CHALMERS
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Majorana Fermions and Topological Superconductivity

1D Topological classification of CII phases

Master's thesis in Physics and Astronomy

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Department of Physics
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2019

MASTER'S THESIS 2019

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Typeset in LaTeX
Printed by Chalmers Reproservice
Gothenburg, Sweden 2019

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Abstract

In the last decades, topology has established itself as a fundamental principle in condensed matter physics. Not only does topology explain the incredible robustness of certain physical quantities such as the Hall conductivity, but as a result of the bulk-boundary correspondence it also accounts for robust exotic fermionic edge states, e.g. Majorana zero modes in superconductors. In this thesis the field of topological quantum matter is reviewed with particular emphasis on one-dimensional non-interacting superconducting systems and symmetry-protected topological phases. By taking off from Kitaev's model of p-wave superconductivity and the tenfold classification of topological superconductors and insulators, we also investigate the notion of gapless phases of matter addressing the issue what happens at a topological phase transition in one dimension. For the symmetry classes BDI and CII, which both are known to host topological superconductors in 1D, we obtain an $\mathbf{N} \times \mathbf{Z}$-classification of gapless phases. In addition to the conventional topological $\mathbf{Z}$-invariant, the other classification is provided by conformal field theory, a framework frequently used when studying critical phenomena.

Keywords: topological superconductors, Majorana zero modes, Majorana bound states, symmetry classes, gapless phases of matter

Acknowledgements

Few theses are written in complete isolation. This is not an exception and I would therefore like to distribute my thankfulness to those who made the past months endurable. Firstly and most importantly, I want to express my sincere gratitude to my thesis supervisor, Henrik Johannesson. The long weekly meetings have been truly rewarding and your passion for theoretical physics, lust for telling historical anecdotes and your kindness and positive attitude has rubbed off on me. Secondly, I must not forget to pay my regards to my fellow compadres in “Teorikorridoren”: Simon, Sebastian, Torbjörn and Magdalena. Thank you for bearing with me during the latest six months and for always having your doors open for a discussion on life, the Universe and everything. Furthermore, the numerous long lunches with the rest of the “MPPAS gang” must not go unmentioned. Although rather contraproductive for the writing of this thesis, they have served as excellent therapeutical sessions and given the possibility of sharing the anxiety between peers and intellectuals.
Lastly, I am glad for having been able to discuss the topic of topological quantum matter with those who practice the subject on a daily basis. Ruben Verresen, Abhishodh Prakash, Christian Spånslätt, Eddy Ardonne and Oleksandr Balabanov have all been very helpful in conveying their expertise. My family and friends outside academia deserve the remainder of my gratitude for supporting me when walking down this road.

Göteborg, June 2019
Daniel Erkensten

Contents

1 Introduction

1.1 Background and motivation

Recently, the notion of unconventional phases of matter has become an established area of research ranging from topological insulators to superconductivity. As evidenced by the 2016 Nobel Prize in Physics to Thouless, Kosterlitz and Haldane for their groundbreaking discoveries in the field of topological quantum matter and topological phase transitions, there is a consensus that the experimental signature of these exotic phases of matter has been well-established [1]–[3]. On the one hand topology is an abstract branch in mathematics which manifests itself through topological invariants, summarized in the statement that geometrical objects remain the same under continuous deformations. On the other hand it has lately turned up as a buzzword in the condensed matter physics community as a way of describing measurable quantities which are robust under smooth perturbations.

In this thesis, we focus on non-interacting one-dimensional topological systems with particular emphasis on topological superconductors. Such systems are interesting not only because of their peculiar topological properties but also since they are associated with the emergence of so called Majorana zero edge modes (MZMs), quasiparticle excitations interpreted as Majorana fermions - particles which are their own anti-particles [4]. This statuates a prime example of the bulk-boundary correspondence, which establishes a direct connection between the bulk topological invariant and edge states at the boundary [5]. The concept of Majorana fermions was introduced by Ettore Majorana already in 1937 but still the particles are nowhere to be found in nature [6]. In particular, all fermions in the theory we use to classify particles, the Standard Model, are Dirac fermions although it has been widely debated whether neutrinos are in fact Majorana fermions [7].[1] Moreover, establishing the existence of Majorana fermions would be consistent with supersymmetric theories in particle physics, where the Majoranas are suggested as superpartners to the spin-0 and spin-1 bosons respectively [6], [7]. However, the main motivation of looking for Majoranas in condensed matter systems is of practical rather than fundamental nature. This is since the robustness of the topologically protected zero modes can be of potential use in future technological applications. In particular, in two spatial dimensions they are non-abelian anyons and demonstrate interesting

[1] For almost a quarter of a century particle physicists believed that the neutrinos were Weyl fermions, i.e. massless and real fermions. However, this changed in the beginning of the 1960s when the consequences of the neutrinos having small but non-zero masses were investigated. Since the discovery of neutrino oscillations it has now been proven that neutrinos are massive [8].

exchange statistics[2], which points to the fact that simple exchange operations in physical space can generate complex motions in the quantum-mechanical infinite-dimensional Hilbert space [9][12] . Moreover, since complex fermion modes can be decomposed into two real Majorana modes in the same way a complex number can be expressed in terms of its real and imaginary part, the spatial separation of Majorana modes is protected by the fermionic degree of freedom, enabling the Majoranas to store information non-locally. These properties in combination with the modes being insensitive to external noise due to topological protection, make the condensed matter version of Majoranas constitute robust building blocks of a topological quantum computer [13].[3]

In this work, we will (perhaps unfortunately) not provide a recipe for the construction of a topological quantum computer using Majoranas but only be concerned with the existence of Majorana edge modes in one-dimensional systems and their relation to topological invariants and symmetries. More precisely, we would like to get an understanding for the robustness of Majorana edge modes when a system undergoes a phase transition from one type of topological superconductor to another. When it comes to systems with an energy gap, the existence of topological invariants is neatly summarized in the so called tenfold classification of topological insulators and superconductors, associating Hamiltonians with a combination of the discrete symmetries $\mathcal{T}$ (time-reversal symmetry), $\mathcal{P}$ (particle-hole symmetry) and $\mathcal{C}$ (sublattice symmetry) to a particular topological invariant [16][17]. In fact, the conventional understanding is that only systems with a non-zero bulk energy gap can support topological edge modes, but this has recently been questioned by Verresen, Jones and Pollmann who have established a classification for gapless Hamiltonians in the BDI symmetry class [18]. As much as this thesis serves to review the compelling field of topological quantum matter it thus also serves to provide some new insights on other gapless one-dimensional BdG chains[4] and extend the work done by Verresen

[2]The term anyon coined by Frank Wilczek is often used when a particle does not obey solely fermionic (Fermi-Dirac) or bosonic (Bose-Einstein) exchange statistics but rather something in between. Typically, exchanging two anyons gives rise to a complex phase $\mathrm{e}^{i\theta}$ such that $|\psi_1\psi_2\rangle = \mathrm{e}^{i\theta}|\psi_2\psi_1\rangle$. Clearly, the anyon demonstrates Fermi-Dirac statistics when $\theta = \pi$ and Bose-Einstein statistics when $\theta = 2\pi$. However, in two spatial dimensions Majorana modes are *non-abelian* anyons and therefore not only does the exchange of particles induce a complex phase, but the internal states $|\psi_1\rangle$ and $|\psi_2\rangle$ are affected as well [9]. Note that non-abelian exchange statistics is impossible in three spatial dimensions, since then the exchange of two particles is topologically equivalent to having the particles fixed, i.e. any loop can be deformed into a point. In one spatial dimension the particles have to pass through each other upon an exchange, which is an ill-defined operation in an interacting system. There have been successful attempts to cheat these topological constraints by allowing particles to move along discrete 1D paths in a higher-dimensional space, by e.g. Alicea et al. in [10], [11].

[3]The Russian-American physicist Alexei Kitaev proposed the construction of a topological quantum computer based on anyonic excitations already in the early 2000s [14]. However, this construction did not rely on the anyonic excitations being Majoranas. A couple of years later Kitaev demonstrated the existence of Majorana edge modes in a spinless p-wave superconductor, pioneering the field of topological superconductivity with his model [15]. The Kitaev model will be of substantial importance in this thesis.

[4]In this language, a BdG chain is described by a Hamiltonian which respects particle-hole symmetry.

et al to other symmetry classes. Due to its striking resemblance with the BDI-case, particular emphasis is put on Hamiltonians in the symmetry class CII.

1.2 Thesis outline

In the next chapter a minor introduction to topology and its relation to condensed matter systems and Hamiltonians is provided. Topological invariants and topological phases of matter are given special attention, the latter culminating in the motivation of symmetry protected topological phases of matter, of immense importance in the remainder of the thesis. In Chapter 3, the concept of symmetries in physics is briefly discussed and the importance of the discrete charge-conjugation (particle-hole), chiral (sub-lattice) and time-reversal symmetries is highlighted. In particular, taking combinations of these symmetries gives rise to symmetry classes, forming the basis for the tenfold classification of topological insulators and superconductors. Having discussed symmetries and topological invariants in detail it is in order to provide some examples in which these concepts are illustrated. Therefore, Chapter 4 is devoted to toy models and realizations of topological quantum systems. Here, particular emphasis is put on Kitaev's one-dimensional model of topological superconductivity, since this is a key ingredient when discussing gapless systems in the BdG and chiral symmetry classes. In the following chapter, gapless topological superconductors in the BDI-class is discussed in terms of Kitaev chains and the work by Verresen, Jones and Pollmann is reviewed. In the final chapter, Chapter 6, the extension and generalization of Verresen et al's results to the symmetry class CII is investigated. The discussion on gapless systems requires knowledge of conformal field theory, critical systems and phase transitions and therefore short introductions to these vast subjects are included as appendices. When it comes to prerequisites, the reader is assumed to be somewhat comfortable with superconductivity, second quantization and many-body theory in general.

2

Hamiltonians and Topology

The study of topological quantum matter dates back to the discovery of the Integer Quantum Hall Effect in 1980 [19]. Before the concepts of topology and topological invariants entered the minds of condensed matter theorists, mathematicians were well-acquainted with them since centuries ago.[1] In this concise chapter, we provide the bare minimum of mathematical rigor when it comes to the vast topic of topology and demonstrate its connection to physics through Berry phases and Berry curvatures. This culminates in a discussion of topological phases of matter. It turns out that, by imposing symmetries on the quantum system, one arrives at the concept of symmetry protected topological phases (SPTs) which have been studied extensively the latest years [24], [25].

2.1 A short note on topology

Although topology has established itself as a fundamental principle in unconventional phases of quantum matter in condensed matter physics systems nowadays, it has its origin in abstract mathematics. Topology can be summarized as the study of geometric properties which remain invariant under smooth continuonus deformations, for instance stretching and twisting. The canonical examples of objects with a non-trivial topology are the sphere and the 1-torus. These objects can not be continuously deformed into one another and are as such part of topologically distinct equivalence classes. This can easily be seen by counting the number of holes, g, in the objects, as illustrated in Figure 2.1. This number, also referred to as the *genus* can not be changed under smooth continuous deformations and is therefore said to be a *topological invariant*. Topologically distinct objects necessarily have different topological invariants.

[1] This is, historically, not the whole truth. In fact, topology and physics has been closely connected since the 19th century. Some fundamental examples concern Lord Kelvin's vortex theory of atoms in the late 1800s [20], the geometrical interpretation of the Schwarzschild singularity in general relativity in 1916 [21] and the discovery of the observable effects of the electromagnetic vector potential through the Aharanov-Bohm effect in 1959 [22]. More recently, topology has played a vital role in the construction of so called topological quantum field theories [23].

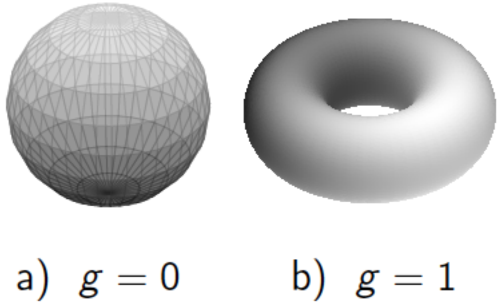

Figure 2.1: A sphere has genus $g = 0$ and a (flat) torus has genus $g = 1$ leaving the objects in different equivalence classes. Hence, a topologist does not differ between an orange and an apple or a doughnut and a coffee cup.

Formally, a topological invariant can be expressed as an integral of a geometrical quantity. The *Gauss-Bonnet theorem* provides a connection between the local (Gaussian) curvature and the global topology of a two-dimensional Riemann surface and gives an integral representation of the topological invariant. Assuming the surface, S, to be closed and orientable it follows that

$$\int_S \kappa dS = 2\pi\chi(S) = 2\pi(2 - 2g) \ , \tag{2.1}$$

with κ being the Gaussian curvature[2] and $\chi(S)$ the *Euler characteristic*[3]. It is easily checked that the theorem holds for a sphere with curvature $\kappa = \frac{1}{r^2}$ and $g = 0$. Remarkably, by continuously deforming the sphere, that is, changing the local Gaussian curvature at a number of points, the surface integral of the curvature remains unchanged and since the Euler characteristic is an integer it is also a topological invariant.

This is all we will say about topology in mathematics. Now, we turn our attention to physics and in particular the concepts of *Berry curvature* and the *Berry phase*, the latter being an analogue of the Gauss-Bonnet theorem arising in adiabatic quantum mechanics. Although not as short as the note above, we only scratch the surface when it comes to topological invariants in physics. For a detailed treatment of topology in physics, see the canonical work by Nakahara [26].

[2]The Gaussian curvature can be seen as an intrinsic measure of curvature which depends only on distances measured on the surface. It can be further expressed as $\kappa = \kappa_1\kappa_2$, with κ_1, κ_2 being the *principal curvatures* at a given point. These quantities measure the maximum and minimal bending at each point of the surface.

[3]The concept of Euler characteristic was in fact historically introduced by Euler in another setting. In 1751, he observed that by triangulating a sphere onto V vertices, E edges and F faces one can combine these quantities as $V - E + F = 2$. More generally, for *any* surface the Euler characteristic can be written as $\chi = V - E + F$ independent of how the triangulation is performed.

2.2 Berry curvature

The concept of Berry curvature and Berry phases was introduced by Michael Berry in 1984, who highlighted the fact that geometrical phases are of physical importance in quantum mechanics [27]. We will here outline the derivation of such phases and make a connection between such phases and topological invariants. To do so, we consider a system described by some Hamiltonian $H(\vec{R})$ with $\vec{R}(t) = (R_1(t), R_2(t), ..., R_D(t))$ being a D-component vector of parameters.[4] Assuming that $\vec{R}(t)$ varies slowly in time compared to the energy scale E of the system, that is, the system undergoes *adiabatic* evolution we may find instantenous eigenstates $|n(\vec{R}(t))\rangle$ and eigenvalues $E_n(\vec{R}(t))$ from the time-independent Schrödinger equation:

$$H(\vec{R}(t))|n(\vec{R}(t))\rangle = E_n(\vec{R}(t))|n(\vec{R}(t))\rangle \ . \tag{2.2}$$

There is a (local) gauge freedom in $|n(\vec{R}(t))\rangle \to \mathrm{e}^{-i\varphi_n(\vec{R}(t))}|n(\vec{R}(t))\rangle$. Now, a general quantum state $|\psi\rangle$ evolves in time according to the *adiabatic theorem*[5]

$$|\psi(t)\rangle = \mathrm{e}^{-i\theta_n(t)}|n(\vec{R}(t))\rangle \ , \tag{2.3}$$

due to the assumption that $\vec{R}(t)$ varies slowly. Note that we introduced the phase-factor $\theta_n(t)$, which we want to investigate further. Returning to the time-dependent Schrödinger equation and making use of the gauge freedom in the instantaneous eigenstates we may write

$$H(\vec{R}(t))|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle \Rightarrow E_n(\vec{R}(t))|n(\vec{R}(t))\rangle = \hbar\theta_n'(t)|n(\vec{R}(t))\rangle + \frac{d}{dt}|n(\vec{R}(t))\rangle i\hbar \ ,$$

where primes indicate derivatives with respect to time. Taking the inner product with $\langle n(\vec{R}(t))|$ then results in

$$E_n(\vec{R}(t)) = \hbar\theta_n'(t) + i\hbar\langle n(\vec{R}(t))|\frac{d}{dt}n(\vec{R}(t))\rangle \ . \tag{2.4}$$

Now, rearranging terms and integrating the equation above with respect to time t gives us an equation for the total phase $\theta_n(t)$:

$$\theta_n(t) = \frac{1}{\hbar}\int_0^t dt' E_n(\vec{R}(t')) - i\int_0^t dt'\langle n(\vec{R}(t'))|\frac{d}{dt'}n(\vec{R}(t'))\rangle \ . \tag{2.5}$$

The first phase-term is due to the ordinary dynamic evolution. However, the second term defines the Berry phase:

$$\gamma_n = i\int_0^t dt'\langle n(\vec{R}(t'))|\frac{d}{dt'}n(\vec{R}(t'))\rangle \ . \tag{2.6}$$

[4] Note that the letter R does not necessarily refer to position, but could really be any parameter.

[5] We provide a formulation of the adiabatic theorem here according to Griffiths [28]. Given that a Hamiltonian, H^i, is prepared with the instantenous eigenstate $|n\rangle$ and, by smooth external perturbations, changes *gradually* to H^f, a particle will remain in the instantenous eigenstate $|n\rangle$ of $H^{f\to i}$. The original proof of the theorem was constructed by Born and Fock in 1928 [29].

By invoking the chain rule such that $\frac{d}{dt'} = \frac{d}{d\vec{R}}\frac{d\vec{R}}{dt'}$ we may write

$$\gamma_n = i \int_C \langle n(\vec{R}(t'))|\nabla_{\vec{R}} n(\vec{R}(t'))\rangle \cdot d\vec{R} \;, \tag{2.7}$$

where C is a curve in the parameter space of $\vec{R}(t)$. The expression above is a purely geometrical quantity in parameter space which essentially describes where the quantum system is located in that space. The Berry phase is, in fact, purely real. This is easily shown by using the fact $\frac{d}{d\vec{R}}\langle n(\vec{R}(t))|n(\vec{R}(t))\rangle = 0$, i.e.

$$\frac{d}{d\vec{R}}\langle n(\vec{R}(t))|n(\vec{R}(t))\rangle = \langle n(\vec{R}(t))|\frac{d}{d\vec{R}}n(\vec{R}(t))\rangle + \langle\frac{d}{d\vec{R}}n(\vec{R}(t))|n(\vec{R}(t))\rangle = 0 \;,$$

and therefore

$$\langle n(\vec{R}(t))|\frac{d}{d\vec{R}}n(\vec{R}(t))\rangle = -\langle\frac{d}{d\vec{R}}n(\vec{R}(t))|n(\vec{R}(t))\rangle = -(\langle n(\vec{R}(t))|\frac{d}{d\vec{R}}n(\vec{R}(t))\rangle)^* \;,$$

and thus the quantity $\langle n(\vec{R}(t))|\frac{d}{d\vec{R}}n(\vec{R}(t))\rangle$ is purely imaginary. Combined with a factor of i (and an integration, see (2.7)) it defines the Berry phase, which then is purely real. In particular, this means that the Berry phase vanishes when the instantaneous eigenstates $|n(\vec{R}(t))\rangle$ are real. Returning to the expression for the Berry phase we may also introduce the *Berry connection*, $\vec{\mathcal{A}}_n(\vec{R}(t))$, according to

$$\vec{\mathcal{A}}_n(\vec{R}) = i\langle n(\vec{R})|\nabla_{\vec{R}}|n(\vec{R})\rangle \;, \tag{2.8}$$

such that

$$\gamma_n = \int_C \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R} \;. \tag{2.9}$$

There is no coincidence that the Berry connection is denoted by the first letter of the alphabet. This is since it bears a striking resemblance to the electromagnetic vector potential $\vec{A}$: if $\vec{R}$ is restricted to position space the objects even coincide. Recall that the electromagnetic vector potential is not gauge invariant and transforms as

$$\vec{A} \to \vec{A} + \nabla\Lambda \;, \tag{2.10}$$

for some scalar function Λ under a gauge transformation. Similarly, by performing the gauge transformation $|n(\vec{R})\rangle \to \mathrm{e}^{if(\vec{R})}|n(\vec{R})\rangle$, the Berry connection transforms as

$$\begin{aligned}\vec{\mathcal{A}}_n(\vec{R}) = i\langle n(\vec{R})|\nabla_{\vec{R}}|n(\vec{R})\rangle \to i\langle n(\vec{R})\mathrm{e}^{-if(\vec{R})}|i\frac{df}{d\vec{R}}\mathrm{e}^{if(\vec{R})}|n(\vec{R})\rangle + i\langle n(\vec{R})|\nabla_{\vec{R}}|n(\vec{R})\rangle \\ = -\nabla_{\vec{R}}f(\vec{R}) + i\langle n(\vec{R})|\nabla_{\vec{R}}|n(\vec{R})\rangle \\ = \vec{\mathcal{A}}_n(\vec{R}) - \nabla_{\vec{R}}f(\vec{R}) \;,\end{aligned}$$

that is, in the same way as the electromagnetic vector potential in (2.10) with $\Lambda = -f$. Now, we have proven that the Berry connection is not a physical quantity. Then, let us perform the gauge transformation on the Berry phase, γ_n, instead:

$$\gamma_n \to \gamma_n - \int_C \nabla_{\vec{R}}f(\vec{R}) \cdot d\vec{R} = \gamma_n + f(\vec{R}(0)) - f(\vec{R}(T)) \;. \tag{2.11}$$

It thus seems as if we could naively cancel the Berry phase completely by choosing $f(\vec{R}(T)) - f(\vec{R}(0)) = \gamma_n$. However, if we demand the eigenstates to be single-valued, this does not work for *closed* paths C. For such paths it follows from the gauge transformation that $f(\vec{R}(0)) - f(\vec{R}(T)) = 2\pi m$, m being an integer. This also means that the Berry phase is a gauge invariant (physical) quantity modulo 2π when C is a closed path. Let us, in the following, restrict to this case. Then, we may write

$$\gamma_n = \oint_{C=\partial S} \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R} = \int_S \nabla_{\vec{R}} \times \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{S} \ , \tag{2.12}$$

by invoking Stokes' theorem and introducing the surface S. The curl of the Berry connection is given its own name, the *Berry curvature* and is defined by

$$\vec{\mathcal{F}}_n(\vec{R}) = \nabla_{\vec{R}} \times \vec{\mathcal{A}}_n(\vec{R}) \ . \tag{2.13}$$

Note that $\vec{\mathcal{F}}_n(\vec{R})$ plays the same role in parameter space as the magnetic field $\vec{B}$ does in position space. Then, the Berry phase, γ_n, is the analogue of the famous Aharonov-Bohm phase in parameter space [22].
Now, we want to relate the Berry phase, Berry connection and Berry curvature to topological invariants. It turns out that the Berry curvature is a crucial ingredient in the *Chern theorem*:

$$\zeta = \frac{1}{2\pi} \int_S \vec{\mathcal{F}}_n(\vec{R}) \cdot d\vec{S} \ , \tag{2.14}$$

where $\zeta \in \mathbf{Z}$ is called the *Chern number* and S is a closed surface in $\vec{R}$-space. The Chern theorem relates the characteristic Chern number (denoted by ζ) of a fiber bundle[6] composed by γ_n and $\vec{R}$ to the curvature $\vec{\mathcal{F}}_n$. Note that this theorem is very similar to the Gauss-Bonnet theorem, in which the Gaussian curvature plays the role of $\vec{\mathcal{F}}_n$, cf. equation (2.1). In fact, the Chern theorem is often referred to as a generalization of the aforementioned theorem. The Chern number ζ is really a topological index and an invariant for a 2D manifold S. It is a crucial quantity when it comes to quantization effects of a physical system. In particular, the robustness of the Hall conductivity in the Integer Quantum Hall Effect (IQHE) on which much of the research in topological quantum matter is based on, is explained by the fact that the integer, n, in the Hall conductivity is a Chern number [30]. This will be the topic of section 4.3 in the chapter on toy models and realizations.

In order to elaborate further on the connection between Berry phases and topological insulators and superconductors it is natural to consider the effect of the Berry phase on crystalline solids. Then, we take the parameter space to be $\vec{k}$-space (more precisely, the first Brillouin zone) and the instantaneous eigenstates $|n(\vec{R})\rangle$ are given by the Bloch factors $|u(\vec{k})\rangle$ according to Bloch's theorem. Therefore,

[6] A fiber bundle can be thought of as an object which is composed of a manifold (here often referred to as a base space) and a set of tangent spaces, that is the fiber. Each point at the manifold has a tangent space attached to it. A simple physical example of a fiber bundle concerns the temperature of a surface. The two-dimensional surface described by the coordinates x and y then constitute the base space and at every position coordinate one can measure a temperature, which takes its values in an external (tangent) space.

the Berry connection or equivalently the Berry curvature (explicitly written out in components) for the m:th band reads

$$\vec{\mathcal{A}}_m(\vec{k}) = i\langle u_m(\vec{k})|\nabla_{\vec{k}}|u_m(\vec{k})\rangle \ , \mathcal{F}^m_{IJ} = \partial_{k_I}\mathcal{A}^m_{k_J} - \partial_{k_J}\mathcal{A}^m_{k_I} \ , I, J = 1...d \ , \tag{2.15}$$

d being the dimension of the parameter space. Now, the corresponding Berry phase, γ_m, is given by the phase acquired by the wavefunction when $\vec{k}$ sweeps over the first Brillouin zone:

$$\gamma_m = \oint_C \vec{\mathcal{A}}_m(\vec{k}) \cdot d\vec{k} \ . \tag{2.16}$$

For 1D systems the expression above collapses to

$$\gamma_m^{(1D)} = \int_{-\pi}^{\pi} dk\mathcal{A}_m(k) = i\int_{-\pi}^{\pi} \langle u_m(k)|\frac{d}{dk}u_m(k)\rangle dk \ , \tag{2.17}$$

assuming the lattice constant a to be equal to unity. This specific case of a Berry phase in momentum space in one spatial dimension defines the so called *Zak phase*, after Joshua Zak who first applied the concept of Berry phase on crystalline solids in 1989 [31].

2.3 Chern numbers and the need for symmetry

Let us go back to (2.14) and try to motivate the Chern theorem. By specifying the parameter space to be momentum space:

$$\zeta = \frac{1}{2\pi}\int \vec{\mathcal{F}}(\vec{k}) \cdot d\vec{S} \ , \tag{2.18}$$

and restricting ourselves to two spatial dimensions, i.e. $\vec{k} = (k_x, k_y)$ we may compute a Chern number for the m:th energy band according to

$$\zeta^{(m)} = \frac{1}{2\pi}\int_{\text{2DBZ}} dk_x dk_y \mathcal{F}^m_{xy}(\vec{k}) \ . \tag{2.19}$$

The integral is carried out on the two-dimensional periodic Brillouin zone (2DBZ) and is as such only non-zero if the Berry connection, $\vec{\mathcal{A}}_m(\vec{k})$, has singularities on the domain. However, such singularities can be easily avoided by means of a gauge transformation:

$$\vec{\mathcal{A}}_m(\vec{k}) \to \vec{\mathcal{A}}_m(\vec{k}) - \vec{\nabla}_{\vec{k}} f_m(\vec{k}) \ , \tag{2.20}$$

and hence, by virtue of Stokes' theorem

$$\frac{1}{2\pi}\int dk_x dk_y \mathcal{F}^m_{xy}(\vec{k}) \to \frac{1}{2\pi}\int_{\partial\text{2DBZ}} d\vec{k} \cdot \vec{\nabla}_{\vec{k}} f_m(\vec{k}) = \zeta \in \mathbf{Z} \ , \tag{2.21}$$

since $\mathrm{e}^{if(\vec{k})}$ is a unique function on ∂2DBZ, $\phi(\vec{k}) = 2\pi\zeta$, ζ being an integer [32]. In particular, the total Chern number of a two-dimensional band insulators is easily obtained by summing the contributions from each band up to the Fermi energy, E_F:

$$\zeta = \sum_{m, E_m < E_F} \zeta^{(m)} \ . \tag{2.22}$$

Being a Chern number, ζ constitutes a fundamental example of a topological invariant and characterizes topological phases of matter. There was no coincidence we chose to work in a two-dimensional parameter space. This is since the Chern number is only well-defined in even dimensions $d = 2s$, $s \in \mathbf{N}$.[7] Surely, we must be able to have quantum systems with non-zero topological invariants also in odd dimensions. As discussed above, the connection between Chern numbers and topological phases of matter was first established through the Integer Quantum Hall Effect. However, the quantum Hall phases of matter have turned out not to be the only phases of matter which are topologically interesting. By imposing symmetries on the physical system a completely different kind of topological phases of matter and invariants emerges, which can not be described by Chern numbers. For instance, if *time-reversal symmetry*, $\mathcal{T}$, is naively implemented in a 2D quantum Hall system it immediately follows that the Chern number vanishes:

$$\zeta = \frac{1}{2\pi}\int dk_x dk_y \sum_m \mathcal{F}^m_{xy}(\vec{k}) \xrightarrow{\mathcal{T}} -\frac{1}{2\pi}\int dk_x dk_y \sum_m \mathcal{F}^m_{xy}(-\vec{k}) = -\zeta \ , \tag{2.23}$$

since

$$\mathcal{A}_{k_I}(\vec{k}) \xrightarrow{\mathcal{T}} \mathcal{A}_{k_I}(-\vec{k}) \ , \mathcal{F}_{IJ}(\vec{k}) \xrightarrow{\mathcal{T}} -\mathcal{F}_{IJ}(-\vec{k}) \ , \tag{2.24}$$

easily verified from the construction in (2.15). Hence, time-reversal has to necessarily be broken in quantum Hall systems in order to get a non-zero Chern number. This does not imply that symmetries must be absent in topological quantum matter. On the contrary, we have established that allowing for systems with certain symmetries forces us to abandon quantum Hall phases and Chern numbers, requiring us to investigate new exotic topological phases of matter.

This leads us to the concept of *symmetry protected* topological phases of matter (SPTs). Still, the topological phase may be characterized by a $\mathbf{Z}$-invariant although it is more restricted in the sense that it is insensitive only to perturbations which respect certain symmetries.[8] In particular, as we will argue extensively in the next chapter, the symmetries of a physical system are encoded in the Hamiltonian, H, and given that the perturbation respects the same symmetries as H, the system will remain in a topological phase. However, if that is not the case the system will be rendered trivial. Excluding the section on the Quantum Hall Effect in Chapter 4, the majority of the thesis serves to investigate these phases further. First, we need to be more specific on which symmetries (besides time-reversal symmetry, $\mathcal{T}$) are considered relevant in this context. This is the topic of the next chapter.

[7] In general (even) dimension $d = 2s$ the Chern theorem is expressed in the language of differential forms as $\zeta^{(s)} = \frac{1}{2s!}\int_{\mathrm{BZ}} \mathrm{Tr}(F^s)$, with $\zeta^{(s)} \in \mathbf{Z}$ being the s:th Chern number and $F^s = F \wedge ... \wedge F$, $F = F_{IJ} dk_I \wedge dk_J$ being a differential two-form [33].

[8] Formally, if only symmetry preserving deformations are allowed, two distinct SPT phases cannot be deformed into each other without going through a phase transition. On the other hand, if symmetry breaking perturbations are allowed, the phases can be deformed to the same trivial (non-topological) product state.

3
Symmetries

Nature as we know it exhibits symmetry. Restricting to physical systems, a symmetry is often defined as something which remains invariant under a transformation of the system. Such transformations can be either continuous or discrete and are well described by the language of group theory. For instance, the statement that the speed of light is constant in all reference frames, which is the foundation of the theory of special relativity, is encoded in the Poincaré group. Similarly, electromagnetism exhibits gauge symmetry with (gauge) group $U(1)$. These continuous symmetries are often considered the most fundamental when discussing symmetries in physics, but they will not be of much use to us in this thesis. This is since the symmetry-protected topological phases that appear in condensed matter systems are associated with exclusively discrete symmetries. Three discrete symmetries will be of particular interest and are seen to alter the topological properties dramatically: time-reversal symmetry, $\mathcal{T}$, particle-hole symmetry, $\mathcal{P}$, and chiral (sublattice) symmetry, $\mathcal{C}$.[1] Therefore, each of the symmetries has been given their own section below. Note that a combination of these symmetries are manifest in a topological system in general. This will be the subject of the last section in this chapter and will eventually lead to the ten-fold classification of topological insulators and superconductors.

3.1 Time-reversal symmetry, $\mathcal{T}$

It should come as no surprise that time-reversal symmetry, $\mathcal{T}$, is manifest if a time-dependent physical system remains the same if the system is run backwards in time. Macroscopically, the universe is said to break time-reversal symmetry due to the fact that time-reversal symmetry implies the conservation of entropy and the entropy of the universe is not conserved due to the second law of thermodynamics.[2] Quantum mechanically, the story is different and observables, S, which are odd under a time-reversal symmetry transformation, i.e. $\mathcal{T}S\mathcal{T}^{-1} = -S$ are for instance $S = p$ (momentum) or $S = l$ (angular momentum), meanwhile $S = x$ (position) is even under time-reversal. In fact, using these properties and demanding that the canonical commutation relation $[x, p] = i\hbar$ holds under $\mathcal{T}$ it follows that $\mathcal{T}$ must be

[1] Note that the notation $\mathcal{T}$, $\mathcal{P}$ and $\mathcal{C}$ for the different symmetries is obviously conventional. Another popular notation is T (time-reversal), C (particle-hole) and S (chiral/sublattice).

