chain is described by

$$\begin{aligned}\hat{H}(\mu, \nu, t) = &- \sum_{j=1}^{N} (\mu + (-1)^j \nu) c_j^\dagger c_j - \sum_{j=1}^{N-1} t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \\ &+ \sum_{j=1}^{N-1} (\Delta c_j^\dagger c_{j+1}^\dagger + \Delta^* c_{j+1} c_j),\end{aligned} \tag{9.25}$$

where $\mu \in \mathbb{R}$ the chemical potential, $\nu \in \mathbb{R}$ a perturbation of that potential, $t \in \mathbb{R}$ the hopping amplitude, and $\Delta \in \mathbb{C}$ the superconducting gap.

Exploiting the sublattice structure we can introduce the sublattice op-



(a) $T = 9\pi/8$ ***(b)*** $T = 9\pi/8$

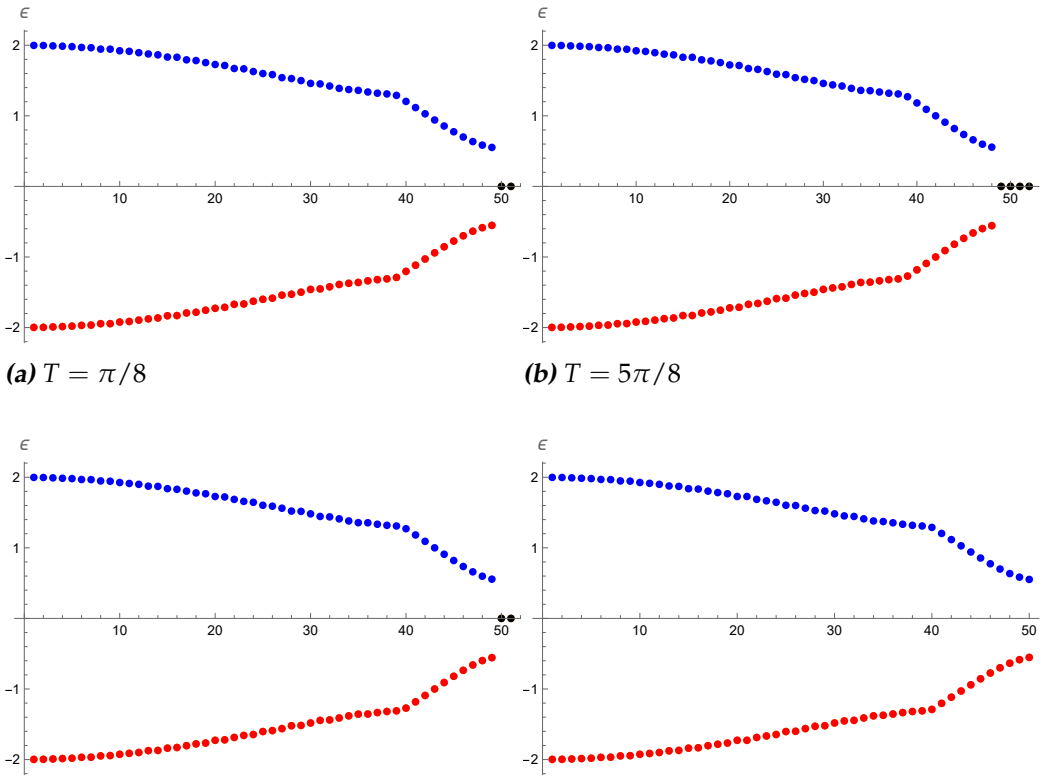
(c) $T = 13\pi/8$ ***(d)*** $T = 13\pi/8$

Figure 9.5: *(a),(b) The edge states corresponding to the point of the loop described by Eq. 9.24 at* $T = 5\pi/8$*. (c),(d) The edge states corresponding to the point at* $T = 13\pi/8$ *on that loop. These states are not MZMs. The x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state.*

erator as in Eq. 9.3 and Eq. 9.4, and rewrite the Hamiltonian

$$\begin{aligned}\hat{H}(\mu, t, \delta, \Delta) = \sum_{m=1}^{M=N/2} \Big[&- (\mu - \nu) b_m^\dagger b_m - (\mu + \nu) a_m^\dagger a_m \\ &- t(a_m^\dagger b_m + b_m^\dagger a_m + b_{m+1}^\dagger a_m + a_m^\dagger b_{m+1}) \\ &+ (\Delta a_m^\dagger b_m^\dagger + \Delta^* b_m a_m + \Delta b_{m+1}^\dagger a_m^\dagger + \Delta^* a_m b_{m+1}) \Big]. \end{aligned} \tag{9.26}$$

Similar to Eq. 9.5 we can perform a Fourier transform. The Fourier transform of the hopping term is easily found as a specific case of the hopping term in section 9.1, and the Fourier transform of the superconducting term is exactly the same as the one in section 9.1. Therefore we only have to perform the Fourier transform of the chemical potential, but that is similar to the transformation in section 7.3, albeit with k equally spaced in $[-\pi/2d, \pi/2d]$ instead of $[-\pi/d, \pi/d]$.



(a) $T = \pi/8$ **(b)** $T = 5\pi/8$

(c) $T = 9\pi/8$ **(d)** $T = 13\pi/8$

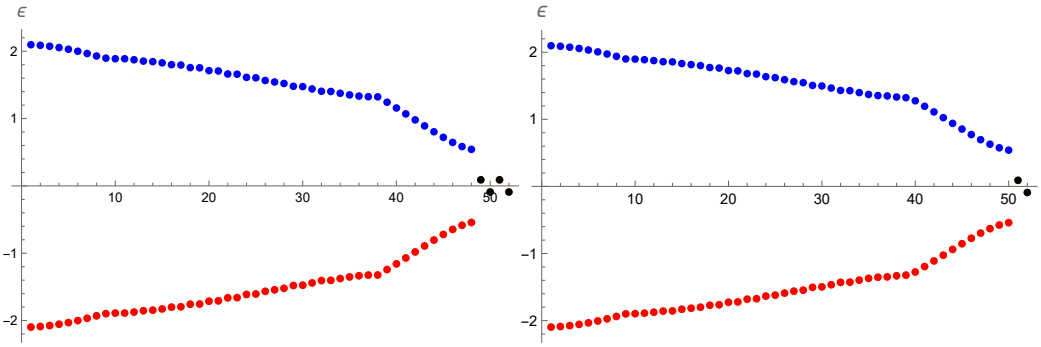
Figure 9.6: *(a),(b),(c),(d) The spectra of a superconducting SSH-model with* 50 *sites along a loop described by Eq. 9.24 at* $T = \pi/8$, $T = 5\pi/8$, $T = 9\pi/8$, *and* $T = 13\pi/8$ *respectively.*

The Fourier transform of Eq. 9.26 is then found to be

$$\begin{aligned}\hat{H}(k) = \sum_k \Big[&-(\mu-\nu)b_k^\dagger b_k + -(\mu+\nu)a_k^\dagger a_k \\ &+ 2t\cos(kd)b_k a_k^\dagger + 2t\cos(kd)a_k b_k^\dagger \\ &- i\Delta\sin(kd)b_k^\dagger a_{-k}^\dagger - i\Delta\sin(kd)a_k^\dagger b_{-k}^\dagger \\ &+ i\Delta^*\sin(kd)b_{-k}a_k + i\Delta^*\sin(kd)a_{-k}b_k\Big],\end{aligned} \tag{9.27}$$

which after a Bogoliubov tranformation with the Nambu spinor of Eq. 9.10 can be represented, up to an unimportant constant, by

$$\hat{H}(k) = \frac{1}{2}\sum_k \hat{\psi}_k^\dagger \mathcal{H}_{Stag.Chem.}\hat{\psi}_k, \tag{9.28}$$



(a) *50 sites,* $T = 5\pi/8$ ***(b)*** *51 sites,* $T = 5\pi/8$

Figure 9.7: *(a) The spectrum of a superconducting SSH-model with* 50 *sites along a loop described by Eq. 9.24 and an additional chemical potential,* $\mu = 0.1$*, at* $T = 5\pi/8$*. (b) The spectrum of a superconducting SSH-model with* 51 *sites with the same parameters.*

here the BdG Hamiltonian is given by

$$\mathcal{H}_{Stag.Chem.}(k) = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{9.29}$$

where

$$C = \begin{pmatrix} -(\mu - \nu) & -2t\cos(kd) \\ -2t\cos(kd) & -(\mu + \nu) \end{pmatrix}, \tag{9.30}$$

and S is given by Eq. 9.14.

Similar to section 9.1 the BdG Hamiltonian can be written in a more concise way using Pauli spin matrices, assuming Δ is real,

$$\begin{aligned} \mathcal{H}_{\text{Stag.Chem.}}(k) =& \mu\sigma_z \otimes \mathbb{1}_2 + \nu\sigma_z \otimes \sigma_z + 2t\cos(kd)\sigma_z \otimes \sigma_x \\ &+ 2\Delta\sin(kd)\sigma_y \otimes \sigma_x. \end{aligned} \tag{9.31}$$

Just as for the superconducting SSH-model we are interested in the closings of the gap. This can be investigate by finding the critical manifold, and to be able to study the critical manifold calculated the determinant of $\mathcal{H}_{\text{Stag.Chem,}}$

$$\begin{aligned} \det(\mathcal{H}_{Stag.Chem.}) =& (\mu^2 - \nu^2 - 4t^2\cos^2(kd))^2 \\ &+ 8\Delta^2\sin^2(kd)(\mu^2 - \nu^2 + 2\Delta^2\sin^2(kd)) \\ &+ 8\Delta^2 t^2\sin^2(2kd). \end{aligned} \tag{9.32}$$

Furthermore, the energy spectrum of the bulk is given by

$$\varepsilon(k) = \pm \Big[\mu^2 + \nu^2 + 4t^2\cos^2(kd) + 4\Delta^2\sin^2(kd) \pm 4\left[\Delta^2\nu^2\sin^2(kd) + \mu^2\nu^2/4 + \mu^2t^2\cos^2(kd)\right]^{1/2}\Big]^{1/2}. \tag{9.33}$$

We notice some similarities between Eq. 9.32 and Eq. 9.17, but a significant difference with the superconducting SSH-model is that the perturbation on the chemical potential, ν, always occurs together with μ. This in contrast with Eq. 9.17 where the perturbation of the hopping amplitude, δ, occurs in combination with the superconducting gap. The latter most probably leads to more unexpected closings and openings of the gap due to the interplay of the different mechanisms that influence the gap, i.e. periodic perturbation and superconductivity, than the periodic perturbation of the chemical potential that we study now. Nevertheless, we will identify some of the structure of the parameter space of this superconductive chain with staggering chemical potential.

To obtain some understanding of the critical manifold of this model we first consider the specific cases $kd = 0$ and $kd = \pm\pi/2$.

From substituting $kd = 0$ into Eq. 9.32 and setting it to zero we obtain

$$(\mu^2 - \nu^2 - 4t^2)^2 = 0. \tag{9.34}$$

This can be rewritten to an expression in μ

$$|\mu| = \sqrt{\nu^2 + 4t^2}, \tag{9.35}$$

which in the homogeneous case, i.e. $\nu = 0$, reduces to the know condition for closing of gap $|\mu| = 2|t|$. Fig. 9.8 shows how this condition leads to a cone in the parameter space where now Δ is just to normalise. It seems that we have more freedom in varying the hopping amplitude in this model, and perhaps even perform a loop around the just found cone. However, when we consider $t = 0$ Eq. 9.32 reduces to

$$(\mu^2 - \nu^2 + 4\Delta^2\sin^2(kd))^2 = 0, \tag{9.36}$$

which has a solution for a $kd \in [-\pi/2, \pi/2]$ when

$$\mu^2 \leq \nu^2 \leq \mu^2 + 4\Delta^2. \tag{9.37}$$

To understand how the requirement of Eq. 9.37 relates to the closing of the gap, we consider the part of the critical manifold that arises from $kd = \pm\pi/2$. For that value Eq. 9.32 reduces to

$$(\mu^2 - \nu^2 + 4\Delta^2)^2 = 0, \tag{9.38}$$

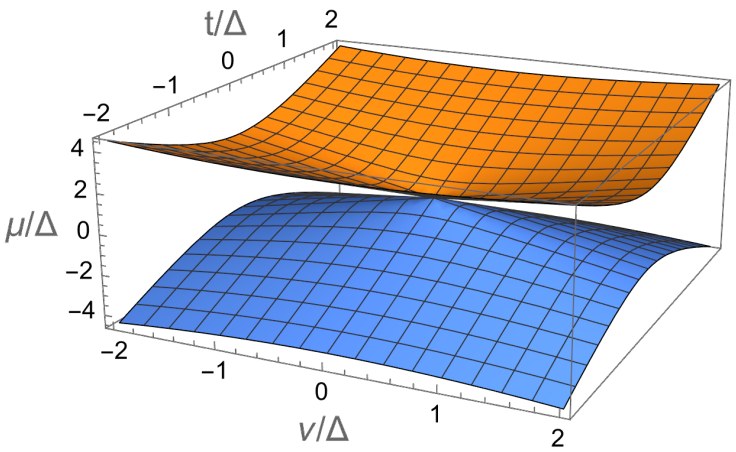


Figure 9.8: *The level set of* $\det(\mathcal{H}_{Stag.Chem}(0) = 0$ *normalised by* Δ *by substituting* $\Delta = 1$ *in Eq. 9.17. This is a part of the critical manifold of the superconducting chain with staggering chemical potential.*

which can be solved for $|v|$

$$|v| = \sqrt{\mu^2 + 4\Delta^2}, \tag{9.39}$$

where we recognise the upper bound on v imposed by Eq. 9.37.