[2] In his thought experiment in 1871, James Clerk Maxwell famously claimed to have challenged the second law of thermodynamics with his Maxwell demon. Although it has remained a thought experiment it certainly spurred the interest in information theory, which has become a well-established area of research in physics [34].

an *anti-unitary* operator:

$$\mathcal{T}[x,p]\mathcal{T}^{-1} = \mathcal{T}i\mathcal{T}^{-1}\hbar = -[x,p] \Rightarrow \mathcal{T}i\mathcal{T}^{-1} = -i \ , \tag{3.1}$$

i.e. $\mathcal{T}$ can be represented as an anti-unitary operator

$$\mathcal{T} = \mathcal{U}\mathcal{K} \ , \tag{3.2}$$

where $\mathcal{U}$ is a unitary operator and $\mathcal{K}$ is the complex-conjugation operator with $\mathcal{K}^2 = 1$. This can be made more general by invoking Wigner's theorem which states that any symmetry operation $\mathcal{S}$ can be represented by a unitary operator $\mathcal{S} = \mathcal{U}$ or an anti-unitary operator $\mathcal{S} = \mathcal{U}\mathcal{K}$. It is these kind of operators which preserve the norms of inner products. However, inner products may still not be invariant under symmetry transformations. In particular, an anti-unitary symmetry operation performs complex-conjugation on inner products. Thankfully, it is the norms of the inner products which are the measurable observables, that is, probabilities [35].
The characteristic symmetries of a physical system sit in the Hamiltonian, H, often expressed in momentum space as a function of k. In particular, since $\mathcal{T}$ is anti-unitary it follows that it must commute with the single-particle Bloch Hamiltonian according to

$$\mathcal{T}H(k)\mathcal{T}^{-1} = H(-k) \ . \tag{3.3}$$

Moreover, due to the fact that performing a time reversal symmetry transformation involves taking a complex conjugate a purely real Hamiltonian must exhibit time-reversal symmetry. Now, this does not imply that all Hamiltonians which are time-reversal symmetric have to be real, but it certainly puts constraints on the entries in H, when represented as a matrix.[3]
A peculiar feature of time-reversal symmetry which is of immense relevance for the physics in the system, is that it comes in two flavors. Either $\mathcal{T}^2 = +1$ or $\mathcal{T}^2 = -1$. This can be proven by requiring that applying $\mathcal{T}$ twice on a physical state gives back the same state up to a phase:

$$\mathcal{T}^2 = \alpha\mathbf{1} \ , \alpha = \mathrm{e}^{i\varphi} \ . \tag{3.4}$$

Invoking the representation in (3.2) then leads to

$$\mathcal{T}^2 = \mathcal{U}\mathcal{U}^* = \alpha\mathbb{1} \Rightarrow \mathcal{U} = \alpha\mathcal{U}^T \ , \tag{3.5}$$

or

$$\mathcal{U} = \alpha\mathcal{U}\alpha \ , \tag{3.6}$$

from which we deduce that the diagonal matrix of phases, $\alpha\mathbf{1}$, must have entries ± 1 and therefore $\mathcal{T}^2 = \pm 1$. Remarkably, considering $\mathcal{T}$ as a single-particle operator,

[3]This is not the case with regular *unitary* symmetries. A unitary symmetry transformation $\mathcal{U}$ simply brings the Hamiltonian matrix to a block-diagonal form and has in general no impact on the topology of the system. Of interest are instead the remaining anti-unitary symmetries which act non-trivially on the irreducible representations of the Hamiltonian. Additionally, such symmetries remain unaffected by introducing disorder and impurities in the Hamiltonian [36]. Since we have picked a matrix representation of the Hamiltonian it is implicitly understood that we are dealing with a single-particle Hamiltonian. The action of $\mathcal{T}$ on the full many-body Hamiltonian will be addressed in section 3.4.

bosonic systems (integer spin) or spinless fermionic systems have $\mathcal{T}^2 = +1$ and half-integer spin systems have $\mathcal{T}^2 = -1$. A system with spin $\frac{1}{2}$ constitutes an important example in this discussion. Recall that the spin s changes sign under $\mathcal{T}$. Then a time-reversal symmetry transformation can be represented by a rotation π about some axis, which we choose to be the y-axis:[4]

$$\mathcal{T} = \mathrm{e}^{-i\pi\frac{\sigma_y}{2}}\mathcal{K} \ , \tag{3.7}$$

where σ_y is the second Pauli matrix.[5] However, the unitary part of the operator can be written in a nicer way by making use of the Taylor series of an exponential:

$$\begin{aligned}\mathrm{e}^{-i\pi\frac{\sigma_y}{2}} &= \sum_{n=0}^{\infty}\frac{1}{n!}(-\frac{i\pi\sigma_y}{2})^n = 1 - \frac{1}{2}(\frac{\pi\sigma_y}{2})^2 + \frac{1}{4!}(\frac{\pi\sigma_y}{2})^4 - \frac{i\pi\sigma_y}{2} + \frac{i}{3!}(\frac{\pi\sigma_y}{2})^3 + ... \\ &= \cos(\frac{\pi}{2})\mathbf{1} - i\sin(\frac{\pi}{2})\sigma_y = -i\sigma_y \ ,\end{aligned}$$

where we recognized the Taylor series for the sine and the cosine and made use of the fact that the Pauli matrices square to unity. Clearly, with $\mathcal{T} = -i\sigma_y\mathcal{K}$ it follows that $\mathcal{T}^2 = -1$.[6] Hamiltonians with this kind of time-reversal symmetry then fulfill the condition

$$-i\sigma_y H^*(k) i\sigma_y = H(-k) \ , \tag{3.8}$$

which gives a crucial consequence for the energy levels of the system, namely they are (at least) two-fold degenerate. Systems with $\mathcal{T}^2 = -1$ exhibit a so called *Kramer's degeneracy.*[7] This will also be reflected in the topological properties of the system. In particular, Kramer's degeneracy forces the topological invariant to only take even (integer) values, which makes it a so called $2\mathbf{Z}$ invariant. It also shows up in other time-reversal symmetric (spinful) systems with $\mathbf{Z}_2$-invariants [37]. Moreover, this has a consequence that the edge state states of a spinful system always come in pairs. It is simple to show Kramer's degeneracy by using a proof of contradiction. That is, we assume that $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ are the *same* states up to a phase, $\mathrm{e}^{i\theta}$. Then, it must follow that

$$\mathcal{T}^2|\psi\rangle = \mathcal{T}\mathrm{e}^{i\theta}|\psi\rangle = \mathrm{e}^{-i\theta}\mathcal{T}|\psi\rangle = \mathrm{e}^{-i\theta}\mathrm{e}^{i\theta}|\psi\rangle = |\psi\rangle \Rightarrow -|\psi\rangle = |\psi\rangle \ , \tag{3.9}$$

and the last equality only holds for $|\psi\rangle = 0$. Thus, the states $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ have to be different states and in a time-reversal symmetric system $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ have the same energy.

[4]This is not an arbitrary choice. By demanding that the spin $\vec{s} = (\frac{\sigma_x}{2}, \frac{\sigma_y}{2}, \frac{\sigma_z}{2})$ is odd under time-reversal one gets the constraints $U\sigma_x U^{-1} = -\sigma_x$, $-U\sigma_y U^{-1} = -\sigma_y$ and $U\sigma_z U^{-1} = -\sigma_z$, that is U has to commute with σ_y and anti-commute with σ_x and σ_z. Then, since every 2×2 matrix U can be written as a linear combination of Pauli matrices such that $U = \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta\mathbf{1}$ and invoking the constraints it follows that the coefficients α, γ and δ are eliminated and we are, in fact, left with $U = \beta\sigma_y$. The remaining constant β is determined from $UU^\dagger = 1$ and often choosen to be $\pm i$.

[5]The Pauli matrices should be familiar to the reader, but here is a reminder:
$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

[6]One has to be careful when taking the square. Consider for instance $\mathcal{T} = i\mathcal{K}$. Taking the square gives $\mathcal{T}^2 = i\mathcal{K}i\mathcal{K} = i(-i)\mathcal{K}^2 = +1$, and not -1 as one would perhaps think naively.

[7]The degeneracy is also referred to as *Kramer's degeneracy theorem*, stated by the Dutch physicist Hendrick Anton Kramers in 1930.

3.2 Chiral (sub-lattice) symmetry, $\mathcal{C}$

Consider a physical system in which we may split all degrees of freedom into two different groups, A and B. This is the situation in for instance graphene, where the hexagonal lattice can be divided into two distinct sublattices, or in the SSH-model presented in section 4.1. Then, the corresponding (single-particle) Hamiltonian is off-diagonal according to

$$H = \begin{pmatrix} 0 & H_{AB} \\ H_{AB}^{*} & 0 \end{pmatrix} , \tag{3.10}$$

assuming $H_{AA} = H_{BB} = 0$. Now, introducing the diagonal (Pauli) matrix σ_z such that $\sigma_z = +1$ on site A and $\sigma_z = -1$ on site B the sublattice symmetry transformation is given by

$$\sigma_z H \sigma_z = -H , \tag{3.11}$$

i.e. the sublattice symmetry $\mathcal{C}$ can be represented by σ_z and is clearly unitary and hermitian. Thus, it also means that $\mathcal{C}$ *anti-commutes* with the Hamiltonian H.[8] Moreover, the chiral symmetry, in contrast to $\mathcal{T}$ (and $\mathcal{P}$ as we shall see), only comes in one flavor:

$$\mathcal{C}^2 = 1 . \tag{3.12}$$

The sublattice symmetry has an impact on the eigenstates to the Hamiltonian in (3.10). In particular, given that $\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$ is an eigenstate to H with energy E it follows by sublattice symmetry that $\begin{pmatrix} \psi_A \\ -\psi_B \end{pmatrix}$ is also an eigenstate to H but with energy $-E$. From this fact we deduce that the energy spectrum of a sublattice symmetric Hamiltonian is symmetric around zero energy, i.e. the number of states below the zero level is equal to the number of states above the zero level. In other words, chiral symmetry influences the topological properties of the system.

3.3 Particle-hole symmetry, $\mathcal{P}$

Particle-hole symmetry is often discussed in relation to superconducting systems. In a superconductor, so called Cooper pairs of electrons are created and annihilated due to electron-phonon interactions. This process is described by a (BCS) Hamiltonian [38]:

$$H_{\mathrm{BCS}} = \sum_{i,j}^{N} H_{ij} c_i^{\dagger} c_j + \frac{1}{2}(\Delta_{ij} c_i^{\dagger} c_j^{\dagger} + \mathrm{h.c.}) , \tag{3.13}$$

where H_{ij} are matrix elements in a real matrix H and Δ_{ij} is a superconducting order parameter which describes the formation and annihilation of Cooper pairs of electrons at site i and j of the lattice. By introducing a vector $C = (c_1, ...c_N, c_1^{\dagger}, ..., c_N^{\dagger})^T$,

[8] Note that the chiral symmetry is not implemented as an ordinary symmetry in the single-particle Hilbert space due to the fact that it anti-commutes rather than commutes with the Hamiltonian, H. However, in the Fock space of many-body Hamiltonians H_{mp}, the situation is different and the chiral symmetry commutes with H_{mp}. This issue is addressed in the next section.

the Hamiltonian above can be rewritten in a Bogoliubov-de Gennes-form:

$$H = \frac{1}{2} C^\dagger H_{\mathrm{BdG}}(k) C \ , \tag{3.14}$$

where H_{BdG} is the *Bogoliubov-de Gennes Hamiltonian* given by:

$$H_{\mathrm{BdG}}(k) = \begin{pmatrix} H & \Delta \\ -\Delta^* & -H^* \end{pmatrix} \ . \tag{3.15}$$

Now, H_{BdG}, is an example of a particle-hole symmetric Hamiltonian which acts on the vector C, whose first half is composed by fermionic annihilation operators and second half of fermionic creation operators of electrons. The latter can also be interpreted as annihilation operators of holes doubling the degrees in the system resulting in an emergent particle-hole symmetry. The particle-hole symmetry $\mathcal{P}$ is represented by an anti-unitary operator defined as

$$\mathcal{P} = \sigma_x \mathcal{K} \ , \tag{3.16}$$

where $\mathcal{K}$ is the complex-conjugation operator which appears also in $\mathcal{T}$. Performing a $\mathcal{P}$-transformation of H_{BdG} gives then

$$\mathcal{P} H_{\mathrm{BdG}}(k) \mathcal{P}^{-1} = -H_{\mathrm{BdG}}(-k) \ , \tag{3.17}$$

i.e. $\mathcal{P}$ anti-commutes with the single-particle Hamiltonian. It should be noted that H_{BdG} is symmetric around zero energy. This can be shown by assuming that $\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigenstate of H_{BdG} with energy E. Then, it follows that $\mathcal{P} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} v^* \\ u^* \end{pmatrix}$ is also an eigenstate but with energy $-E$.[9]

[9]Note that the eigenstates of a superconducting Hamiltonian are not purely electronic eigenstates, but are rather described by a superposition of electrons and holes which is referred to as Bogolons or Bogoliubov quasiparticles.

3.4 A word on multi-particle Hamiltonians versus single-particle Hamiltonians

The observant reader should have noticed that the symmetry operators $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{C}$ act on the single-particle Hamiltonian, that is the *Bloch Hamiltonian* or the Bogoliubov-de Gennes Hamiltonian in the case of superconductors, rather than the full multi-particle Hamiltonian. We also saw that the symmetry operators are either unitary or anti-unitary which has the consequence that the symmetries either commute or anti-commute with the single-particle Hamiltonian. It may seem counter-intuitive that this is what defines the Hamiltonian to be invariant under some symmetry transformation. However, in the multi-particle language the story is different and all the symmetry operators commute with the Hamiltonian, in agreement with physical intuition. Let us consider a generic multi-particle Hamiltonian written in second quantization acting in Fock space:

$$H_{\text{mp}} = \sum_{A,B} \Psi_A^\dagger H_{AB} \Psi_B \ , \tag{3.18}$$

with H_{AB} being matrix elements of the single-particle Hamiltonian. Now, by demanding the symmetry operators to commute with the multi-particle Hamiltonian, the peculiar (anti)-commutation relations with the single-particle Hamiltonian follow by acting with $\mathcal{P}$ and $\mathcal{T}$ on the creation and annihilation operators:

$$\begin{aligned} \mathcal{T}\Psi_A\mathcal{T}^{-1} &= \sum_B (U_T)_{AB}\Psi_A \ , \\ \mathcal{P}\Psi_A\mathcal{P}^{-1} &= \sum_B (U_P^*)_{AB}\Psi_A^\dagger \ , \end{aligned}$$

where we expressed $\mathcal{T} = U_T\mathcal{K}$ and $\mathcal{P} = U_P\mathcal{K}$, U_T and U_P being unitary. Moreover, $\mathcal{T}$ is anti-unitary and $\mathcal{T}i\mathcal{T}^{-1} = -i$. Having this in mind, we are ready to perform the full symmetry transformations on H_{mp}:[10]

$$\mathcal{T}H_{\text{mp}}\mathcal{T}^{-1} = \mathcal{T}\Psi_A^\dagger\mathcal{T}^{-1}\mathcal{T}H_{AB}\mathcal{T}^{-1}\mathcal{T}\Psi_B\mathcal{T}^{-1} = (U_T^*)_{AC}\Psi_C^\dagger H_{AB}^*(U_T)_{BD}\Psi_D = \Psi_C^\dagger H_{CD}\Psi_D \ ,$$

and by comparing the left-hand side and right-hand side we deduce that

$$(U_T^*)_{AC}H_{AB}^*(U_T)_{BD} = H_{CD} \ , \tag{3.19}$$

which can be summarized in

$$U_T^\dagger H^* U_T = H \ , \tag{3.20}$$

that is, the time-reversal symmetry operator commutes with the single-particle Hamiltonian. Similarly,

$$\begin{aligned} \mathcal{P}H_{\text{mp}}\mathcal{P}^{-1} &= (U_P)_{AD}\Psi_D H_{AB}(U_P^*)_{BC}\Psi_C^\dagger \\ &= -\Psi_C^\dagger (U_P^t)_{DA} H_{AB} (U_P^*)_{BC}\Psi_D \\ &= \Psi_C^\dagger H_{CD}\Psi_D \ , \end{aligned}$$

[10]Summation over A and B is implied.

where, in the second step, we made use of the fact that Ψ and $\Psi^\dagger$ are Grassmann-variables and non-commuting quantities, $\{\Psi, \Psi^\dagger\} = 0$. The letter "$t$" denotes transpose. This leaves us with

$$-(U_P^t)_{DA}H_{AB}(U_P^*)_{BC} = H_{CD} \leftrightarrow U_P^t H U_P^* = -H^t \ . \tag{3.21}$$

Taking the complex conjugate of both sides yields the peculiar anti-commutator between $\mathcal{P}$ and H:

$$U_P^\dagger H^* U_P = -H^\dagger = -H \ , \tag{3.22}$$

since H is assumed hermitian. Similarly, one can show that the chiral symmetry operator $\mathcal{C} = \mathcal{P}\mathcal{T} = U_S$, $U_S = U_T U_C^*$ acting on the single-particle Hamiltonian gives rise to the anti-commutator relation

$$\mathcal{C}H\mathcal{C}^{-1} = -H \ , \tag{3.23}$$

which is proven by demanding the (anti-unitary) chiral symmetry to commute with the many-body Hamiltonian $[\mathcal{C}, H_{\text{sp}}] = 0$ [39].
We have thus, perhaps affront to our physical intuition, unraveled the mystery that some symmetries are seen to anti-commute rather commute with the single-particle Hamiltonian. Hence, one has to be careful and distinguish between the action of a symmetry operator acting on a single-particle Hamiltonian and the action on a many-body Hamiltonian.

Let us also comment on the difference between the square of symmetry operators in the single-particle langugage and the multi-particle language. In the previous subsections we have seen that particle-hole symmetry and time-reversal symmetry come in two flavors, $\mathcal{P}^2 = \pm 1$ and $\mathcal{T}^2 = \pm 1$. This is valid in the single-particle picture, but in the many-body picture the corresponding statement for $\mathcal{P}^2 = \mathcal{T}^2 = -1$ is that

$$\mathcal{T}_{\text{mp}}^2 = \mathcal{P}_{\text{mp}}^2 = (-1)^{N_F} \ , \tag{3.24}$$

where N_F is the number of fermions in the system. This can be justified by seeing the many-body Fock space as being composed by N_F single-particle Hilbert spaces. Then, $\mathcal{T}_{\text{mp}}^2$ is formed by taking N_F tensor products of $T^2 = -1$ resulting in (3.24).[11]

Finally, it is in order to discuss the breaking of symmetries when moving from a many-body picture to a single-particle picture. Consider a generic fermionic many-body Hamiltonian in second quantization. Such a Hamiltonian always commutes with the *fermionic parity*[12]

$$\mathcal{P}_f = (-1)^{N_F} \ , \tag{3.25}$$

[11] The argument is quite superficial. Of course, the tensor products have to be taken in such a way that they respect anti-symmetrization in the many-body Hilbert space.

[12] This can be be explained by the fact that the creation operators and annihilation operators always come in pairs in the non-interacting Hamiltonian, i.e. only terms of the type $cc^\dagger$, cc and $c^\dagger c^\dagger$ are allowed. This is due to locality: consider a Hamiltonian which is odd in the number of fermionic operators, $H_n = c_n + c_n^\dagger$, and assume that there exists a state $|\psi\rangle$ such that $\langle\psi|H_n|\psi\rangle = \xi \neq 0$, with ξ being a fixed number. Then, if locality is enforced we require the condition $\lim_{|n-m|\to\infty}\langle H_n H_m\rangle = \langle H_n\rangle\langle H_m\rangle$ to hold. However, the right-hand side is a finite number but the left-hand side is anti-commuting in n and m, giving a contradiction.

and therefore it is often an implicitly assumed symmetry in the literature. However, not all fermionic Hamiltonians commute with the particle number N_F, that is have a $U(1)$ symmetry expressing charge conservation or particle number conservation. In particular, mean-field superconducting Hamiltonians of BCS-type necessarily break $U(1)$ symmetry through its superconducting order parameter Δ, see equation (3.13). Moreover, in the single-particle language the breaking of $U(1)$-symmetry is reflected in a particle-hole symmetric BdG Hamiltonian. However, the particle-hole symmetry is really a result of performing a Bogoliubov transformation and introducing redundant degrees of freedom into the system. Thus, in some sense the particle-hole symmetry of the BdG-Hamiltonian is artificial and very similar to a gauge symmetry.

Now, it might seem strange that we have not discussed the $U(1)$ symmetry before in the context of single-particle Hamiltonians. Whenever the $U(1)$ symmetry expresses particle number conservation in the many-body langauge it is, however, a trivial symmetry in the single-particle langugage. This is so since the $U(1)$-symmetry is generated by a scalar, 1, when acting on a single-particle Hamiltonian, H_{sp}.

3.5 A glimpse of the ten-fold classification of topological insulators and superconductors

Returning to the single-particle picture, we summarize the previous sections by listing the most fundamental properties of the (single-particle) symmetries $\mathcal{T}$, $\mathcal{P}$ and $\mathcal{C}$:[13]

$$\begin{aligned}
\mathrm{Time-reversal\ symmetry}\ \mathcal{T}: &\ \textit{anti-unitary}\ , [\mathcal{T}, H_{\mathrm{sp}}] = 0,\ ,\mathcal{T}^2 = \pm 1\ , \\
\mathrm{Particle-hole\ symmetry}\ \mathcal{P}: &\ \textit{anti-unitary}\ , \{\mathcal{P}, H_{\mathrm{sp}}\} = 0,\ ,\mathcal{P}^2 = \pm 1\ , \\
\mathrm{Chiral/sublattice\ symmetry}\ \mathcal{C} = \mathcal{T}\mathcal{P}: &\ , \textit{unitary}\ , \qquad \{\mathcal{C}, H_{\mathrm{sp}}\} = 0,\ ,\mathcal{C}^2 = 1\ .
\end{aligned}$$

Note that we have indicated that $\mathcal{C} = \mathcal{T}\mathcal{P}$, meaning that whenever particle-hole symmetry *and* time-reversal symmetry is apparent in a system so is sublattice symmetry. However, $\mathcal{C}$ can also appear by its own if both $\mathcal{P}$ and $\mathcal{T}$ are absent. Given these facts it is quite straightforward to count the number of ways the symmetries $\mathcal{C}$, $\mathcal{P}$ and $\mathcal{T}$ can be combined into different *symmetry classes*. Since $\mathcal{P}$ and $\mathcal{T}$ both can appear in three different ways (square to $+1$, square to -1, or be absent), there are $3^2 - 1 = 8$ different combinations in which anti-unitary symmetries can appear. Then the remaining combinations are those of solely unitary symmetries, i.e. where only $\mathcal{C}$ appears or where all three symmetries are absent. In total, this gives 10 different symmetry classes, which is used to form the *ten-fold classification* of non-interacting topological insulators and superconductors. In Table 3.1, these classes are given along with their names or *Cartan label*. Interestingly, the names of the different symmetry classes comes from an elegant classification of symmetric spaces due to Elie Cartan in 1927 [40]. More than eighty years later the explicit connection to topological quantum matter was made when Schnyder, Ludwig, Furusaki and

[13]The fermionic parity, $\mathcal{P}_f$, could in principle be included as well but it is trivial in the sense that $N_F = 1$.

Ryu completed and summarized the classification of topological invariants in the ten-fold way, see section 4.4 and Table 4.1 [17].[14]

class	$\mathcal{C}$	$\mathcal{P}$	$\mathcal{T}$
A	-	-	-
AI	-	-	1
AII	-	-	-1
BDI	1	1	1
C	-	-1	-
CI	1	-1	1
CII	1	-1	-1
D	-	1	-
DIII	1	1	-1
AIII	1	-	-

Table 3.1: The ten Cartan symmetry classes forming the basis for the tenfold classification of topological insulators and superconductors. ± 1 indicate the square of the operators $\mathcal{T}$, $\mathcal{P}$ or $\mathcal{C}$ and $-$ denote that symmetries are absent. Note that the complete table involve topological invariants in different dimensions as well. This will be addressed in section 4.4.

[14]Already in 1996, Altland and Zirnbauer classified mesoscopic systems in contact with superconductors using Cartan's classification of symmetric spaces [41]. In particular, they identified that the systems could be associated with the symmetry classes C, CI, D and DIII. Therefore, although Schnyder et al. put together the complete puzzle, the tenfold classification table of TSCs and TIs is sometimes referred to as the Altland-Zirnbauer table.

4

Famous Toy Models and Realizations

Having introduced the concepts of discrete symmetries in condensed matter physics and topological invariants it is fruitful to consider toy models and realizations which statuate prime examples of topological insulators and superconductors. In the first two sections, perhaps the most famous toy models in the field of topological quantum matter are investigated: the SSH model and Kitaev's Majorana chain. Although the models are simple and considered in a non-interacting setting in one spatial dimension, they exhibit remarkable topological properties and give a basic understanding for topological band insulators and superconductors. The discussion of toy models is followed by an introduction to the Integer Quantum Hall Effect (IQHE) which culminates in the TKNN-invariant, connecting the quantized Hall conductivity to topology and Chern numbers. Finally, we return to the tenfold classification of topological insulators and superconductors, and associate the investigated toy models and IQHE with particular symmetry classes and topological invariants.

4.1 SSH model

The one-dimensional Su-Schrieffer-Heeger model constitutes the most simple yet non-trivial example of a topological insulator, that is, a model which is insulating in the bulk but which supports conducting edge states. It describes spinless fermions hopping on a lattice with staggered (alternating) hopping amplitudes.[1] In Figure 4.1, the lattice structure and hopping is apparent. In particular, we are considering N unit cells with each unit cell hosting two atoms at different atomic sites A (filled ovals) and B (unfilled ovals). The hopping can occur intercell or intracell, that is, atoms can jump from a site $A(B)$ to a site $B(A)$ either in its own unit cell or to the next unit cell. The intracell hopping amplitude is described by the parameter $v = t + \delta t$ and the intercell hopping amplitude by the parameter $w = t - \delta t$, so that for $\delta t \neq 0$, $v \neq w$. We assume these parameters to be real and larger than zero and neglect interactions between electrons.[2]

[1]In fact, this type of hopping is energetically favourable and occurs in nature due to a phenomenon called *Peierls instability* [5].

[2]If we allow v and w to be complex, i.e. $v = |v|e^{i\phi_1}$ and $w = |w|e^{i\phi_2}$ the phases can be gauged away by redefining the basis states. However, if we consider v and w to be real the Hamiltonian H_{SSH} in (4.1) is time-reversal symmetric with $\mathcal{T}^2 = +1$.

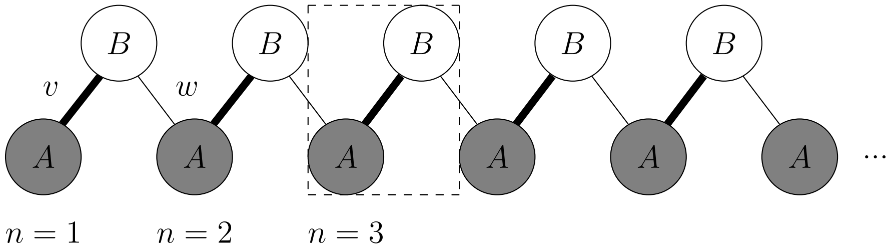

Figure 4.1: Illustration of the SSH model. The A(B) atoms are denoted by a filled (unfilled) circle and the parameters v and w describe intracell hopping (thick line) and intercell hopping (thin line) respectively. Each unit cell $n = 1...N$ hosts an A-site and a B-site.

By introducing fermionic ladder operators $c_{A,i}, c^\dagger_{A,i}$ and $c_{B,i}, c^\dagger_{B,i}$ at the sites A and B we are able to write down the SSH Hamiltonian:

$$H_{\text{SSH}} = \sum_{i=1}^{N}(t+\delta t)c^\dagger_{A,i}c_{B,i} + \sum_{i=1}^{N-1}(t-\delta t)c^\dagger_{A,i+1}c_{B,i} + \text{h.c.} \ , \tag{4.1}$$

where h.c. denotes Hermitian conjugate. Note that this Hamiltonian does not take spin into account, which obviously is needed to describe a real fermionic system. In fact, the SSH model was developed in 1979 to describe soliton excitations in the carbon-based polymer polyacetylene [42]. To do so, Su, Schreiffer and Heeger had to take two copies of their model, one copy for each fermionic spin degree of freedom. Since this chapter is mainly about toy models of topological systems it is justified for us to consider the spinless SSH chain.

By inspection of Figure 4.1 it is evident that the SSH model has a bulk and a boundary. However, if we allow the number of unit cells to be very large, i.e. $N \to \infty$, that is the thermodynamic limit, only the bulk becomes important. By setting periodic boundary conditions and close the bulk part into a ring it is possible by Bloch's theorem and translation invariance to translate the Hamiltonian into a momentum space Hamiltonian. For brevity, we will drop the sublattice index A and B on the fermionic ladder operators and instead let $c_{A,i} \to c_i$ and $c_{B,i} \to d_i$. In terms of these operators the SSH Hamiltonian reads

$$H_{\text{SSH}} = \sum_{j=1}^{N}(t+\delta t)c^\dagger_j d_j + \sum_{j=1}^{N-1}(t-\delta t)c^\dagger_{j+1}d_j + \text{h.c.} \ . \tag{4.2}$$

Now, expressing each degree of freedom, c_j and d_j via the Fourier transform gives

$$c_j = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} \mathrm{e}^{ijk\frac{2\pi}{N}} c_k \ , \tag{4.3}$$

$$d_j = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} \mathrm{e}^{ijk\frac{2\pi}{N}} d_k \ , \tag{4.4}$$

assuming the lattice spacing $a = 1$. Note that the expressions include the factor $\frac{2\pi}{N}$, taking into account the fact that the momentum k is in the first Brillouin zone.

Note that $1 \leq k \leq N$. However, due to periodicity the range can be extended. For instance, $-k$ can equivalently be interpreted as $N-k$. Fourier transforming the first term of the SSH Hamiltonian in (4.2) gives us

$$\sum_{j=1}^{N} c_j^\dagger d_j = \frac{1}{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{k'=1}^{N} \mathrm{e}^{ij(k'-k)\frac{2\pi}{N}} c_k^\dagger d_{k'} = \frac{1}{N}\sum_{k=1}^{N}\sum_{k'=1}^{N} N\delta_{k'-k,0} c_k^\dagger d_{k'} = \sum_{k=1}^{N} c_k^\dagger d_k \ ,$$

where the sum over j evaluates to a Kronecker delta due to

$$\sum_{j=1}^{N} \mathrm{e}^{ij(k'-k)\frac{2\pi}{N}} = N\delta_{k,k'} \ . \tag{4.5}$$

Similarly, for the second term,

$$\sum_{j=1}^{N-1} c_{j+1}^\dagger d_j = \frac{1}{N}\sum_{j=1}^{N-1}\sum_{k=1}^{N}\sum_{k'=1}^{N} \mathrm{e}^{ij(k'-k)\frac{2\pi}{N}} \mathrm{e}^{-ik\frac{2\pi}{N}} c_k^\dagger d_{k'} = \sum_{k=1}^{N} \mathrm{e}^{-ik\frac{2\pi}{N}} c_k^\dagger d_k \ ,$$

and thus the Fourier-transformed total Hamiltonian reads

$$\tilde{H}_{\mathrm{SSH}} = \sum_{k=1}^{N} (t+\delta t)(c_k^\dagger d_k + d_k^\dagger c_k) + \sum_{k=1}^{N} (t-\delta t)(\mathrm{e}^{-ik\frac{2\pi}{N}} c_k^\dagger d_k + \mathrm{e}^{ik\frac{2\pi}{N}} d_k^\dagger c_k) \ . \tag{4.6}$$

Next, introduce $k' = \frac{2\pi}{N}k$ such that $k' \in [\frac{2\pi}{N}, 2\pi]$ (for N large this is the first Brillouin zone) and relabel $k' \to k$. Then, we may write the expression above neatly in matrix form:

$$\tilde{H}_{\mathrm{SSH}} = \sum_{k\in 1\mathrm{BZ}} \begin{pmatrix} c_k^\dagger, d_k^\dagger \end{pmatrix} \underbrace{\begin{pmatrix} 0 & t+\delta t + \mathrm{e}^{-ik}(t-\delta t) \\ t+\delta t + \mathrm{e}^{ik}(t-\delta t) & 0 \end{pmatrix}}_{=H(k)} \begin{pmatrix} c_k \\ d_k \end{pmatrix} \ . \tag{4.7}$$

Now, $H(k)$ can be written more neatly using Euler's formula and the definition of the Pauli matrices:

$$\begin{aligned} H(k) &= \begin{pmatrix} 0 & t+\delta t + \mathrm{e}^{-ik}(t-\delta t) \\ t+\delta t + \mathrm{e}^{ik}(t-\delta t) & 0 \end{pmatrix} \\ &= (t+\delta t + (t-\delta t)\cos(k)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + (t-\delta t)\sin(k) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \vec{d}\cdot\vec{\sigma} \ , \end{aligned}$$

with $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ being Pauli matrices acting on the sublattice index (A and B) and $\vec{d} = (d_x, d_y, d_z)$ such that

$$d_x = v + w\cos(k) \ , d_y = w\sin(k) \ , d_z = 0 \ , \tag{4.8}$$

with $v = t + \delta t$ and $w = t - \delta t$. The expression $H(k) = \vec{d}\cdot\vec{\sigma}$ is in fact a general way of writing the Bloch Hamiltonian for a two-level system. This is since the Pauli matrices constitute a basis for all 2×2 hermitian matrices. However, often a fourth component is included in $\vec{d}$ and $\vec{\sigma}$, i.e. $\vec{d} = (d_0, d_x, d_y, d_z)$ and $\vec{\sigma} = (\sigma_0, \sigma_x, \sigma_y, \sigma_z)$ where σ_0 is the 2×2 identity matrix. The piece $d_0\sigma_0$ in the Bloch Hamiltonian is however regarded as constant and has no impact on the topological properties of

the system.
Having expressed the SSH Hamiltonian in terms of the Bloch Hamiltonian $H(k) = \vec{d}\cdot\vec{\sigma}$ it is now in order to investigate its symmetries. Due to the construction of the SSH chain depicted in Figure 4.1 there is a sublattice symmetry, $\mathcal{C}$, associated with the atoms at site A and the atoms at site B. Recall, from (3.11) in the chapter on symmetries, that the condition

$$\sigma_z H(k)\sigma_z = -H(k) \ , \tag{4.9}$$

needs to hold for the SSH Hamiltonian for chiral symmetry to be manifest. This is clearly the case for our Hamiltonian:

$$\sigma_z H(k)\sigma_z = \sigma_z(d_x\sigma_x + d_y\sigma_y)\sigma_z = -id_x\sigma_y\sigma_z + id_y\sigma_x\sigma_z = -(d_x\sigma_x + d_y\sigma_y) = -H(k) \ ,$$

where we made use of the $su(2)$-algebra $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$, ϵ_{ijk} being the totally anti-symmetric Levi-Civita symbol. Note that if $d_z \neq 0$ sublattice symmetry would be violated. This proves that two-level Bloch Hamiltonians of the form $H(k) = \vec{d}\cdot\vec{\sigma}$ need to be off-diagonal and have $d_z = 0$ in order to exhibit chiral symmetry. $H(K)$ is also invariant under a time-reversal symmetry $\mathcal{T}$ which, in the absence of spin, acts simply as complex conjugation. Consequently, particle-hole symmetry, being the product of chiral and time-reversal symmetry, is apparent as well.

4.1.1 Topological invariant of the SSH model

It turns out that, given $d_z = 0$, it is particularly simple to extract a topological invariant for the SSH model directly from the Bloch Hamiltonian, $H(k)$. First, we need to comment on the fact that the system is in general gapped. The band structure of the SSH Hamiltonian is easily read off from $H(k)$ as

$$E_\pm(k) = |\vec{d}| = \pm\sqrt{v^2 + w^2 + 2vw\cos(k)} \ , \tag{4.10}$$

since the Pauli matrices square to unity. In particular, we identify an energy band gap, Δ, from the two energy bands in (4.10) such that

$$\Delta = \min(E_+) - \max(E_+) = 2|v - w| \ . \tag{4.11}$$

Note, that whenever the gap is non-zero ($v \neq w$) the SSH chain describes an insulator. At the gap-closings the system is conducting. In Figure 4.2, the two bands, $E_+(k)$ and $E_-(k)$, are shown for different choices of parameters v and w. Note that equation (4.10) is symmetric in the hopping parameters, and therefore the dispersion relations in a) and c) of Figure 4.2 are identical. We have here omitted the (rather uninteresting) cases with $v = 0$ or $w = 0$, which gives a constant dispersion relation for all k. Clearly, case b) has a gap-closing at the points $k = \pm\pi$. We refer to such a system as *gapless*. This is fundamentally different from the *gapped* cases a) and c) not only in the sense that the system is conducting rather than insulating but it will also have more exotic consequences when it comes to topological properties.

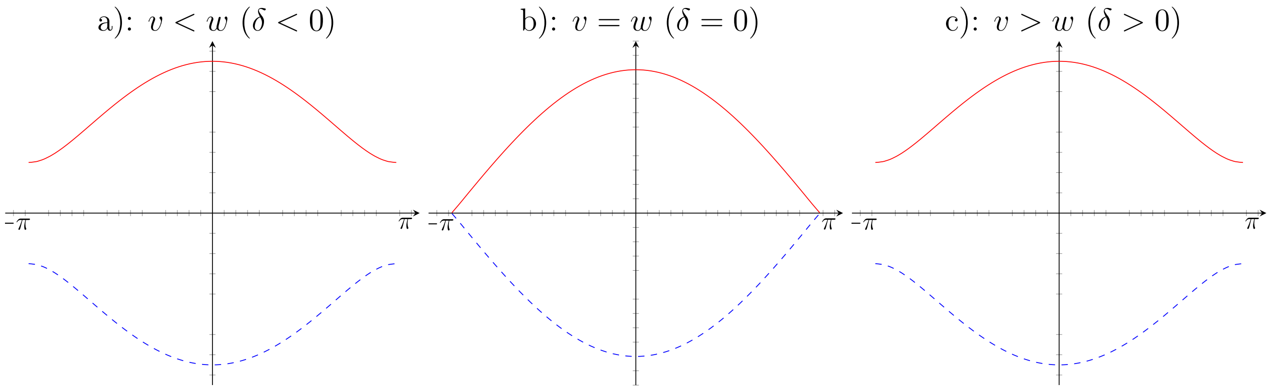

Figure 4.2: Dispersion relations $E_+(k)$ (—) and $E_-(k)$ (- - -) of the SSH model for different values of the hopping parameters v and w. To generate the case a) we used the parameters $v = \frac{w}{2}$ (and the reverse relationship $w = \frac{v}{2}$ for case c)) and the parameters $v = w$ for case b). Note that the cases a) and c) have a non-zero band-gap, $\Delta \neq 0$, but case b) demonstrates a gap-closing for $k = \pm\pi$.

Since k runs from $-\pi$ to π or equivalently 0 to 2π, the vector $\vec{d}(k)$ (with components given in equation (4.8)) traces out a circle in the d_x, d_y-plane. This is easily seen from equation (4.8):

$$d_x = v + w\cos(k) \Rightarrow (d_x - v)^2 = w^2\cos^2(k) \ , \tag{4.12}$$

$$d_y = w\sin(k) \Rightarrow d_y^2 = w^2\sin^2(k) \ , \tag{4.13}$$

which by adding the two equations give the equation for a circle with radius w centered in $(v, 0)$:

$$(d_x - v)^2 + d_y^2 = w^2 \ . \tag{4.14}$$

This is a special property of the SSH model but not a generic feature in a two-band Bloch Hamiltonian. In general, the path $\vec{d}$ traces out does not need to be a circle but only a closed loop which avoids the origin when the system is gapless. The fact that $d_z = 0$ enables us to extract the topological invariant of the SSH model as a winding number, ν, an integer which counts how many times the closed loop winds *around* the origin in the d_x, d_y-plane. Depending on the relationship between the parameters v and w, it is possible to get three distinct (interesting) cases. These are indicated in Figure 4.3. The case a) corresponding to $v > w$ or equivalently $\delta t < 0$ has a non-zero winding number, that is, it is topologically non-trivial. Similarly, the case c) has zero winding number and such a phase is called trivial. The phase between case a) and case c) is perhaps the most interesting. Since the origin is a point on the circle it becomes impossible to define a winding number ν in case b).

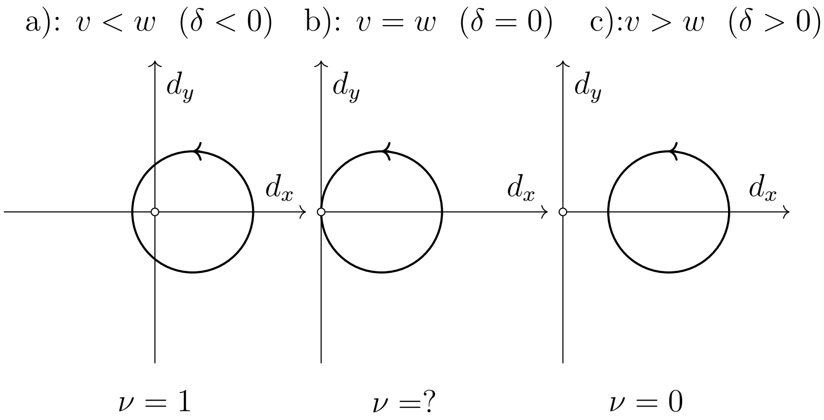

Figure 4.3: The three limiting cases a), b) and c) yield three topologically distinct phases. The case a) has a non-zero winding number, corresponding to a non-trivial topological phase and in case c) the winding number is zero, corresponding to a trivial phase. Case b) is peculiar and the fact that the loop goes through the origin makes the winding number undefined. The direction of the curve is indicated as anti-clockwise.

The winding numbers in the three cases a), b) and c) should be compared with the notion of the system being gapped or gapless. By comparing Figures 4.2 and 4.3 we note that the winding number, ν, becomes undefined at the topological phase transition, at which the system also becomes gapless. This is a generic feature in topological systems and attempts to resolve the issue will be addressed in the next chapter. Generally, moving from one topological phase to another requires a gap-closing. However, a system can also undergo a phase transition between two gapless phases as we also shall see in the next chapter.

The graphical approach to extract the topological invariant of the SSH model is not in any way general and relies heavily on the fact that there is no d_z-component in the Bloch Hamiltonian. It is clear that we need to find a more systematic way of extracting topological properties and winding numbers in one spatial dimension. Following the logic of Asboth et al. [5], we will make use of an analytic expression for the winding number, ν, in terms of an integral. By introducing the normalized vector $\vec{e}_{\vec{d}} = \frac{\vec{d}}{|\vec{d}|}$, which is the projection of $\vec{d}$ onto the unit circle, the winding number can be written as [5]

$$\nu = \frac{1}{2\pi} \int \vec{e}_{\vec{d}} \times \frac{d}{dk} \vec{e}_{\vec{d}} \, dk \ , \tag{4.15}$$

where k is one-dimensional momentum. In the case of the SSH model (which, as we have seen, has an off-diagonal Bloch Hamiltonian with $d_z = 0$), the integral can be rewritten as

$$\nu = \frac{1}{2\pi i} \int_0^{2\pi} dk \frac{d}{dk} (\log(h(k))) \ , \tag{4.16}$$

where $h(k)$ can be read off from the Bloch Hamiltonian $H(k)$ as

$$H(k) = d_x \sigma_x + d_y \sigma_y = \begin{pmatrix} 0 & d_x - i d_y \\ d_x + i d_y & 0 \end{pmatrix} = \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix} \ . \tag{4.17}$$

Details on how to get from the general expression in (4.15) to (4.16) can be found in Appendix A. The quantity $h(k)$ is a complex number and can as such be expressed as $h(k) = |h(k)|\mathrm{e}^{i\arg(h)}$. Therefore, the logarithm of $h(k)$ is given by $\log(h(k)) = \log|h| + i\arg(h)$. When evaluating the integral in (4.16), the branch cut of the logarithm is shifted in a way that the derivative with respect to k is always well-defined. Moreover, the integral is ensured to be real since $|h(k=0)| = |h(k=2\pi)|$. However, it still looks quite tedious. Therefore, we do the standard procedure when dealing with a difficult integral: perform an analytical continuation of the integral to the complex plane.[3] Since $k \in [0, 2\pi]$ it makes sense to do the change of variables $z = \mathrm{e}^{ik}$, where z goes around the unit circle. Now, with slight abuse of notation, $h(k)$ becomes $h(z = \mathrm{e}^{ik})$ and

$$\nu = \frac{1}{2\pi i}\int_0^{2\pi} dk \frac{d}{dk}(\log(h(k))) \underbrace{\rightarrow}_{z=\mathrm{e}^{ik}} \frac{1}{2\pi i}\oint_{|z|=1} dz \frac{d}{dz}(\log(h(z))) \ . \tag{4.18}$$

The new formula we have arrived at is very neat:

$$\nu = \frac{1}{2\pi i}\oint_{|z|=1} dz \frac{h'(z)}{h(z)} \ , \tag{4.19}$$

since Cauchy's famous argument principle comes in hand here:

$$\frac{1}{2\pi i}\oint_{|z|=1} dz \frac{h'(z)}{h(z)} = N_Z - N_P \ , \tag{4.20}$$

where N_Z is the number of zeros $h(z)$ has *inside* the unit circle $|z| = 1$ and N_P is the number of poles inside the unit circle taking multiplicity into account. Note that the winding number, once again, becomes ill-defined and breaks down when $h(z)$ has zeros or poles *on* the unit circle. Writing $h(k)$ as a function of z forces us to reconsider the cases a), b) and c) in Figure 4.3 again:

$$\begin{aligned} h(z = \mathrm{e}^{ik}) = d_x - id_y &= v + \frac{w}{2}(\mathrm{e}^{ik} + \mathrm{e}^{-ik}) - \frac{w}{2}(\mathrm{e}^{ik} - \mathrm{e}^{-ik}) \\ &= v + w\frac{1}{z} \ , \end{aligned}$$

using $d_x = v + w\cos(k)$ and $d_y = w\sin(k)$ and Euler's formula. Apparently, there is a pole at $z = 0$ regardless of the parameters v and w, that is $N_P = 1$ (neglecting the case $w = 0$). However, for the zeros we have to distinguish between the three cases *a*), *b*) and *c*):

$$\begin{aligned} &a) : v < w \ , h(z) = 0 \Rightarrow z_0 = -\frac{w}{v}, |z_0| > 1, N_Z = 0 \ , \\ &b) : v = w \ , h(z) = 0 \Rightarrow z_0 = -1, |z_0| = 1, N_Z = ? \ , \\ &c) : v > w \ , h(z) = 0 \Rightarrow z_0 = -\frac{w}{v}, |z_0| < 1, N_Z = 1 \ , \end{aligned}$$

[3] Analytic continuation works whenever there is only one momentum variable k.

where we note for case b) that $v = w$ corresponds to having a zero on the unit circle. Therefore, the winding number for the different cases becomes

$$\begin{aligned} a) &: \nu = 0 - 1 = -1 \ , \\ b) &: \nu = ? \ , \\ c) &: \nu = 1 - 1 = 0 \ . \end{aligned}$$

Clearly, these results are in agreement with the graphical analysis above, even though the winding number for case a) is negative rather than positive. However, the sign of ν is not physically relevant, it is only a matter of choosing the direction of the enclosed curve to be anti-clockwise or clockwise.

4.1.2 Fermionic edge states in the SSH model

We have not yet made a physical interpretation of the non-zero winding numbers of the SSH model obtained in the previous sections. This is provided by the bulk-boundary correspondence, stating that a non-zero topological invariant implies the existence of fermionic edge states [43]. As shown above, there are three distinct cases to investigate: $\delta < 0$, $\delta = 0$ and $\delta > 0$, with the case $\delta = 0$ being a boundary between the topological and non-topological phase of the model. Now, the analysis of edge states is most easily done by specifying the value of the parameter δ. In particular, we may choose $\delta = 0$ or ± 1 and get a representative for each case. Then, since Hamiltonians within a topological phase are adiabatically connected, it follows that the analysis holds for general values of the parameters. The parameter choice $\delta = -1$ corresponding to the topological phase of the model is particularly convenient since the SSH Hamiltonian in (4.1) reduces to

$$H_{\text{SSH}} = 2t \sum_{j=1}^{N-1} c^{\dagger}_{A,j+1} c_{B,j} + \text{h.c.} \ . \tag{4.21}$$

Clearly, the fermionic operators $c^{\dagger}_{A,1}$ and $c^{\dagger}_{B,N}$ are absent from the Hamiltonian. This means that there exists a fermionic state that can be added to each end of the SSH chain without energy cost. Tuning the parameter δ away from $\delta = -1$ results in the edge states overlapping and splitting apart in energy at a scale which is exponentially small dependent on the length of the chain, N [44]. Similarly, $\delta = +1$ results in the Hamiltonian

$$H_{\text{SSH}} = 2t \sum_{j=1}^{N} c^{\dagger}_{A,j} c_{B,j} + \text{h.c.} \ , \tag{4.22}$$

indicating that there exists a strong bond between the sites in all unit cells $n = 1...N$. Hence, no fermionic edge states appear, which also is reflected in the fact that the winding number ν vanishes for positive values of the parameter δ, compare with Figure 4.3.

4.2 Kitaev's model and Majorana edge states

Another model of vital importance when it comes to the discussion of topological phases and invariants is the Kitaev model, constituting a prototype of a topological superconductor in one spatial dimension [15]. However, the Kitaev model is also of interest since it displays the existence of so called Majorana zero energy edge modes (MZMs), which may be interpreted as Majorana fermions bound to a defect at zero energy.[4] It should be stated that such fermions are nowhere to be found in nature and are not (as we know) part of the Standard Model. The idea of Majoranas was considered by Ettore Majorana already in 1937, who came up with a real wave equation similar to the Dirac equation describing fermionic particles which were their own anti-particles [46].[5] Back then the "zen particles"[6] were merely seen as a mathematical curiosity and Majorana received hardly any acclaim for his discoveries.[7] Today, engineering systems hosting Majoranas is a very active area of research. It turns out that they tend to show up, although in the form of bound states and zero modes, in condensed matter systems and more precisely in (topological) superconductors [9]. The mathematical framework of superconductivity relies on so called Bogoliubov quasiparticle excitations, formed by superpositions of negatively charged electrons and positively charged holes causing them to be charge neutral and fermionic. As argued by Beenakker, the Majorana nature of such quasiparticles can be experimentally probed [45]. Chamon et al. took it one step further and claimed that the Majorana fermions do not necessarily have to be confined to zero energy in the form of MZMs in superconductors, but the full quantum field (similar to the real field found by Majorana himself) emerges solely as a result of fermionic statistics and superconductivity [47]. Hence, superconductors are suitable candidates when it comes to finding Majorana fermions as well as MZMs. The latter will however be of most interest to us due their robust nature in topological systems. The first section below is therefore devoted to the exotic Majoranas and edge modes, which play a key role in the Kitaev model. In particular, the intimate connection between topology and Majorana edge states will become apparent.

[4]The MZMs are often referred to simply as Majorana fermions, but this is really a misnomer since the zero modes are not fermions but rather non-abelian anyons [45].

[5]More precisely, he found a real solution $\tilde{\psi}$ to the equation $(i\tilde{\gamma}^{\mu}\partial_{\mu} - m)\tilde{\psi} = 0$, where the γ-matrices are expressed in a basis where they are purely imaginary.

[6]This term for Majorana fermions is jokingly used by renowned physicists in the field, e.g. by Beenakker and Frolov, who compare the particles with the Higgs boson commonly referred to as the God particle. Since the Majorana zero modes have zero energy and charge and moreover are massless making them immensely difficult to find in nature, the naming can probably be justified.

[7]In fact, the existence of Majorana particles has remained as elusive as Majorana himself, who disappeared without a trace during a boat trip between Naples and Palermo less than a year after he came up with his equation.

4.2.1 Majorana edge modes

Using the regular fermionic ladder operators c_n and $c_n^\dagger$ in second quantization[8] we may introduce another set of (real) operators γ_n and $\tilde{\gamma}_n$ such that[9]

$$c_n = \frac{1}{2}(\gamma_n + i\tilde{\gamma}_n) \ , c_n^\dagger = \frac{1}{2}(\gamma_n - i\tilde{\gamma}_n) \ , \tag{4.23}$$

which are easily inverted as

$$\gamma_n = c_n + c_n^\dagger \ , \tilde{\gamma}_n = i(c_n^\dagger - c_n) \ . \tag{4.24}$$

The operators above are called *Majorana operators* and describe Majorana fermions, which essentially have half the fermionic degrees of freedom of the electron. Due to this fact, Majoranas must always come in pairs in a physical fermionic system (since the Majorana modes must necessarily combine into a complex fermion). From the construction, it is obvious that the operators are real, i.e. $\gamma_n = \gamma_n^\dagger$ and $\tilde{\gamma}_n = \tilde{\gamma}_n^\dagger$ and they also obey the (anti)-commutation relations:

$$\begin{aligned}
\{\gamma_n, \gamma_m\} &= \{c_n + c_n^\dagger, c_m + c_m^\dagger\} = 2\delta_{n,m} \ , \\
\{\tilde{\gamma}_n, \tilde{\gamma}_m\} &= -\{c_n^\dagger - c_n, c_m^\dagger - c_m\} = 2\delta_{n,m} \ , \\
\{\gamma_n, \tilde{\gamma}_m\} &= i\{c_n + c_n^\dagger, c_m^\dagger - c_m\} = 0 \ ,
\end{aligned}$$

i.e. the operators γ and $\tilde{\gamma}$ anti-commute and square to unity independently. Now, let us consider a system with $n = N$ unit cells (sites), where each site can host one fermion described by the fermionic operator $c_n^\dagger$. Equivalently, due to the construction above, the site hosts two different Majorana modes γ_n and $\tilde{\gamma}_n$. The modes are referred to as *real* and *imaginary* respectively, referring to how they transform under complex conjugation, $\mathcal{K}$:[10]

$$\mathcal{K}\gamma_n\mathcal{K} = \gamma_n \ , \mathcal{K}\tilde{\gamma}_n\mathcal{K} = -\tilde{\gamma}_n \ . \tag{4.25}$$

Having made the distinction between the modes explicit, we are effectively considering the one-dimensional “domino model” in Figure 4.4. Conventionally, the modes to the left in a unit cell are chosen to be real (γ_n) and the modes to the right are imaginary ($\tilde{\gamma}_n$).

[8]The operators $c_n^\dagger$ and c_n are creation and annihilation operators which create or destroy a fermion at a fermionic site n respectively. They obey the fermionic algebra $\{c_n^\dagger, c_m\} = \delta_{n,m}$ and $\{c_n^\dagger, c_m^\dagger\} = \{c_n, c_m\} = 0$. We could also be more general and assign a spin index $\sigma =\uparrow,\downarrow$ to the operators. However, in this chapter (and the next) we will exclusively deal with spinless fermions making such an index superfluous.

[9]The factors $\frac{1}{2}$ in front are conventional.

[10]This should not be confused with the fact that the Majorana operators are real under hermitian conjugation.

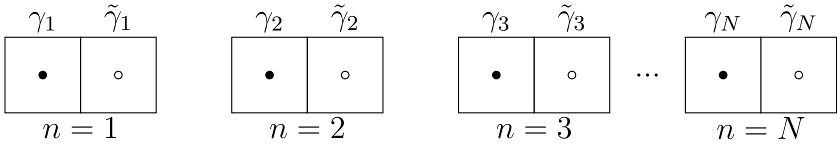

Figure 4.4: Schematic illustration of the domino model. Each fermionic site n hosts one fermion or equivalently two Majoranas.

Now, interesting physics emerge if we try to pair up the Majoranas. Let us consider two vastly different cases. In the first case, we pair up Majoranas intracell, that is Majoranas only pair up with modes at the same site n. This is illustrated in Figure 4.5. Note that no Majoranas are isolated from each other.

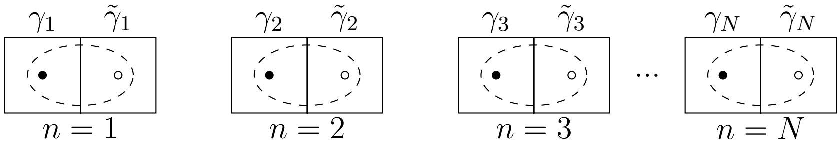

Figure 4.5: Pairing of Majoranas only occurs in the same unit cell n. This corresponds to a topologically trivial phase and no Majorana edge modes appear.

This corresponds to a topologically trivial phase as we shall see later on. Assuming that the energy cost of putting an electron at site n is given by μ, the corresponding Hamiltonian is easily written down as

$$H_0 = \frac{i\mu}{2} \sum_{n=1}^{N} \tilde{\gamma}_n \gamma_n \ . \tag{4.26}$$

The subscript "0" will be given an explanation later. However, if we instead allow ourselves to pair up the Majoranas intercell, that is the modes couple to adjacent (nearest), neighboring, sites, the situation is radically different. See Figure 4.6.

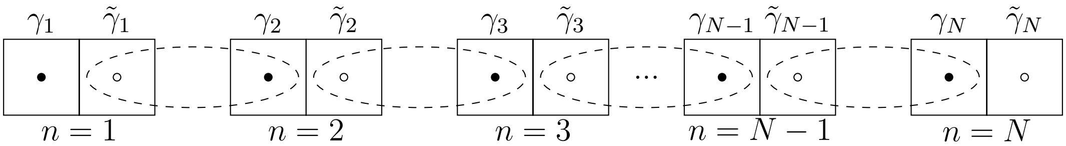

Figure 4.6: Pairing of Majoranas occur only *between* unit cells and adjacent sites (nearest neighbors). Note that pairing in this fashion results in two Majorana edge modes, γ_1 and $\tilde{\gamma}_N$.

Now, the Majorana modes γ_1 and $\tilde{\gamma}_N$ are unpaired! This is evident also in the Hamiltonian:

$$H_1 = it \sum_{n=1}^{N-1} \tilde{\gamma}_n \gamma_{n+1} \ , \tag{4.27}$$

where we introduced the hopping parameter t (resulting in an energy difference $2t$ between filled and unfilled states).[11] Clearly, γ_1 and $\tilde{\gamma}_N$ are absent from the

[11] The hopping parameter t can be real or complex.

Hamiltonian, and therefore the edge modes can be added without any energy cost, i.e. they are so called *zero-energy Majorana modes* or *Majorana zero modes* (MZMs). In this case, we are thus considering a system with a gapped bulk flanked by two zero-energy edge states. The two cases of the domino model in fact constitute extreme limits of a more general model, the *Kitaev model*, which we consider in the next section.

4.2.2 Kitaev's model and the emergence of Majorana zero modes

The Kitaev model is the most simple one-dimensional toy model of a topological superconductor which illustrates the concept of Majorana edge modes and topological phases. It was proposed by the Russian-American physicist Alexei Kitaev in 2001. Kitaev considered the tight-binding Hamiltonian [15][12]

$$H_{\mathrm{K}} = -\mu \sum_n c_n^\dagger c_n - t \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) + \sum_n (\Delta c_n c_{n+1} + \Delta^* c_{n+1}^\dagger c_n^\dagger) \ , \tag{4.28}$$

where μ is the on-site energy (chemical potential), t is the nearest-neighbor hopping amplitude and $\Delta = |\Delta| \mathrm{e}^{i\theta}$ is the (complex) superconducting pairing potential. Note that (4.28), in contrast to the BCS-Hamiltonian describing superconductivity, does not depend on spin or have an even superconducting order parameter.

In his derivation, Kitaev assumed the electrons to have one fixed spin direction, which is equivalent to considering an effectively spinless system. This has the consequence that the superconducting order parameter is odd under the exchange of particles and holes, which makes the Kitaev model constitute a p-wave superconductor.[13]

We redefine our Majorana operators in (4.24) to get rid of the phase $\mathrm{e}^{i\theta}$ in Δ according to

$$\gamma_n = \mathrm{e}^{i\frac{\theta}{2}} c_n + \mathrm{e}^{-i\frac{\theta}{2}} c_n^\dagger \ , \tilde{\gamma}_n = i(\mathrm{e}^{-i\frac{\theta}{2}} c_n^\dagger - \mathrm{e}^{i\frac{\theta}{2}} c_n) \ , \tag{4.29}$$

which can be inverted as

$$c_n^\dagger = \frac{\mathrm{e}^{i\theta/2}}{2}(\gamma_n - i\tilde{\gamma}_n) \ , c_n = \frac{\mathrm{e}^{-i\theta/2}}{2}(\gamma_n + i\tilde{\gamma}_n) \ . \tag{4.30}$$

[12]One can in fact derive this Hamiltonian directly from the superconducting BCS-Hamiltonian $H_{\mathrm{BCS}} = \sum_k (\epsilon_k - \mu) c_k^\dagger c_k + (\Delta_k^* c_{-k} c_k + \text{h.c.})$ (omitting the spin dependence), with $\epsilon_k = \frac{\hbar^2 k^2}{2m}$, by putting it on a lattice. In practice moving from the continuum model to the lattice model involves performing the substitutions $k \to \sin(k)$ and $k^2 \to 2(1 - \cos(k))$, with the expressions coinciding at long wave lengths [48]. Then, by taking the inverse Fourier transformation from k-space to real space and setting $\frac{\hbar^2}{2m} = t$ results in (4.28).

[13]To those with little knowledge of superconductivity but having some experience with quantum mechanics, we provide an alternative explanation here. The total wavefunction of a spinful system, $\psi(r_1, r_2, \sigma_1, \sigma_2)$, can be decomposed into two parts, an orbital part, $g(r_1, r_2)$, and a part taking spin degrees of freedom into account, $\chi(\sigma_1, \sigma_2)$. By assuming the electrons to be spinless one is left with the orbital part and due to the Pauli exclusion principle the total wavefunction has to be anti-symmetric. In our case, $g(r_1, r_2) = -g(r_2, r_1)$, i.e. the orbital wavefunction is odd under the exchange of particles. Moreover, the superconducting order parameter Δ is directly proportional to $g(r_1, r_2)$ and therefore $\Delta(k) = -\Delta(-k)$ (it does not matter if we consider the order parameter in k-space rather than real space, the proportionality still holds).

Inserting these relations into the Hamiltonian above then results in

$$\begin{aligned} H_{\mathrm{K}} &= -\frac{\mu}{2}\sum_n (1 - i\tilde{\gamma}_n\gamma_n) - \frac{it}{2}\sum_n (\gamma_{n+1}\tilde{\gamma}_n + \gamma_n\tilde{\gamma}_{n+1}) + \frac{i|\Delta|}{2}\sum_n \tilde{\gamma}_n\gamma_{n+1} + \gamma_n\tilde{\gamma}_{n+1} \\ &= \frac{i\mu}{2}\sum_n \tilde{\gamma}_n\gamma_n + \frac{i}{2}(|\Delta| + t)\sum_n^{N-1} \tilde{\gamma}_n\gamma_{n+1} + \frac{i}{2}(|\Delta| - t)\sum_n^{N-1} \gamma_n\tilde{\gamma}_{n+1} \ , \end{aligned}$$

where we made use of the fermionic (anti)-commutation relations and dropped the constant term in the Hamiltonian. Now, it is in order to consider some special cases. Note that for the case $t = |\Delta| = 0$ and $\mu \neq 0$ the Hamiltonian becomes

$$H_{0\mathrm{K}} = \frac{i\mu}{2}\sum_n \tilde{\gamma}_n\gamma_n \ , \tag{4.31}$$

which is precisely the Hamiltonian H_0 in (4.26), corresponding to the situation in Figure 4.5 where there are no unpaired Majorana modes. For $|\Delta| = t \neq 0$ and $\mu = 0$ we are instead left with

$$H_{1\mathrm{K}} = it\sum_{n=1}^{N-1} \tilde{\gamma}_n\gamma_{n+1} \ , \tag{4.32}$$

which is precisely H_1 in (4.27). We saw that this case corresponds to Figure 4.6 , where we have two unpaired Majorana edge modes γ_1 and $\tilde{\gamma}_N$. Now it seems that $\mu = 0$ and $|\Delta| = t$ is a very exotic choice of parameters. However, it is possible to tune μ up to $2t$ and the zero energy modes will still persist. In other words, the Majorana modes are protected as long as the bulk energy gap is finite. When μ takes the value $2t$ the first empty energy band (when $\mu < 2t$) becomes populated, in effect closing the band gap. The Majorana edge state levels will now mix with the levels of the bulk states, making them recombine into ordinary electrons.
It will prove useful to express the Kitaev Hamiltonian in (4.28) in a Bogoliubov-de Gennes fashion. That is, we write

$$H_{\mathrm{K}} = \frac{1}{2}C^\dagger H_{\mathrm{BdG}} C \ , \tag{4.33}$$

where $C = (c_1 ... c_N, c_1^\dagger ... c_N^\dagger)^T$ and H_{BdG} is the $2N \times 2N$ BdG Hamiltonian. H_{BdG} can be expressed in terms of Pauli matrices τ in particle-hole space acting on basis states $|n\rangle = (0, ..., 1, ...0)^T$, which corresponds to the n:th site of the chain. Then, it follows that

$$H_{\mathrm{BdG}} = -\mu\sum_n \tau_z|n\rangle\langle n| - \sum_n (t\tau_z + i\Delta\tau_y)|n\rangle\langle n+1| + \mathrm{h.c.} \ , \tag{4.34}$$

which acts on basis states $|n\rangle|\tau\rangle$, with $\tau = +1$ for electronic states and $\tau = -1$ for hole states. Particle-hole symmetry is manifest in H_{BdG}, i.e. $\mathcal{P}H_{\mathrm{BdG}}\mathcal{P}^{-1} = -H_{\mathrm{BdG}}$ with $\mathcal{P} = \tau_x\mathcal{K}$. Now, we allow ourselves to connect the ends of the Kitaev chain and form a "Kitaev ring". This implies that the Hamiltonian exhibits translational symmetry $|n\rangle \to |n{+}1\rangle$. In the presence of translational symmetry we invoke Bloch's theorem and express the BdG Hamiltonian in Fourier modes, i.e. in momentum space. A state with momentum k is then given by

$$|k\rangle = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} \mathrm{e}^{-ikn}|n\rangle \Rightarrow |n\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} \mathrm{e}^{ikn}|k\rangle \ , \tag{4.35}$$

where we let $|k\rangle$ obey periodic boundary conditions. Therefore, k is a conserved quantum number taking values $\frac{2\pi p}{N}$ with $p = 0, 1....$ For N large, k is more or less continuous and restricted to take values in the first Brillouin zone. Let us substitute (4.35) into the BdG Hamiltonian:

$$\begin{aligned}
H_{\mathrm{BdG}} &= -\frac{\mu\tau_z}{N}\sum_n\sum_k\sum_{k'} \mathrm{e}^{i(k-k')n}|k\rangle\langle k'| - \sum_n\sum_k\sum_{k'}((t\tau_z + i\Delta\tau_y)\mathrm{e}^{i(k-k')n}\mathrm{e}^{-ik}|k\rangle\langle k'| + \mathrm{h.c.}) \\
&= -\mu\tau_z\sum_k |k\rangle\langle k| - \sum_k((t\tau_z + i\Delta\tau_y)\mathrm{e}^{-ik} + \mathrm{h.c.})|k\rangle\langle k| \\
&= -\mu\tau_z\sum_k |k\rangle\langle k| - \sum_k\left(t\tau_z(\mathrm{e}^{-ik} + \mathrm{e}^{ik}) + i\Delta\tau_y(\mathrm{e}^{-ik} - \mathrm{e}^{ik})\right)|k\rangle\langle k| \\
&= \sum_k(-\mu - 2t\cos(k))\tau_z|k\rangle\langle k| + \sum_k 2\Delta\sin(k)\tau_y|k\rangle\langle k| \ ,
\end{aligned}$$

i.e.

$$H(k) = \langle k|H_{\mathrm{BdG}}|k\rangle = -(\mu + 2t\cos(k))\tau_z + 2\Delta\sin(k)\tau_y \ . \tag{4.36}$$

This is the 2×2 Bloch Hamiltonian for the Kitaev model.[14] Although the Hamiltonian formally looks very similar to the Bloch Hamiltonian of the SSH model in (4.7) it is important to remember that they act on different single-particle degrees of freedom. The Kitaev Bloch Hamiltonian acts in the space of real Majorana operators, in contrast to the Bloch Hamiltonian of the SSH model which lives in the space of complex fermionic operators. From the Bloch Hamiltonian, $H(k)$, the band structure is easily obtained from the secular equation $\det(H - EI) = 0$ as

$$E(k) = \pm\sqrt{(2t\cos(k) + \mu)^2 + 4|\Delta|^2\sin^2 k} \ . \tag{4.37}$$

Obviously, we do not expect any Majorana edge states since we are dealing with a circular structure, but still the energy gap closes at $k = 0$ and $k = \pi$ for $\mu = 2t$ and $\mu = -2t$ respectively.