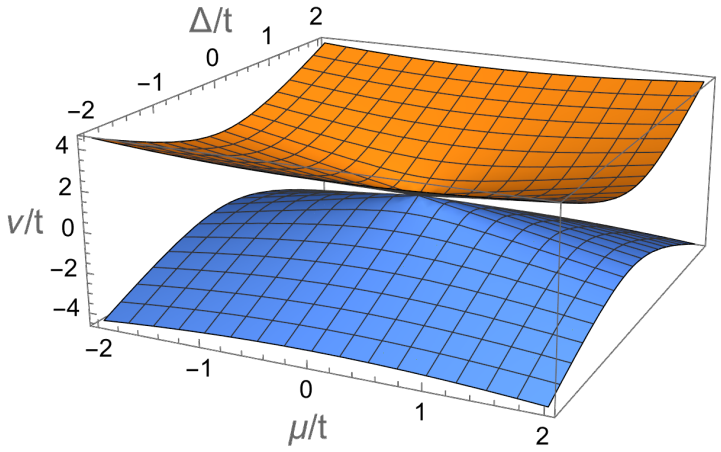


Figure 9.9: *The level set of* $\det(\mathcal{H}_{Stag.Chem.}(\pm\pi/2) = 0$ *normalised by* t *by substituting* $t = 1$ *in Eq. 9.17. This is a part of the critical manifold of the superconducting chain with staggering chemical potential.*

That means that when we are in the not simply connected part of the parameter space as seen in Fig. 9.9, there will be a closing of the gap at

$t = 0$ when $|\nu| \geq |\mu|$, and this implies that the gap surely closes when $t = \mu = 0$.

The most natural solution is to take $t \neq 0$, and to try to perform a loop in the not simply connected part of the parameter space as a result of the cone in Fig. 9.8. When doing this one inevitably crosses the plane described by $\Delta = 0$. Substituted in Eq. 9.32 this leaves us with

$$(\mu^2 - \nu^2 - 4t^2 \cos^2(kd))^2 = 0, \tag{9.40}$$

which has solution for some $kd \in [-\pi/2, \pi/2]$ when

$$\nu^2 \leq \mu^2 \leq \nu^2 + 4t^2. \tag{9.41}$$

Eq. 9.41 is extremely similar to Eq. 9.37, and it implies that when we are in the not simply connected part of Fig. 9.8 there will surely be a gap closing when $|\mu| \geq |\nu|$. Therefore we conclude that it is not possible to perform a loop in the seemingly not simply connected subspace of the parameter space without closing of the gap along the loop.

Nevertheless, the different topological phase transitions in this parameter space can be very interesting. Despite the fact that more analysis of the existence edge states is needed to obtain a full understanding of all transitions, one can observe very intriguing critical manifolds, e.g. when assumed that $\Delta = t$ as we have seen in Eq. 7.29 the two cones of Fig. 9.8 and Fig. 9.9 will become perpendicular and divide the parameter space in six regions which have different topological properties.

9.3 Superconducting Rice-Mele model

In Section 9.1 and Section 9.2 we have seen how simple perturbations of the chemical potential and the hopping amplitude influenced the critical manifold. However, the perturbation were not enough to open gaps in such a way that a noncontractible loop would be possible. Since the perturbations on the chemical potential and the hopping amplitude open the gap via different physical mechanisms it is thought that combining them in one chain might lead to new regions of the parameter space where the gap remains open.

A Kitaev chain with a staggering chemical potential and hopping amplitude is a simple superconducting generalisation of a combined off-diagonal and diagonal Harper model. Moreover, it can be called a *superconducting SSH-model with periodic kicking* or a *superconducting generalisation of the Rice-Mele model*.

Firstly we will describe such a system with the Hamiltonian

$$\begin{aligned}\hat{H}(\mu,\nu,t,\delta) = &-\sum_{j=1}^{N}(\mu+(-1)^j\nu)c_j^\dagger c_j - \sum_{j=1}^{N-1}(t+(-1)^j\delta)(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j)\\ &+\sum_{j=1}^{N-1}(\Delta c_j^\dagger c_{j+1}^\dagger + \Delta^* c_{j+1}c_j),\end{aligned} \tag{9.42}$$

where $\mu \in \mathbb{R}$ the chemical potential, $\nu \in \mathbb{R}$ the perturbation of the chemical potential, $t \in \mathbb{R}$ the hopping amplitude, $\delta \in \mathbb{R}$ the perturbation of the hopping amplitude, and $\Delta \in \mathbb{C}$ the superconducting gap.

Just as with the superconducting SSH-model and the Kitaev chain with staggering chemical potential the Hamiltonian in Eq. 9.42 can be expressed in sublattice operators, and Fourier transformed. Fortunately, in section 9.1 and 9.2 we have already transformed each term of this Hamiltonian. Therefore we immediately obtain

$$\hat{H}(k) = \frac{1}{2}\sum_k \hat{\psi}_k^\dagger \mathcal{H}_{RM1}\hat{\psi}_k, \tag{9.43}$$

where the BdG Hamiltonian is given by

$$\mathcal{H}_{RM1} = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{9.44}$$

with

$$C = \begin{pmatrix} -(\mu-\nu) & -2(t\cos(kd) - i\delta\sin(kd)) \\ -2(t\cos(kd)+i\delta\sin(kd)) & -(\mu+\nu) \end{pmatrix} \tag{9.45}$$

and S is given by Eq. 9.14. If we assume Δ to be real, this BdG Hamiltonian can be written in terms of Pauli matrices

$$\begin{aligned}\mathcal{H}_{\mathrm{RM1}}(k) =&\mu\sigma_z\otimes\mathbb{1}_2 + \nu\sigma_z\otimes\sigma_z + 2t\cos(kd)\sigma_z\otimes\sigma_x\\ &-2\delta\sin(kd)\sigma_z\otimes\sigma_y + 2\Delta\sin(kd)\sigma_y\otimes\sigma_x.\end{aligned} \tag{9.46}$$

We expect the critical manifold of this superconducting Rice-Mele model to be more complicated than the previous ones, because there might be some interplay between the different perturbations. We predict that the interaction between the two periodic perturbations will not close many gaps, as different physical mechanisms are relevant, but they might open the gap more often.

To verify this prediction we consider the determinant of the relevant BdG Hamiltonian

$$\begin{aligned}\det(\mathcal{H}_{RM1}(k)) = &-(\mu^2-\nu^2)^2+8t^2(\Delta^2+\delta^2)\sin^2(2kd)\\ &+(\mu^2-\nu^2-4t^2\cos^2(kd))^2\\ &+(\mu^2-\nu^2+4(\Delta^2-\delta^2)\sin^2(kd))^2,\end{aligned} \tag{9.47}$$

where one recognises terms from both Eq. 9.17 and Eq. 9.32, and the bulk spectrum reads

$$\begin{aligned}\varepsilon(k) = \pm\Big[&\mu^2+4t^2\cos^2(kd)+4(\Delta^2+\delta^2)\sin^2(kd)\\ &\pm 4\Big[\mu^2(\delta^2\sin^2(kd)+t^2\cos^2(kd)+\nu^2/4)\\ &+\Delta^2\sin^2(kd)(\nu^2+4\delta^2\sin^2(kd))\Big]^{1/2}\Big]^{1/2}.\end{aligned} \tag{9.48}$$

In line with the previous section we consider the middle and edges of the Brillouin zone in more detail. For $kd = 0$ setting Eq. 9.47 to 0 yields

$$\mu^2 = \nu^2 + 4t^2, \tag{9.49}$$

which also occurs in the superconducting chain with staggering chemical potential as obtained from Eq. 9.34.

On the other hand, at the edges of the Brillouin zone, i.e. $kd = \pm\pi/2$,

$$\mu^2 + 4\Delta^2 = \nu^2 + 4\delta^2, \tag{9.50}$$

where we see both periodic perturbations occur.

Instead of studying this model in much depth in the way how it is formulated here, we can reformulate this intuitive generalisation of the SSH-model to a better know system, the Rice-Mele model.

An alternative formulation

A model with staggering chemical potential and a periodic modulation of the hopping potential is also known as the Rice-Mele model [59]. This model is of special interest to us since Thouless and Niu where able to construct a protocol for adiabatic charge pumping in this model [55], which

was experimentally realised in photons [35] and cold atoms [42]. The formulation of the model is a little different then Eq. 9.47. The periodic perturbation is only applied to the odd sites. Now we are able to formulate the superconducting generalisation of the Rice-Mele model

$$\hat{H}(\mu,\nu,t,\delta) = -\sum_{j=1}^{N}(\mu+(-1)^j\nu)c_j^\dagger c_j - \sum_{j=1}^{N-1}(t+(j \bmod 2)\delta)(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j) + \sum_{j=1}^{N-1}(\Delta c_j^\dagger c_{j+1}^\dagger + \Delta^* c_{j+1}c_j), \tag{9.51}$$

where $\mu \in \mathbb{R}$ the chemical potential, $\nu \in \mathbb{R}$ a perturbation of that potential, $t \in \mathbb{R}$ the hopping amplitude, $\delta \in \mathbb{R}$ a perturbation on that parameter and $\Delta \in \mathbb{C}$ the superconducting gap. Notice that Eq. 9.42 can be recovered from Eq. 9.51 by redefining t and δ in the following way

$$\begin{aligned} t &\mapsto t-\delta \\ \delta &\mapsto 2\delta. \end{aligned}$$

By performing a Fourier transformation and a Bogoliubov transformation, where we can make use of the results of the previous chapter and leave the transformation of the perturbation as an exercise to the reader, we immediately obtain

$$\hat{H}(k) = \frac{1}{2}\sum_k \hat{\psi}_k^\dagger \mathcal{H}_{RM2}\hat{\psi}_k, \tag{9.52}$$

where the BdG Hamiltonian is given by

$$\mathcal{H}_{RM2} = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{9.53}$$

with

$$C = \begin{pmatrix} -(\mu-\nu) & -2t\cos(kd)-\delta e^{ikd} \\ -2t\cos(kd)-\delta e^{-ikd} & -(\mu+\nu) \end{pmatrix} \tag{9.54}$$

and S is given by Eq. 9.14.

The critical manifold is quite complicated at first sight

$$\begin{aligned}\det \mathcal{H}_{RM2}(k) =&((\mu^2-\nu^2)-\delta(\delta+t+e^{2ikd}t))^2\\ &-4e^{-ikd}\delta t(\mu^2-\nu^2-\delta^2)\cos(kd)\\ &-4t^2(2\mu^2-2\nu^2-(4+e^{-2ikd})\delta^2)\cos^2(kd)\\ &+16t^3(t+2\delta)\cos^4 8\Delta^2(\mu^2-\nu^2\\ &+\delta^2\cos(2kd))\sin^2(kd)+16\Delta^4\sin^4(kd)\\ &+8\Delta^2 t(t+\delta)\sin^2(2kd),\end{aligned} \tag{9.55}$$

where one should keep in mind that despite the complex terms the critical manifold will only take real values. This can be made explicit by working out Eq. 9.55. However, we omit doing this here, since the result is not much more insightful than considering the cases in the middle and the edge of the Brillouin zone, i.e. $kd = 0$ and $kd = \pm\pi/2$.

For the case of $kd = 0$ we obtain the condition

$$\mu^2-\nu^2-(\delta+2t)^2=0. \tag{9.56}$$

This results in a shifted cone in the parameter space when we assume $t \neq 0$, and we normalise by it, Fig. 9.10.

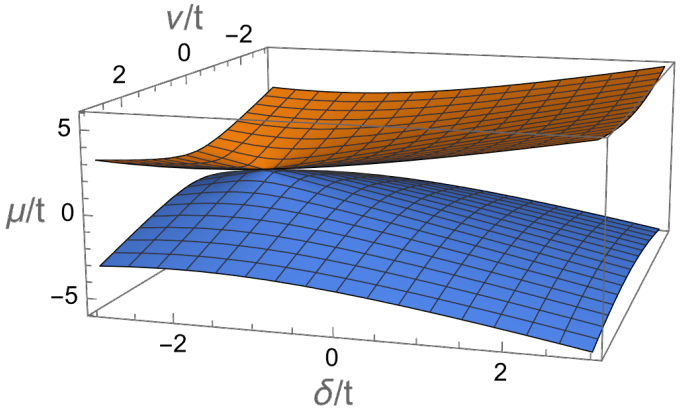


Figure 9.10: *The level set of* $\det(\mathcal{H}_{RM2}(0) = 0$ *normalised by* t *by substituting* $t = 1$ *in Eq. 9.55. This is a part of the critical manifold of the superconducting Rice-Mele model.*

Fig. 9.10 seems to admit a loop through a not simply connected subspace of $\mathbb{R}^3$. However, at $\delta = 2t$ the gap closes. Although it is not easily perceived from Eq. 9.55, it can be explained by the observation that the case of $\delta = 2t$ corresponds to the case of a vanishing hopping amplitude

in our previous formulation of this model. At vanishing hopping amplitude, or bandwidth, the gap closes in the model described by Eq. 9.42 and so it does here.

At the edge of the Brillouin zone the critical manifold reads

$$(\mu^2 - v^2 + 4\Delta^2 - \delta^2)^2 = 0, \tag{9.57}$$

which leaves us with a condition for the closing of the gap similar to Eq. 9.50

$$\mu^2 + 4\Delta^2 = v^2 + \delta^2. \tag{9.58}$$

This condition leads to different cones of hyperboloids in parameter space depending on the choice of the fourth parameter which can be zero or non-zero. Fig. 9.11 shows the case of a hyperboloid for non-zero Δ.

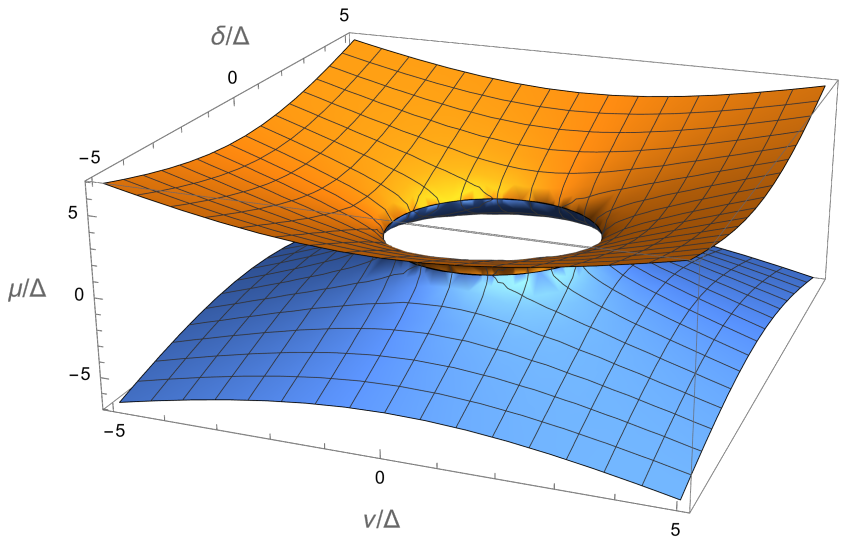


Figure 9.11: *The level set of* $\det(\mathcal{H}_{RM2}(\pm\pi/2) = 0$ *normalised by* Δ *by substituting* $\Delta = 1$ *in Eq. 9.55. This is a part of the critical manifold of the superconducting Rice-Mele model.*

From previous sections we can deduce that the parts where MZMs can occur are not simply connected. One case cannot be deduced from previous section, namely if a loop around the the cone or hyperboloid described by Eq. 9.58 for a constant μ would be possible. However, one can check, with a topological invariant or by numerically calculating the spectrum of a finite-sized chain, that only inside the cone or hyperboloid MZMs are present. This provides us from preforming a loop in a not simply connected space.

Nevertheless, their is interesting behaviour to be discovered in this model. To observe that behaviour we need to look into the loop of Thouless charge pump first. This loop is performed adiabatically slow and can be described by

$$\nu = \sin(t), \quad t = 1, \quad \delta = \cos(t). \tag{9.59}$$

The spectrum and the positive energy edge state of some points around this point are visualised in Fig. 9.12, the negative energy edge state can be found in Appendix B. The pumping of charge corresponds to the edge state moving from one side of the the chain as a particle to the other side as a hole and vice versa. As said earlier this loop is proposed, and experimentally realised, in a Rice-Mele model, which originally does not have a superconducting term, but what happens if we turn on the superconductivity in this model?

In a finite-dimensional chain this can be tested. It is important to notice however that the parity of the number of sites is extremely important. In numerical calculations with an even number of sites there are parts of the Thouless loop without edge states and parts with $4n$-fold degenerate edge states. This indicates some topological phase transition in the finite chain. A careful reader might be suspicious about the use of the word phase transition in a finite-sized chain. However, we use a intuitive notation of those transition characterised by the existence of edge states.

On the other hand, in a chain with an odd number of sites we can observe the Thouless loop and the influence of a superconducting gap. Fig. 9.13 shows that at first the original edge states persist, and that the superconducting gap tends to close that gap. When the loop from above is performed for this Δ similar behaviour is observed. After a closing of the gap, exactly when Eq. 9.58 is fulfilled, increasing the superconducting gap leads to an increase of the gap, to a certain extent. Moreover, by comparing Fig. 9.13c and Fig. 9.13e with Fig. 9.13d and Fig. 9.13f we observe that the nature of edge states changed. It can be numerically shown that performing the loop described by Eq. 9.59 does not change the energy of the edge states anymore. Moreover, along the loop the lowest bulk energy is constant as well. This can be understood in by the fact that turning on the superconducting gap introduces a topological phase transition where the nature of the edge states does change and MZMs are introduced.

9.4 A review

In this chapter we have studied essentially three different extensions of the Kitaev chain with as common factor the periodic, or alternating, perturba-

tion of the chemical potential or the hopping amplitude. This perturbation lead to a distortion of the lattice and a corresponding opening of the gap.

Indeed we observed MZMs in all three of the extensions for nonzero perturbations. Despite the fact not for all values of the parameter space the system exhibited MZMs, this means that extensions of the Kitaev chain inspired by topological insulators are possible, just as expected.

It is known that the periodic perturbations and the superconducting gap open the gap in the spectrum via different physical mechanisms. In the proposed extensions we observed how the mechanisms competed. This lead to the existence of different types of edge states for different parameter regimes of the same model.

In the superconducting SSH-model we discovered how different edge states exist in the $\mu = 0$ plane. In finite-sized chains we observed how MZMs were present for $|\delta| < |\Delta|$, this would be the region where the superconducting gaps dominated. For $|\delta| > |\Delta|$ the number of edge states differed between finite-sized chains with different parity, and the spectrum exhibited a splitting of the energy of the edge modes, this would be the region where the perturbation of the hopping amplitude dominated. These phase transition gave insight in the topological structure of the superconducting SSH-model.

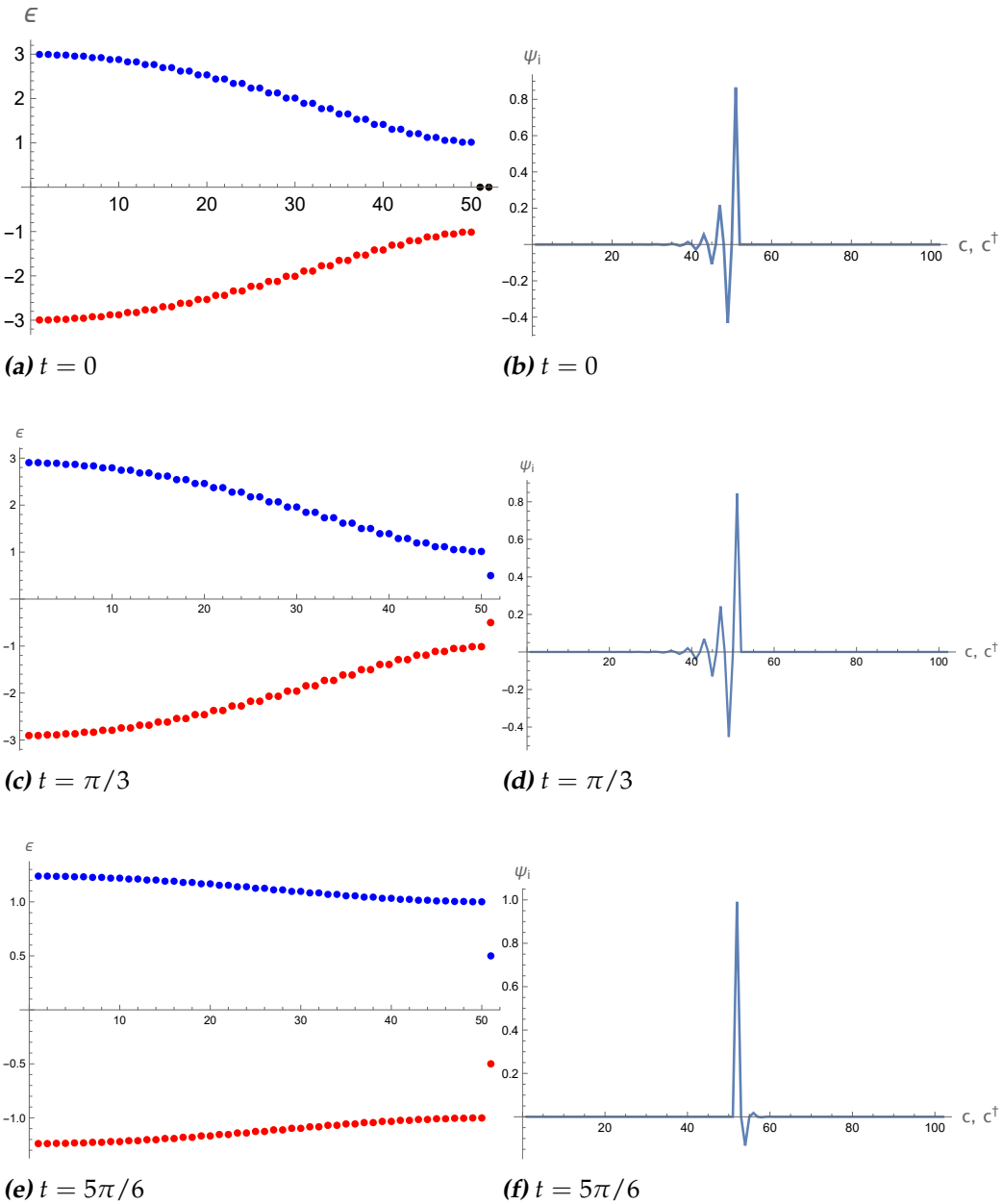
In the superconducting Rice-Mele model we studied the effect of superconductivity on the edge states that play a crucial role in the well-known Thouless charge pump. For a small superconducting gap the edge states persist, but when Eq. 9.58 was satisfied the gapped closed and for a larger superconducting gap MZMs were present. These had zero-energy independent of nonzero, but small enough, chemical potential, which distinguishes them from the other edge states.