4.2.3 Integral representation of the topological invariant of the Kitaev model

It is possible to extract the topological invariant ν for the Kitaev model using the integral expression

$$\nu = \frac{1}{2\pi i}\int_{k=0}^{2\pi}\frac{d}{dk}(\log(h(k)))dk \ , \tag{4.38}$$

i.e. the one used to compute the winding number for the SSH model analytically. Note that this required us to have a Bloch Hamiltonian $H(k)$ which is off-diagonal. This is not the case for the Kitaev model in the basis implied by the construction in section 4.2.2. Recall that the Bloch Hamiltonian for the Kitaev model was there given by

$$H(k) = \vec{h}\cdot\vec{\tau} = (-\mu - 2t\cos(k))\tau_z + 2\Delta\sin(k)\tau_y = \begin{pmatrix} -\mu - 2t\cos(k) & -2i\Delta\sin(k) \\ 2i\Delta\sin(k) & \mu + 2t\cos(k)\end{pmatrix} \ ,$$

[14] We could of course also Fourier transform (4.28) directly (as we did for the SSH model) instead of introducing basis states and arrive at the BdG Hamiltonian in (4.36).

where τ_z and τ_y act on the particle-hole degrees of freedom (since the fermions are assumed to be spinless). We will also restrict to the case where the superconductivity parameter Δ and the hopping parameter t are *real*. This implies that time-reversal symmetry is manifest in the Hamiltonian (with $\mathcal{T}^2 = 1$ for $\mathcal{T} = \mathcal{K}$) and thus the Kitaev chain can be placed in symmetry class BDI, rather than D.[15] In particular, as we shall see, this greatly simplifies the calculation of the topological invariant of the model. In general, finding the topological invariant of the Kitaev model involves computing a Pfaffian, but choosing the parameters to be real enables us to use the winding number definition in (4.38) instead. Before doing so, we have to recast the Bloch Hamiltonian into the off-diagonal form

$$H(k) = \begin{pmatrix} 0 & h(k) \\ h(-k)^* & 0 \end{pmatrix} .= \begin{pmatrix} 0 & h_x - ih_y \\ h_x + ih_y & 0 \end{pmatrix} . \tag{4.39}$$

Note that we have $\vec{h} = (0, h_y, h_z)$ and therefore we want to rotate h_y and h_z to the $x-y$-plane, i.e. $h_z \to h_x$. The unitary transformation

$$U = \mathrm{e}^{-\frac{i\pi}{2\hbar}S_y} = \mathrm{e}^{-\frac{i\pi}{4}\tau_y} , \tag{4.40}$$

which performs a rotation by $\frac{\pi}{2}$ around the y-axis does the trick. This gives us

$$\tilde{H}(k) = UH(k)U^\dagger = \mathrm{e}^{-\frac{i\pi}{4}\tau_y} H(k) \mathrm{e}^{\frac{i\pi}{4}\tau_y} . \tag{4.41}$$

This object looks quite complicated. However, note that we may write

$$\begin{aligned}
\mathrm{e}^{-\frac{i\pi}{4}\tau_y} = \sum_{n=0}^{\infty} (\frac{-i\pi}{4}\tau_y)^n \frac{1}{n!} &= 1 - \frac{i\pi}{4}\tau_y + (\frac{-i\pi}{4})^2 \frac{1}{2!} + (\frac{-i\pi}{4})^3 \frac{1}{3!}\tau_y + ... \\
&= \underbrace{1 - (\frac{\pi}{4})^2 \frac{1}{2!} + ...}_{=\cos(\frac{\pi}{4})} - i\tau_y \underbrace{(\frac{\pi}{4} - (\frac{\pi}{4})^3 \frac{1}{3!} + ...)}_{=\sin(\frac{\pi}{4})} \\
&= \cos(\frac{\pi}{4}) - i\sin(\frac{\pi}{4})\tau_y .
\end{aligned}$$

In a matrix representation, it reads

$$U = \mathrm{e}^{-\frac{i\pi}{4}\tau_y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} . \tag{4.42}$$

Now, the transformation reduces to computing a product of matrices to find $\tilde{H}(k)$:

$$\begin{aligned}
\tilde{H}(k) &= \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} h_z & -ih_y \\ ih_y & -h_z \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} h_z - ih_y & -ih_y + h_z \\ h_z + ih_y & -ih_y - h_z \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & h_z - ih_y \\ h_z + ih_y & 0 \end{pmatrix} ,
\end{aligned}$$

[15] Assigning a Hamiltonian to a certain symmetry class is a matter of choice and highly dependent on which symmetry preserved perturbations we allow in our model.

which clearly is off-diagonal. The topological invariant ν is defined up to a unitary transformation U and therefore we conclude that $\tilde{H}(k)$ can be used to compute the topological invariant of $H(k)$. For the SSH model we used $h(k) = d_x - id_y$ and now we identify h_z with d_x and h_y with d_y. We also perform an analytical continuation to the complex plane in order to be able to tackle the winding integral:

$$\nu = \frac{1}{2\pi i} \int dk \frac{d}{dk}(\log(h(k))) \rightarrow \nu = \frac{1}{2\pi i} \oint_{|z|=1} dz \frac{d}{dz} \log(h(z)) \;, \tag{4.43}$$

where we set $z = \mathrm{e}^{ik}$ (i.e. all points k in the Brillouin zone are mapped onto the unit circle in the complex plane) and let $h(k) \rightarrow h(z) = h(\mathrm{e}^{ik})$ and allowed ourselves a slight abuse of notation. The sign of the integral is ambiguous and depends on the direction of the curve (clockwise or anti-clockwise), but it does not matter for our purposes. Thus we have

$$\nu = \frac{1}{2\pi i} \oint_{|z|=1} dz \frac{h'(z)}{h(z)} \;. \tag{4.44}$$

Note that $|h(z)| \neq 0$ for the integral to be well-defined. This corresponds to closing the energy-gap, thus breaking time-reversal symmetry and moving away from the topological phase. By Cauchy's argument principle the integral above is easily evaluated:

$$\nu = \frac{1}{2\pi i} \oint_{|z|=1} dz \frac{h'(z)}{h(z)} = N_Z - N_P \;, \tag{4.45}$$

where N_Z denote the number of zeros of $h(z)$ *inside* the unit circle and N_P denote the number of poles (including multiplicity) inside the unit circle. Note that if $h(z)$ has poles *on* the unit circle the winding number definition above breaks down and becomes undefined.[16] For the Kitaev model we have $h_z = -\mu - 2t\cos(k)$ and $h_y = 2\Delta \sin(k)$. In terms of the variable $z = \mathrm{e}^{ik}$ these read

$$\begin{aligned} h_y &= -i\Delta(\mathrm{e}^{ik} - \mathrm{e}^{-ik}) = -i\Delta(z - \frac{1}{z}) \;, \\ h_z &= -\mu - t(\mathrm{e}^{ik} + \mathrm{e}^{-ik}) = -\mu - t(\frac{1}{z} + z) \;, \end{aligned}$$

and therefore

$$h(z) = h_z - ih_y = -\mu - t(\frac{1}{z} + z) - \Delta(z - \frac{1}{z}) = -\mu + (\Delta - t)\frac{1}{z} - (\Delta + t)z \;. \tag{4.46}$$

Clearly, we will have a pole at $z = 0$ for all $\Delta \neq t$. In the following, let us consider two extreme cases:

$$\text{a)} : \Delta = t \;, \mu = 0 \Rightarrow h(z) = -2tz \;, N_Z = 1 \;, N_P = 0 \tag{4.47}$$

$$\text{b)} : \Delta = t = 0 \;, \mu \neq 0 \Rightarrow h(z) = -\mu = \text{const} \;, N_Z = N_P = 0 \;. \tag{4.48}$$

[16] The case when $h(z)$ has zeros on the unit circle corresponds to a *gapless* topological system. Such systems will be discussed extensively in the remaining chapters. The classification of topological phases in gapless systems is a current area of research and not fully understood, which is outlined by this thesis.

Case a) has a non-trivial winding number. This corresponds to a topological phase. Similarly, case b) corresponds to a topologically trivial superconductor. a) is of interest when discussing Majorana edge modes. Finally, we comment on the transition from a topological phase to a non-topological phase. This occurs when the energy gap closes, i.e. when $|h(z)| = \pm\sqrt{h_y^2 + h_z^2} = 0$ and the winding number integral becomes undefined. Since,

$$|h(k)| = \pm\sqrt{(\mu + 2t\cos(k))^2 + 4|\Delta|^2 \sin^2(k)}\ , \tag{4.49}$$

it follows that for $\mu = -2t$ ($k = 0, 2\pi$) and $\mu = +2t$ ($k = \pi$) the energy gap closes. By considering the gap closing in the vicinity of $k = 0$ it will be possible to understand the topological phase transition more in detail. Then, the original (non-rotated) Bloch Hamiltonian becomes

$$H(k) = (-\mu - 2t\cos(k))\tau_z + 2\Delta\sin(k)\tau_y \approx (-\mu - 2t)\tau_z + 2\Delta k\tau_y\ , \tag{4.50}$$

just by taking the first-order terms in the Taylor expansion. Note that this is precisely a Dirac Hamiltonian which is linear in momentum k with mass-term $m = -\mu - 2t$.[17] The topology is now encoded in m since

$$\begin{cases} m > 0 & : \ \mu > -2t \Rightarrow \text{ topological phase in open chain with Majorana edge modes}\ , \\ m < 0 & : \ \mu - 2t \Rightarrow \text{trivial phase in open chain without Majorana edge modes}\ , \end{cases}$$

and the case $m = 0$ corresponds to a critical point, that is, the topological phase transition at which the bulk energy gap closes and the mass-term switches sign. Now, we allow the mass-term to vary with position x in such a way that

$$\lim_{x\to\pm\infty} m(x) = \pm m\ , m(0) = 0\ . \tag{4.51}$$

Then $x = 0$ corresponds to a domain wall separating two regions of space where m is negative ($x < 0$) and m is positive ($x > 0$). To be able to use this mass-term in the Hamiltonian, the Bloch Hamiltonian has to be transformed to real space. Moreover, we introduce the parameter $v = 2\Delta$ as the speed of the Majorana modes[18]

$$H(x) = -vi\tau_y\partial_x + m(x)\tau_z\ , \tag{4.52}$$

using the position representation of the momentum operator, $k \to -i\partial_x$ in one dimension. We have already established previously that the case $m = 0$ supports zero-energy Majorana edge states. This also becomes apparent when solving the Schrödinger equation for zero-energy states with $H(x)$:

$$H(x)\psi = 0 \Rightarrow (-v\tau_y i\partial_x + m(x)\tau_z)\psi(x) = 0\ . \tag{4.53}$$

[17] Perhaps sloppily, in condensed matter physics we call every Hamiltonian which is linear in momentum a Dirac Hamiltonian.

[18] If the mass-term $m = 0$, the Dirac Hamiltonian has two energy eigenstates with energy $E_\pm = \pm 2\Delta k$. This describes left-moving Majorana modes with energy $E_- = -2\Delta k$ and right-moving Majorana modes with energy $E_+ = 2\Delta k$. Thus, it makes sense to interpret 2Δ as a velocity.

The first-order differential equation above is easily solved by multiplying the equation from the left with τ_y and making use of $\tau_y\tau_z = i\tau_x$ and $\tau_y^2 = 1$, giving us:

$$\partial_x\psi(x) = \frac{m(x)}{v}\tau_x\psi(x) \ . \tag{4.54}$$

The solution to the equation is easily deduced as

$$\psi(x) = \exp(\pm\int_0^x \frac{m(x')}{v}dx'\tau_x)\psi(0) \ , \tag{4.55}$$

with $\psi(0)$ being the eigenstates of τ_x:

$$\psi(0) = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \ . \tag{4.56}$$

However, due to the fact that $m(x)$ changes sign at $x = 0$, only one of the solutions $\psi(x)$ will be normalizable ($\int dx|\psi(x)|^2 < \infty$). This yields a solution which is localized at $x = 0$ with two exponential tails for $x < 0$ and $x > 0$ respectively. The sign-change in $m(x)$ is really crucial to get this kind of behavior and if this would not have been the case there would be no normalizable solutions. At the domain wall $x = 0$ there is a zero-energy bound state corresponding to the Majorana edge mode. The solution in (4.55) is a special case of a solution first obtained by Jackiw and Rebbi in 1976 which formed the mathematical basis for topological excitations in systems described by an effective Dirac Hamiltonian [49]. In Figure 4.7, the situation is depicted with $m(x > 0) = +m$ and $m(x < 0) = -m$. Above we have seen that the solution for $x < 0$ corresponds to the topological phase and the solution for $x > 0$ corresponds to the trivial phase. At the interface between these regions there is a Majorana zero energy mode.

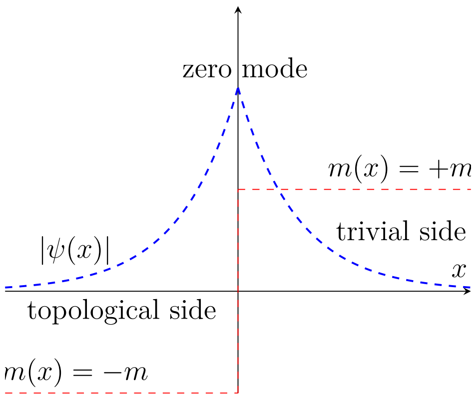

Figure 4.7: The solution $\psi(x)$ admits a zero-energy mode at the interface between two regions $x < 0$ and $x > 0$. The region $x < 0$ corresponds to the topological phase and the region $x > 0$ to the trivial phase. Here $m(x)$ is set to $m(x < 0) = -m$ and $m(x > 0) = +m$ but one could of course be more general and take an arbitrary function $m(x)$ as long as it fulfills $\lim_{x\pm\infty} m(x) = \pm m$.

4.2.4 Realizing Kitaev's model

Although Kitaev's model is of conceptual interest and constitutes a pedagogical example when it comes to the emergence of Majorana zero modes and non-trivial topology, it still remains a toy model. To please the more experimentally inclined reader we therefore comment on the attempts to realize Kitaev's model. Firstly, the model assumes spinless electrons which has the consequence that the superconducting order parameter Δ must be odd, i.e. we are considering a p-wave superconductor. Superconductors of intrinsic p-wave type are extremely rare in nature[19] and moreover, as discussed by e.g. Kallin [51], zero modes are neither easily detected or manipulated in such systems. Hence, it may seem hopeless to realize Kitaev's model with a system of spinful electrons. However, if one spin degree of freedom can be "frozen out" we are effectively considering a spinless system. This necessarily requires the lifting of Kramer's degeneracy and typically the breaking of time-reversal symmetry [6]. Arguably, the most celebrated realization of Majorana zero modes in a topological superconductor was proposed by Fu and Kane in 2007 [52]. In fact, they did not use a superconductor of p-wave type but instead more conventional building blocks. In particular, they made use of the *proximity effect* between an ordinary s-wave superconductor and the edge states of a topological insulator.[20] However, Fu and Kane concluded that they had engineered a spinless two-dimensional superconducting state of $p_x + ip_y$-type, with the Majorana bound states emerging at vortices.

When it comes to the realization of precisely Kitaev's model and Majorana zero modes in one dimension, the proposals of Lutchyn, Sau, Das Sarma [53] and Oreg, Refael and van Oppen [54] were instrumental for the first attempts to experimentally probe the signatures of MZMs performed by Kouwenhoven and his group in Delft 2012 [55].[21] This work relied on superconducting nanowires with strong Rashba/-Dresselhaus spin-orbit interactions exposed to an external magnetic field. Here, the nanowire is a gated semiconductor deposited on an s-wave superconductor which by the application of a magnetic field results in a topological superconducting state [58]. A pedagogical and more formal treatment of this realization can be found in Christian Spånslätt's doctoral thesis on low-dimensional topological quantum matter, see [36].

[19]The layered oxide superconductor Sr_2RuO_4 and the superfluid ^3He are two examples that stand out when it comes to intrinsic p-wave superconductors [50].

[20]The (superconducting) proximity effect is a phenomenon which arises when a superconductor gets in contact with a conventional material. It enables the Cooper pairs in the superconductor to tunnel into the normal material causing a layer of the material to be superconducting. In Fu and Kanes' system the Cooper pairs diffuse into the surface edge states of the topological insulator, resulting in a topological superconducting surface state.

[21]More recently, one-dimensional Majorana zero modes have seen to emerge also in chains of magnetic (iron) atoms [56], [57]. The atoms are placed on a superconducting lead-substrate of s-wave type. By making use of scanning tunneling spectroscopy one found experimental signature of possible Majorana zero modes at the ends of the chain.

4.3 Integer Quantum Hall Effect

Any thesis which serves to review topological matter and invariants should be considered incomplete if a section on the integer quantum Hall effect is not included. This is by no means a section devoted to toy models but rather to realizations (which the name of this chapter also hints about). In 1980, von Klitzing, Dorda and Pepper provided the experimental motivation for the entire field of topological quantum matter [19]. Their experiment on the integer quantum Hall effect has been of crucial importance in the theory development of using topological invariants in physics, and, in particular, for understanding and topologically protected edge states.[22] The conventional Hall effect had been discovered a century earlier by Edwin Hall, who observed that the application of an electrical field in the presence of a magnetic field generated a current perpendicular to the electrical and magnetic fields [59]. Moreover, the ratio between the voltage, V_H, and the current, I, is described by a linear relationship through the Hall resistance, R_H, and Ohm's law:

$$R_H = \frac{V_H}{I} \ . \tag{4.57}$$

By considering a similar two-dimensional electron system in a strong magnetic field ($B > 5$ T) at very low temperatures ($T < 4$ K), von Klitzing noticed that the Hall resistivity was quantized in integer multiples n and that flat plateaus of the voltage would occur in the voltage-current spectrum at the same voltage regardless of the quality of the sample. In particular, he found that

$$R_{QH} = \frac{1}{n}\frac{e^2}{\hbar} \ , \tag{4.58}$$

in a precision better than 1 part in 10^5. The theoretical explanation for the quantized behavior and plateaus of the resistivity relies on the concept of filled *Landau levels*. Quantum mechanically, the motion of electrons being exposed to a strong magnetic field follows, due to the Lorentz force, cyclotron orbits which are quantized with energy

$$E_n = \hbar\omega(n + \frac{1}{2}) \ , \tag{4.59}$$

with the cyclotron frequency $\omega = \frac{eB}{m_e}$, m_e being the electron mass. Although they are very similar to the energy levels of the harmonic oscillators, these energy levels are referred to as Landau levels and are highly degenerate for strong magnetic fields. This means that for sufficiently large magnetic fields, i.e. $B > 5$ T as in the quantum Hall experiment, giving highly degenerate energy levels, there will be only a few filled Landau levels of relevance. Before introducing disorder in the two-dimensional electron system, we should justify how von Klitzing arrived at the astonishing result for the Hall resistance in (4.58). Neglecting the possibility of a substrate potential, the Hamiltonian for a two-dimensional non-interacting electron system in a magnetic field $\vec{B} = B\hat{z}$ is easily written down as[60]

$$H = \frac{1}{2m_e}(-i\hbar\frac{\partial}{\partial x} + eA_x)^2 + \frac{1}{2m_e}(-i\hbar\frac{\partial}{\partial y} + eA_y)^2 + V(x,y) \ , \tag{4.60}$$

[22] In fact, the main motivation of von Klitzing et al. was to accurately determine the value of the fine structure constant $\alpha = \frac{1}{137}$, of immence importance in the field of quantum electrodynamics.

where $V(x,y) = -eE_y y$ (assuming the electrical field to be in the y-direction). The inclusion of the electrical field forces the electrons to move not only in a cyclotron motion but they are also exposed to a linear drift. The setup for the corresponding quantum Hall experiment is illustrated in Figure 4.8.

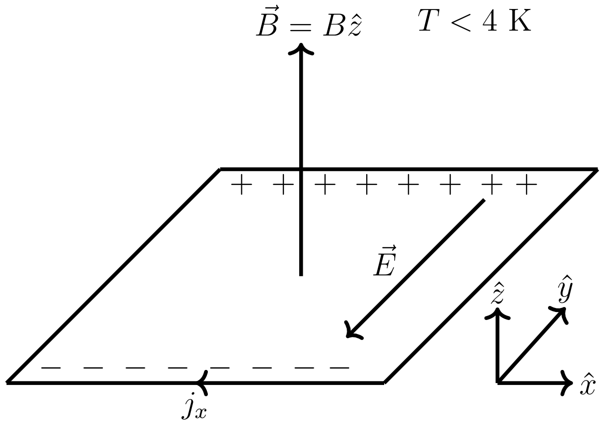

Figure 4.8: Schematic illustration of the quantum Hall experiment. The application of an electric field generates a current density perpendicular to the field. A crucial difference between this experiment and the original Hall experiment performed in 1879 is the temperature of the sample.

By imposing the *Landau gauge* $A_y = 0$, $A_x = -By$, with the x-dependence of the wavefunction being $\sim \mathrm{e}^{ik_x x}$ (plane wave), we may rewrite the Hamiltonian as

$$H = \frac{1}{2m_e}(\hbar k_x - eBy)^2 - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial y^2} - eE_y y = \frac{1}{2m_e}(\hbar k_x - eBy)^2 + \frac{p_y^2}{2m_e} - eE_y y \ , \quad (4.61)$$

which, if we neglect the last (linear) drift term, and shift the y-coordinate $y \to y - \frac{\hbar k_x}{eB}$, is precisely the Hamiltonian of a harmonic oscillator.[23] This motivates the striking resemblance betwen the Landau levels and the energy levels of the harmonic oscillator. Including all terms, the solution for the eigenenergies reads

$$E_n = \hbar\omega(n + \frac{1}{2}) - eE_y(y - \frac{p_y}{eB}) + \frac{m_e}{2}(\frac{E_y}{B})^2 \ . \quad (4.62)$$

Now, recall that the current density operator for a charged particle in a magnetic field with Hamiltonian $H = \frac{1}{2m_e}(\vec{p} - e\vec{A})^2 + V(\vec{r})$ in a potential $V(\vec{r})$ can obtained from

$$\hat{\vec{j}}(\vec{r}) = \frac{e}{m_e}\mathrm{Re}(\psi^*(\vec{r})(\vec{p} - e\vec{A})\psi(\vec{r})) \ , \quad (4.63)$$

and thus the x-component of the current density operator with our Hamiltonian is given by

$$\hat{j}_x = \frac{e}{m_e}(\hbar k_x + eBy) \ . \quad (4.64)$$

This current corresponds to the electrons having a drift velocity $v_d = -\frac{E_y}{B}$ in the x-direction, readily apparent in the last term in the energy spectrum in (4.62). By

[23]Translating the harmonic oscillator in position space does not affect the eigenenergies.

the Drude model the current density is given by

$$\vec{j}(\vec{r}) = en_e(\vec{r})\vec{v}_d \ , \tag{4.65}$$

n_e being the electron density, and, in particular, with the (absolute) magnitude of j_x given by

$$j_x = en_e \frac{E_y}{B} \ . \tag{4.66}$$

It remains to express the electron density in terms of the known variables. The density of a single electron flux quantum is given by

$$n_1 = \frac{1}{2\pi l^2} \ , l^2 = \frac{\hbar}{eB} \ , \tag{4.67}$$

with l being the *Larmor length.* Note that we assumed that each electron takes up an area πl^2, with the factor of 2 in the denominator of the single electron density taking spin degrees of freedom into account. Considering n filled Landau levels the electron number density is then given by

$$n_e = \frac{n}{2\pi l^2} = \frac{neB}{h} \ , \tag{4.68}$$

resulting in the current density

$$j_x = e(\frac{nBe}{h})(\frac{E_y}{B}) = \frac{ne^2}{h} E_y \ . \tag{4.69}$$

Finally, we need to turn our attention to Ohm's law, which in its most general form reads

$$j_\alpha = \sum_\beta \sigma_{\alpha\beta} E_\beta \ , \tag{4.70}$$

with $\sigma_{\alpha\beta}$ being the conductivity tensor. The only non-vanishing component of this tensor is σ_{xy}:

$$\sigma_{xy} = -\sigma_{yx} = \frac{j_x}{E_y} = \frac{ne^2}{h} \ , \tag{4.71}$$

assuming an isotropic material. Consequently, the longitudinal resistivity ρ_{xy} is simply the inverse of the conductivity:

$$\rho_{xy} = \frac{1}{\sigma_{xy}} = \frac{1}{n}\frac{h}{e^2} \ , \tag{4.72}$$

which checks out with the results of von Klitzing et al [19]. Having established that the Hall conductance is quantized at a quantum mechanical level, a note on the existence of plateaus in the Hall spectrum is in order. Introducing disorder in the system results in a broadening of the degenerate Landau levels. Each broadened Landau level has the non-perturbed Landau level in the center and away from the center there exists localized states. When sweeping the Fermi level (by tuning the gate-voltage) across these localized states we do not expect a change in the Hall current (since these states are assumed not to carry current) giving rise to plateaus in the conductance spectrum [61][62].

We have yet not discussed the relation between the quantum Hall effect and topology. The connection was made explicit by Thouless, Kohomoto, Nightingale and den Nijs in 1982 and is neatly summarized in the *TKNN-formula* [30]. Thouless et al. (indirectly) managed to relate the conductivity, σ_{xy}, in the integer quantum Hall effect to the Berry curvature and Chern numbers, discussed in Chapter 2.[24] By computing the conductivity on a torus[25] T^2 in a periodic potential and by making use of the famous Kubo formula they obtained[30]

$$\sigma_{xy} = \frac{e^2}{2\pi\hbar}\sum_{k=1}^{n}\int_{T^2}\vec{\mathcal{F}}_k \cdot d\vec{S} = \frac{e^2}{h}\sum_{k=1}^{n}\zeta_k = \frac{ne^2}{h}\ , \tag{4.73}$$

with $\vec{\mathcal{F}}_k$ being the Berry curvature and $\zeta_k = 1$ being the Chern number of each filled band k. The Hall conductivity thus constitutes a topological invariant and as such we may explain the robustness of the integer quantum Hall effect. Being an integer, the Chern number can not change continuously and therefore the Hall conductivity remains unchanged under smooth deformations. In particular, as we have seen in the SSH model and the Kitaev chain, a non-zero topological invariant is also accompanied by the existence of edge states, in agreement with the bulk-boundary correspondence. In the IQHE, these edge states are referred to as *Halperin states* [64]. The connection between the number of gapless chiral edge states and the TKNN topological invariant was made explicit by Hatsugai in the early 1990s [65]. These edge states are chiral since they move in one direction on one edge and the opposite direction on the other edge.

As of today, numerous of experiments similar to that of von Klitzing et al. have indicated the robust nature of the quantum Hall effect. Remarkably, the shape and condition of the sample does not influence the conductivity in any way. Comparisons between different materials have been made, for instance in gallium arsenide and silicon, where the agreement between the Hall resistance in the two systems has been found with a precision of a few parts in 10^{10} [66].

As stated in the introductory paragraph, the integer quantum Hall effect paved the way for the search for unconventional states of matter. In particular, it led to the discovery of other remarkable topological phenomena such as the fractional quantum Hall effect (FQHE) and the anomalous quantum Hall effect (AQHE) [67]–[69]. Perhaps most importantly, by making use of Duncan Haldane's model of graphene exhibiting an IQHE, Kane and Mele were able to establish the theoretical existence of so called *quantum spin Hall states* [70][71].[26] Their work, which eventually lead

[24] In fact, the real connection between the Berry phase and the TKNN-formula was provided by the American mathematical physicist Barry Simon in 1983 [63]. However, it should not come as a surprise that the word Berry curvature or Berry phase is not mentioned by Thouless et al. given the fact that Michael Berry introduced the concepts of geometrical phases in quantum physics a year after the TKNN-paper was published [27].

[25] One can also consider the two-dimensional magnetic Brillouin zone as the integration domain. Once imposing (twisted) periodic boundary conditions, this is topologically equivalent to the torus T^2.

[26] Bernevig and Zhang also proposed a quantum spin Hall model during the same time period, independent of the work by Kane and Mele [72].

to the realization of topological insulators, can be summarized in the *Quantum Spin Hall Effect* (QSHE), a cousin of the effect we have been considering in this section.[27] However, in contrast to the fractional or integer quantum Hall effect, achieving the quantum spin Hall effect does not require the application of a large magnetic field. The role of the magnetic field is instead played by spin-orbit interactions in the material. This means that quantum spin Hall systems respect time-reversal symmetry. Moreover, if time-reversal invariance is manifest in a spinful system we have seen in section 3.1 that the edge states come in pairs due to Kramer's degeneracy. By taking two copies of an IQHE-system, one copy with only spin down electrons and one copy with only spin up electrons with the magnetic fields of the systems having the same magnitude but opposite directions, the magnetic field of the combined system cancels. In particular, the edge states of the separated systems have different chiralities and combine into a single Kramer's pair. This is the recipe of engineering a spin Hall system in theory. In practice, Kane and Meles' proposal of graphene as a candidate for QSHE has proven not to be successful due to the small spin-orbit gap of the material. It should be stressed though that, already in 2007, just a year after Kane and Meles' discoveries the quantum spin Hall effect was experimentally realized in HgTe quantum wells [73].

4.4 Returning to the ten-fold way

So far, we have by no means covered all toy models or realizations of topological insulators or superconductors even in one dimension. However, in 2008, Schnyder, Ludwig, Furusaki and Ryu provided a framework for the classification of gapped systems in different symmetry classes in the ten-fold classification of topological insulators and superconductors [17]. By starting from Altland and Zirnbauers' work a decade earlier which discussed the different symmetry classes in the context of random matrix theory, and interpreting the random matrices as representations of non-interacting fermionic Hamiltonians, Schnyder and his collaborators managed to show that, in particular, three-dimensional topological insulators and superconductors can exist in five of the ten symmetry classes [41], [74].

We touched upon the framework already in the previous chapter, but then we were only able to discuss the classification in terms of symmetries. Now, we complete Table 3.1 by providing the possible topological invariants in specific dimensions for each symmetry class of non-interacting single-particle fermionic Hamiltonians.

[27] Kane and Meles' work in the field of topological quantum matter has been highly acclaimed. In the year of writing this thesis (2019) they were awarded the prestigious *Breakthrough Prize in Fundamental Physics*.

class	$\mathcal{C}$	$\mathcal{P}$	$\mathcal{T}$	$d = 1$	$d = 2$	$d = 3$
A (unitary)	-	-	-	-	$\mathbf{Z}$	-
AI (orthogonal)	-	-	1	-	-	-
AII (symplectic)	-	-	-1	-	$\mathbf{Z}_2$	$\mathbf{Z}_2$
AIII (chiral unitary)	1	-	-	$\mathbf{Z}$	-	$\mathbf{Z}$
BDI (chiral orthogonal)	1	1	1	$\mathbf{Z}$	-	-
CII (chiral symplectic)	1	-1	-1	$\mathbf{Z}$	-	-
D	-	1	-	$\mathbf{Z}_2$	$\mathbf{Z}$	-
C	-	-1	-	-	$\mathbf{Z}$	-
DIII	1	1	-1	$\mathbf{Z}_2$	$\mathbf{Z}_2$	-
CI	1	-1	1	-	-	$\mathbf{Z}$

Table 4.1: The tenfold classification of topological insulators and superconductors. The leftmost column indicates the Cartan label of the symmetry class followed by the different symmetries $\mathcal{C}$, $\mathcal{P}$ and $\mathcal{T}$ (chiral/sublattice symmetry, particle-hole symmetry and time-reversal symmetry respectively). If a symmetry is absent it is indicated with "-" and if it is present the entries are either ± 1 depending on whether the symmetry operators square to $+1$ or -1. Recall that the chiral symmetry, $\mathcal{C}$, only comes in one flavor, $\mathcal{C}^2 = +1$. The additional three columns indicate whether there exists topological invariants in the corresponding symmetry class in $d = 1, 2$ and 3 dimensions. If a $\mathbf{Z}$-entry is present it means that the topological invariant in the symmetry class can take any integer value. However, the $\mathbf{Z}_2$ invariant is more restricted and only takes two values, typically 0 or 1 or ± 1 depending on convention. Entries with "-" in the last three columns indicate that the system has no topological phase. Theoretically there exists topological invariants in dimensions $d > 3$ as well, but we only consider the physically interesting cases here.

The symmetry classes A, AI and AII are referred to as the standard *Wigner-Dyson classes* and have been well-investigated in physics in terms of Anderson localization of electrons in disordered solids [17] . By enforcing a sublattice symmetry on the classes one ends up with the symmetry classes AIII, BDI and CII which constitute the *chiral* classes. The remaining four symmetry classes D, C, CI and DIII are listed by Schnyder et al. as the superconducting *Bogoliubov-de Gennes classes* or the *BdG classes* [17]. This is since the non-interacting fermionic Hamiltonians in these classes can only be realized as superconductors. The other six classes (Wigner-Dyson and chiral) can host non-superconducting topological systems, e.g. topological insulators or band insulators as well. This does not imply that, for instance, the chiral classes BDI and CII can not have superconducting realizations. In fact, it is fairly standard to make use of the BdG formalism when dealing with these symmetry classes as well (since particle-hole symmetry is present), and therefore we may choose to refer to the classes as (chiral) BdG classes whenever BDI or CII has a superconducting realization.

In fact, in our discussion on the (one-dimensional) Kitaev model we chose the parameters Δ, t and μ to be real in order to be able to use the winding number as a topological invariant. By this choice the spinless Kitaev chain is transferred from symmetry class D to the chiral symmetry class BDI.[28] In agreement with Table 4.1, we obtained a $\mathbf{Z}$ topological invariant in section 4.2.3. In his original paper, Kitaev allowed his parameters to be complex and was thus required to compute a $\mathbf{Z}_2$ topological invariant (Pfaffian), readily apparent as an entry in the class D-row in Table 4.1 [15]. Moreover, by considering a *spinful* Kitaev chain and enforcing a time-reversal symmetry $\mathcal{T}$ with $\mathcal{T}^2 = -1$ one can even end up with a $\mathbf{Z}_2$-classification in symmetry class DIII.

Similarly, most conventionally the SSH model of polyacethyelene discussed in section 4.1 is put in the symmetry class AIII with a $\mathbf{Z}$ topological invariant. This is due to the apparent sublattice symmetry between A and B-atoms of the model. However, as we saw in section 4.1, the single-particle Hamiltonian of the model, $H_{\mathrm{SSH}}(k)$, also exhibits a time-reversal symmetry and a charge-conjugation symmetry why it may also be tempting to put it in the symmetry class BDI. In fact, it is really a matter of choice where to put the model and it depends on which symmetries are being enforced and which are considered accidental. When assigning a symmetry class to a particular model the rule of thinking is really based on what terms (associated with a certain type of symmetry) we allow to add to the Hamiltonian rather than what symmetries the model exhibit. With this basis of thinking it is also possible to put the SSH model in the symmetry classes BDI (all perturbations are required to have chiral, time-reversal symmetry,and particle-hole symmetry), D (all perturbations that are charge-conjugation symmetric are allowed but time-reversal symmetry or chiral symmetry can be broken), AI or A (only time-reversal symmetric perturbations allowed or all perturbations are allowed but the symmetries can be broken). However, in the latter case we can not say that the edge modes of the SSH model are topologically protected by symmetry.