All of the proposed models contained a mean field superconductivity term. In such models the PHS is present, since the Bogoliubov transformation imposes it. The existence of different types of edges states might indicate that the studied models are in different symmetry classes for different parameter regimes.

We did not succeed in fully describing the topological phases of the proposed extension substantiated by the calculation of topological quantum numbers, nor have we found a explicit and comprehensible expression for the critical manifold. This is partial due to the complexity of the critical manifold, and partial because the focus of our research lies on finding a region of the parameter space where MZMs are present in the chain and where we can perform a noncontractible loop.

Such a not simply connected subspace of the parameter space without gap closings and with the presence of MZMs in the chain was not found. It

might be that our initial thought, that another mechanism than that of superconductivity could open a gap at crucial points and therefore creating a not simply connected subspace, was completely wrong. It might also be that this is just not possible in the cases of the underlying mechanisms of these three extension of the Kitaev chain. However, that a different mechanism would open the gap at vanishing Δ while preserving the MZMs is extremely unlikely, since in that case no one stops us from forgetting about the superconductivity at all. That would mean a discovery of MZMs in a not superconductive system, which would be a major surprise.

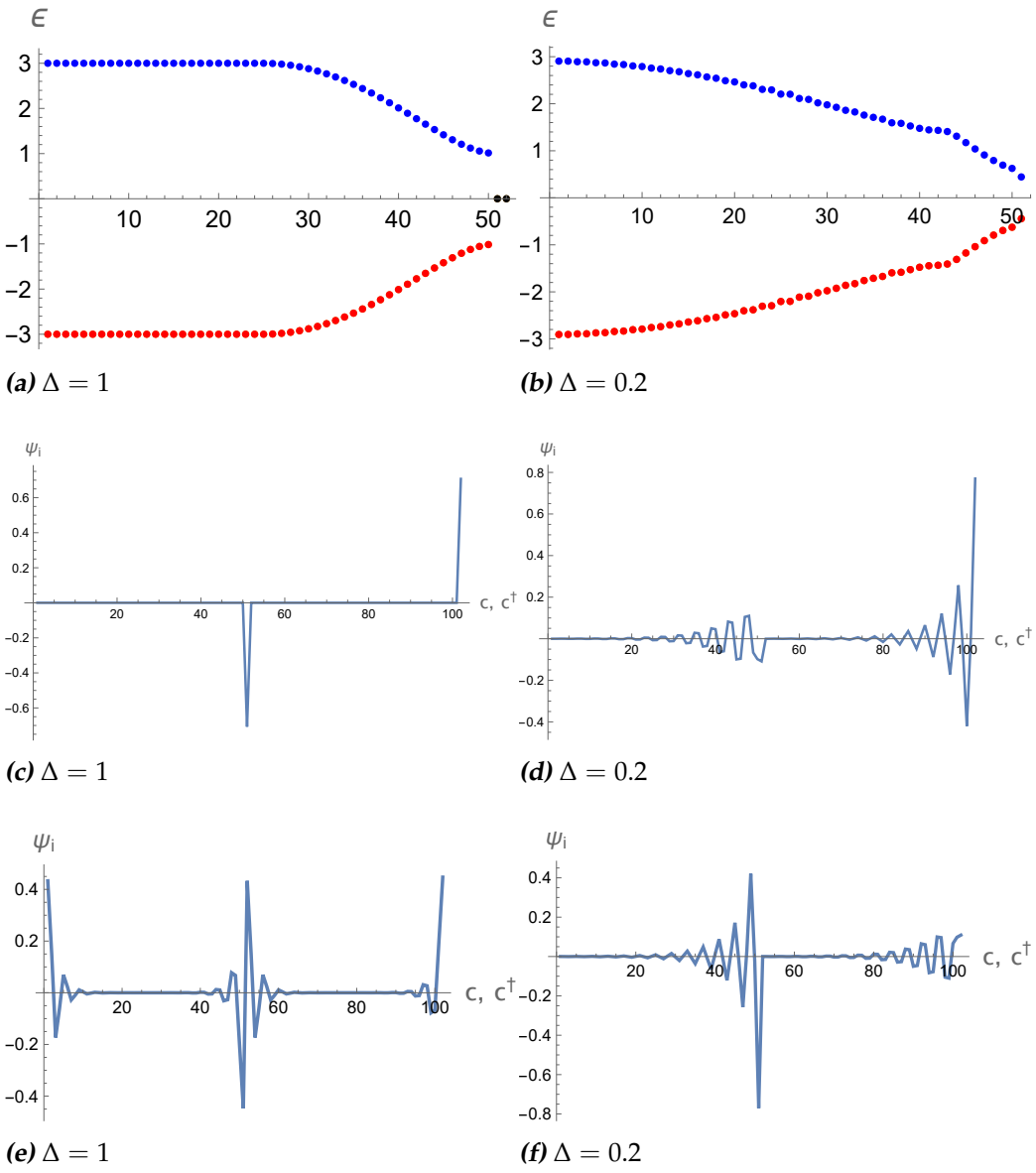


(a) $t = 0$ **(b)** $t = 0$

(c) $t = \pi/3$ **(d)** $t = \pi/3$

(e) $t = 5\pi/6$ **(f)** $t = 5\pi/6$

Figure 9.12: *(a),(c),(e) The spectrum of a Rice-Mele model with* 51 *sites performing a loop described by Eq. 9.59 at* $t = 0$, $t = \pi/3$, *and* $t = 5\pi/6$ *respectively. The spectra show how throught the loop the energies of the edge states are lifted to the bulk and brought back. (b),(d),(f) The positive energy edge state corresponding to the spectra. The* x*-axis depicts the Nambu spinor, Eq. 7.31, and the* y*-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state.*



(a) $\Delta = 1$ **(b)** $\Delta = 0.2$

(c) $\Delta = 1$ **(d)** $\Delta = 0.2$

(e) $\Delta = 1$ **(f)** $\Delta = 0.2$

Figure 9.13: *(a) The spectrum of a superconducting Rice-Mele model with* 51 *sites with* $\mu = 0.5$, $t = 1$, $\delta = \sqrt{3}/2$, *and* $\Delta = 1$. *(c),(e) The corresponding (Majorana) edge modes. (b) The spectrum of the same superconducting Rice-Mele model with* $\Delta = 0.2$. *(d),(f) The corresponding edge modes are shown, and these are not Majorana modes. The* x*-axis depicts the Nambu spinor, Eq. 7.31, and the* y*-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state.*

Chapter 10

Superconducting extensions of the Kitaev chain

Until thus far we have looked into models with alternating chemical potential and hopping amplitude. These models do not exhibit topological non-trivial connected subspaces, i.e. connected subspaces that are not simply connected. Therefore we need to consider further extensions of the Kitaev chain.

10.1 A fully staggering model

Firstly, we will consider a model with a simple periodic perturbation in all parameters. This utilises the full capacity of the Peierls distortion by creating larger unit cells, consisting of two sites, with alternating chemical potential, hopping amplitude, and superconducting gap. Such a model is described by the following Hamiltonian

$$\begin{aligned}\hat{H}(\mu,\nu,t,\delta,\Delta,\zeta) = &-\sum_{j=1}^{N}(\mu+(-1)^j\nu)c_j^\dagger c_j - \sum_{j=1}^{N-1}(t+(-1)^j\delta)(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j)\\ &+\sum_{j=1}^{N-1}(|\Delta|+(-1)^j\zeta)e^{i\theta}c_j^\dagger c_{j+1}^\dagger + (|\Delta|+(-1)^j\zeta)e^{-i\theta}c_{j+1}c_j),\end{aligned} \tag{10.1}$$

where $\mu \in \mathbb{R}$ the chemical potential, $t \in \mathbb{R}$ the hopping amplitude, $\Delta \in \mathbb{C}$ the superconducting gap, $\nu, \delta, \zeta \in \mathbb{R}$ the corresponding perturbations and $\theta = \mathrm{Arg}(\Delta)$, and assume $\theta = 0$. One could consider a perturbation that

differs in phase with the superconducting gap. However, this would make the analysis more difficult, and it turns out that this kind of perturbation on the magnitude of the superconducting gap gives rise to interesting structures already.

To study the bulk we can express Eq. 10.1 in sublattice operators, Fourier transform it. In section 9.3 we have already performed this transformation for all terms except for the periodic changing superconducting gap. Since the Fourier transform is a linear operation we can solely focus on the ζ-term. Fourier transforming this term immediately yields

$$\begin{aligned}&\sum_k \left[\zeta(e^{-ikd}b_k^\dagger a_{-k}^\dagger - e^{-ikd}a_k^\dagger b_{-k}^\dagger + \zeta(e^{ikd}a_{-k}b_k - e^{ikd}b_{-k}a_k)\right]\\ =&\sum_k 2\cos(kd)(\zeta b_k^\dagger a_{-k}^\dagger + \zeta a_{-k}b_k),\end{aligned} \tag{10.2}$$

where we again made elaborate use of of the fact that k is summed over equally spaces values in he interval $[-\pi/2d, \pi/2d]$.

Using Eq. 10.2 we find the Fourier transform of Eq. 10.1 up to an insignificant constant

$$\hat{H}(k) = \frac{1}{2}\sum_k \hat{\psi}_k^\dagger \mathcal{H}_{Full}\hat{\psi}_k, \tag{10.3}$$

where the BdG Hamiltonian is given by

$$\mathcal{H}_{Full} = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{10.4}$$

where

$$S = \begin{pmatrix} 0 & -2i\Delta\sin(kd) + 2\zeta\cos(kd) \\ 2i\Delta\sin(kd) - 2\zeta\cos(kd) & 0 \end{pmatrix} \tag{10.5}$$

and C is given by Eq. 9.45. Remember the assumption that both ζ and Δ are real, then in terms of Pauli matrices this BdG Hamiltonian reads

$$\begin{aligned}\mathcal{H}_{\text{Full}}(k) =&\mu\sigma_z\otimes\mathbb{1}_2 + \nu\sigma_z\otimes\sigma_z + 2t\cos(kd)\sigma_z\otimes\sigma_x - 2\delta\sin(kd)\sigma_z\otimes\sigma_y\\ &+ 2\Delta\sin(kd)\sigma_y\otimes\sigma_x + 2\zeta\sigma_x\otimes\sigma_y.\end{aligned} \tag{10.6}$$

Notice that the assumption that Δ and ζ are real here does not change the physical properties of our model, since we started with the assumption that both superconducting gaps had the same phase.

To obtain some elementary insight in the possible topological phase transitions that could occur in this model the critical manifold has to be studied. Hence we examine the level of 0 of the following expression

$$\begin{aligned}\det(\mathcal{H}_{\text{Full}}) = &-(\mu^2-\nu^2)^2+8\sin^2(2kd)((t^2+\zeta^2)(\Delta^2+\delta^2)-4t\delta\Delta\zeta)\\ &+(\mu^2-\nu^2-4(t^2-\zeta^2)\cos^2(kd))^2\\ &+(\mu^2-\nu^2+4(\Delta^2-\delta^2)\sin^2(kd))^2. \end{aligned} \tag{10.7}$$

Moreover the energy spectrum of the bulk is given by

$$\begin{aligned}\varepsilon(k) = \pm\Big[&\mu^2+\nu^2+4(t^2+\zeta^2)\cos^2(kd)+4(\Delta^2+\delta^2)\sin^2(kd)\\ &\pm 4\Big[\mu^2(\delta^2\sin^2(kd)+t^2\cos^2(kd)+\nu^2/4)\\ &+\Delta^2\sin^2(kd)(\nu^2+4\delta^2\sin^2(kd))\\ &+\nu^2\zeta^2/2+4t^2\zeta^2\cos^4(kd)+8t\delta\Delta\zeta\sin^2(2kd)\Big]^{1/2}\Big]^{1/2}. \end{aligned} \tag{10.8}$$

The first thing that catches our eyes is the pairing of t and ζ in Eq. 10.7 and Eq. 10.8. So besides the pairing of the superconducting gap and the perturbation on the hopping amplitude, the pairing between the hopping amplitude and the perturbation on the superconducting gap also occurs. On top of that there is exists a term that depends on all four of them.

When the standard case of $kd = 0$ and $kd = \pm\pi/2$ are studied, we obtain the conditions

$$\mu^2-\nu^2-4t^2+4\zeta^2=0 \tag{10.9}$$

and

$$\mu^2-\nu^2+4\Delta^2-4\delta^2=0 \tag{10.10}$$

respectively.

Unfortunately, these standard cases do not provide a parameter space that is om much interest to or goal of performing a noncontractible loop without crossing a manifold. Nevertheless, such properties are hidden in this model, but we need to consider some minor changes which we will do shortly in Section 10.2.

Before we will dive deeper into those changes of this model, let us do some simple observation. Firstly, it is clear that there exist regions in the parameter space where there are 2 MZMs because turning of ζ reduces the model to an already studied case of the superconducting Rice-Mele model. The interesting part however is that in this the fully staggering chain one

can find MZMs for zero chemical potential and hopping amplitude, and no perturbation on both, and anon-zero superconducting gap and corresponding perturbation. The most interesting part is that the spectrum in Fig. 10.1 shows a 4-fold degenerate ground state, i.e. 4 MZMs, without any defects. We have noticed that for non-zero chemical potential a splitting of the ground state energies is introduced.

Despite the fact that we have to omit a description of the whole parameter space this 4-fold degeneracy in a chain without topological defect is still worth mentioning.

10.2 A superconducting equivalent of the Rice-Mele model

In an attempt to deform the fully staggering model and to endow a chain with multiple independent p-wave superconductivity terms we consider a superconducting equivalent of the Rice-Mele model. This means that we have a tight binding chain with periodically perturbed chemical potential and homogeneous hopping amplitude, and two superconducting terms. One of these is present between all of the nearest neighbours, while the other alternates. The Hamiltonian of this system can be described by

$$\begin{aligned}\hat{H}(\mu,\nu,t,\Delta_1,\Delta_2) = &-\sum_{j=1}^{N}(\mu+(-1)^j\nu)c_j^\dagger c_j \\ &-\sum_{j=1}^{N-1} t(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j) \\ &+\sum_{j=1}^{N-1}(\Delta_1 c_j^\dagger c_{j+1}^\dagger+\Delta_1^* c_{j+1}c_j) \\ &+\sum_{j=1}^{N-1}(\Delta_1 c_{2j}^\dagger c_{2j-1}^\dagger+\Delta_1^* c_{2j}c_{2j-1}),\end{aligned} \tag{10.11}$$

where $\mu \in \mathbb{R}$ the chemical potential, $t \in \mathbb{R}$ the hopping amplitude, and $\Delta_1, \Delta_2 \in \mathbb{C}$ p-wave superconductivity terms. Here we have simplified further analysis by assuming that they have the same phase and in fact are real, otherwise the interaction of the two terms adds to the complexity of the model by introducing interference. Contrary to the fully staggering model, the perturbation of the hopping amplitude is taken to be zero.

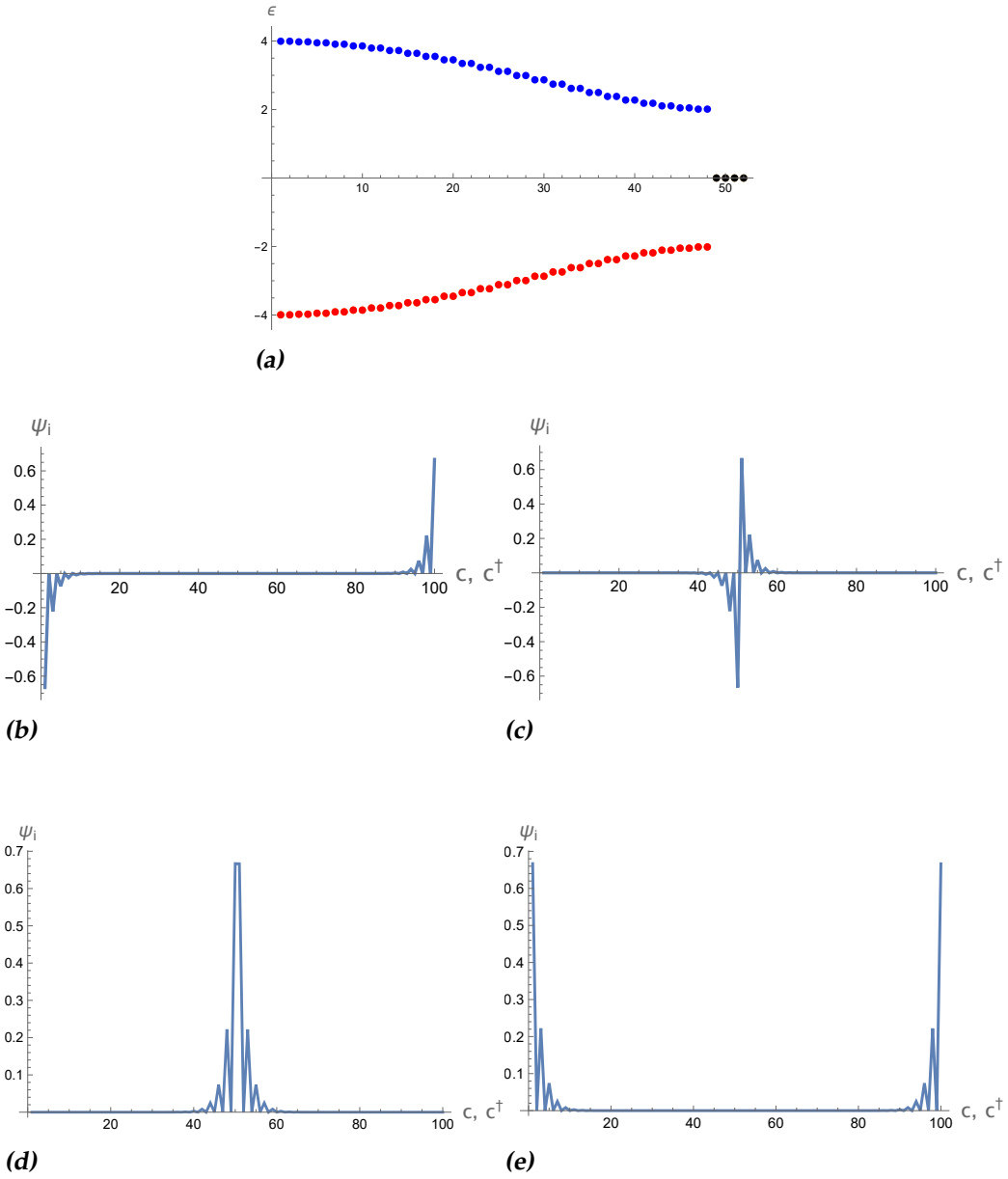


Figure 10.1: *(a) The edge states of a finite-sized fully staggering model with 50 sites where $\mu = \nu = t = \delta = 0, \Delta = 2$, and $\zeta = 1$. (b),(c),(d),(e) The corresponding MZMs present in the chain without topological defect.*

By performing the usual transformations, Fourier aand Bogoliubov, and making use of results obtained earlier we obtain

$$\hat{H}(k) = \frac{1}{2}\sum_{k} \hat{\psi}_k^{\dagger} \mathcal{H}_{SC2} \hat{\psi}_k, \tag{10.12}$$

where the BdG Hamiltonian is given by

$$\mathcal{H}_{SC2} = \begin{pmatrix} C & S \\ S^\dagger & -C \end{pmatrix}, \tag{10.13}$$

with

$$S = \begin{pmatrix} 0 & -2i\Delta_1 \sin(kd) + \Delta_2 e^{ikd} \\ -2i\Delta_1 \sin(kd) - \Delta_2 e^{-ikd} & 0 \end{pmatrix} \tag{10.14}$$

and C is given by Eq. 9.30. Notice that we omit explicitly working out the transformation since this is not especially insightful and previous section make the general idea perfectly clear.

To understand the topological phases for different regions in the parameter space we need to consider the 0 level set of the determinant of $\mathcal{H}_{SC2}(k)$

$$\begin{aligned} \det(\mathcal{H}_{SC2}(k)) = &\Big[\mu^2 - \nu^2 - 4t^2\cos^2(kd) + (|\Delta_2| - \sin^2(kd)|\Delta_1|)^2 \\ &- 2i(|\Delta_2| - 2|\Delta_1|)t\sin(2kd)\Big] \cdot \Big[\mu^2 - \nu^2 - 4t^2\cos^2(kd) \\ &+ (|\Delta_2| - \sin^2(kd)|\Delta_1|)^2 + 2i(|\Delta_2| - 2|\Delta_1|)t\sin(2kd)\Big], \end{aligned} \tag{10.15}$$

which is obviously real despite the occurrence of i because of the multiplication with the complex conjugate.

A quick skim over Eq. 10.15 convinces us that the corresponding critical manifold has an complicated structure. To obtain an elementary understanding this manifold we consider the middle and the edge of the Brillouin zone. At $kd = 0$ Eq. 10.15 reduces to

$$(\mu^2 - \nu^2 + |\Delta_2|^2 - 4t^2)^2 = 0, \tag{10.16}$$

and at $kd = \pm\pi/2$ to

$$(\mu^2 - \nu^2 + (|\Delta_2| - 2|\Delta_1|)^2)^2 = 0. \tag{10.17}$$

Let us consider a specific case where $t = 2\Delta_1$, and Δ_1 is used to normalise al the energies. Then Eq. 10.16 gives rise to a hyperboloid with an radius of 4 at $\nu = 0$. Moreover, Eq. 10.17 induces a shifted cone in the parameter space around $(\mu, \Delta_2) = (0, 2)$. Combining these to manifolds as embeddings of three dimensional parameter space consisting of μ, Δ_2, and ν yields a not-simply connected subspace within the hyperboloid, Fig. 10.2.

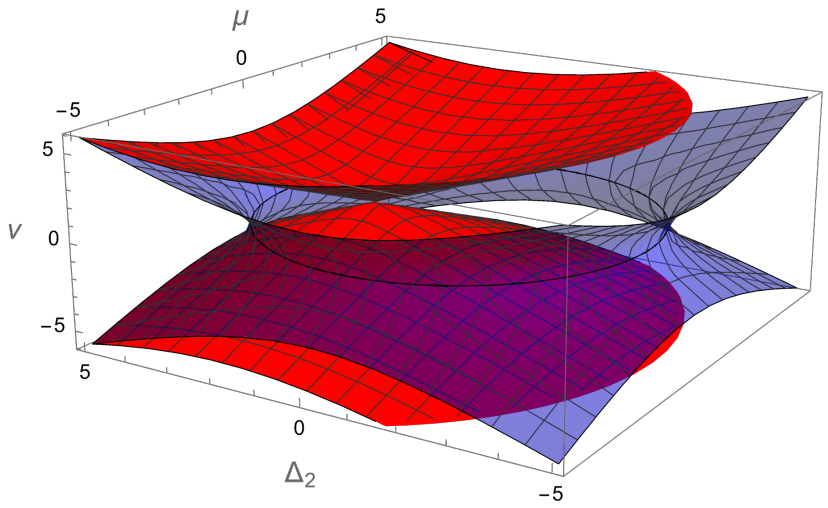


Figure 10.2: *The level set of* $\det(\mathcal{H}_{SC2}(0)) = 0$*, in red, and the level set of* $\det(\mathcal{H}_{SC2}(\pm\pi/2)) = 0$*, in blue, for* $t = 2\Delta_1$ *normalised by* Δ_1 *by substituting* $t = 2$ *and* $\Delta_1 = 1$ *in Eq. 10.16 and Eq. 10.17 respectively. This is a part of the critical manifold of the superconducting equivalent of the Rice-Mele model.*

The not simply connected subspace enclosed by the red and blue level sets in Fig. 10.2 brings with it a little optimism. Let us consider a loop in the $\nu = 0$ plane around the point $(\mu, \Delta_2, \nu) = (0, 0, 2)$, while obeying

$$\mu^2 + \Delta_2^2 < 16, \tag{10.18}$$

which means that the loop does not cross the blue level set in Fig. 10.2. Then the loop can be described by

$$t/2 = \Delta_1 = 1, \quad \nu = 0, \quad \mu = \alpha \sin(t), \quad \Delta_2 = 2 + \alpha \cos(t), \tag{10.19}$$

where $\alpha^2 < 2$.