Lastly, a comment on the quantum Hall insulator is in order. Since the integer quantum Hall effect necessarily requires a (net) magnetic field, time-reversal symmetry must be broken. Consequently, it is put in the symmetry class A with a $\mathbf{Z}$ topological invariant in $d = 2$ dimensions, that is the Chern number apparent in the TKNN-formula, equation (4.73). However, by taking two spinful copies of the quantum Hall insulator one can engineer the *Quantum Spin Hall Effect*, which does not require a magnetic field and respects time-reversal symmetry, see the discussion in section 4.3. This insulator then falls into the class AII with a $\mathbf{Z}_2$ topological invariant as shown by Kane and Mele [71].

Now, we have seemingly skipped to discuss Schnyder, Ryu, Furusaki and Ludwigs' major contribution to the field of topological quantum matter, the classification of *three-dimensional* topological superconductors and insulators. These systems are an active area of research due to their (recent) promising realizations in nature

[28] Here, the Kitaev chain refers to the topological phase of the Kitaev model, with specified parameters $\Delta = t > 0$ and $\mu = 0$, where there are unpaired Majorana edge modes.

[75]–[77]. This is out of scope of this thesis, which covers almost exclusively non-interacting one-dimensional topological systems. However, the thesis reaches beyond the tenfold classification of topological insulators and superconductors in the sense that the following chapters will involve not only the classification of *gapped* but also *gapless* systems. We shall, in particular, see that non-trivial phases in the chiral and non-chiral BdG classes which are gapless are classified not exclusively by a topological invariant (winding number or a Pfaffian) but also by an extensive degree of freedom of the bulk, namely the *central charge* of the bulk conformal field theory.

5

Topology and Edge Modes of Critical Systems in Class BDI

In the previous chapter we swept the notion of topological critical systems under the rug, that is, to address the issue what happens precisely at the topological phase transition, when the energy gap closes and the topological invariant changes from trivial to non-trivial (or vice versa), see for instance the critical case of the SSH model in Figure 4.3. Having established that the tenfold classification of topological insulators and superconductors in Table 4.1 is valid only for gapped quantum systems, it is clear that additional work is needed to be done on gapless chains. Therefore, this chapter purports to review and analyze the very recent work by Verresen, Jones and Pollmann (VJP) who have obtained a classification of superconducting critical systems in the BDI symmetry class, which may possibly be extended to the remaining chiral classes and the BdG classes [18]. The latter (original work) is the topic of the next chapter. The discussion below thus follows the paper "Topology and edge modes in quantum critical chains" closely but also an earlier paper by Verresen, Pollmann and Moessner, "One-dimensional symmetry protected topological phases and their transitions" [78]. Additional details are provided by a third paper by Jones and Verresen, "Asymptotic correlations in gapped and critical topological phases of 1D quantum systems" from 2018 [79].

5.1 α-chains and stacking Kitaev chains

To be able to discuss gapped and gapless topological phases in the BDI symmetry class we employ the notation used by Verresen, Jones and Pollmann and define the translation-invariant spinless *α-chain*:

$$H_\alpha = \frac{i}{2}\sum_{n\leq 1} \tilde{\gamma}_n \gamma_{n+\alpha} \ , \ \alpha \in \mathbf{Z} \ , \tag{5.1}$$

where $\alpha = 1$ corresponds to the topological phase of the Kitaev model, see equation (4.32) with the hopping parameter $t = \frac{1}{2}$ and $\alpha = 0$ is the non-topological phase in equation (4.26) with $\mu = 1$. In general, (5.1) can be seen as a Kitaev chain with range α, see Figure 5.1.[1] In the previous chapter we saw that the Kitaev chain, H_1, exhibits two Majorana zero modes, one real mode γ_1 on the left edge and an

[1] In contrast to the previous chapter, we will refer to the topological phase of Kitaev's model, H_1, simply as the *Kitaev chain* in the following. Similarly, we refer to H_0 as the trivial or non-topological phase.

imaginary mode $\tilde{\gamma}_N$ on the right edge, whereas the trivial chain, H_0, has no edge modes. More generally, H_α has $|\alpha|$ Majorana zero modes per edge.

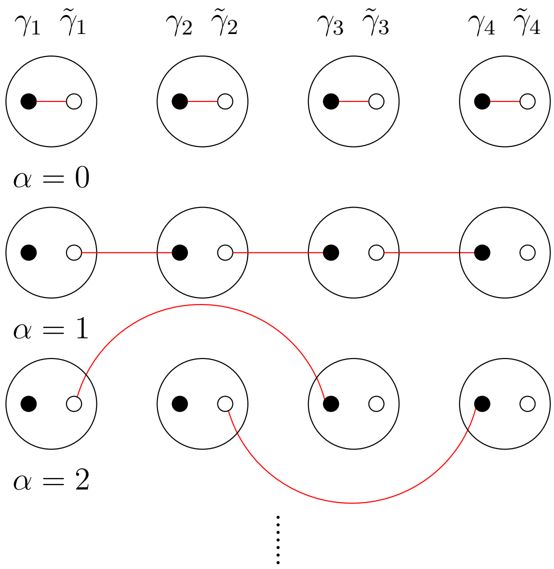

Figure 5.1: Illustration of one-dimensional α-chains. Each fermionic cell indicated with a circle includes two Majoranas, γ_n and $\tilde{\gamma}_n, n = 1, ..., 4$ denoted by a filled and an unfilled circle respectively. Note that H_α represents a Kitaev chain with (coupling) range α.

Note that we also allow the integer α to be negative. This corresponds to a spatially inverted chain, i.e a chain with the left and right ends being swapped. The α-chain is clearly invariant under the spinless (BDI) time-reversal symmetry transformation $\mathcal{T} = \mathcal{K}$, $\mathcal{K}$ being the complex conjugation operator in the occupation number basis:

$$\begin{aligned}\mathcal{T} H_\alpha \mathcal{T}^{-1} &= \mathcal{K}\frac{i}{2}\sum_n \tilde{\gamma}_n \gamma_{n+\alpha}\mathcal{K} = -\frac{i}{2}\mathcal{K}\sum_n \tilde{\gamma}_n \gamma_{n+\alpha}\mathcal{K} \\ &= -\frac{i}{2}\mathcal{K}\sum_n i(c_n^\dagger - c_n)(c^\dagger + c_n)\mathcal{K} = \frac{i}{2}\sum_n i(c_n^\dagger - c_n)(c^\dagger + c_n) = H_\alpha \ ,\end{aligned}$$

that is, H_α commutes with the time-reversal operator $\mathcal{T}$. In fact, we may consider the α-chain as a basis for all translation-invariant Hamiltonians in the BDI class, generated by taking linear combinations of (5.1). This should come as no surprise if we consider a generic non-interacting BDI Hamiltonian:

$$H_{\mathrm{BDI}} = \frac{i}{2}\sum_{n,m} t_{nm}\tilde{\gamma}_n\gamma_m + (\mathcal{T}\text{−preserving interactions}) \ . \tag{5.2}$$

Note that combinations of the type $i\gamma_n\gamma_m$ or $i\tilde{\gamma}_n\tilde{\gamma}_m$ are not allowed since such terms explicitly violate time-reversal symmetry. The coefficients t_{nm} are real by $\mathcal{T}$-symmetry and hermiticity. By also enforcing translational symmetry, $t_{nm} = t_{m-n}$ and performing the change of variables $\alpha = m - n$ we get a neat expression for the full BDI Hamiltonian as

$$H_{\mathrm{BDI}} = \frac{i}{2}\sum_{\alpha,n} t_\alpha \tilde{\gamma}_n \gamma_{n+\alpha} = \sum_\alpha t_\alpha H_\alpha \ , \tag{5.3}$$

where we take the sum over α to be finite and $t_\alpha \in \mathbf{R}$. Since t_α is real it follows that H_{BDI} is time-reversal symmetric (we just checked that so is the case for H_α) and hermitian.
A concept which will prove particularly useful in the generalization of Verresen, Jones and Pollmann to include symmetry class CII (the topic of next chapter) concerns *stacking* of Kitaev chains. As also stressed by Verresen et al. , stacking $\alpha > 0$ Kitaev chains (described by the Hamiltonian H_1) on top of each other can equivalently be seen as a single Kitaev chain with range α.[2] In Figure 5.2, the situation is illustrated for $\alpha = 2$. On the one hand, stacking enforces us to introduce a unit cell (containing multiple "domino" building blocks) but on the other hand the stacked chains can be rewritten in a translation-invariant manner.[3]

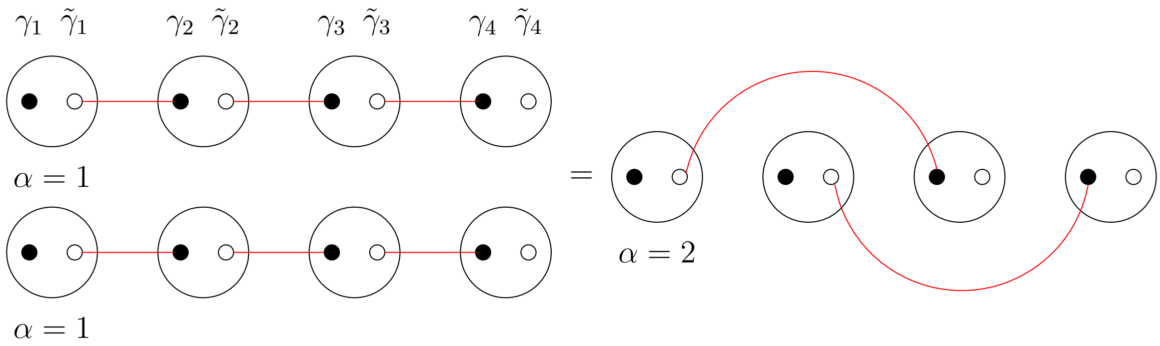

Figure 5.2: Stacking two Kitaev chains on top of each other (H_α with $\alpha = 1$) is equivalent to considering the translation-invariant H_2 chain.

We can also stack more complicated (translation-invariant) Kitaev chains on top of each other, for instance two different BDI chains $H^{(1)}_{\mathrm{BDI}}$ and $H^{(2)}_{\mathrm{BDI}}$ formed by taking linear combinations of Kitaev chains with weighting coefficients $t^{(1)}_\alpha$ and $t^{(2)}_\alpha$. Then, the stacked system is described by the Hamiltonian[4]

$$H = \frac{i}{2}\sum_{n,\alpha}(\tilde{\gamma}_{n,1}, \tilde{\gamma}_{n,2})T_\alpha \begin{pmatrix} \gamma_{n+\alpha,1} \\ \gamma_{n+\alpha,2} \end{pmatrix} \ , \ T_\alpha = \begin{pmatrix} t^{(1)}_\alpha & 0 \\ 0 & t^{(2)}_\alpha \end{pmatrix} \ , \tag{5.4}$$

introducing a unit cell with two sites. In general, in a system with N sites, T_α is a $N \times N$ real matrix and we may write

$$H = \frac{i}{2}\sum_{n}(\tilde{\gamma}_{n,1}, \tilde{\gamma}_{n,2}, \ldots, \tilde{\gamma}_{n,N})T_\alpha(\gamma_{n+\alpha,1}, \gamma_{n+\alpha,2}, \ldots, \gamma_{n+\alpha,N})^T \ . \tag{5.5}$$

[2] To ease potential confusion: although the term Kitaev chain is exclusively used for the $\alpha = 1$-chain, we may still view a generic α-chain ($\alpha > 1$) as a Kitaev chain with range α described by the Hamiltonian H_α.

[3] This is not *generally* true. For instance, consider stacking the Kitaev chain H_1 and the critical Majorana chain $H_0 + H_1$. It is impossible to rewrite the stacked system as a single translation-invariant chain.

[4] Certainly, BDI chains which explicitly break translational invariance, i.e have a unit cell structure can be stacked as well. Then, each chain (i) is described by a set of numbers $T^{(i)}_\alpha$ in a $N \times N$ matrix (N being the number of sites in the unit cell) and the full Hamiltonian is specified by the real matrix $T_\alpha = \mathrm{diag}(T^{(1)}_\alpha, T^{(2)}_\alpha, \ldots)$.

Returning to translation-invariant BDI chains it is clear that the coefficients t_α uniquely define the Hamiltonian, H_{BDI}. In particular, since the basis elements H_α by themselves give rise only to *gapped* topological phases, the relationship between the weighting coefficients becomes crucial in order to obtain a BDI Hamiltonian with *gapless* degrees of freedom. Of course, we could also equivalently consider the Fourier transform of the weighting coefficients as the fundamental object of interest:

$$f(k) := \sum_\alpha t_\alpha \mathrm{e}^{ik\alpha} \ , \tag{5.6}$$

which has a one-to-one correspondence with the Hamiltonian, H_{BDI}. By writing $f(k) = \epsilon_k \mathrm{e}^{i\varphi_k}$, $\epsilon_k, \varphi_k \in \mathbf{R}$[5], one can show that this particular function diagonalizes the BDI Hamiltonian by a Bogoliubov rotation with a single-particle spectrum ϵ_k such that [18]

$$H_{\text{BDI}} = \sum_k \epsilon_k \left(\frac{1}{2} - d_k^\dagger d_k \right) \ , \tag{5.7}$$

with $\begin{pmatrix} d_k \\ d_{-k}^\dagger \end{pmatrix} = \exp(i\varphi_k \frac{\sigma_x}{2}) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}$ being the Bogoliubov-transformed fermionic operators. For gapped systems with $\epsilon_k \neq 0$, $f(k) = \epsilon_k \mathrm{e}^{i\varphi_k}$ is a well-defined function on the unit circle. It therefore makes sense to consider the topological invariant for gapped BDI chains as a winding number, ν, defined by the number of loops $f(k)$ winds around the origin in the complex plane such that

$$\nu = \frac{1}{2\pi i} \int_{1\text{BZ}} dk \frac{f'(k)}{f(k)} \ . \tag{5.8}$$

This definition of a topological invariant breaks down for gapless BDI chains. However, the problem can be solved by performing an analytical continuation of $f(k)$ to the entire complex plane, i.e., with abuse of notation we take $f(k) \to f(z) = f(\mathrm{e}^{ik})$ in such a way that

$$f(z) = \sum_\alpha t_\alpha z^\alpha \ , \tag{5.9}$$

which is a complex meromorphic function with the number of poles and zeros to be determined. In particular, forming a gapless system using e.g. the gapless Hamiltonian $H_{\text{BDI}} = H_0 + H_1$ corresponds to the complex function $f(z) = z + 1$, which has the zero $z_0 = -1$ at the unit circle, or equivalently $f(z_0) = f(\mathrm{e}^{ik_0}) = 0$ for momentum $k_0 = \pm\pi$. Now, the winding number, ν, can be calculated using Cauchy's argument principle as[6]

$$\nu = N_Z - N_P \ , \tag{5.10}$$

N_Z being the number of zeros of $f(z)$ inside the unit circle $|z| = 1$ and N_P being the number of poles (counting multiplicities) inside $|z| = 1$. The right-hand side of equation (5.10) is well-defined also in the gapless case. Still, the introduction of the complex, meromorphic function $f(z = \mathrm{e}^{ik})$ may seem ad-hoc. However, as a

[5] It should come as no surprise that any complex function expressed as a finite sum of weighted exponentials can be written as a single exponential with an amplitude. This is due to the harmonic addition theorem [80].

[6] A more detailed treatment is provided in section 4.2.2.

consistency check we may in fact show, by means of a unitary transformation, that it coincides with the function $h(z)$ in (4.46) we used to compute the winding number of Kitaev's model. The calculation is provided in its entirety in Appendix B.

5.2 Majorana edge modes in gapless systems

It is in order to give a physical interpretation of the topological invariant introduced in the previous section. For gapped systems, e.g. the individual α-chains readily apparent in Figure 5.1, it should probably come as no surprise that the winding number counts Majorana edge modes. H_α has the associated complex, meromorphic function $f(z) = z^\alpha$ with the winding number $\nu = \alpha$ and the (total) number of Majorana edge modes being $2|\alpha|$ as discussed above. However, using our construction of the BDI Hamiltonian, equation (5.3), we will show below that localized Majorana edge modes emerge in gapless BDI systems as well. Verresen, Jones and Pollmann have chosen to summarize these statements in a theorem [18]:

Theorem 1 *If the topological invariant $\nu > 0$, then*

- *each edge has ν Majorana zero modes*
- *the modes have a localization length $\xi_i = -\frac{1}{\ln|z_i|}$ with z_i being the ν largest zeros of $f(z)$ within the unit disk.*
- *the modes on the left (right) are real (imaginary)*

If the topological invariant $\nu < -2c \leq 0$, with $2c$ being the number of zeros of $f(z)$ on the unit circle, the left (right) edge has $|\nu + 2c|$ imaginary (real) edge modes with localization length $\xi_i = \frac{1}{\ln|z_i|}$, with z_i being the $|\nu + 2c|$ smallest zeros outside the unit disk. For any other value of ν, there exists no edge modes.

As of now, it is not obvious why the number of zeros of $f(z)$ *on* the unit circle is chosen to be precisely $2c$, but it will become clear at the end of the next section. In particular, the number c will be given a special meaning and contributes to the topological classification of gapless systems in the BDI class.
Every theorem should be accompanied by a proof. Here, we will provide the proof outlined by Verresen, Jones and Pollmann but be somewhat more explicit [18]. The proof of the case $\nu \leq 0$ relies heavily on the case $\nu > 0$. Starting with the latter, the basic idea of the proof is to construct a Majorana edge mode (at either the left edge or the right edge) which commutes with the BDI Hamiltonian, (5.3) and is normalizable. Let us choose the left edge and construct for the ν largest zeros z_i *inside* the unit circle a *real* edge mode:

$$\gamma^{(i)}_{\text{left}} = \sum_{n \geq 1} b^{(i)}_n \gamma_n \ . \tag{5.11}$$

Assuming the coefficients $b^{(i)}_n$ to be real, it follows that $\gamma^{(i)}_{\text{left}}$ is hermitian and real ($\mathcal{T}\gamma^{(i)}_{\text{left}}\mathcal{T}^{-1} = \gamma^{(i)}_{\text{left}}$). Moreover, we require that the different modes anti-commute such that $\{\gamma^{(i)}_{\text{left}}, \gamma^{(j)}_{\text{left}}\} \sim 2\delta_{ij}$ and $|b^{(i)}_n| \sim |z_i|^n$. The latter condition immediately implies that $\xi_i \sim -\frac{1}{\ln|z_i|}$ since we may write [7]

$$b_n^{(i)} \sim \mathrm{e}^{-n/\xi_i} \ , \tag{5.12}$$

i.e. the $b_n^{(i)}$:s are exponentially localized.
To require that $\gamma_{\text{left}}^{(i)}$ is an edge mode we require the commutator $[\gamma_{\text{left}}^{(i)}, H_{\text{BDI}}]$ to vanish

$$[\gamma_{\text{left}}^{(i)}, H_{\text{BDI}}] = 0 \ , H_{\text{BDI}} = \sum_{\alpha=-\alpha_1}^{\alpha_2} t_\alpha H_\alpha = \frac{i}{2} \sum_{\alpha=-\alpha_1}^{\alpha_2} t_\alpha \Bigg(\sum_{n \in \text{sites}} \tilde{\gamma}_n \gamma_{n+\alpha} \Bigg) \ , \tag{5.13}$$

where $\alpha_1, \alpha_2 \in \mathbf{N}$ $(< \infty)$ are introduced to make the sum over α finite-ranged. Evaluating the commutator explicitly gives us:

$$[\gamma_{\text{left}}^{(i)}, H_{\text{BDI}}] = \frac{i}{2} \sum_{a \geq 1} \sum_{\alpha} t_\alpha \sum_n b_a^{(i)} [\gamma_a, \tilde{\gamma}_n \gamma_{n+\alpha}] = 0 \ , \tag{5.14}$$

where

$$\begin{aligned}
[\gamma_a, \tilde{\gamma}_n \gamma_{n+\alpha}] = [\gamma_a, \tilde{\gamma}_n]\gamma_{n+\alpha} + \tilde{\gamma}_n [\gamma_a, \gamma_{n+\alpha}] &= (\{\gamma_a, \tilde{\gamma}_n\} - 2\tilde{\gamma}_n \gamma_a)\gamma_{n+\alpha} + \tilde{\gamma}_n(\{\gamma_a, \gamma_{n+\alpha}\} - 2\gamma_{n+\alpha}\gamma_a) \\
&= -2\tilde{\gamma}_n \gamma_a \gamma_{n+\alpha} - 2\tilde{\gamma}_n \gamma_{n+\alpha}\gamma_a + 2\tilde{\gamma}_n \delta_{a,n+\alpha} \\
&= -4\tilde{\gamma}_n \delta_{a,n+\alpha} + 2\tilde{\gamma}_n \gamma_{n+\alpha}\gamma_a - 2\tilde{\gamma}_n \gamma_{n+\alpha}\gamma_a + 2\tilde{\gamma}_n \delta_{a,n+\alpha} \\
&= -2\tilde{\gamma}_n \delta_{a,n+\alpha} \ ,
\end{aligned}$$

and therefore (5.14) reduces to

$$[\gamma_{\text{left}}^{(i)}, H_{\text{BDI}}] = -i \sum_{a \geq 1} \sum_{\alpha} t_\alpha \sum_n b_a^{(i)} \tilde{\gamma}_n \delta_{a,n+\alpha} = -i \sum_{n \geq 1} \sum_{a \geq 1} t_{a-n} b_a^{(i)} \tilde{\gamma}_n = 0 \ . \tag{5.15}$$

Introducing $\mathcal{C}_n = \sum_{a \geq 1} t_{a-n} b_a^{(i)}$ we get the condition

$$-\, i \sum_{n \geq 1} \mathcal{C}_n \tilde{\gamma}_n = 0 \ , \tag{5.16}$$

giving us a set of constraints $\{\mathcal{C}_n\} = 0$. Now, it is in order to consider different cases. Considering the case $N_P = 0$ we have $t_{\alpha<0} = 0$ (recall that $\alpha < 0$ corresponds to poles), and therefore $\mathcal{C}_n$ contains all the coefficients $t_{\alpha>0}$ of $f(z)$. This means that, upon taking $b_a^{(i)} = z_i^{a-1}$, we get

$$\mathcal{C}_n = \sum_{a \geq 1} z_i^{a-1} t_{a-n} = \sum_{a \geq 1} z_i^{a-1-n} z_i^n t_{a-n} = z_i^{n-1} f(z_i) \ , \tag{5.17}$$

and thus all constraints are trivially fulfilled. If z_i is real this defines a real Majorana mode which is normalizable:

$$\{\gamma_{\text{left}}^{(i)}, \gamma_{\text{left}}^{(i)}\} = \sum_{n \geq 1} \sum_{m \geq 1} z_i^{n-1} z_i^{m-1} \{\gamma_n, \gamma_m\} = 2 \sum_{n \geq 1} \sum_{m \geq 1} z_i^{n-1} z_i^{m-1} \delta_{nm} = 2 \sum_{n \geq 1} z_i^{2(n-1)} \ .$$

[7] Since z_i is a complex number inside the unit circle it must have $|z_i| < 1$ and thus $|z_i| \sim \mathrm{e}^{-1/\xi_i}$ with $0 < \xi_i < \infty$ should be a fair parametrization.

The sum is easily evaluated as a geometric sum:

$$\{\gamma_{\text{left}}^{(i)}, \gamma_{\text{left}}^{(i)}\} = 2\sum_{n\geq 1} z_i^{2(n-1)} = \frac{2}{z_i^2}\sum_{n\geq 1}(z_i^2)^n = \frac{2}{z_i^2}\left(\frac{1}{1-z_i^2} - 1\right) = \frac{2}{1-z_i^2} \neq 0 \ ,$$

where we had to remove the first term "1" from the sum $\sum_{k=0}^{\infty} x^k$ since we start our summation at $n = 1$ rather than at $n = 0$. The anti-commutator is obviously non-zero for all z_i and therefore we conclude that $\gamma_{\text{left}}^{(i)}$ is normalizable. Note that this is really a result of taking $b_n^{(i)} = z_i^{n-1}$ rather than perhaps the more intuitive form $b_n^{(i)} = z_i^n$. This form would not give a normalized solution for $z_i = 0$. Considering z_i to be complex we may instead pick $b_n^{(i)} = z_i^{n-1} + \bar{z}_i^{n-1}$, which is also a solution since γ_n is hermitian. This is consistent with z_i and $\bar{z}_i$ both being zeros to $f(z)$ (if z_i are complex the zeros come in complex conjugate pairs, since the coefficients t_α are real), i.e. $f(z_i) = f(\bar{z}_i) = 0$. [8] Now, we consider the case when $N_P > 0$. Denote by $\{\tilde{z}_s\}$ the N_P *smallest* zeros of $f(z)$. Then consider the ansatz

$$b_a^{(i)} = z_i^a + \sum_{s=1}^{N_P} \lambda_s^{(i)} \tilde{z}_s^a \ . \tag{5.18}$$

Note that, now, the exponent in z is a rather than $a-1$, which we needed to have normalizability in the previous case when $z_i = 0$. However, since $N_P > 0$ we must have $z_i \neq 0$. Otherwise it would be subtracted by the pole. As in the previous case, we have $t_{\alpha<-N_P} = 0$ and therefore we expect $\mathcal{C}_{n>N_P}$ to be trivially fulfilled by the zeros of $f(z)$. We still have N_P conditions left to consider. Using the ansatz in (5.18) and demanding $[\gamma_{\text{left}}^{(i)}, H_{\text{BDI}}] = 0$, the following condition has to be fulfilled:

$$\sum_{a\geq 1} t_{a-n}(z_i^a + \sum_{s=1}^{N_P} \lambda_s^{(i)} \tilde{z}_s^a) = 0 \Rightarrow -\sum_{a\geq 1} t_{a-n} z_i^a = \sum_{s=1}^{N_P} \underbrace{\sum_{a\geq 1} t_{a-n} \tilde{z}_s^a}_{=A_{ns}} \lambda_s^{(i)} \ , \tag{5.19}$$

giving us a problem of the type $A\lambda = b$ (summation over s is implied):

$$A_{ns}\lambda_s^{(i)} = -\sum_{a\geq 1} t_{a-n} z_i^a \ . \tag{5.20}$$

If z_i is non-degenerate the claim is that the matrix A is invertible. Using the fact that $f(\tilde{z}_s) = 0$ and $\tilde{z}_s \neq 0$ we may rewrite the matrix A_{ns}. Recall that

$$f(\tilde{z}_s) = \sum_{\alpha} t_\alpha \tilde{z}_s^\alpha = \sum_{\alpha\leq n-1} t_{-\alpha}\tilde{z}_s^{-\alpha} + \sum_{\alpha=n}^{N_P} t_{-\alpha}\tilde{z}_s^{-\alpha} = 0 \Rightarrow \sum_{\alpha\leq n-1} t_{-\alpha}\tilde{z}_s^{-\alpha} = -\sum_{\alpha=n}^{N_P} t_{-\alpha}\tilde{z}_s^{-\alpha} \ ,$$

since we must have $t_{\alpha<-N_P} = 0$. By shifting the indices in A_{ns} such that $a-n \to -\alpha$ we have

$$A_{ns} = \sum_{a\geq 1} t_{a-n}\tilde{z}_s^a = \sum_{\alpha\leq n-1} t_{-\alpha}\tilde{z}_s^{n-\alpha} = \tilde{z}_s^n \sum_{\alpha\leq n-1} t_{-\alpha}\tilde{z}_s^{-\alpha} \ , \tag{5.21}$$

[8] Another difficulty arises when z_i is degenerate. We refer the interested reader to the supplemental material in [18].

and combined with the line above, A, reads

$$A_{ns} = -\sum_{\alpha=n}^{N_P} t_{-\alpha} \tilde{z}_s^{n-\alpha} \ , \tag{5.22}$$

which, by row-reduction, can be reduced to a *Vandermonde* matrix with a known determinant $\prod_{1\leq s'<s\leq N_P}(\tilde{z}_s - \tilde{z}_{s'}) \neq 0$.[9] We show this in the case where, for simplicity, all $t_\alpha = -1$. In a matrix representation, A is then given by

$$\begin{aligned} A &= \begin{pmatrix} 1+\tilde{z}_1^{-1}+...+\tilde{z}_1^{1-N_P} & ... & 1+\tilde{z}_{N_P}^{-1}+...+\tilde{z}_{N_P}^{1-N_P} \\ 1+\tilde{z}_1^{-1}+...+\tilde{z}_1^{2-N_P} & ... & ... \\ ... & ... & ... \\ 1+\tilde{z}_1^{-1}+...+\tilde{z}_1^{N_P-N_P} & ... & 1+\tilde{z}_{N_P}^{-1}+...+\tilde{z}_{N_P}^{N_P-N_P} \end{pmatrix} \\ &\sim \begin{pmatrix} 1+\tilde{z}_1^{-1}+...+\tilde{z}_1^{1-N_P} & ... & 1+\tilde{z}_{N_P}^{-1}+...+\tilde{z}_{N_P}^{1-N_P} \\ \tilde{z}_1^{2-N_P} & ... & ... \\ ... & ... & ... \\ \tilde{z}_1^{N_P-N_P} & ... & \tilde{z}_{N_P}^{N_P-N_P} \end{pmatrix} \\ &\sim \begin{pmatrix} \tilde{z}_1^{1-N_P} & ... & \tilde{z}_{N_P}^{1-N_P} \\ \tilde{z}_1^{2-N_P} & ... & ... \\ ... & ... & ... \\ \tilde{z}_1^{N_P-N_P} & ... & \tilde{z}_{N_P}^{N_P-N_P} \end{pmatrix} , \end{aligned}$$

by performing successive row-reduction. Clearly, there is a geometric progression in each column. Therefore there is a unique solution for each $\lambda^{(i)}$. The situation is different if we have degeneracies in $\tilde{z}_s$, then one has to turn to derivatives.[10] The case of complex zeros is dealt with similarly as in the case $N_P = 0$, that is, we take the real and imaginary combination of the solution.[11]

Next, consider the case when the winding number satisfies $\nu < -2c \leq 0$, with $2c \in \mathbf{N}$ being the number of zeros on the unit circle. Then, we can not construct a real edge mode on the left side of the chain, since the modes will not be normalizable (i.e. the anti-commutator between the Majorana edge modes will vanish!). We could instead try to construct an imaginary edge mode on the left, or equivalently a real edge mode on the right. This means that if we are able to construct a real edge mode on the left for the *spatially inverted* system everything is fine. Hence, to prove the theorem, we need to be able to show that if the original system has winding number ν, the spatially inverted system has winding number $\nu_{\text{inv}} = -(\nu+2c)$. Then, indeed, if $\nu_{\text{inv}} > 0$ the number of imaginary edge modes of the original system is $|\nu + 2c|$ (according to the discussion above) and if $\nu_{\text{inv}} \leq 0$ there are no edge modes at all. In the original system we are considering the meromorphic function $f(z)$

[9] A Vandermonde matrix, $V_{ij} = \alpha_i^{j-1}$, is a matrix where the terms are arranged in geometric progression in each row. In our case we work with the transpose, which is also perfectly fine. Its determinant is particularly simple to compute as $\det(V) = \prod_{1\leq i<j\leq n}(\alpha_j - \alpha_i)$.

[10] See [18] for a treatment on degenerate zeros in the case when $N_P = 0$.

[11] We know that $z_i \neq \in \{\tilde{z}_s\}$. However, we may have $\bar{z}_i \in \{\tilde{z}_s\}$ and then the real and imaginary solutions are linearly independent.

which has the topological invariant ν. In the spatially inverted system we instead have $f_{\mathrm{inv}}(z) = f(\frac{1}{z})$ (since spatial inversion comes down to swapping $t_\alpha \leftrightarrow t_{-\alpha}$).[12] Then, according to the fundamental theorem of algebra we may write[13]

$$f(z) = \frac{1}{z^{N_P}} \prod_i (z - z_i) \ , \tag{5.23}$$

where N_P is the number of poles of $f(z)$ inside the unit circle (counting multiplicity). We also define N as the total number of zeros such that

$$N = N_Z + 2c + N_0 \ , \tag{5.24}$$

with $2c$ being the zeros on the unit circle and N_0 being the zeros outside the unit circle. Now, we have to derive an expression for $f_{\mathrm{inv}}(z)$ using (5.23):[14]

$$\begin{aligned} f_{\mathrm{inv}}(z) = f(\frac{1}{z}) = \frac{1}{z^{-N_P}} \prod_{i=1}^{N} (\frac{1}{z} - z_i) &= \frac{1}{z^{N-N_P}} \prod_{i=1}^{N} (1 - z z_i) \\ &= \frac{1}{z^{N-N_P}} \prod_{i \neq j : z_j = 0}^{N} (\frac{1}{z_i} - z) z_i = \frac{(-1)^N}{z^{N-N_P}} \prod_{i=1}^{N} (z - \frac{1}{z_i}) z_i \ , \end{aligned}$$

and therefore we conclude that

$$f_{\mathrm{inv}}(z) \propto \frac{1}{z^{N-N_P}} \prod_{i=1}^{N} (z - \frac{1}{z_i}) \ , \tag{5.25}$$

that is we have $N_{P\mathrm{inv}} = N - N_P$. Moreover, $f(\frac{1}{z})$ must have the same number of zeros inside the unit circle as $f(z)$ has outside the unit circle, that is $N_{Z\mathrm{inv}} = N_0$. Then, the topological invariant for the inverted system is easily computed as

$$\begin{aligned} \nu_{\mathrm{inv}} = N_{Z\mathrm{inv}} - N_{P\mathrm{inv}} &= N_0 - (N - N_P) \\ &= N_0 - (N_Z + N_0 + 2c - N_P) = -(N_Z - N_P) - 2c = -\nu - 2c \ , \end{aligned}$$

and we have proven that $\nu_{\mathrm{inv}} = -\nu - 2c$. This completes the proof of Theorem 1. For gapped systems we note that ν is the only quantity which determines the topological properties. Next, let us discuss the physics of gapless systems forcing us to investigate the $2c$ zeros on the unit circle further.

[12] Note that $H_\alpha \to H_{-\alpha}$ corresponds to a spatial inversion of the chain.

[13] This expression does not take multiplicity into account. On the other hand we do not restrict the zeros z_i to be distinct. A more general expression for a function $g(z)$ with $z_1 ... z_N$ zeros with multiplicities m_j, $j = 1...N$ and $z'_1 .... z'_{N_P}$ poles with multiplicity m'_k, $k = 1...N_P$ reads $g(z) = \mathrm{e}^{h(z)} \frac{\prod_{i=1}^{N} (z - z_i)^{m_i}}{\prod_{j=1}^{N_P} (z - z'_j)^{m'_j}}$, where the exponential is a positive function (note that $h(z)$ is chosen to be zero in (5.23)).