In numerical calculations we can verify that there are MZMs present in the system for every point on the loop in the parameter space, and this observation does not depend on the parity of the number of sites. The existence of MZMs can be concluded, because at $t = 0$ the spectrum of a finite-sized chain indicates the existence of zero-energy edge modes, Fig. 10.3c, these edge modes are indeed MZMs as the edge states in Fig. 10.3a and Fig. 10.3b clearly satisfy the relations of Eq. 7.8 and Eq. 7.9, and Fig. 10.3d shows that the gap does not close along the loop.

Now we have found a noncontractible loop in the parameter space that is complementary to the critical manifold. The question that remain however, is if this loop will give rise to a non-trivial geometrical phase.

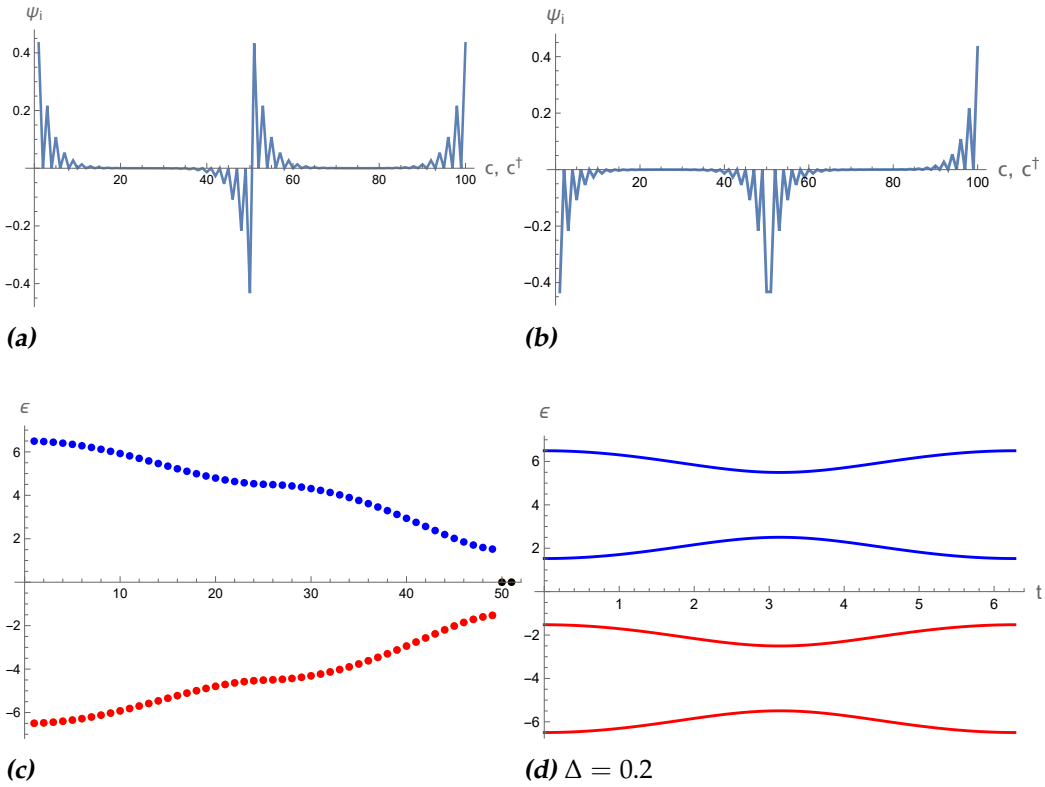


Figure 10.3: *(a),(b) The edge states of a finite-sized superconducting equivalent of the Rice-Mele model with 50 sites where $\mu = \nu = 0$, $t/2 = \Delta_1 = 1$, and $\Delta_2 = 2.5$. (c) The corresponding spectrum of that model with the given parameters. (d) The blue lines indicate the upper and lower bound of the positive bulk energy spectrum around a loop described by Eq. 10.19 with $\alpha = 0.5$, and the red lines boundaries of the negative counterpart.*

Solving the Schrödinger equation numerically

Now we have found the critical manifold we can perform a non-contractable loop. The analytical calculation of the eigenstates in the adiabatic limit however, can still be quite difficult. That leads to a numerical first approach of the problem. Consider SchrÃ¶dinger's equation with an Hamiltonian that depends on μ, ν, t, Δ_1, and Δ_2:

$$i\partial_t \hat{\psi} = \mathcal{H}(\mu, \nu, t, \delta, \Delta_1, \Delta_2)\hat{\psi}, \tag{10.20}$$

and consider a smooth loop $\gamma : [0, T] \to \mathbb{R}^5$ with $\gamma(0) = \gamma(T)$ defined by $t \mapsto (\mu(t), \nu(t), t(t), \Delta_1(t), \Delta_2(t))$, where all the component function are smooth, see Eq. 10.19. Using this loop we can make the Hamiltonian time dependent: $\hat{\mathcal{H}}(t) = H(\mu(t), t(t), \Delta_1(t), \Delta_2(t))$. This enables us to write

down a time dependent Schrödinger equation:

$$i\partial_t \psi(t) = \mathcal{H}(t)\psi(t). \tag{10.21}$$

The question that still stands is how to solve this equation numerically in the adiabatic approximation. First of all, we need to start with a $\psi(0)$ in the ground state. This boils down to solving $H(0)\psi(0) = E_0\psi(0)$ with E_0 the lowest non-negative eigenvalue of $H(0)$. Equipped with this starting position point of the wave function, we are almost ready to do calculation. However, it is important to look at the time scale of the varying of the parameters and the time scale of the splitting, i.e. the eigenvalue not being exactly zero due to the finite-sized of the system.

The splitting energy is the difference between the lowest non-negative and highest non-positive eigenvalue of $\mathcal{H}(t)$. This is called the splitting since we expect a degenerate zero-energy ground state and the finite size lead, together with the PHS, to a $+\delta E$ and $-\delta E$ pair instead of two 0 energies. This value can be roughly estimated, as only it order of magnitude is really of importance. To go from an energy to a time we use the energy-time uncertainty principle, 4.36. Substituting the splitting energy, $2\delta E$, in Eq. 4.36 yields the time scale of the splitting:

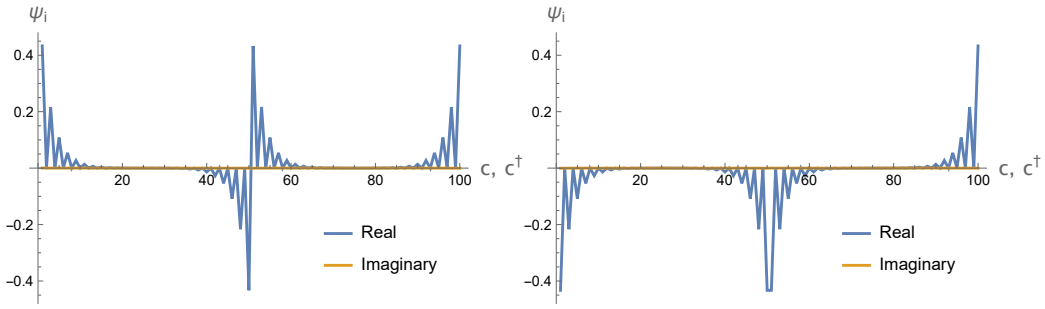
$$t = \frac{1}{2\delta E}. \tag{10.22}$$

In our case the splitting is of the order 10^{-8} and hence the loop should be performed in a time of an order much smaller than 10^8.

From Fig. 10.4 it becomes clear that the edge states do not acquire a non-trivial geometrical phase, and after repeating the loop numerous times the noise increases without any indication of a small geometrical phase showing up. So despite the fact that we solve the Schrödinger equation on a time scale much large then the time scale of the gap, on the order of 1, and much smaller then the time scale of the splitting, on the order of 10^8, no geometrical phase occurs.

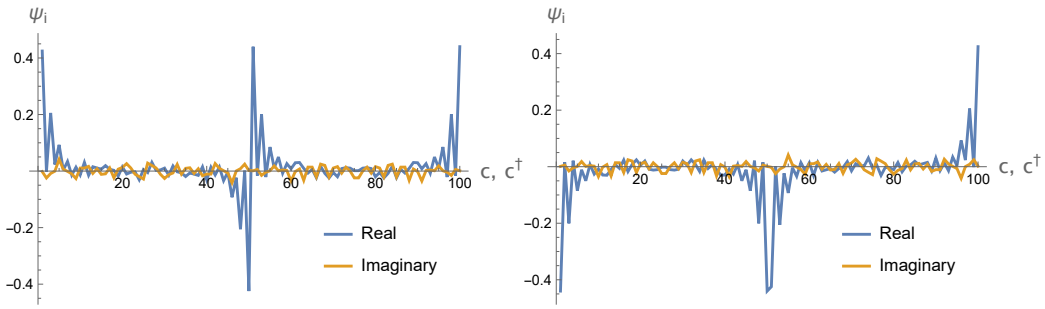
10.3 A review

In this chapter we have studied some topological properties of two models, and in both models there were two slightly different terms in the Hamiltonian which made the chain a p-wave superconductor. Just like the superconducting SSH-model with periodic kicking and the Rice-Mele model the models in this chapter were related by a similar transformation.



(a) *1 loop*

(b) *1 loop*



(c) *20 loops*

(d) *20 loops*

Figure 10.4: *(a),(b) The edge states of a finite-sized superconducting equivalent of the Rice-Mele model with 50 sites after one loop described by Eq. 10.19. (c),(d) The edge states of a finite-sized superconducting equivalent of the Rice-Mele model with 50 sites after twenty loops described by Eq. 10.19. In both cases the imaginary and real part of the wave function are shows seperatly. The loop takes place in* $T = 100$.

In both these models we observed the existence of MZMs. In addition, in the first one we have also looked for different edge modes. For zero hopping and chemical potential only the superconducting gap and the corresponding perturbation have play a role. It is interesting to see that the gap does not necessarily closes at $t = 0$, in contrary to all other models that we have studied so far. In this case we observed a 4-fold degenerate ground state. The edge states are not MZMs, because a nonzero chemical potential introduces a splitting, and linear combinations of the states in Fig. 10.4 are not MZMs. This again indicates that the different mechanisms that create edge states in a chain are competing. Again the distortion of the one-dimensional lattice places a role here.

Again the models contained a mean field superconductivity term. Hence the models exhibit PHS. The existence of different types of edges states indicates that the chains are in different symmetry classes for different pa-

rameter regimes.

In the superconducting equivalent of the Rice-Mele model we found a subspace of the parameter space without closings of the gap, where MZMs were present in the chain, and that was not simply connects. In this subspace bounded by two parts of the critical manifold it was possible to construct a noncontractible loop. Then we solved the Schrödinger equation along that loop, to numerically determine the geometrical phase that a state would acquire from adiabatic movement along that loop. In Fig. 10.4 the eigenstate after the loop is shown, and from comparison with Fig. 10.3 it is clear that the obtained phase is zero. Since the obtained geometrical phase is essential for braiding in the parameter space, this would mean that braiding is such a way cannot be achieved in this particular subspace.

Be aware that the geometrical phase turning out to be zero is perfectly in line with the theory. Since the holonomy of a loop is dependent on the connection, which we do not explicitly know here, it can be the unit even though the loop is noncontractible. The other way around is not possible, the holonomy of a contractible loop will always be the unit element in the holonomy group.

All in all, a definite answer to the main question of this thesis if it is possible to braid Majorana modes in the parameter space, cannot yet be provided. In the next chapter we will do some recommendations for further research, and how to go forward from here.

Chapter 11

Conclusion and outlook

In this thesis we provided the elementary mathematical background for studying of geometrical phases in many-body systems. This heavily relies on the concept of connections and we have seen how the adiabatic theorem gives rise to a connection on the parameter space of appropriate Hamiltonians [12, 75].

Furthermore, we gave a construction of the formalism second quantisation for fermionic many-body systems from first principles. It turned out that this formalism is uniquely defined, up to unitary transformations, by the creation and annihilation operators and their anticommutation relations according to the Stone-Von Neumann theorem [28]. One key advantage of this formalism is that the relevant symmetries of second-quantised Hamiltonian can be studied in a comprehensive manner, as demonstrated in Chapter 6. These symmetries could be used to classify Hamiltonian, and according to Kitaev [32] certain topologically protected properties could be assigned to every symmetry class.