[14] The case when there are z_i :s equal to zero has to be treated carefully. This corresponds to $N_P = 0$, cf. the first part of the proof.
Then one has to write $f_{\mathrm{inv}}(z) = \frac{1}{z^{N-N_P}} \left(\prod_{i \neq j : z_j = 0, j \in [1,r]}^{N} (\frac{1}{z_i} - z) z_i + \underbrace{\prod_{j=1}^{r} 1}_{=1} \right)$ which still gives the same $N_{P\mathrm{inv}}$.

5.3 Conformal Field Theory and Low-Energy Theory

In this section we turn our attention to the gapless case at which $f(z)$ necessarily has zeros *on* the unit circle. For now, assume these zeros to be *non-degenerate*. Then, since the weighting coefficients t_α are real it follows by the fundamental theorem of algebra that the zeros of $f(z)$, $\{z_0\}$, are either purely real or come in complex conjugated pairs.[15] Focusing on the latter case this means that $f(z_0) = f(\mathrm{e}^{\pm ik_0}) = 0$, but since $f(k) = \epsilon_k \mathrm{e}^{i\varphi_k}$ it also implies that

$$\epsilon_k \sim (k \pm k_0) \ , \tag{5.26}$$

assuming the zeros to be non-degenerate. The linear low-energy dispersion relation implies that the *dynamical critical exponent*, $z = 1$ for the critical system, i.e. the *correlation length* ξ and the *relaxation time* τ are directly proportional to each other, $\xi \sim \tau$, and Lorentz symmetry is manifest. The quantities ξ and τ are characteristic length and time scales for any critical system (not only topological ones) and are covered in detail in the appendix on phase transitions, see Appendix C.
Now, the claim is that each zero contributes with a (massless) Majorana fermion to the *bulk conformal field theory* with *central charge* $c = \frac{1}{2}$ in the low-energy limit.[16] More generally, one-dimensional gapless systems with small short-ranged interactions have an emerging conformal symmetry in this limit [81]. A short introduction to conformal field theory (CFT) with particular emphasis on the central charge is provided in Appendix D. The claim is by no means trivial and requires a justification. Let us start by considering the free Hamiltonian for a non-interacting spinless system:[17]

$$H = \sum_k \epsilon_k a_k^\dagger a_k \ , \tag{5.27}$$

with $a_k^\dagger$ and a_k being the fermionic creation and annihilation operators and ϵ_k being the single-particle spectrum in $f(k)$. By considering electronic states in the vicinity

[15] The points $k_0 = \pm\pi$ and $k_0 = 0$ give zeros on the real axis ($z_0 = \pm 1$). The following discussion holds for these special cases as well, which will be indicated on the way. Note that $\mathrm{e}^{\pm i\pi} = -1$ and hence it may seem as if $z_0 = -1$ is a degenerate zero. However, this does not imply a quadratic dispersion relation but rather $\epsilon_k^L \sim (k-\pi)$, $\epsilon_k^R \sim (k+\pi)$ and hence the reasoning below holds even for this case.

[16] If we would have m *degenerate* complex zeros, we would instead have $\epsilon_k \sim (k-k_0)^m$, implying a dynamical critical exponent $z = m$. This follows immediately by making use of the fact that the energy gap $\Delta \sim |\lambda - \lambda_c|^{\nu z} \sim (k - k_0)^m \sim (\frac{1}{\xi})^m$ using the notation introduced in Appendix C. However, $|\lambda - \lambda_c|^{\nu z} \sim (\frac{1}{\xi})^z$, gives $z = m$ by comparing the right-hand side and the left-hand side of the equation. This means that Lorentz symmetry is not manifest in the system, making it impossible to use conformal field theory to get a physical interpretation of the zeros.

[17] This is the correct expression up to some additive constant, which we omit.

of the zeros of ϵ_k we may perform the Taylor expansions

$$\epsilon_k^L = \underbrace{\epsilon_{k_0}}_{=0} + (k-k_0)\frac{d\epsilon_k}{dk}|_{k=k_0} + \mathcal{O}(k^2)\ , k \approx k_0\ ,$$
$$\epsilon_k^R = \underbrace{\epsilon_{-k_0}}_{=0} + (k+k_0)\frac{d\epsilon_k}{dk}|_{k=-k_0} + \mathcal{O}(k^2)\ , k \approx -k_0\ ,$$

where we attached the subscripts L and R for left and right-moving fermions respectively. Moreover, assuming $k_0 = k_F$, k_F being the Fermi momentum[18], we may interpret the derivative $\frac{d\epsilon_k}{dk}|_{k=k_0}$ as the Fermi velocity v_F of right-movers, reducing the expressions above to

$$\epsilon_k^R = v_F(k-k_0) + \mathcal{O}(k^2)\ ,$$
$$\epsilon_k^L = -v_F(k+k_0) + \mathcal{O}(k^2)\ .$$

Now, consider the low-energy limit in which the electronic states are located in small intervals near the Fermi energy $\epsilon_F = \epsilon_{\pm k_0} = 0$. This means that we are considering states and low-energy excitations in k-space in the intervals $[-\Lambda - k_0, -k_0 + \Lambda]$ and $[k_0 - \Lambda, k_0 + \Lambda]$, with Λ being a momentum cut-off (thus $v_F\Lambda$ is the energy cut-off) as indicated in Figure 5.3. Then, the Hamiltonian in the low-energy limit reads[19]

$$H = \sum_{k'} \epsilon_{k'} a_{k'}^\dagger a_{k'} \approx -\sum_{-k_0-\Lambda}^{-k_0+\Lambda} v_F(k'+k_0) a_{k'}^\dagger a_{k'} + \sum_{k_0-\Lambda}^{k_0+\Lambda} v_F(k'-k_0) a_{k'}^\dagger a_{k'}\ . \tag{5.28}$$

Performing the index change $k = k' + k_0$ in the first sum and $k = k' - k_0$ in the second sum leaves us with

$$H_{\mathrm{LE}} = -\sum_{-\Lambda}^{\Lambda} k v_F a_{k-k_0}^\dagger a_{k-k_0} + \sum_{-\Lambda}^{\Lambda} k v_F a_{k+k_0}^\dagger a_{k+k_0}\ . \tag{5.29}$$

Next, introduce another set of ladder operators, d_k^L and d_k^R separating the left-movers and right-movers such that

$$d_k^R = a_{k+k_0}\ , d_k^L = a_{k-k_0}\ . \tag{5.30}$$

This results in the low-energy Hamiltonian

$$H_{\mathrm{LE}} = \sum_{k=-\Lambda}^{\Lambda} k v_F \left(d_k^{R\dagger} d_k^R - d_k^{L\dagger} d_k^L \right)\ . \tag{5.31}$$

Now, although it may seem strange, we take the (continuum) limit $\Lambda \to \infty$ and then the sum above turns into an integral such that

$$H_{\mathrm{LE}} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk k v_F \left(d_k^{R\dagger} d_k^R - d_k^{L\dagger} d_k^L \right)\ . \tag{5.32}$$

[18] In the continuum limit (which we will consider later on), the Fermi momentum is related to the number of particles, N, in the system according to $k_F = \frac{\pi N}{L}$, L being the size [82]. This implies that the case $k_F = k_0 = 0$ is physically uninteresting.

[19] The Hamiltonian in this limit is also referred to as the linearized effective Hamiltonian [83].

The limit $\Lambda \to \infty$ can be justified by the fact that we are considering a low-energy theory where only low-energetic states in the vicinity of the Fermi energies matter. Extending the momentum cut-off to be infinite should not affect the behavior of the low-energy theory [83] .[20]

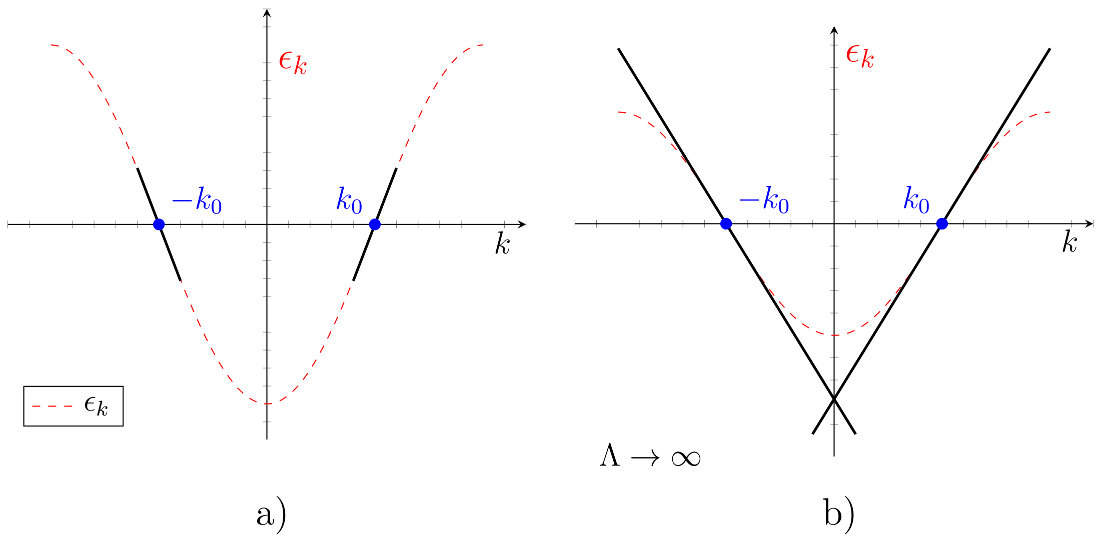

Figure 5.3: In situation a) the dispersion relation ϵ_k for non-interacting electrons and its linearization around the momenta $\pm k_0$ is readily apparent. Each zero in momentum space corresponds to a zero of $f(z)$ on the unit circle $|z| = 1$ in the complex plane. In Figure b) we have extended the linearized dispersion relation around the Fermi points to all momenta k and taken the cut-off parameter $\Lambda \to \infty$. As a consequence, the electronic ground state is an infinite Dirac sea. The infinities can be taken care of by normal-ordering the fermionic operators in the continuum Dirac Hamiltonian, (5.35).

[20] To assure that divergences are removed when extending the range of the momentum cut-off one has to normal-order the fermionic operators, but let us be sloppy here [84]. In fact, similar cut-off procedures were performed by Luttinger and Tomanaga in the context of bosonization [85], [86]. Their procedures differed in the sense that Luttinger extended the dispersion relation to infinity in contrast to Tomonaga who kept it finite. For a more detailed treatment of the two cut-off procedures, we refer to the acclaimed work by Solyom and Apostol, [87] and [88] respectively.

Now, using the ladder operators d_k^L and d_k^R, it is possible to find the one-dimensional position-dependent, slowly varying, continuum right and left-moving fields $\psi_L(x)$ and $\psi_R(x)$ according to

$$\psi_L(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk d_k^L \mathrm{e}^{ikx} \ , \tag{5.33}$$

$$\psi_R(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk d_k^R \mathrm{e}^{ikx} \ , \tag{5.34}$$

and similar for their hermitian conjugates. Note that the continuum fields obey the regular anti-commutation relations

$$\{\psi_L(x), \psi_L^\dagger(x')\} = \{\psi_R(x), \psi_R^\dagger(x')\} = 2\pi\delta(x-x') \ ,$$
$$\{\psi_L(x), \psi_L(x')\} = \{\psi_R(x), \psi_R(x')\} = 0 \ ,$$

which follow by direct insertion of the expressions above. To be able to write the low-energy Hamiltonian, H_{LE}, in terms of $\psi_L(x)$ and $\psi_R(x)$ one could invert (5.34), but we will instead do it backwards and consider

$$H_L = iv_F \int dx \psi_L^\dagger(x)\partial_x\psi_L(x) \ ,$$

$$H_R = iv_F \int dx \psi_R^\dagger(x)\partial_x\psi_R(x) \ .$$

Inserting the expansions in (5.34) into the equation above we deduce that

$$H_L = iv_F \int dx \psi_L^\dagger(x)\partial_x\psi_L(x) = \frac{iv_F}{(2\pi)^2}\int dx \int dk' \int dk d_{k'}^{L\dagger} d_k^L (ik)\mathrm{e}^{i(k-k')x} = -\frac{v_F}{2\pi}\int dk k d_k^{L\dagger} d_k^L \ ,$$
$$H_R = iv_F \int dx \psi_R^\dagger(x)\partial_x\psi_R(x) = \frac{iv_F}{(2\pi)^2}\int dx \int dk' \int dk d_{k'}^{R\dagger} d_k^R (ik)\mathrm{e}^{i(k-k')x} = -\frac{v_F}{2\pi}\int dk k d_k^{R\dagger} d_k^R \ ,$$

where one factor of $\frac{1}{2\pi}$ cancels due to the integral $\int dx \mathrm{e}^{i(k-k')x} = 2\pi\delta(k-k')$. Hence, by comparing to H_{LE} in (5.32) we get

$$H_{\mathrm{LE}} = \int dx \mathcal{H}_{\mathrm{LE}} = iv_F \int dx \Big(\psi_L^\dagger(x)\partial_x\psi_L(x) - \psi_R^\dagger(x)\partial_x\psi_R(x) \Big) \ . \tag{5.35}$$

This is precisely the Hamiltonian of right-moving and left-moving massless Dirac fermions [89]. By introducing a time-dependence in the continuum fields, i.e. $\psi_L(x) = \psi_L(x,t)$ and $\psi_R(x) = \psi_R(x,t)$[21] we may make an ansatz for the corresponding Lagrangian (density), $\mathcal{L}_{LE}$:[22]

$$\mathcal{L}_{\mathrm{LE}} = -iv_F \Big(\psi_R^\dagger(x,t)(\frac{1}{v_F}\partial_t - \partial_x)\psi_R(x,t) + \psi_L^\dagger(x,t)(\frac{1}{v_F}\partial_t + \partial_x)\psi_L(x,t) \Big) \ , \tag{5.36}$$

[21] Including a time-dependence in the fermionic fields modifies the expansion $\psi_{L/R}(x) = \frac{1}{2\pi}\int dk d_k^{L/R}\mathrm{e}^{ikx} \to \psi_{L/R}(x,t) = \frac{1}{2\pi}\int dk d_k^{L/R}\mathrm{e}^{i(kx - v_F k t)}$.

[22] If one introduces 1+1-dimensional Dirac matrices and combine $\psi_L(x,t)$ and $\psi_R(x,t)$ into a two-component spinor $\Psi(x,t) = (\psi_L(x,t), \psi_R(x,t))$ the expression can be written in a nicer form.

which is seen to hold since $\mathcal{H}_{\text{LE}}$ is related to $\mathcal{L}_{\text{LE}}$, via the Legendre transformation

$$\mathcal{H}_{\text{LE}} = \frac{\partial \mathcal{L}_{\text{LE}}}{\partial \dot{\psi}_i}\dot{\psi}_i - \mathcal{L}_{\text{LE}} \ , \tag{5.37}$$

with implied summation over $i = L, R$ and $\dot{\psi}_i = \frac{\partial \psi_i}{\partial t}$. The Lagrangian in (5.36) can be expressed in terms of the complex coordinates (familiar from CFT) $z = -i(x - v_F t)$ and $\bar{z} = i(x + v_F t)$ using [90]:

$$\partial_z = -\frac{i}{2}(\frac{1}{v_F}\partial_t - \partial_x) \ , \ \partial_{\bar{z}} = -\frac{i}{2}(\frac{1}{v_F}\partial_t + \partial_x) \ , \tag{5.38}$$

and therefore

$$\mathcal{L}_{\text{LE}} = 2v_F\left(\psi_R^\dagger(z)\partial_z\psi_R(z) + \psi_L^\dagger(\bar{z})\partial_{\bar{z}}\psi_L(\bar{z})\right) \ . \tag{5.39}$$

We still have not made the connection to Majorana fermions explicit. Let us turn to this task now. By writing the fermionic fields as complex linear combinations of (real) Majorana fields χ_1 and χ_2 we have

$$\psi_L(\bar{z}) = \frac{1}{\sqrt{2}}(i\chi_1(\bar{z}) + \chi_2(\bar{z})) \ , \psi_R(z) = \frac{1}{\sqrt{2}}(\bar{\chi}_1(z) + i\bar{\chi}_2(z)) \ , \tag{5.40}$$

where the factor $\frac{1}{\sqrt{2}}$ assures that ψ fulfills the anti-commutation relations $\{\psi_i(z), \psi_i^\dagger(z')\} = \delta(z - z')$. Note that we could also have written $\chi_1 = \chi_1^L$ and $\bar{\chi}_1 = \chi_1^R$ (and similar for χ_2 and $\bar{\chi}_2$). Now, it remains to plug in the Majorana fields into (5.39):

$$\begin{aligned}
\mathcal{L}_{\text{LE}} &= v_F\left((\bar{\chi}_1 - i\bar{\chi}_2)\partial_z(\bar{\chi}_1 + i\bar{\chi}_2) + (\chi_2 - i\chi_1)\partial_{\bar{z}}(\chi_2 + i\chi_1)\right) \\
&= v_F\left(\bar{\chi}_1\partial_z\bar{\chi}_1 + \bar{\chi}_2\partial_z\bar{\chi}_2 + i(\bar{\chi}_1\partial_z\bar{\chi}_2 - \bar{\chi}_2\partial_z\bar{\chi}_1) + \bar{\chi} \leftrightarrow \chi\right) \\
&= v_F\left(\bar{\chi}_1\partial_z\bar{\chi}_1 + \bar{\chi}_2\partial_z\bar{\chi}_2 + i(\partial_z(\bar{\chi}_1\bar{\chi}_2) - \partial_z(\bar{\chi}_1)\bar{\chi}_2 - \bar{\chi}_2\partial_z\bar{\chi}_1) + \bar{\chi} \leftrightarrow \chi\right) \\
&= v_F\left(\bar{\chi}_1\partial_z\bar{\chi}_1 + \bar{\chi}_2\partial_z\bar{\chi}_2 + \chi_1\partial_{\bar{z}}\chi_1 + \chi_2\partial_{\bar{z}}\chi_2\right) \ ,
\end{aligned}$$

where in the last step we made use of the anti-commutator relation between Majorana fermions and omitted the total derivative term.[23] This term will be considered a boundary term in the action and is of no use to us. We have thus been able to write the Dirac Lagrangian as a sum of two Majorana Lagrangians:

$$\mathcal{L}_{\text{LE}} = \mathcal{L}_{M_1} + \mathcal{L}_{M_2} \ , \tag{5.41}$$

with $\mathcal{L}_{M_1} = v_F\left(\bar{\chi}_1\partial_z\bar{\chi}_1 + +\chi_1\partial_{\bar{z}}\chi_1\right)$ and $\mathcal{L}_{M_2} = v_F\left(\bar{\chi}_2\partial_z\bar{\chi}_2 + +\chi_2\partial_{\bar{z}}\chi_2\right)$, and consequently the following low-energy (Majorana) action, $\mathcal{S}_{\text{LE}}$, is obtained as

$$\mathcal{S}_{\text{LE}} = v_F\int d^2z\left(\bar{\chi}_1\partial_z\bar{\chi}_1 + \chi_1\partial_{\bar{z}}\chi_1 + \bar{\chi}_2\partial_z\bar{\chi}_2 + \chi_2\partial_{\bar{z}}\chi_2\right) \ . \tag{5.42}$$

[23] Note that we really used $\{\chi_1, \partial_{\bar{z}}\chi_2\} = 0$, but since $\partial_{\bar{z}}$ is a bosonic operator (which commutes with fermionic fields) the relation should still hold.

In this action, *conformal symmetry* is manifest, in the sense that it is invariant under conformal coordinate transformations in the complex plane [81]. More precisely, under a conformal transformation $z \to g(z)$, $g(z)$ being a holomorphic function and $\chi_i \to (\frac{dg}{dz})^{1/2}\chi_i(g(z))$ since the Majorana field has scaling dimension $h = \frac{1}{2}$, cf. Appendix D (and similar for the anti-holomorphic coordinate $\bar{z}$).
To summarize, we have now shown that each of the (two) non-degenerate zeros $\mathrm{e}^{\pm ik_0}$ on the unit circle $|z| = 1$ contributes a massless Majorana fermion field theory.[24] This suggests that there must be an intimate connection between the number of zeros and the degrees of freedom in a CFT, measured by the central charge c. The fact that each Majorana fermion contributes with central charge $c = \frac{1}{2}$ is established in Appendix D. In particular this means that systems with $2c$ zeros on the unit circle result in a total central charge c. In our calculation with zeros $z_0 = \mathrm{e}^{\pm ik_0}$ we expect the central charge $c = 1$ (which is indeed true since the central charge is additive under stacking and each Majorana fermion contributes with $c = \frac{1}{2}$, see Appendix D).

[24]More precisely, there are both left-moving and right-moving Majorana fields in a single Majorana field theory.

5.4 Classification of topological phases

One may define and classify different phases of matter in terms of equivalence classes of ground states under smooth (continuous) deformations of the Hamiltonian. Then, two ground states are said to be equivalent if they can be smoothly connected without going through a phase transition [79]. As we have seen, a topological phase transition between gapped phases is accompanied by the closing (and re-opening) of the energy-gap. We have not yet established how to realize such smooth changes in the BDI Hamiltonian, (5.3). Since the weighting coefficients t_α clearly determine the physical behavior of the superconducting BDI system, smooth changes in our language corresponds to tuning on/off a finite number of these coefficients. This also implies, due to its one-to-one correspondence with the Hamiltonian, that the zeros of $f(z)$ move around in the complex plane under such deformations.
Similarly, it is possible to transit between gapless phases of matter as well. In the previous section we established that we needed to introduce another degree of freedom, the central charge c of the bulk conformal field theory, in addition to the winding number, in order to fully characterize the topological phase of a gapless BDI system. Then of course a topological phase transition is not associated with a gap-closing (the spectrum is always gapless!), but the central charge c, and hence the number of zeros on the unit circle, has to change. In agreement with the *c-theorem*, states of matter with different central charges cannot be smoothly connected, and therefore the phases before and after the transition have to be topologically distinct [91].[25]

By now, it should be clear that two different invariants come into play when describing H_{BDI} for gapped and gapless phases respectively:

$$c = \frac{1}{2}(\text{number of zeros on } |z| = 1)\ , \nu = N_Z - N_P\ , \tag{5.43}$$

treated in the two previous sections. For gapped systems, we have $c = 0$, while gapless systems have a non-zero central charge *if* the zeros on the unit circle are non-degenerate. Clearly, ν is an invariant since it cannot change under smooth motion without changing c. Moreover, it manifests itself through symmetry-protected edge modes as seen in Theorem 1. The theorem also implies that a generic gapped phase in the BDI class can be represented simply by H_ν (which is really the α-chain with $\alpha = \nu$), and a gapless phase as $H_\nu + H_{2c+\nu}$.
The discussion above leads us to making the claim that gapless phases can be labeled by the *semigroup* $\mathbf{N} \times \mathbf{Z}$ with $c \in \frac{1}{2}\mathbf{N}$ ($c \neq 0$) and $\nu \in \mathbf{Z}$.[26] It is really a semigroup since c, as seen in Appendix D, can only increase under stacking. The operation of stacking corresponds to addition when it comes to the central charge. The special case, $c = 0$, gives the classification $\mathbf{Z}$ for gapped phases or $\{0\} \times \mathbf{Z} \subset \mathbf{N}$. We repeat once again that the first classification is only valid when the zeros on $|z| = 1$ are non-degenerate. Then, and only then, is the bulk described by a CFT and a central charge $c \in \frac{1}{2}\mathbf{N}$.

[25] A formulation of Zamolodchikov's famous c-theorem is provided in Appendix D.
[26] This claim is summarized in a theorem later.

Returning to the translation-invariant gapless chain $H_{2c+\nu}+H_\nu$ (or H_ν in the gapped case), the corresponding complex (meromorphic) function $f(z)$ can be turned into the canonical form[27]

$$f(z) = (z^{2c} + 1)z^\nu \ , \tag{5.44}$$

without causing a phase transition. However, due to translational invariance we could in fact be more general and let $H = \pm(H_\nu \pm H_{\nu+2c})$. This modifies $f(z)$ into

$$f(z) = \pm(z^{2c} \pm 1)z^\nu \ . \tag{5.45}$$

In addition to the central charge, c, and the winding number ν, we thus get a $\mathbf{Z}_2 \times \mathbf{Z}_2$-classification for the overall and intermediate sign due to translational invariance. Note that $f(z)$ reduces to $\pm z^\nu$ in the case $c = 0$, giving only an additional $\mathbf{Z}_2$-classification. These findings can be summarized in another theorem due to [18]:

Theorem 2 *The phases in the BDI class described by a bulk CFT have a* $\mathbf{N} \times \mathbf{Z}$ *semigroup classification, labeled by the central charge* $c \in \frac{1}{2}\mathbf{N}$ *and the topological invariant* $\nu \in \mathbf{Z}$*. Translational invariance gives an extra* $\mathbf{Z}_2$*-classification if* $c = 0$ *and a* $\mathbf{Z}_2 \times \mathbf{Z}_2$*-classification if* $c \neq 0$*.*
Moreover, one can show that topological phases in two chains with identical c and ν but with different $\mathbf{Z}_2$-signs can be connected by means of a unitary transformation given that we have introduced a unit cell breaking the translational invariance.[28]

The phase transition between two topological phases with topological invariants ν_1 and ν_2 is then described by a central charge which is given by the difference in winding number between the two phases (i.e. the number of zeros that must cross the unit circle at the transition). This is neatly summarized in another theorem:

Theorem 3 *A phase transition between two gapped phases with topological invariants* ν_1 *and* ν_2 *obeys* $c \geq \frac{|\nu_1 - \nu_2|}{2}$.

The inequality may be slightly surprising, but can be explained by the fact that one can fine-tune the transition to move zeros off the unit circle. Recall that $2c$ counts the number of zeros on the unit circle and that, given that these zeros are non-degenerate, the bulk is a CFT with central charge c.

[27] Given that $f(z)$ has $2c$ zeros $\{z_0\}$ on the unit-disk $|z| = 1$, due to time-reversal symmetry, these zeros cannot be moved off the real axis. This has the consequence that $\{z_0\}$ has to fulfill $z_0^{2c} = \pm 1$.

[28] In Appendix E, we show how Hamiltonians $H_1 = +(H_{2c+\nu} + H_\nu)$ can be connected to $H_2 = -(H_{2c+\nu} + H_\nu)$ with a unitary transformation, $U(\alpha)$. Connecting Hamiltonians with different intermediate signs can also be done as shown by Verresen et al. [18]

6

Topological Edge Modes At Criticality in Class CII

The discussion in the previous chapter provided a topological classification of one-dimensional non-interacting gapless superconducting models in the symmetry class BDI, and a natural question to ask is then whether a similar classification can be made for other symmetry classes. According to the tenfold way for gapped systems, see Table 4.1, we should expect a non-trivial classification of topological superconductors also in classes D, DIII, AIII and CII.[1] Due to its striking resemblance with BDI, the latter should be the most straightforward to provide a classification of, which is the main topic of this chapter. In the last section of the chapter, the difficulties of providing a topological classification for gapless phases in the classes D and DIII will be addressed.

6.1 Representative CII models

There are many ways of constructing a (single-particle) Hamiltonian which can be assigned a particle-hole symmetry and a time-reversal symmetry with operators $\mathcal{P}$ and $\mathcal{T}$ such that $\mathcal{T}^2 = \mathcal{P}^2 = -1$ and a chiral symmetry $\mathcal{C}$ with $\mathcal{C}^2 = +1$. We would, however, like to rely on the construction by Verresen, Jones and Pollmann, as much as possible and make use of Kitaev chains to form representative gapped and gapless phases in the class. We will consider two different approaches in order to arrive at an appropriate set of models representing the CII class. As will be indicated on the way, the first approach does not give representative CII Hamiltonians of the desired form, but the ingredients are still important building blocks in the (presumably) successful models.

6.1.1 Approach I: Zhao and Wang Hamiltonian

By taking off from general index theorems [92], Zhao and Wang show that four topologically distinct types of Majorana zero modes can emerge at the ends of one-dimensional superconducting wires in the symmetry classes D, DIII, AIII, BDI and CII. In particular, they provide a representative model for the symmetry class CII, which can be seen as a spinful analogue of Kitaev's model. In the BdG-formalism,

[1]The BdG classes CI and C have a trivial classification in one dimension as can be seen in Table 4.1.

the Hamiltonian can be written as [93]

$$H_{\mathrm{ZW}}^{\mathrm{CII}} = \sum_k \Psi_k^\dagger H_{\mathrm{ZW}}(k)\Psi_k \ , H_{\mathrm{ZW}}(k) = -\Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x \ , \quad (6.1)$$

with $\Psi_k^\dagger = (\hat{a}_k^\dagger, \hat{a}_{-k}(-i\sigma_y))^2$ and $t, \mu, \Delta \in \mathbf{R}$. Here, the spin dependence in the fermionic operators is made explicit through the notation $\hat{a}_k^\dagger = (a_{\uparrow,k}^\dagger, a_{\downarrow,k}^\dagger)$ (similar for $\hat{a}_k$). Note that the Pauli matrices σ_i and τ_i act on the spin and particle-hole degrees of freedom respectively. Expressed in this way, it is simple to read off a time-reversal symmetry $\mathcal{T}$ and a particle-hole symmetry $\mathcal{P}$ of the model such that

$$\mathcal{T} = \sigma_y \otimes \mathbf{1}\mathcal{K} \ , \mathcal{P} = \mathbf{1} \otimes \tau_y \mathcal{K} \ , \quad (6.2)$$

obeying $\mathcal{T}^2 = \mathcal{P}^2 = -1$. Hence, we may put the model in symmetry class CII. Let us check explicitly that the Bloch Hamiltonian $H_{\mathrm{ZW}}(k)$ transforms correctly under $\mathcal{T}$ and $\mathcal{P}$:

$$\begin{aligned}
\mathcal{T} H_{\mathrm{ZW}}(k)\mathcal{T}^{-1} &= -\sigma_y \otimes \mathbf{1}\mathcal{K}(-\Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x)\sigma_y \otimes \mathbf{1}\mathcal{K} \\
&= \sigma_y \otimes \mathbf{1}(\Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x)\sigma_y \otimes \mathbf{1} \\
&= \Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x \\
&= H_{\mathrm{ZW}}(-k) \ ,
\end{aligned}$$

in agreement with (3.3). Similarly,

$$\begin{aligned}
\mathcal{P} H_{\mathrm{ZW}}(k)\mathcal{P}^{-1} &= -\mathbf{1} \otimes \tau_y\mathcal{K}(-\Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x)\mathbf{1} \otimes \tau_y\mathcal{K} \\
&= \mathbf{1} \otimes \tau_y(\Delta \sin k\sigma_y \otimes \tau_z + (t\cos k - \mu)\mathbf{1} \otimes \tau_x)\mathbf{1} \otimes \tau_y \\
&= -\Delta \sin k\sigma_y \otimes \tau_z - (t\cos k - \mu)\mathbf{1} \otimes \tau_x \\
&= -H_{\mathrm{ZW}}(-k) \ ,
\end{aligned}$$

as expected according to (3.17). Now, the Hamiltonian, $H_{\mathrm{ZW}}^{\mathrm{CII}}$ is easily written in real space via the inverse Fourier transformation:

$$H_{\mathrm{ZW}}^{\mathrm{CII}} = \sum_j \left(t\hat{a}_{j+1}^\dagger \sigma_x \hat{a}_j - \Delta \hat{a}_{j+1}\sigma_x\hat{a}_j - \mu \hat{a}_j^\dagger \sigma_x \hat{a}_j + \text{h.c.} \right) \ , \quad (6.3)$$

with the full calculation provided in Appendix F. This will be used later when discussing the emergence of Majorana zero modes. First, we turn our attention to topological invariants of the model. In accordance with the Kitaev model, there are two topological phases described by a topological invariant, ν. However, due to the spin degrees of freedom, the topological invariant takes the values $\nu = \pm 2$ (in contrast to $\nu = \pm 1$ of the Kitaev model). To arrive at this result we make use of Zhao and Wangs' neat formula for computing the CII-topological invariant in one spatial dimension [93]

$$\nu_{\mathrm{CII}} = \frac{1}{4\pi i}\int_{-\pi}^{\pi} dk \mathrm{tr}\left(\sigma_y \otimes \tau_y (H_{\mathrm{ZW}}(k))^{-1}\partial_k H_{\mathrm{ZW}}(k)\right) = \frac{1}{4\pi i}\int_{-\pi}^{\pi} dk f(k) \ , \quad (6.4)$$

[2] This defines a *Nambu spinor*, commonly introduced in superconducting BdG systems. Matrices acting on such spinors must be 4×4, e.g. $\sigma_i \otimes \tau_j$ or $\tau_i \otimes \sigma_j$ [4].

which is quite similar to the winding number integral we used to compute the topological invariant for the SSH model and the Kitaev model, cf. equation (4.38). The integrand, $f(k)$, is easily (but tediously) computed as

$$f(k) = \frac{4i\Delta(t - \mu\cos k)}{\mu^2 - 2\mu t\cos k + t^2\cos^2 k + \Delta^2\sin^2 k} \ . \tag{6.5}$$

Specifying the parameters $t = \Delta > 0$ and $\mu = 0$ gives the integrand $f(k) = 4i$ and a trivial integral to solve with a non-zero topological invariant:

$$\nu = \frac{4i}{4\pi i}\int_{-\pi}^{\pi} dk = 2 \ , \tag{6.6}$$

in agreement with the topological phase of the conventional Kitaev model (which has $\nu = 1$ for the same choice of parameters). However, note that we may also have $\mu \neq 0$ and still get $\nu \neq 0$. To get $\nu = +2$, t is restricted to be strictly larger than μ. This can be seen by turning the integral in (6.4) with $\Delta = t$ into a complex integral by the substitution $z = \mathrm{e}^{ik}$:

$$\nu = \frac{1}{4\pi i}\int_{-\pi}^{\pi} dk f(k) = \frac{-i}{4\pi i}\int_{|z|=1} dz\frac{f(z)}{z} = -\frac{1}{4\pi i}\int_{|z|=1} dz\frac{4t(tz - \mu/2(z^2+1))}{\mu t z(z - \frac{\mu}{t})(z - \frac{t}{\mu})} \ ,$$

where Euler's formula has been used to write $f(k)$ as a polynomial of the variable $z = \mathrm{e}^{ik}$. Considering $t > \mu$ only the poles at $z = 0$ and $z = \frac{\mu}{t}$ are inside the unit circle and contribute to the integral and therefore

$$\begin{aligned}\nu_{\mathrm{CII}}\Big|_{t>\mu} &= -\frac{4t2\pi i}{4\pi i\mu t}\Bigg(\frac{(tz - \mu/2(z^2+1))}{(z - \frac{\mu}{t})(z - \frac{t}{\mu})}\Bigg|_{z=0} + \frac{(tz - \mu/2(z^2+1))}{z(z - \frac{t}{\mu})}\Bigg|_{z=\frac{\mu}{t}}\Bigg) \\ &= -\frac{2}{\mu}\Bigg(-\frac{\mu}{2} + \frac{\mu/2(1 - \frac{\mu^2}{t^2})}{\frac{\mu}{t}(\frac{\mu}{t} - \frac{t}{\mu})}\Bigg) = -\frac{2}{\mu}\Bigg(-\frac{\mu}{2} - \frac{\mu}{2}\Bigg) = 2 \ ,\end{aligned}$$

invoking Cauchy's integral formula (alternatively the residue theorem). However, for $t < \mu$ we instead have

$$\begin{aligned}\nu_{\mathrm{CII}}\Big|_{t<\mu} &= -\frac{4t2\pi i}{4\pi i\mu t}\Bigg(\frac{(tz - \mu/2(z^2+1))}{(z - \frac{\mu}{t})(z - \frac{t}{\mu})}\Bigg|_{z=0} + \frac{(tz - \mu/2(z^2+1))}{z(z - \frac{\mu}{t})}\Bigg|_{z=\frac{t}{\mu}}\Bigg) \\ &= -\frac{2}{\mu}\Bigg(-\frac{\mu}{2} + \frac{(\mu/2(\frac{t^2}{\mu^2} - 1)}{\frac{t}{\mu}(\frac{t}{\mu} - \frac{\mu}{t})}\Bigg) = -\frac{2}{\mu}\Bigg(-\frac{\mu}{2} + \frac{\mu}{2}\Bigg) = 0 \ .\end{aligned}$$