In Chapter 7 we defined topologically protected properties as properties of a Hamiltonian that could not vanish by continuous deformation of the Hamiltonian without closing the gap. This is where we arrived at the main topic of this thesis, braiding. The noncommutative exchange of Majorana zero modes gave rise to this concept, but utilising it was still not possible. In the first place because of the fact that the existence of MZMs has not yet been experimentally verified, and secondly because the protocols for braiding in real space have their experimental impracticalities. Therefore we proposed to utilise the geometrical phases obtained by adiabatic movement to perform braiding in the parameter space. However, we encountered two problems. First of all, for braiding we need at least a $2n$-fold degenerate ground state of MZMs, with $n > 1$, so we needed to

increase the degeneracy. Furthermore, for braiding a non-trivial geometrical phase is needed, therefore a noncontractible loop should be found in the parameter space.

In Chapter 8 we showed how MZMs can occur at domain walls in finite-sized chains without influencing the MZMs that were already present at the edges of the chain. This would solve the problem of the degeneracy. Although our analysis considered defects in the homogeneous Kitaev chain, it is assumed that this generalises to extensions of the chain.

To solve the problem of the noncontractible loop we had to find a not simply connected connected component of the parameter space were the gap in the spectrum did not close and MZMs were present. To achieve this we proposed different extensions of the Kitaev chain. The first category of extension were superconducting generalisations of topological insulators, which did not exhibited the relevant not simply connected subspaces. However, we observed interesting topological behaviour of transitions between phases with different types of edge states.

The second category of extensions were models with different superconducting terms in the Hamiltonian, each term should prevent the gap from closing when the other term vanishes. In this models we observed some topologically interesting behaviour, and again the coexistence of different types of edge states in the same model, albeit at different parameter regimes. Furthermore, a not simply connected connected subspace was found. Unfortunately, the numerical calculation of the corresponding Wilczek-Zee factor of that loop yielded zero.

Therefore, we cannot conclude that braiding MZMs via the parameter space is possible. Further extensions are necessary. One could try to introduce periodic perturbations with a longer period. Moreover, Kitaev chains and extensions could be considered with longer range interactions [3], interactions on different ranges might open unexpected gaps. Alternatively, one could look into the phase of the superconductive gap. While in the case of one superconducting term the superconducting gap can always chosen to be real by a trivial transformation of the creation and annihilation operators, this is not necessarily true for two or more terms of superconductivity, which might introduce interesting behaviour which resembles interference. On top of that, the phase of the superconducting gap could be varied along the chain [76], which give rise to Cooper pairs where the momenta of the electrons do not cancel out.

When a extension of the Kitaev chain is found with the desired properties, there is one step in the analysis that is of major importance. To translate the observations done on eigenstates of the Bogoliubov-de-Gennes Hamiltonian to physical eigenstates, one should discard the unphysical

eigenstate that is found solely because of the particle-hole symmetry. However, for states with zero energy the distinction between physical and unphysical is not easily made. A approach is to select the eigenstate corresponding to the positive energy in a finite-sized chain where the splitting is still obvious, and follow this state as the size of the chain goes to infinity.

Let us finish this thesis with relating this work with the most recent developments in research. Besides the elaborate theoretical research on Majorana particles, the experiments are also still evolving. One example is the search for p-wave superconductivity, a cornerstone of the Kitaev chain. Although we still require a more conclusive proof, experiments on the two-dimensional material UTe_2 showed promising results for the discovery of unconventional, p-wave, superconductivity in 2023 [2, 21, 27].

For those who are concerned about the influence of dissipation on the occurrence of MZMs, theoretical predictions from 2024 say that even a dissipative Rashba nanowire can host MZMs , albeit with a finite life-time [18].

Further research on experimental implementations of the Kitaev chain include coupling quantum dots through a two-dimensional electron gas in a region proximitised by a superconductor [67]. Although only two dots were coupled and therefore a chain with only two sites was created in 2024, the quantum dots are ideal for tuning to the interesting spots of the parameter space. Being able to tune the parameters of a chain are essential for braiding via the parameter space, therefore this is a promising step in that direction.

The interest in the Kitaev chain reaches further than research groups that are interested in its properties for quantum computing. This year an bosonic equivalent, i.e. optomechanical Kitaev chain, was realised [63]. This chain is an example of a topological metamaterial which has promising applications in signal manipulation and sensing.

All in all, research to the Kitaev chain and Majorana quasiparticles is still worth doing. Despite the difficulties in experimentally realising the theoretical models there is progress, and with this possibility of experimental realisation on the horizon, it would be interesting to further investigate the topological properties of extensions of the Kitaev chain.

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Appendix A

Eigenstates and spectra of Kitaev chains with defects

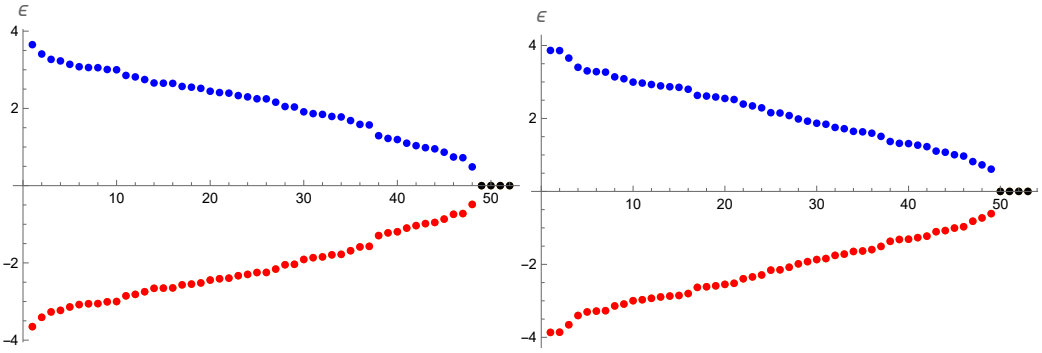
In Chapter 8 defects in the homogeneous Kitaev chain are studied. Here we provided the spectra and eigenstates of chains complementary to the figures in Chapter 8. Finite-sized Kitaev chains with different parity and with a centralised and non-centralised defects are considered for both defects in the superconducting gap as the hopping amplitude. Because of the topological protection, it is not fruitful consider many variations of parameters for which MZMs exist at the edges. Hence only the configuration $\mu = t = \Delta = 1$ is considered. To reduce the number of figures in this appendix the spectra and edge states are only provided for chains with additional noise.

Notice that in all plots of edge states the x-axis depicts the Nambu spinor, Eq. 7.31, and the y-axis the coefficients such that $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ is a normalised state, and the shaded areas mark the position of the defect.

From the figures of this appendix it is clear that the zero-energy modes at the edges and domain walls persist a Kitaev chain with noise. The eigenstates can be heavily disturbed, but both the position and the relation between the coefficients of creation and annihilation operators are approximately what we expected from Eq. 7.8 and Eq. 7.9. We can conclude that the MZMs at edges and domain walls still exist in the chain with noise, despite the noise level of the perturbation being high, i.e. almost of the order of the parameters in the Hamiltonian..

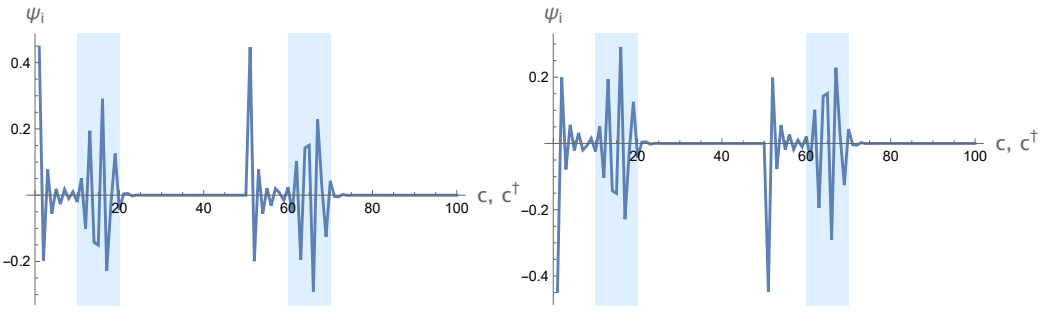
Defect of the superconducting gap

Fig. A.1, A.2, and A.3 are related to chains with a defect in the superconducting gap.

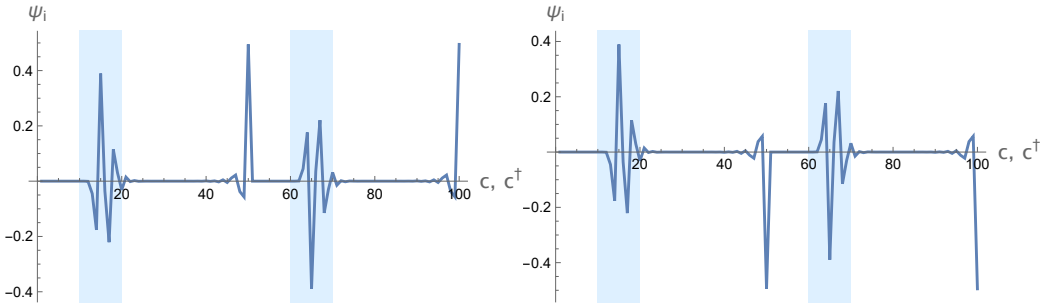


(a) *Unperturbed spectrum with defect* ***(b)***

Figure A.1: *(a) The numerical energy spectrum of the perturbed inhomogeneous Kitaev chain with* 50 *sites and open boundary conditions for the parameters* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 15th site that is effecting* 11 *sites, i.e.* $n = 15$ *and* $l = 10$. *These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32 and four zero-energy states with energies of the order of* 10^{-10}. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq. 7.32 with noise level* $t/2$. *(b) The numerical energy spectrum of a similar chain, but consisting of 51 sites with the defect centred around the 25th site. The zero-energy states have energies of the order of* 10^{-7}

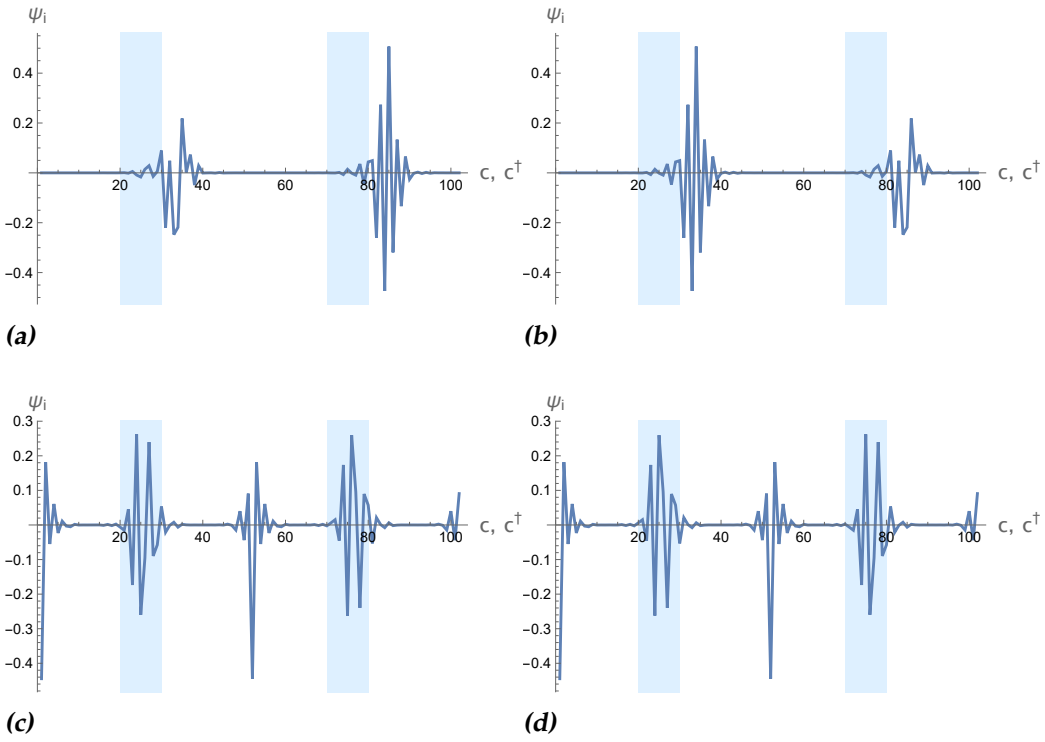


(a) ***(b)***



(c) **(d)**

Figure A.2: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 15th site that is effecting* 11 *sites, i.e.* $n = 15$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32.*



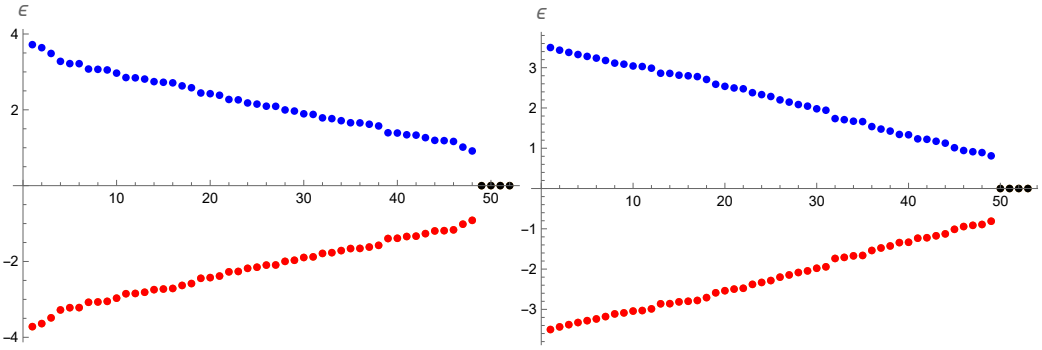
(a) **(b)**

(c) **(d)**

Figure A.3: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 51 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the superconducting gap centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32.*

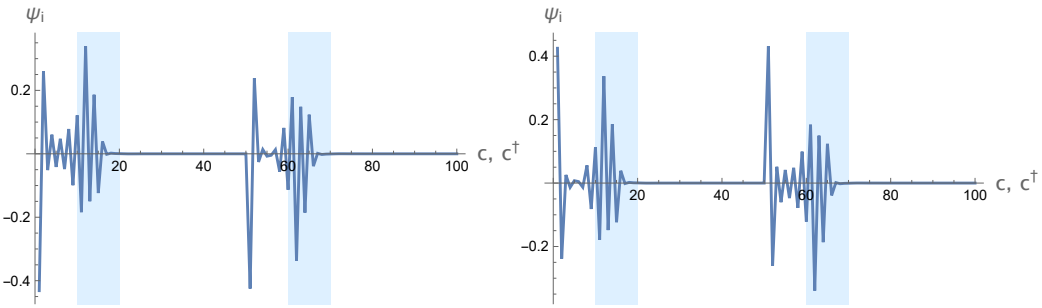
Defect in the hopping amplitude

Fig. A.4, A.5, and A.6 are related to chains with a defect in the hopping amplitude.

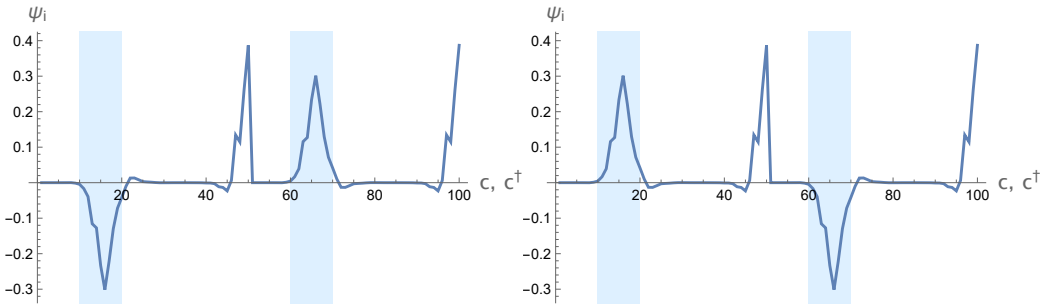


(a) *Unperturbed spectrum with defect* ***(b)***

Figure A.4: *(a) The numerical energy spectrum of the perturbed inhomogeneous Kitaev chain with* 50 *sites and open boundary conditions for the parameters* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the hopping amplitude centred around the 15th site that is effecting* 11 *sites, i.e.* $n = 15$ *and* $l = 10$. *These are the eigenvalues of the BdG Hamiltonian from Eq. 7.32 and four zero-energy states with energies of the order of* 10^{-8}. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq. 7.32 with noise level* $t/2$. *(b) The numerical energy spectrum of a similar chain, but consisting of 51 sites with the defect centred around the 25th site. The zero-energy states have energies of the order* 10^{-11}

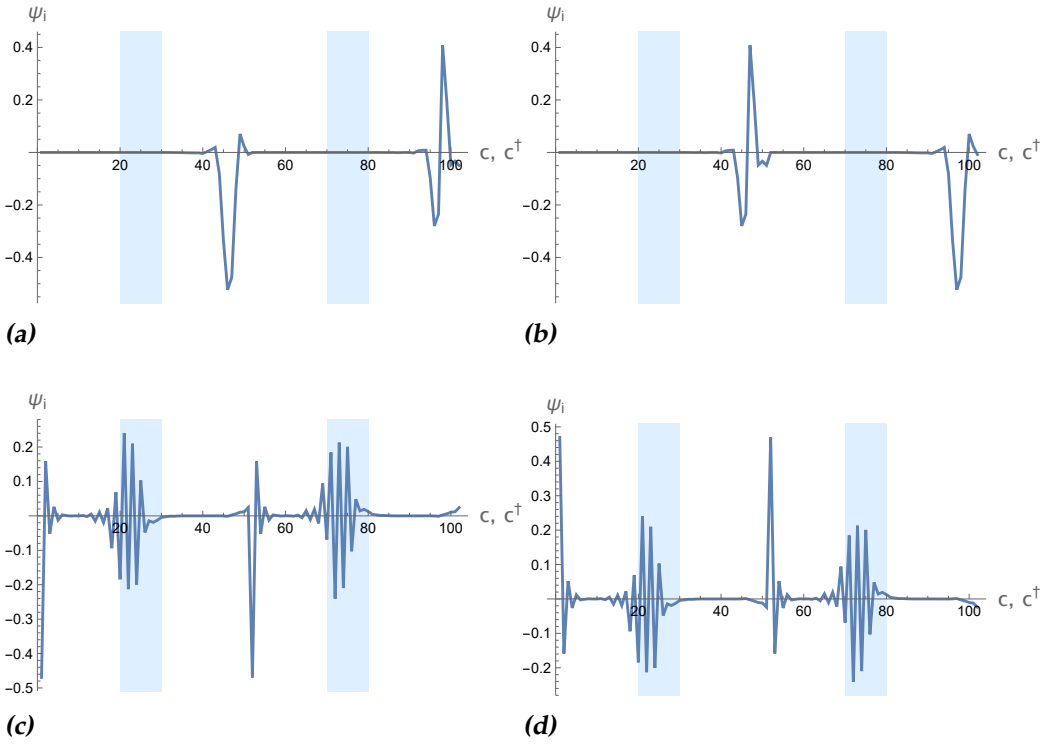


(a) ***(b)***



(c) **(d)**

Figure A.5: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 50 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the hopping amplitude centred around the 15th site that is effecting* 11 *sites, i.e.* $n = 15$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32.*



(a) **(b)**

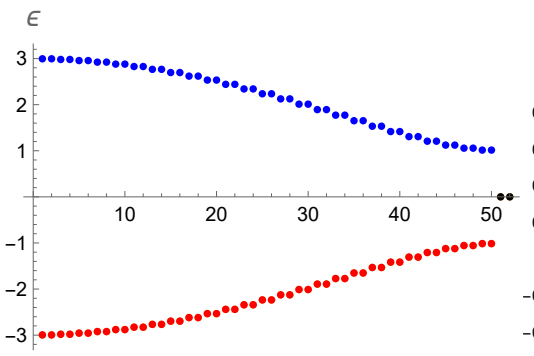
(c) **(d)**

Figure A.6: *(a),(b),(c),(d) The perturbed eigenstates corresponding to the zero-energy modes of Kitaev chain of* 51 *sites with* $\mu = 1$, $t = 1$, *and* $\Delta = 1$ *with a defect in the hopping amplitude centred around the 25th site that is effecting* 11 *sites, i.e.* $n = 25$ *and* $l = 10$. *The perturbation consists of random noise with noise level* $t/2$ *that is added to every parameter in Eq.7.32.*

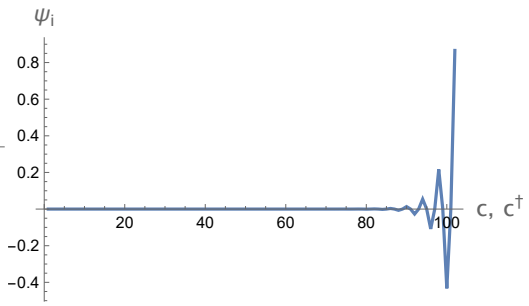
Appendix B

Negative eigenstates along a Thouless loop

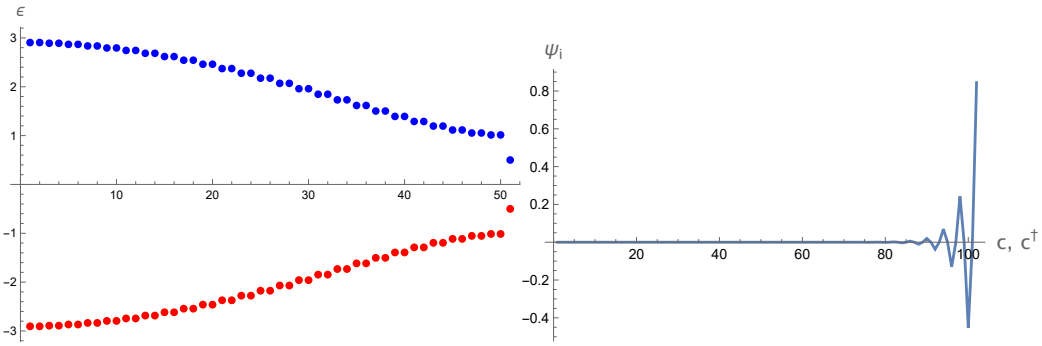
The Thouless loop is described by Eq. 9.59. In Section 9.3 we have seen some of the eigenstates along loop corresponding to positive energy in Fig. 9.12. Here the eigenstates corresponding to the negative energy are shown in Fig. B.1.



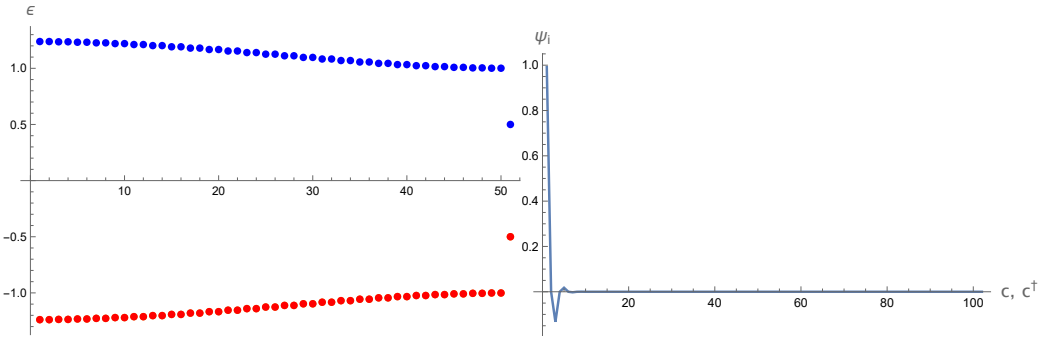
(a) $t = 0$



(b) *t=0*



(c) $t = \pi/3$ **(d)** $t = \pi/3$



(e) $t = 5\pi/6$ **(f)** $t = 5\pi/6$

Figure B.1: *(a),(c),(e) The spectrum of a Rice-Mele model with* 51 *sites performing a loop described by Eq. 9.59 at* $t = 0$, $t = \pi/3$, *and* $t = 5\pi/6$ *respectively. (b),(d),(f) The negative energy edge state corresponding to the spectra. The* x*-axis depicts the Nambu spinor, Eq. 7.31, and the* y*-axis the coefficients such that* $(\psi_1, ..., \psi_{2N})(c_1, ..., c_N, c_1^\dagger, ..., c_N^\dagger)^T$ *is a normalised state.*