Similarly, by putting $t = -\Delta < 0$ and $\mu = 0$ we arrive at $\nu_{\mathrm{CII}} = -2$. To summarize, for $\mu \neq 0$ we need $|t| > |\mu|$ in order to belong to a topological phase. In analogy with the conventional Kitaev model, one can find topologically protected Majorana modes in this phase by recasting the Hamiltonian in terms of spinful Majorana operators[3]

$$\gamma_{js} = a_{js} + a_{js}^\dagger \ , \tilde{\gamma}_{js} = i(a_{js}^\dagger - a_{js}) \ , \tag{6.7}$$

[3]In general, we could include a phase in the definition of the Majorana operators according to $\gamma_{js} = \mathrm{e}^{i\theta/2}a_{js} + \mathrm{e}^{-i\theta/2}a_{js}^\dagger$ and $\tilde{\gamma}_{js} = i(\mathrm{e}^{-i\theta/2}a_{js}^\dagger - \mathrm{e}^{i\theta/2}a_{js})$. In this setting θ is chosen to be zero.

where $j \in [1, N-1]$ and s is the spin index, i.e. $s = \uparrow, \downarrow$. Moreover, $\gamma_{js} = \gamma_{js}^\dagger$ and $\tilde{\gamma}_{js} = \tilde{\gamma}_{js}^\dagger$. Putting $\Delta = t > 0$ and $\mu = 0$ in (6.3), and decomposing $\hat{a}_j = (a_{j\uparrow}, a_{j\downarrow})$ (and similar for the hermitian conjugate) we deduce that

$$
\begin{aligned}
H_{\text{Majorana}}^{\text{CII}} &= \sum_j t\left(\hat{a}_{j+1}^\dagger \sigma_x \hat{a}_j - \hat{a}_{j+1}\sigma_x \hat{a}_j + \text{h.c.}\right) \\
&= \sum_j t\left(a_{j\uparrow}^\dagger a_{j+1\downarrow} + a_{j\downarrow}^\dagger a_{j+1\uparrow} + a_{j+1\uparrow}^\dagger a_{j\downarrow} + a_{j+1\downarrow}^\dagger a_{j\uparrow}\right. \\
&\qquad \left. - a_{j+1\downarrow}^\dagger a_{j\uparrow}^\dagger - a_{j+1\uparrow}^\dagger a_{j\downarrow}^\dagger - a_{j\uparrow}a_{j+1\downarrow} - a_{j\downarrow}a_{j+1\uparrow}\right) \\
&= \sum_j t\left((a_{j\uparrow}^\dagger - a_{j\uparrow})(a_{j+1\downarrow} + a_{j+1\downarrow}^\dagger) + (a_{j\downarrow}^\dagger - a_{j\downarrow})(a_{j+1\uparrow} + a_{j+1\uparrow}^\dagger)\right) \\
&= -it\sum_j \left(\tilde{\gamma}_{j\uparrow}\gamma_{j+1\downarrow} + \tilde{\gamma}_{j\downarrow}\gamma_{j+1\uparrow}\right) ,
\end{aligned}
$$

where $\tilde{\gamma}_j = i(a_j^\dagger - a_j)$ and $\gamma_j = a_j^\dagger + a_j$. Thus, in terms of Majorana operators the Hamiltonian reads

$$
H_{\text{Majorana}}^{\text{CII}} = -it\sum_{j=1}^{N-1}\left(\tilde{\gamma}_{j\uparrow}\gamma_{j+1\downarrow} + \tilde{\gamma}_{j\downarrow}\gamma_{j+1\uparrow}\right) . \tag{6.8}
$$

Now, by comparing the expression above with H_1 in (5.1), it seems as if the representative Kitaev-like CII model can be seen as two copies of the Kitaev chain. However, the spins in (6.8) are coupled in an exotic way and in contrast to H_1, $H_{\text{Majorana}}^{\text{CII}}$ has two Majorana zero modes on *each* edge. On the left edge $\gamma_{1\uparrow}$ and $\gamma_{1\downarrow}$ serve as Majorana zero modes and similar for $\tilde{\gamma}_{N\uparrow}$ and $\tilde{\gamma}_{N\downarrow}$ on the right edge. To confidently be able to argue that the CII Hamiltonian in (6.8) is just two copies of the BDI Kitaev chain, we would like Majorana operators with the same spin to couple to each other. Then, a representative CII model can be obtained by stacking two BDI copies, one with spin up and one with spin down, on top of each other and we may make use of the stacking procedure described by Verresen, Jones and Pollmann [18] and in the previous chapter. This complication will be resolved in the next section.

6.1.2 Approach II: PWW Hamiltonian

Another set of representative CII models is provided by Prakash, Wang and Wei (PWW) who make use of stackings of Kitaev chains to form general *short-range entangled*[4] symmetry-protected fermionic phases in the BdG and chiral classes [95]. The construction by Prakash et al. is however really more general than we need since it is also valid in the presence of interactions. Moreover, the model relies on

[4]This is superfluous terminology here since all symmetry-protected states can be seen as short-range entangled states with a symmetry ($\mathcal{T}, \mathcal{P}$ or $\mathcal{C}$). By contrast, states with intrinsic *topological order* are long-range entangled [94].

having four (rather than two) fermion species per unit cell labeled by the indices $a = 1, 2$ and the spin index $\sigma =\uparrow, \downarrow$ with the PWW Hamiltonian reading [95]

$$H_{\mathrm{CII}}^{\mathrm{PPW}} = i \sum_{n,\sigma} (\gamma_{\sigma,2,n}\gamma_{\sigma,1,n+1} - \tilde{\gamma}_{\sigma,2,n}\tilde{\gamma}_{\sigma,1,n+1}) \; . \tag{6.9}$$

It is clear that this Hamiltonian is difficult to interpret in the light of the previous chapter. In contrast to the BDI Hamiltonian in (5.3), the Majorana operators γ and $\tilde{\gamma}$ couple to themselves rather than to each other and they are also decorated with extra indices $a = 1, 2$. The exotic couplings can be taken care of by means of a unitary basis-transformation, M_s, such that

$$M_s = \prod_n \exp\left(\frac{\pi}{4} \sum_{\sigma=\uparrow,\downarrow} \gamma_{\sigma,2,n}\tilde{\gamma}_{\sigma,1,n}\right) = \prod_n \frac{(1 + \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n})}{\sqrt{2}} \frac{(1 + \gamma_{\downarrow,2,n}\tilde{\gamma}_{\downarrow,1,n})}{\sqrt{2}} = M_\uparrow M_\downarrow \; ,$$

where the second step follows by noting that the quantities $A = \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}$ and $B = \gamma_{\downarrow,2,n}\tilde{\gamma}_{\downarrow,1,n}$ are commuting quantities, i.e. the identity $\exp(A + B) = \exp(A)\exp(B)$ holds. One can then make use of the Taylor series expansion of each exponential to arrive at the neat expression above. The unitary operators $M_\uparrow$ and $M_\downarrow$ are easily read off as

$$M_\sigma = \prod_n \frac{(1 + \gamma_{\sigma,2,n}\tilde{\gamma}_{\sigma,1,n})}{\sqrt{2}} \; , \sigma =\uparrow, \downarrow \; ,$$

which gives

$$M_s^\dagger H_{\mathrm{CII}} M_s = \tilde{H}_{\mathrm{CII}} = M_\uparrow^\dagger H_{\mathrm{CII}}^\uparrow M_\uparrow + M_\downarrow^\dagger H_{\mathrm{CII}}^\downarrow M_\downarrow \; , \tag{6.10}$$

since $M_\uparrow^\dagger H_{\mathrm{CII}}^\downarrow M_\uparrow = H_{\mathrm{CII}}^\downarrow$, $M_\downarrow^\dagger H_{\mathrm{CII}}^\uparrow M_\downarrow = H_{\mathrm{CII}}^\uparrow$. Let us, at least once, do the basis transformation explicitly with $\sigma =\uparrow$ acting on $H_{\mathrm{CII}}^\uparrow$. First, it is convenient to rewrite the Hamiltonian:

$$H_{\mathrm{CII}}^\uparrow = i \sum_n (\gamma_{\uparrow,2,n}, \tilde{\gamma}_{\uparrow,2,n}) \begin{pmatrix} \gamma_{\uparrow,1,n+1} \\ -\tilde{\gamma}_{\uparrow,1,n+1} \end{pmatrix} \; ,$$

and thus

$$M_\uparrow^\dagger H_{\mathrm{CII}}^\uparrow M_\uparrow = i \sum_n M_\uparrow^\dagger (\gamma_{\uparrow,2,n}, \tilde{\gamma}_{\uparrow,2,n}) \underbrace{M_\uparrow M_\uparrow^\dagger}_{=1} \begin{pmatrix} \gamma_{\uparrow,1,n+1} \\ -\tilde{\gamma}_{\uparrow,1,n+1} \end{pmatrix} M_\uparrow \; .$$

The problem thus reduces to computing

$$\begin{aligned}
M_\uparrow^\dagger \begin{pmatrix} \gamma_{\uparrow,2,n} & \tilde{\gamma}_{\uparrow,2,n} \end{pmatrix} M_\uparrow &= \left(\prod_{n'} \frac{(1 + \gamma_{\uparrow,2,n'}\tilde{\gamma}_{\uparrow,1,n'})}{\sqrt{2}}\right)^\dagger \begin{pmatrix} \gamma_{\uparrow,2,n} \\ \tilde{\gamma}_{\uparrow,2,n} \end{pmatrix} \prod_{n''} \frac{(1 + \gamma_{\uparrow,2,n''}\tilde{\gamma}_{\uparrow,1,n''})}{\sqrt{2}} \\
&= \frac{1}{2}(1 - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \begin{pmatrix} \gamma_{\uparrow,2,n} \\ \tilde{\gamma}_{\uparrow,2,n} \end{pmatrix} (1 + \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \\
&= \frac{1}{2} \begin{pmatrix} \gamma_{\uparrow,2,n} + \tilde{\gamma}_{\uparrow,1,n} \\ \tilde{\gamma}_{\uparrow,2,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\tilde{\gamma}_{\uparrow,2,n} \end{pmatrix} (1 + \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \\
&= \frac{1}{2} \begin{pmatrix} \tilde{\gamma}_{\uparrow,1,n} + \gamma_{\uparrow,2,n} + \tilde{\gamma}_{\uparrow,1,n} + \tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} \\ \tilde{\gamma}_{\uparrow,2,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\tilde{\gamma}_{\uparrow,2,n} + \tilde{\gamma}_{\uparrow,2,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\tilde{\gamma}_{\uparrow,2,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} \end{pmatrix} \\
&= \begin{pmatrix} \tilde{\gamma}_{\uparrow,1,n} \\ \tilde{\gamma}_{\uparrow,2,n} \end{pmatrix} \; ,
\end{aligned}$$

where we made use of the fermionic anti-commutator relations $\{\gamma_{js}, \gamma_{j's'}\} = \{\tilde{\gamma}_{js}, \tilde{\gamma}_{j's'}\} = 2\delta_{jj'}\delta_{ss'}$ and $\{\gamma_{js}, \tilde{\gamma}_{j's'}\} = 0$. The products over n' and n'' could be removed right away since

$$\begin{aligned}\left(\prod_{n'} M_{\uparrow,n'}\right)^{\dagger} \vec{\gamma}_2(n) \prod_{n''} M_{\uparrow,n''} &= M^{\dagger}_{\uparrow,N} M^{\dagger}_{\uparrow,N-1} \cdot ... \cdot M^{\dagger}_{\uparrow,n} \cdot ... M^{\dagger}_{\uparrow,1} \vec{\gamma}_2(n) M_{\uparrow,1} M_{\uparrow,2} \cdot ... \cdot M_{\uparrow,n} \cdot ... \\ &= M^{\dagger}_{\uparrow,n} \vec{\gamma}_2(n) M_{\uparrow,n} \ ,\end{aligned}$$

with $\vec{\gamma}_2(n) = \begin{pmatrix} \gamma_{\uparrow,2,n} \\ \tilde{\gamma}_{\uparrow,2,n} \end{pmatrix}$. All factors $M_{\uparrow,n'}$ with $n' \neq n$ can be moved to the left of $\vec{\gamma}_2(n)$ (since $[M_{\uparrow,n'}, \vec{\gamma}_2(n)] = 0 \ , n' \neq n$), and using $M^{\dagger}M = 1$ successively gives the end result. Similarly,

$$\begin{aligned} M^{\dagger}_{\uparrow} \begin{pmatrix} \gamma_{\uparrow,1,n} \\ -\tilde{\gamma}_{\uparrow,1,n} \end{pmatrix} M_{\uparrow} &= \frac{1}{2}(1 - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \begin{pmatrix} \gamma_{\uparrow,1,n} \\ -\tilde{\gamma}_{\uparrow,1,n} \end{pmatrix} (1 + \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \\ &= \frac{1}{2} \begin{pmatrix} \gamma_{\uparrow,1,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,1,n} \\ \gamma_{\uparrow,2,n} - \tilde{\gamma}_{\uparrow,1,n} \end{pmatrix} (1 + \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}) \\ &= \frac{1}{2} \begin{pmatrix} \gamma_{\uparrow,1,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,1,n} + \gamma_{\uparrow,1,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} - \gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,1,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} \\ \gamma_{\uparrow,2,n} - \tilde{\gamma}_{\uparrow,1,n} + \tilde{\gamma}_{\uparrow,1,n} - \tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,2,n}\tilde{\gamma}_{\uparrow,1,n} \end{pmatrix} \\ &= \begin{pmatrix} \gamma_{\uparrow,1,n} \\ \gamma_{\uparrow,2,n} \end{pmatrix} \ , \end{aligned}$$

and therefore

$$M^{\dagger}_{\uparrow} H^{\uparrow}_{\mathrm{CII}} M_{\uparrow} = i \sum_n (\tilde{\gamma}_{\uparrow,1,n}, \tilde{\gamma}_{\uparrow,2,n}) \begin{pmatrix} \gamma_{\uparrow,1,n+1} \\ \gamma_{\uparrow,2,n+1} \end{pmatrix} = i \sum_n \left(\tilde{\gamma}_{\uparrow,1,n}\gamma_{\uparrow,1,n+1} + \tilde{\gamma}_{\uparrow,2,n}\gamma_{\uparrow,2,n+1} \right) \ ,$$

and analogously for $M^{\dagger}_{\downarrow} H^{\downarrow}_{\mathrm{CII}} M_{\downarrow}$. Thus, we may recast $H^{\mathrm{PPW}}_{\mathrm{CII}}$ into the form [5]

$$\tilde{H}^{\mathrm{PPW}}_{\mathrm{CII}} = i \sum_n \sum_{\sigma=\uparrow,\downarrow} \left(\tilde{\gamma}_{\sigma,1,n}\gamma_{\sigma,1,n+1} + \tilde{\gamma}_{\sigma,2,n}\gamma_{\sigma,2,n+1} \right) \ . \tag{6.11}$$

Now, we allow ourselves to be naive and check whether the index $a = 1, 2$ is really necessary in order to put the Hamiltonian in the symmetry class CII. Hence, we remove the second term in (6.11) and suppress the remaining site index:

$$\tilde{H}^{\mathrm{PPW}}_{\mathrm{CII}} \xrightarrow{\text{drop } a} H^{1}_{\mathrm{CII}} = i \sum_n \sum_{\sigma=\uparrow,\downarrow} \tilde{\gamma}_{\sigma,n}\gamma_{\sigma,n+1} \ , \tag{6.12}$$

and thus the CII chain hosts Majorana zero modes $\tilde{\gamma}_{\uparrow,N}$, $\tilde{\gamma}_{\downarrow,N}$ on the right edge of the chain and $\gamma_{\uparrow,1}$, $\gamma_{\downarrow,1}$ on the left edge of the chain. Generically, when a spinful time-reversal symmetry is present, the pairs of Majorana zero modes on each edge are referred to as *Kramers pairs* due to Kramers theorem discussed briefly in section

[5] The basis transformation, M_s, and this representation of the PPW Hamiltonian is nowhere to be found in [95]. However, the correctness of the expression has been verified by one of the authors (Prakash) [96].

3.1.[6] To easier analyze the symmetries of the model, we turn our attention to the corresponding single-particle BdG Hamiltonian as in the previous section. In this case, the entire calculation will be provided in the main text. First, the CII Hamiltonian has to be expressed in terms of fermionic creation and annihilation operators:

$$
\begin{aligned}
H^1_{\text{CII}} &= i\sum_j \sum_{\sigma=\uparrow,\downarrow} i(c^\dagger_{\sigma,j} - c_{\sigma,j})(c^\dagger_{\sigma,j+1} + c_{\sigma,j+1}) \\
&= -\sum_j \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{\sigma,j} - c_{\sigma,j})(c^\dagger_{\sigma,j+1} + c_{\sigma,j+1}) \\
&= -\sum_j \sum_{\sigma=\uparrow,\downarrow} \left(c^\dagger_{\sigma,j} c^\dagger_{\sigma,j+1} + c^\dagger_{\sigma,j} c_{\sigma,j+1} - c_{\sigma,j} c^\dagger_{\sigma,j+1} - c_{\sigma,j} c_{\sigma,j+1} \right) ,
\end{aligned}
$$

and by expressing the fermionic operators in momentum space according to

$$
c_{\sigma,j} = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{-ijk} c_{\sigma,k} \ , \tag{6.13}
$$

it is a simple matter to write the CII model in a Bogoliubov-de Gennes fashion:

$$
\begin{aligned}
H^1_{\text{CII}} = &-\frac{1}{N} \sum_{j,k,k',\sigma} \Big(c^\dagger_{\sigma,k} c^\dagger_{\sigma,k'} \mathrm{e}^{ij(k'+k)+ik'} + c^\dagger_{\sigma,k} c_{\sigma,k'} \mathrm{e}^{ij(k-k')-ik'} \\
&\qquad - c_{\sigma,k} c^\dagger_{\sigma,k'} \mathrm{e}^{ij(k'-k)+ik'} - c_{\sigma,k} c_{\sigma,k'} \mathrm{e}^{-ij(k'+k)-ik'} \Big) \\
= &-\sum_{k,\sigma} \left(c^\dagger_{\sigma,k} c^\dagger_{\sigma,-k} \mathrm{e}^{-ik} + c^\dagger_{\sigma,k} c_{\sigma,k} \mathrm{e}^{-ik} - c_{\sigma,k} c^\dagger_{\sigma,k} \mathrm{e}^{ik} - c_{\sigma,k} c_{\sigma,-k} \mathrm{e}^{ik} \right) \\
= &-\frac{1}{2} \sum_{k,\sigma} \Big(c^\dagger_{\sigma,k} c^\dagger_{\sigma,-k} \mathrm{e}^{-ik} + c^\dagger_{\sigma,-k} c^\dagger_{\sigma,k} \mathrm{e}^{ik} + c^\dagger_{\sigma,k} c_{\sigma,k} \mathrm{e}^{-ik} + c^\dagger_{\sigma,-k} c_{\sigma,-k} \mathrm{e}^{ik} \\
&\qquad - c_{\sigma,k} c^\dagger_{\sigma,k} \mathrm{e}^{ik} - c_{\sigma,-k} c^\dagger_{\sigma,-k} \mathrm{e}^{-ik} - c_{\sigma,k} c_{\sigma,-k} \mathrm{e}^{ik} - c_{\sigma,-k} c_{\sigma,k} \mathrm{e}^{-ik} \Big) \\
= &\sum_k \begin{pmatrix} c^\dagger_{\uparrow,k} \\ c^\dagger_{\downarrow,k} \\ c_{\downarrow,-k} \\ -c_{\uparrow,-k} \end{pmatrix}^T
\begin{pmatrix}
-(\frac{\mathrm{e}^{-ik}+\mathrm{e}^{ik}}{2}) & 0 & 0 & -(\frac{\mathrm{e}^{ik}-\mathrm{e}^{-ik}}{2}) \\
0 & -(\frac{\mathrm{e}^{-ik}+\mathrm{e}^{ik}}{2}) & -(\frac{\mathrm{e}^{-ik}-\mathrm{e}^{ik}}{2}) & 0 \\
0 & -(\frac{\mathrm{e}^{ik}-\mathrm{e}^{-ik}}{2}) & \frac{\mathrm{e}^{-ik}+\mathrm{e}^{ik}}{2} & 0 \\
\frac{\mathrm{e}^{-ik}-\mathrm{e}^{ik}}{2} & 0 & 0 & -(\frac{\mathrm{e}^{-ik}+\mathrm{e}^{ik}}{2})
\end{pmatrix}
\begin{pmatrix} c_{\uparrow,k} \\ c_{\downarrow,k} \\ c^\dagger_{\downarrow,-k} \\ -c^\dagger_{\uparrow,-k} \end{pmatrix} , \\
= &\sum_k \begin{pmatrix} c^\dagger_{\uparrow,k} \\ c^\dagger_{\downarrow,k} \\ c_{\downarrow,-k} \\ -c_{\uparrow,-k} \end{pmatrix}^T
\underbrace{\begin{pmatrix}
-\cos(k) & 0 & 0 & -i\sin(k) \\
0 & -\cos(k) & i\sin(k) & 0 \\
0 & -i\sin(k) & \cos(k) & 0 \\
i\sin(k) & 0 & 0 & \cos(k)
\end{pmatrix}}_{=H(k)}
\begin{pmatrix} c_{\uparrow,k} \\ c_{\downarrow,k} \\ c^\dagger_{\downarrow,-k} \\ -c^\dagger_{\uparrow,-k} \end{pmatrix} ,
\end{aligned}
$$

[6] In the introduction, Chapter 1, of this thesis we argued that long-range separation of Majorana zero modes obeying non-abelian statistics can be useful to store information non-locally. Clearly, this is the case for the regular spinless Kitaev chain with two isolated Majorana edge modes with large separation in the thermodynamic limit. However, the cautious reader may be worried that a Kramer's pair of Majoranas combine into a fermion, thereby loosing its exotic statistics. Fortunately, this is not the case: in spinful TRS systems Kramer pairs of Majorana can still be braided in a non-commutative fashion [37][97].

where we adapted the Nambu spinor-convention introduced by Zhao and Wang [93].[7] The Bloch Hamiltonian, $H(k)$, can be written more elegantly by introducing Pauli matrices σ_i and τ_i acting on spin degrees of freedom and particle-hole degrees of freedom respectively.[8] One obtains:

$$H(k) = \sin(k)\sigma_x \otimes \tau_y - \cos(k)\sigma_z \otimes \mathbf{1} \ , \tag{6.14}$$

which is seen to be invariant under the time-reversal transformation $\mathcal{T} = \mathbf{1} \otimes \tau_y \mathcal{K}$ and the particle-hole symmetry transformation $\mathcal{P} = -\sigma_y \otimes \mathbf{1}\mathcal{K}$, $\mathcal{K}$ being the complex conjugation operator. In other words,

$$\mathcal{T}H(k)\mathcal{T}^{-1} = H(-k) \ , \mathcal{P}H(k)\mathcal{P}^{-1} = -H(-k) \ . \tag{6.15}$$

Note that $\mathcal{T}^2 = \mathcal{P}^2 = -1$, which confirms that $H(k)$ in the CII symmetry class. However, one might also choose the particle-hole operator $\mathcal{P} = \sigma_y \otimes \tau_y \mathcal{K}$ and still fulfill (6.15), giving $\mathcal{C}^2 = +1$ and putting the model in symmetry class DIII. Remarkably, (6.14) can be related to the CII Hamiltonian suggested by Zhao and Wang, $H_{\mathrm{ZW}}(k)$, equation (6.1) with $\Delta = t = 1$ and $\mu = 0$, via a unitary transformation, U, such that

$$UH(k)U^\dagger = H_{\mathrm{ZW}}(k) \ , \tag{6.16}$$

where U, in matrix representation, can be taken as[9]

$$U = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 \end{pmatrix} = \frac{1}{2}\mathbf{1} \otimes \tau_z + \frac{1}{2}\sigma_x \otimes \mathbf{1} + \frac{i}{2}\sigma_y \otimes \tau_x + \frac{i}{2}\sigma_z \otimes \tau_y \ . \tag{6.17}$$

The latter representation makes the connection between $H(k)$ and $H_{\mathrm{ZW}}(k)$ more explicit (since these are expressed as linear combinations of Kronecker products of Pauli matrices in spin space and particle-hole space). This shows that our discussion of topological invariants in the previous section will now serve as well. In particular, we do not have to provide a new calculation of the topological invariant for the CII model in the setting of Prakash et al. but can rely on the discussion in 6.1.1. Now we return to H^1_{CII} and use this Hamiltonian to form the corresponding translation-invariant α-chain for Hamiltonians in symmetry class CII in analogy with (5.1) in Chapter 5:

$$H^\alpha_{\mathrm{CII}} = i\sum_n \sum_{\sigma=\uparrow,\downarrow} \tilde{\gamma}_{\sigma,n}\gamma_{\sigma,n+\alpha} \ , \tag{6.18}$$

which, due to spin-degeneracy, hosts $2|\alpha|$ Majoranas at *each* edge. These chains may now be used as basis elements when forming a general CII Hamiltonian:

$$H_{\mathrm{CII}} = \sum_\alpha t_\alpha H^\alpha_{\mathrm{CII}} \ , t_\alpha \in \mathbf{R} \ . \tag{6.19}$$

As before, basis elements of the type $i\gamma_n\gamma_m$ or $i\tilde{\gamma}_n\tilde{\gamma}_m$ are not allowed in H_{CII} due to time-reversal symmetry.

---

[7] Another popular convention for the Nambu spinor, $\Psi^\dagger$, is given by $\Psi^\dagger = (a^\dagger_{k\uparrow}, a^\dagger_{k\downarrow}, -a_{-k\downarrow}, a_{-k\uparrow})$.

[8] It is a matter of choice whether to write the Hamiltonian as $H(k) = f_{ij}(k)\sigma_i \otimes \tau_j$ or $H(k) = f_{ij}(k)\tau_i \otimes \sigma_j$.

[9] It should be noted that the proposed unitary transformation is by no means unique. However, U fulfills the conditions $UH(k) = H_{\mathrm{ZW}}(k)U$ and $UU^\dagger = \mathbf{1}$ which is all we require.

6.2 Classifying critical phases of CII

We have now justified that the representative CII Hamiltonian can be seen as two copies of the BDI Hamiltonian, assigning a spin index to each copy, cf. equation (5.3). In other words, H_{CII}, can equivalently be written as

$$H_{\mathrm{CII}} = H_{\mathrm{BDI}}^{(1)} + H_{\mathrm{BDI}}^{(2)} \;, \tag{6.20}$$

with (1) and (2) referring to $\uparrow$ and $\downarrow$ respectively. Considering the different decoupled chains we may use the concept of stacking BDI chains to describe the CII model. In particular, given that $H_{\mathrm{BDI}}^{(1)}$ and $H_{\mathrm{BDI}}^{(2)}$ have a one-to-one correspondence with the complex functions $g(z)$ and $h(z)$, the function used to calculate the topological invariant of the stacked system is provided by Verresen et al. as [18]

$$f(z) = \begin{vmatrix} g(z) & 0 \\ 0 & h(z) \end{vmatrix} = g(z)h(z) \;. \tag{6.21}$$

Let us take the canonical example with the stacking of two H_{BDI}^{1}-chains to see that this construction holds. Recall that we calculated the topological invariant of H_{CII}^{1} to be equal to $\nu = 2$ in (6.6) for parameters $\Delta = t$ and $\mu = 0$. Now, our claim is that H_{CII}^{1} can be seen as two copies of the regular (BDI) Kitaev chain, H_1 in (5.1). Such a chain has a complex function $g(z) = z$ associated to it and consequently the topological invariant $\nu = 1$. Thus, the corresponding function $f(z)$ of H_{CII}^{1} is given by

$$f(z) = \begin{vmatrix} z & 0 \\ 0 & z \end{vmatrix} = z^2 \;, \tag{6.22}$$

according to the recipe above. This naturally gives a topological invariant $\nu = 2$, which coincides with our result in (6.6). For gapped systems, in which $f(z)$ has no zeros on the unit circle, it seems as the main difference between topological phases in the symmetry class CII and the symmetry class BDI is reflected in the degree of the poles and the degeneracies of the zeros of $f(z)$. Since $f(z)$ is the product of two identical functions $h(z) = g(z)$ (each associated to a gapped BDI chain), the zeros of $f(z)$ identically coincide with the zeros of $g(z)$ although they are at least two-fold degenerate.[10]

Turning our attention to *gapless* systems, we have to be very careful. The construction of stacking BDI copies on top of each other necessarily requires the inclusion of a unit cell (if we neglect the possibility of rewriting the resulting CII chain in a translation-invariant manner). Then, since the complex function $f(z)$ can be expressed as the product of energy bands [18] such that $|f(\mathrm{e}^{ik})| = \prod_n^N \epsilon_k^{(n)}$, with N being the number of bands (i.e. the number of BDI copies), it is clear that zero-degeneracies in $f(z)$ has another interpretation than in the translation-invariant case. In particular, we have seen that in the translation-invariant case the classification of gapless phases in terms of the central charge of the bulk CFT fails when the zeros on the unit circle are degenerate. This does not have to be the case with a unit cell. In fact, if all BDI copies are described by a CFT in the bulk (that is,

[10] We have omitted the rather uninteresting trivial case $f(z) = 1$ here.

they are each associated to complex functions with non-degenerate zeros on the unit circle), we should have no reason to worry about the stacked system. For instance, $f(z) = (z+1)^2$ does *not* in general imply a dynamical critical exponent $z_{\text{dyn}} = 2$. However, if the composition of $f(z)$ is unknown one can not use $f(z)$ to distinguish a CFT with $c = 1$ from a gapless quadratic point with $z_{\text{dyn}} = 2$.

6.3 Topological classification of remaining BdG classes

Given that the bulk of the two BDI chains labeled by the spin index $\sigma =\uparrow, \downarrow$ is described by a CFT, we have been able to perform an extension of Verresen, Jones and Pollmann's arguments to include symmetry class CII giving an $2\mathbf{N}\times 2\mathbf{Z}$-classification for gapless phases. The factor "2" is due to the spin degeneracy. It still remains to classify gapless phases in the symmetry classes D and DIII, which both have a non-trivial gapped $\mathbf{Z}_2-$classification in one dimension, see Table 4.1. It is clear that the winding number-description outlined in [18] can not be immediately used in these cases to compute $\mathbf{Z}_2$-invariants, which rather are commonly computed as Pfaffians [15]. However, as shown by Ardonne and Budich for the Kitaev chain in class D, the $\mathbf{Z}_2$-invariant can equivalently be computed in terms of a Zak-Berry phase [27][31] and consequently a winding number [98]. Moreover, in a presence of an additional $U(1)$ spin rotation symmetry, Budich and Ardonne argue (in another paper) that a 1D topological superconductor in class DIII can be understood as two copies of the TSC in class D, each copy being assigned one spin direction [99]. This is analogous to the construction of a representative CII model using two BDI chains presented in the previous section. Hence, it seems plausible that it is possible to provide a topological classification for gapped and gapless phases in classes D and DIII in the light of Verresen, Jones and Pollman as well. However, focusing on symmetry class D, Ardonne and Budich allow for fermionic chains which are neither translation-invariant or time-reversal invariant forcing us to introduce terms of the type $i\gamma_n\gamma_m$ and $i\tilde{\gamma}_n\tilde{\gamma}_m$ such that a general superconducting (mean field) Hamiltonian without any physical symmetries[11] can be expressed as[100]

$$H_{\text{D}} = \frac{i}{4}\sum_{j,k}\gamma_j t_{jk}\gamma_k \ , \gamma_{2j} = i(c_j^\dagger - c_j) \ , \gamma_{2j-1} = c_j^\dagger + c_j \ , j = 1...N \ , \tag{6.23}$$

where $t_{ij} = -t_{ji} \in \mathbf{R}$ are matrix elements in an $2N \times 2N$ real matrix, T. In our notation, $\gamma_{2j} \leftrightarrow \tilde{\gamma}_j$ and $\gamma_{2j-1} \leftrightarrow \gamma_j$ and (6.23) can be rewritten according to

$$H_{\text{D}} = \frac{i}{4}\sum_{j,k}\tilde{\gamma}_j a_{jk}\tilde{\gamma}_k + \frac{i}{4}\sum_{j,k}\gamma_j b_{jk}\gamma_k + \frac{i}{2}\sum_{j,k}\tilde{\gamma}_j g_{jk}\gamma_k \ , \tag{6.24}$$

with $a_{jk} = t_{2j,2k}$, $b_{jk} = t_{2j-1,2k-1}$ and $g_{jk} = t_{2j-1,2k}$. The last term was our starting-point for the generic, time-reversal symmetric, BDI Hamiltonian, equation (5.2), before demanding translation-invariance. Now, it is by no means obvious how to

[11] As stressed earlier Hamiltonians in class D have a particle-hole symmetry. This symmetry emerges as a result of introducing Bogoliubov quasiparticles, which is a mathematical construction.

relate the entries in the matrix T to a complex, meromorphic function $f(z)$ which is one-to-one with the Hamiltonian H_D. Naively, we may follow the logic by Ardonne and Budich and make use of the fact that T, being real and anti-symmetric, have purely imaginary eigenvalues which come in complex-conjugated pairs, i.e. $\pm i\epsilon_\lambda$, $\epsilon_\lambda > 0$. Note that this reasoning is only valid for gapped systems ($\epsilon_\lambda \neq 0$). Hence, T can be brought to an off-diagonal *Jordan form* using an orthogonal transformation, W $(WW^T = \mathbf{1})$[98]:

$$\tilde{T} = WTW^T = \mathrm{diag}\begin{pmatrix} 0 & \epsilon_\lambda \\ -\epsilon_\lambda & 0 \end{pmatrix} . \tag{6.25}$$

Now, as outlined in detail in [98], one can show that the $\mathbf{Z}_2$ Pfaffian invariant, $\mathcal{M}$, introduced by Kitaev [15] can be related to a winding integral over half the Brillouin zone of the quantity, $\det(\tilde{W}(k))$, which is the determinant of the Fourier transform of W:

$$\mathcal{M} = (-1)^\nu \ , \nu = i\int_0^\pi dk\partial_k \mathrm{log}(\det(\tilde{W}(k))) \ , \tag{6.26}$$

where ν is seen to be an integer since $\det(\tilde{W}(k))) = \mathrm{e}^{i\varphi_k}$ and $\varphi_k = \varphi_{-k}$. This implies that Kitaev's $\mathbf{Z}_2$-invariant takes two values, ± 1 with one sign (-) being attributed to a topological phase and one sign (+) attributed to a trivial phase. At first glance it may seem as if we are not able to give this winding number the same physical interpretation as in the BDI-case, that is, the winding number counts the number of Majorana edge modes. This is since, $\nu = 2m$, $m \in \mathbf{N}$, corresponds to the trivial phase and $\nu = 2m - 1$ to the topological phase, and naively it seems as if we only can have an odd number of MZMs in the topological phase. However, since time-reversal symmetry is not present in the symmetry class D, phases of matter with different topological invariants $\nu_1 = 2m - 1$ and $\nu_2 = 2n - 1$, $n, m \in \mathbf{N}$, $n \neq m$ can be adiabatically connected without closing the energy gap [101]. Using the same argument, (non-topological) phases with an even non-zero topological invariant can be considered equivalent to a trivial phase with $\nu = 0$. Hence, ν still counts Majorana edge modes in class D. Still the construction does not hold for gapless systems. As such, the analysis of the symmetry classes D and DIII is incomplete, although it seems reasonable to expect a single topological phase with $\mathcal{M} = -1$ per central charge c as also concluded by Verresen, Jones and Pollmann [18].

7

Conclusion

This thesis has served to review the nowadays well-established field in condensed matter physics – topological quantum matter. This field provides a bridge between abstract mathematics and measurable quantities. In contrast to much of the introductory literature on the subject, the emphasis has been put on topological superconductors rather than on topological insulators. The fact that such superconductors may host Majorana bound states, which are exotic quasiparticle excitations obeying non-abelian anyon statistics, is truly remarkable and hence, doing basic research on the topic is well-motivated by desirable future technological applications.

We have been concerned with the existence of Majorana zero modes in the simplest setting possible: one-dimensional and non-interacting systems. In fact, we have seen that already these toy models demonstrate rich physics in the sense that they well illustrate the concepts of symmetry-protected topological phases and their relation to topological invariants and boundary states. Moreover, although the gapped classification of topological classification of one-dimensional TSCs is fully understood and neatly summarized in the tenfold table, we have indicated that the comprehension of gapless critical systems is lacking. Therefore, this thesis can also be seen as an attempt of addressing the issue of what happens precisely at a topological phase transition. Following the logic by Verresen, Jones and Pollmann, we have been able to extend their topological classification for gapless superconductors in the BDI symmetry class to CII in terms of the conventional $\mathbf{Z}$-invariant, the winding number, complemented by the central charge c in the bulk conformal field theory. In particular, it was shown that the winding number counts Majorana zero modes, although the extension to the CII-class introduces a doubling of the edge modes due to spin degeneracy. This is also reflected in the winding number only taking even integer values in the CII-case. Finally, we also commented on the difficulties of extending the classification of gapless phases to the remaining BdG-classes with a non-trivial topological invariant in one dimension. However, in classes D and DIII, these are $\mathbf{Z}_2$-invariants commonly computed as Pfaffians, making them difficult to interpret in the context of our earlier discussion based on a winding number construction.

More importantly, it should be noted that realistic topological systems are expected to be more complex than implied by the simple toy models studied above. Firstly, it would be favourable to classify topological phases of matter in a larger number of dimensions and secondly, interactions between electrons have to be taken into account. Unfortunately, this Master's thesis resides almost exclusively in a one-dimensional universe with electrons that interact only at mean-field level to form Cooper pairs. On the other hand, just a couple of decades ago there would be no material at all to fill this thesis with and that would be truly dissatisfying. The journey starting in 1980 with the discovery of the (integer) quantum Hall effect, eventually leading to the detection of the first experimental signals of possible Majorana zero modes and a couple of Nobel prizes[1] on the way, has only begun. Additionally, and optimistically, the experimental realization of topological quantum computing might soon be made successful. Thus, to conclude, from a physics perspective, these are truly interesting times.

[1]von Klitzing was awarded the prize for the experimental discovery of the quantization of the Hall conductivity in 1985, and a cousin of IQHE, the Fractional Quantum Hall Effect was rewarded in 1998 when Laughlin, Störmer and Tsu received the prize. More recently, in 2016, the entire field of topological quantum matter was celebrated and exposed to the public, when Thouless, Haldane and Kosterlitz got their Nobel medals [102].

A
Alternative Form of Winding Number Integral

In Asboth et al. [5], the following definition of the winding number ν is given:

$$\nu = \frac{1}{2\pi} \int_{k \in 1\mathrm{BZ}} \vec{e}_{\vec{d}}(k) \times \frac{d}{dk} \vec{e}_{\vec{d}}(k) dk \ , \tag{A.1}$$

where $\vec{e}_{\vec{d}}(k) = \frac{\vec{d}(k)}{|\vec{d}(k)|}$ is the projection of $\vec{d} = (d_x, d_y, d_z)$ onto the unit circle. Moreover, $\vec{e}_{\vec{d}}$ is well-defined since it is assumed that $|\vec{d}| \neq 0$. The claim is then that, in the case of the SSH model (or any other model with an off-diagonal Bloch Hamiltonian), the integral above is equivalent to

$$\nu = \frac{1}{2\pi i} \int_{k \in 1\mathrm{BZ}} dk \frac{d}{dk} (\log(h(k))) \ , \tag{A.2}$$

with $h(k) = d_x - i d_y$. Showing this equivalence is the topic of this appendix. Since $d_z = 0$ by chiral symmetry, it follows that the result of taking the cross-product in (A.1) is a vector in the $\hat{z}$-direction:

$$\vec{e}_{\vec{d}}(k) \times \frac{d}{dk} \vec{e}_{\vec{d}}(k) = \frac{(d_x, d_y, 0)}{|\vec{d}|} \times \frac{d}{dk} (\frac{(d_x, d_y, 0)}{|\vec{d}|}) = (\tilde{d}_x \frac{d}{dk} \tilde{d}_y - \tilde{d}_y \frac{d}{dk} \tilde{d}_x) \hat{z} \ ,$$

where we introduced $\tilde{d}_x = \frac{d_x}{|\vec{d}|}$ (and similar for $\tilde{d}_y$). Now, we have to write the expression out explicitly and be careful about signs:

$$\begin{aligned}
\tilde{d}_x \frac{d}{dk} \tilde{d}_y &= \frac{d_x}{\sqrt{d_x^2 + d_y^2}} (\frac{d'_y}{\sqrt{d_x^2 + d_y^2}} + d_y \frac{d}{dk} (\frac{1}{\sqrt{d_x^2 + d_y^2}})) \ , \\
\tilde{d}_y \frac{d}{dk} \tilde{d}_x &= \frac{d_y}{\sqrt{d_x^2 + d_y^2}} (\frac{d'_x}{\sqrt{d_x^2 + d_y^2}} + d_x \frac{d}{dk} (\frac{1}{\sqrt{d_x^2 + d_y^2}})) \ ,
\end{aligned}$$

and when taking the difference between the two terms, the terms with derivatives on $\frac{1}{|\vec{d}|}$ cancel yielding

$$\tilde{d}_x \frac{d}{dk} \tilde{d}_y - \tilde{d}_y \frac{d}{dk} \tilde{d}_x = \frac{d_x d'_y - d_y d'_x}{d_x^2 + d_y^2} \ . \tag{A.3}$$

Next, note that

$$\frac{d}{dk} \Big(d_x - i d_y \Big) (d_x + i d_y) = d'_x d_x + d_y d'_y - i (d'_y d_x - d'_x d_y) \ , \tag{A.4}$$

and therefore

$$\nu = \frac{i}{2\pi} \int \frac{\frac{d}{dk}(d_x - id_y)(d_x + id_y)}{d_x^2 + d_y^2} dk - \frac{i}{2\pi} \int \frac{d_x' d_x + d_y' d_y}{d_x^2 + d_y^2} dk \ . \tag{A.5}$$

The second term is easily evaluated:

$$\frac{i}{2\pi} \int_{k \in 1\mathrm{BZ}} \frac{d_x' d_x + d_y' d_y}{d_x^2 + d_y^2} dk = \frac{i}{4\pi} [\log(d_x^2 + d_y^2)]_{k=0}^{2\pi} = 0 \ , \tag{A.6}$$

since $h(k) = d_x^2 + d_y^2$ and $|h(0)| = |h(2\pi)|$. The remaining term gives the final formula (up to a sign)

$$\begin{aligned}
\nu &= \frac{i}{2\pi} \int_{k \in 1\mathrm{BZ}} \frac{\frac{d}{dk}(d_x - id_y)(d_x + id_y)}{(d_x + id_y)(d_x - id_y)} dk \\
&= \frac{i}{2\pi} \int_{k \in 1\mathrm{BZ}} \frac{\frac{d}{dk}(h(k))}{h(k)} dk = \frac{i}{2\pi} \int_{k \in 1\mathrm{BZ}} dk \frac{d}{dk} \log(h(k)) \ .
\end{aligned}$$

We are therefore left with

$$\nu = -\frac{1}{2\pi i} \int_{k \in 1\mathrm{BZ}} dk \frac{d}{dk} \log(h(k)) \ , \tag{A.7}$$

which agrees with Asboth up to an (irrelevant) sign. The sign is quite arbitrary in the sense that it depends on whether the curve $\vec{e}_{\vec{d}}(k)$ is traversed clockwise or anti-clockwise around the origin. Going back to (A.4), we could get rid of the sign by considering $h^*(k)$ rather than $h(k)$ by noting

$$\frac{d}{dk}\Big((d_x + id_y)\Big)(d_x - id_y) = d_x' d_x + d_y d_y' + i(d_y' d_x - d_x' d_y) \ , \tag{A.8}$$

and therefore

$$\nu = -\frac{i}{2\pi} \int_0^{2\pi} \frac{\frac{d}{dk}(d_x + id_y)}{d_x + id_y} dk = \frac{1}{2\pi i} \int_0^{2\pi} \frac{\frac{d}{dk} h^*(k)}{h^*(k)} dk \ , \tag{A.9}$$

concluding that

$$\nu = -\frac{1}{2\pi i} \int_0^{2\pi} dk \frac{h'(k)}{h(k)} = \frac{1}{2\pi i} \int_0^{2\pi} dk \frac{\frac{d}{dk} h^*(k)}{h^*(k)} \ . \tag{A.10}$$

This means that it does not matter if we work with $h(k)$ or $h^*(k)$. The resulting winding numbers will only differ by a total sign.

B

Connecting $f(z)$ of VJP to $h(z)$ of the Kitaev Model

In this section we will demonstrate a connection between the function $h(z)$ in the Kitaev model, cf. equation (4.46), and the complex, meromorphic $f(z)$ introduced by Verresen, Jones and Pollmann to classify topological phases in symmetry class BDI [18]. Recall that the non-topological phase of the Kitaev model sits in H_0 and the topological phase sits in H_1, see equations (4.26) and (4.27) respectively. Recall the Bloch Hamiltonian for the Kitaev model:

$$H(k) = \begin{pmatrix} -\mu - 2t\cos(k) & -2i\Delta\sin(k) \\ 2i\Delta\sin(k) & \mu + 2t\cos(k) \end{pmatrix} = \begin{pmatrix} h_z & -ih_y \\ ih_y & -h_z \end{pmatrix} , \tag{B.1}$$

with $h_z = -\mu - 2t\cos(k)$ and $h_y = 2\Delta\sin(k)$. Now, by a unitary transformation $U = \mathrm{e}^{-i\varphi_k\sigma_x/2}$ we will be able to diagonalize $H(k)$ according to

$$UH(k)U^\dagger = \begin{pmatrix} E(k) & 0 \\ 0 & -E(k) \end{pmatrix} , \tag{B.2}$$

where $E(k) = \pm\sqrt{(\mu + 2t\cos(k))^2 + 4\Delta^2\sin^2(k)}$ is the bandstructure, cf. equation (4.37), equal to the single-particle energy, ϵ_k. The unitary transformation can be rewritten as

$$U = \mathrm{e}^{-i\varphi_k\sigma_x/2} = \cos(\frac{\varphi_k}{2}) - i\sin(\frac{\varphi_k}{2})\sigma_x , \tag{B.3}$$

which is easily proven by expressing the exponential as a Taylor series, cf. the derivation leading up to (4.42). Written out, U reads

$$U = \begin{pmatrix} \cos(\frac{\varphi_k}{2}) & -i\sin(\frac{\varphi_k}{2}) \\ -i\sin(\frac{\varphi_k}{2}) & \cos(\frac{\varphi_k}{2}) \end{pmatrix} . \tag{B.4}$$

Now, we need to compute the matrix product $UH(k)U^\dagger$:

$$UH(k)U^\dagger = \begin{pmatrix} h_z\cos(\varphi_k) + h_y\sin(\varphi_k) & -ih_y\cos(\varphi_k) + ih_z\sin(\varphi_k) \\ ih_y\cos(\varphi_k) - ih_z\sin(\varphi_k) & -h_z\cos(\varphi_k) - h_y\sin(\varphi_k) \end{pmatrix} . \tag{B.5}$$

Comparing this with the diagonal matrix $\mathrm{diag}(E, -E)$ we immediately see that

$$\begin{aligned} h_z\cos(\varphi_k) + h_y\sin(\varphi_k) &= E \\ h_y\cos(\varphi_k) &= h_z\sin(\varphi_k) . \end{aligned}$$

Assuming $h_z \neq 0$ ($\mu \neq -2t$) we may solve for $\sin(\varphi_k) = \frac{h_y}{h_z}\cos(\varphi_k)$ and plug the result into the first equation:

$$(h_z + \frac{h_y^2}{h_z})\cos(\varphi_k) = E \Rightarrow \cos(\varphi_k) = \frac{Eh_z}{h_z^2 + h_y^2} = \pm\frac{h_z}{|E|} \ , \tag{B.6}$$

using the fact $E^2 = h_y^2 + h_z^2$. Similarly, we can solve for $\cos(\varphi_k) = \frac{h_z}{h_y}\sin(\varphi_k)$ (assuming $h_y \neq 0$) and get an expression for $\sin(\varphi_k)$:

$$(\frac{h_z^2}{h_y} + h_y)\sin(\varphi_k) = E \Rightarrow \sin(\varphi_k) = \pm\frac{h_y}{|E|} \ . \tag{B.7}$$

Therefore, we have

$$f(k) = E(k)\mathrm{e}^{i\varphi_k} = \pm(h_z + ih_y) \ . \tag{B.8}$$

Note that if we pick the $+$ sign for h_z and the $-$ sign for h_y $f(z)$ reduces to precisely $h(z)$ in (4.46). This is remarkable! We have thus found out that $f(z)$ seems like a plausible candidate for computing winding numbers (at least this holds for the Kitaev model).

C

Phase Transitions and Critical Systems

Most readers are probably well acquainted with the concept of phase transitions from a course in thermodynamics or even from elementary level physics. A familiar example of a phase transition is when water freezes to ice, but Nature exhibits many other types of phase transitions, as when a metal is cooled down to low temperatures and becomes superconducting. These examples have in common that both transitions occur by varying an external parameter, in this case temperature. The topological phase transitions discussed in this thesis, however, are *non-thermal*, happening at zero temperature and so called *quantum phase transitions.* A phase transition is here induced by changing a non-thermal control parameter, such as a magnetic field, chemical potential, or coupling constant. In the discussion below, we have closely followed the canonical work by Sachdev [103] and the review by Vojta [104] (although Vojta has benefited a lot from Sachdev).

Conventionally, one distinguishes between *first-order* transitions and *continuous* transitions. In the realm of classical thermal phase transitions, first-order transitions involve a discrete jump in energy, i.e. latent heat, at the transition temperature, a characteristic feature well-known from the water-vapor and ice-water phase transitions. Continuous transitions instead demonstrate a discontinuity or a singular behavior in the derivatives of thermodymamic quantities. In particular, such transitions are described by some order parameter which is non-zero in one phase (ordered phase) and zero in the other phase referred to as the disordered phase or the high-symmetric phase.[1] This is since conventional phase transitions are associated with broken symmetries. For instance, the spins in a paramagnetic material with (spontaneous) magnetization $M = 0$ display rotational symmetry but in a ferromagnetic phase with $M \neq 0$ the spins tend to align with the direction of the magnetization, breaking the rotational symmetry. Above a certain temperature $T > T_C$ the magnetization of a ferromagnetic material vanishes while for $T < T_C$ M is non-zero. As $T \to T_C$ the magnetization goes to zero according to the power-law[81]

$$M \sim (T_C - T)^{\beta} \ , \tag{C.1}$$

with $\beta = \frac{1}{8}$. Note that M is continuous at $T = T_C$. This is not the case for its

[1] It is really the *thermodynamic average* of the order parameter which is zero or non-zero in the disordered or orded phases.

derivative with respect to the magnetic field, h, that is, the magnetic susceptibility:

$$\chi = \frac{\partial M}{\partial h} \sim (T - T_C)^{-\gamma} \ , \tag{C.2}$$

with $\gamma = \frac{7}{4}$. Moreover, although the thermodynamic average of the magnetization is zero for $T > T_c$, the fluctuations of the parameter are non-zero in general. In particular, if $T \to T_C$ the spatial correlations between the fluctuations will be very large and the correlation length, $\xi(T)$, scales as

$$\xi(T) \sim \frac{1}{|T - T_C|} \ . \tag{C.3}$$

For a generic system undergoing a continuous phase transition the correlation length does not have to depend on temperature but rather

$$\xi \sim |t|^{-\nu} \ , \tag{C.4}$$

with $|t| = |\lambda - \lambda_c|$, λ being some external control parameter.[2] The *critical exponent* ν is of crucial importance and determines the divergence of the correlation length. Similarly, one can also define a correlation time, τ_c, which determines the time scale of the decay of correlations between fluctuations of the order parameter,

$$\tau_c \sim \xi^z \sim |t|^{-\nu z} \ , \tag{C.5}$$

in this way introducing the *dynamical critical exponent* z. The parameters ν and z are fundamental characteristics of continuous phase transitions and critical phenomena. At the critical point the correlation length and correlation time are infinite and fluctuations of the order parameter occur at all time scales and length scales, i.e. scale invariance is manifest. Therefore, in the vicinity of the critical point, all thermodynamic functions (such as M and χ) are defined by power-laws. Critical phenomena are thus completely characterized by the different critical exponents (up to amplitudes, which are usually less relevant when comparing theory to experiments). Interestingly, the critical exponents are not independent from each other but are in general connected by the *scaling hypothesis*. In our example with the ferromagnet with magnetization M, the hypothesis states that the free energy density is a *homogenous* function of the parameters t and h near the critical point $T \to T_C$. Introducing the free energy density $f(t, h)$ there must then exist exponents λ^a and λ^b such that

$$f(\lambda^a t, \lambda^b h) = \lambda f(t, h) \ , \tag{C.6}$$

since the correlation length is the only relevant length scale at $T = T_C$. Moreover, note that the quantity $t^{-1/a} f(t, h)$ is invariant under the transformations $t \to \lambda^a t$ and $h \to \lambda^b h$:

$$t^{-1/a} f(t, h) \to (\lambda^a t)^{-1/a} f(\lambda^a t, \lambda^b h) = t^{-1/a} f(t, h) \ , \tag{C.7}$$

according to (C.6). This implies that $t^{-1/a} f(t, h)$ only depends on the scale-invariant parameter $y = h/t^{b/a}$, i.e. $t^{-1/a} f(t, h) = g(y)$ and therefore we must be able to write

$$f(t, h) = t^{1/a} g(y) \ , y = \frac{h}{t^{b/a}} \ , \tag{C.8}$$

[2]One can also renormalize $|t|$ to be dimensionless by writing $|t| = |\lambda - \lambda_c|/|\lambda_c|$.

which is consistent with (C.6) under the transformations $t \to \lambda^a t$ and $h \to \lambda^b h$. Now, the derivatives of the free energy at zero magnetic field, $h = 0$, are related to the spontaneous magnetization and the magnetic susceptibility according to

$$M = -\frac{\partial f}{\partial h}_{h=0} = t^{(1-b)/a} g'(0) \ ,$$
$$\chi = \frac{\partial^2 f}{\partial h^2}_{h=0} = t^{(1-2b)/a} g''(0) \ .$$

By comparing these equations to (C.1) and (C.2) the following constraints have to be obeyed:

$$\gamma = \frac{1-b}{a} \ ,$$
$$\beta = -\frac{(1-2b)}{a} \ .$$

These relations show that the critical exponents γ and β are related through what is called a *scaling law*.

The most remarkable feature about continuous phase transitions concerns the concept of *universality classes*. Near the critical point the behavior of the system is solely determined by the symmetries and dimensionality of the order parameter and not the microscopic properties of the Hamiltonian (which otherwise characterizes the system). This means that there exists entire classes of phase transitions described by certain critical exponents, and thus, systems which describe completely different kinds of physics may belong to the same universality class. Given that the critical exponents are well-investigated for a single simple model it then immediately follows that all other models in the same universality class have the same exponents.

It is now in order to comment on the distinction between quantum phase transitions and the classical phase transitions we have discussed above. In quantum mechanics, the energy scale $\hbar\omega_c$ of quantum fluctuations is important and should be compared to the (classical) thermal energy scale k_BT, with k_B being the Boltzmann constant and T the temperature. Simply put, whenever $\hbar w_c >> k_BT$ quantum mechanical effects have to be taken into account but if $\hbar\omega_c << k_BT$ the system can be treated classically. At zero temperature quantum fluctuations dominate the system's behavior. From (C.5) we note that the characteristic time scale, τ, diverges as the critical point $\lambda \to \lambda_c$ is approached. Similarly, the frequency scale ω_c vanishes at the quantum critical point and the energy scale goes as

$$\hbar\omega_c \sim |t|^{\nu z} \ . \tag{C.9}$$

Now, as soon as $\hbar\omega_c$ is smaller than k_BT, the order parameter fluctuations can be described classically.

The connection between quantum mechanical systems and classical systems in fact goes deeper than the discussion above. In fact, by turning to (quantum) statistical mechanics we may show an intimate connection between d-dimensional quantum systems and $d+1$-dimensional classical systems. In order to understand what happens when the temperature goes to zero and quantum mechanichal effects become important, we consider the partition function

$$Z(\beta) = \mathrm{tr}(\mathrm{e}^{-\beta H}) \ , \tag{C.10}$$

with $\beta = \frac{1}{k_B T}$ and $H = H_{\mathrm{kin}} + H_{\mathrm{p}}$ being the Hamiltonian with its kinetic (H_{kin}) and potential (H_{p}) parts. In a classical system the kinetic and potential part commute and hence the partition function factorizes according to $Z = Z_{\mathrm{kin}} Z_{\mathrm{pot}}$. In this way, the statics and dynamics of the system can be considered decoupled. In contrast, H_{kin} and H_{p} are anti-commuting quantities in a quantum theory, forcing us to consider both space and time-dependent fields in an order parameter field theory [104]. Next, note that the quantity $\mathrm{e}^{-\beta H}$ coincides with the regular time evolution operator $\mathrm{e}^{-iHt/\hbar}$ at (imaginary) time $t = -i\hbar\beta$, implying that

$$Z(\beta) = \sum_n \langle n | \mathrm{e}^{-\beta H} | n \rangle \ , \tag{C.11}$$

can be seen as a sum of (imaginary-time) transition amplitudes [105]. We have thus established that calculating the thermodynamics in the quantum system is equivalent of computing the dynamics in imaginary time. Note that, at zero temperature, the imaginary time-dimension in the quantum system becomes a proper space dimension in the classical system. As a result, the partition function of a d-dimensional quantum system is identical to the classical partition function in a $d+1$-dimensional classical system and in the quantum case the inverse temperature can be interpreted as imaginary time.[3] Note that this equivalence only holds in the so called *scaling limit* $\frac{\xi}{a} \to \infty$, ξ being the correlation length and a the microscopic length (lattice constant).

Let us be more explicit and properly show the equivalence between a 1D classical Ising model and a 0D (quantum) Ising model. The Hamiltonian, H in (C.10) is then given by that of a one-dimensional Ising model:

$$H = H_{\mathrm{Ising}} = -J \sum_i \sigma_i \sigma_{i+1} \ , \sigma_i = \pm 1 \ , \tag{C.12}$$

where σ_i are spins on a one-dimensional lattice and J describes the coupling strength between neighboring sites. Then it follows that the partition function can be expressed as

$$Z(\beta) = \prod_i \sum_{\{\sigma_i\}} \mathrm{e}^{K\sigma_i\sigma_{i+1}} \ , \tag{C.13}$$

introducing $K = J\beta$. Now, with slight abuse of notation, we may interpret $\mathrm{e}^{K\sigma_i\sigma_{i+1}}$ as elements $T_{\sigma_i\sigma_{i+1}}$ in a *transfer matrix*, T:

$$T = \begin{pmatrix} \mathrm{e}^{K} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K} \end{pmatrix} \ , \tag{C.14}$$

with eigenvalues $\epsilon_1 = \cosh K$ and $\epsilon_2 = \sinh K$. Next, we write out (C.13) in its full glory:

$$Z(\beta) = \sum_{\{\sigma_i\}} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \cdot \ldots \cdot T_{\sigma_{M-1}\sigma_1} = \mathrm{tr}(T^M) = \epsilon_1^M + \epsilon_2^M \ , \tag{C.15}$$

[3] Surely, this connection between quantum and classical systems is truly remarkable and, as Polyakov [106] puts it, there might be "deep reasons" for the analogies which have to do with the properties of spacetime.

where we imposed periodic boundary conditions, i.e. $\sigma_M = \sigma_1$. To further investigate the scaling limit $\frac{\xi}{a}$, we turn to correlation functions:

$$\langle\sigma_i\sigma_j\rangle = \frac{1}{Z}\sum_{\{\sigma_\lambda\}} \mathrm{e}^{K\sum_l \sigma_l\sigma_{l+1}}\sigma_i\sigma_j = \frac{1}{Z}\prod_l \sum_{\{\sigma_\lambda\}} \mathrm{e}^{K\sigma_l\sigma_{l+1}}\sigma_i\sigma_j \ , \tag{C.16}$$

where

$$\begin{aligned}
\prod_l \sum_{\{\sigma_\lambda\}} \mathrm{e}^{K\sigma_l\sigma_{l+1}}\sigma_i\sigma_j &= \sum_{\{\sigma_\lambda\}} T_{\sigma_1\sigma_2}T_{\sigma_2\sigma_3}\cdot\ldots\cdot T_{\sigma_{M-1}\sigma_1}\sigma_i\sigma_j \\
&= \sum \langle\sigma_1|T^{i-1}\sigma_z T^{j-i}\sigma_z T^{M-(j-1)}|\sigma_1\rangle \\
&= \mathrm{tr}\Big(T^{i-1}\sigma_z T^{j-i}\sigma_z T^{M-(j-1)}\Big) \ ,
\end{aligned}$$

where we made use of the resolution of identity $\sum_k |\sigma_k\rangle\langle\sigma_k| = \mathbf{1}$, $k \neq i, j$ and noted that $\sum_k \sigma_k|\sigma_k\rangle\langle\sigma_k| = |+\rangle\langle+| - |-\rangle\langle-|$ and $\sigma_z|\pm\rangle = \pm 1$. We also assumed $j \geq i$. Now, it is convenient to compute the trace in the eigenbasis of T. Let us denote the eigenstates of T by $|\rightarrow\rangle$ and $|\leftarrow\rangle$ where

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \ , |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle) \ , \tag{C.17}$$

with $T|\rightarrow\rangle = \epsilon_1|\rightarrow\rangle$ and $T|\leftarrow\rangle = \epsilon_2|\leftarrow\rangle$. Hence,

$$\begin{aligned}
\langle\sigma_i\sigma_j\rangle &= \frac{1}{Z}\sum_{m,n,m',n'=\leftarrow,\rightarrow} \mathrm{tr}\Big(T^{i-1}|m\rangle\langle m|\sigma_z|n\rangle\langle n|T^{j-i}|m'\rangle\langle m'|\sigma_z|n'\rangle\langle n'|T^{M-j+1}\Big) \\
&= \frac{1}{\epsilon_1^M + \epsilon_2^M}\Big(\epsilon_1^{i-1}\epsilon_2^{j-i}\epsilon_1^{M-(j-1)} + \epsilon_2^{i-1}\epsilon_1^{j-i}\epsilon_2^{M-(j-1)}\Big) \ ,
\end{aligned}$$

reducing to

$$\langle\sigma_i\sigma_j\rangle = \frac{\epsilon_1^{M-j+i}\epsilon_2^{j-i} + \epsilon_2^{i-j+M}\epsilon_1^{j-i}}{\epsilon_1^M + \epsilon_2^M} \ . \tag{C.18}$$

In terms of $\epsilon_1 = \cosh K$ and $\epsilon_2 = \sinh K$ the expression can be rewritten as

$$\langle\sigma_i\sigma_j\rangle = \frac{\tanh K^{j-i} + \tanh K^M \tanh K^{i-j}}{1 + \tanh K^M} \ . \tag{C.19}$$

Next, we let the number of sites, M, be very large and take the thermodynamic limit $M \to \infty$. Thus, we need to investigate $\tanh K^M$ as $M \to \infty$. Note that

$$\tanh K^M = (1 - \frac{2}{\mathrm{e}^{2K} + 1})^M = C^M \to 0 \ , C \in (-1, 1) \ . \tag{C.20}$$

Hence, we deduce that

$$\langle\sigma_i\sigma_j\rangle = \tanh K^{j-i} \ , j \geq i \ . \tag{C.21}$$

By introducing the parameter $\tau = ja$, a being the microscopic length and defining

$$\xi^{-1} = -\frac{1}{a}\ln(\tanh K) \Rightarrow \coth K = \mathrm{e}^{a/\xi} \ , \tag{C.22}$$

we note that (C.21) is consistent with the conventional exponential correlation function

$$\langle\sigma(0)\sigma(\tau)\rangle = \mathrm{e}^{-\tau/\xi} \ , \tag{C.23}$$

if we also set $i = 0$. This enables us to consider the scaling limit:

$$\frac{\xi}{a} = \frac{1}{\log(\coth K)} = \frac{1}{\log(1 + \underbrace{\frac{2\mathrm{e}^{-K}}{\mathrm{e}^{K} - \mathrm{e}^{-K}}}_{<<1 \ ,K>>1})} \approx \frac{e^{2K}}{2} \ , K >> 1 \ , \tag{C.24}$$

where we made use of $\log(1 + x) \approx x$, $x << 1$. Finally, we return to the transfer matrix

$$T = \begin{pmatrix} \mathrm{e}^{K} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K} \end{pmatrix} = \mathrm{e}^{K}(1{+}\mathrm{e}^{-2K}\sigma_x) \approx \mathrm{e}^{K}(1 + \frac{a}{2\xi}\sigma_x + ...) = \mathrm{e}^{K}\mathrm{e}^{\frac{a}{2\xi}\sigma_x} = \mathrm{e}^{a(-E_0\cdot\mathbf{1}+\frac{1}{2\xi}\sigma_x)} \ ,$$

introducing $E_0 = -\frac{K}{a}$. Here we have implicitly taken the scaling limit $a \to 0$ (and $M \to \infty$). Hence, we may also introduce another parameter L_τ as the product of a and M, which is constant as $a \to 0$ and $M \to \infty$. As a consequence,

$$Z(\beta) = \mathrm{tr}(T^M) = \mathrm{tr}\left(\mathrm{e}^{-L_\tau H_q}\right) \ , \tag{C.25}$$

with

$$H_q = E_0 \cdot \mathbf{1} - \frac{1}{2\xi}\sigma_x \ , \tag{C.26}$$

being a quantum Hamiltonian with *one* spin. We have thus established the connection between a one-dimensional classical system and a zero-dimensional quantum spin system. Finally, let us set $L_\tau = \frac{1}{T}$ such that

$$Z = \mathrm{tr}\left(\mathrm{e}^{-\frac{1}{T}H_q}\right) \ . \tag{C.27}$$

As mentioned above L_τ becomes a proper length dimension at low temperatures T. A treatment of higher-dimensional analogies of quantum versus classical (Ising) systems can be found in [107].

D

Conformal Field Theory and the Central Charge

D.1 A condensed introduction to CFT

In 1+1 dimensions, time and space are on the same footing in a quantum critical system in the low-energy limit, cf. the situation in section 5.3. In other words, Lorentz invariance is manifest in the system, which in the *imaginary-time formalism* translates into regular rotational-invariance [90].[1] Moreover, such systems also exhibit translation invariance and scale invariance which combines into *conformal invariance*.[2] The unified framework for describing 1+1-dimensional gapless quantum systems in the low-energy limit is therefore provided by a *conformal field theory*. At a quantum level one also has to introduce a scale which renders the theory finite which may break the conformal symmetry except at the *fixed points* of the theory [81]. Still, we should bear in mind that conformal symmetry in a quantum critical system does not follow from a classical system exhibiting conformal invariance. However, perhaps surprisingly, there exists a formal analogy between d-dimensional quantum systems and $d+1$-dimensional classical systems. In fact, the imaginary-time formalism employed in this section enables us to consider a one-dimensional quantum system to be effectively two-dimensional, with the imaginary time acting as an extra spatial dimension in a classical system.[3] In the following, we will make no distinction between the quantum world and the classical world.

Let us move away from one dimension for a while and be more formal and define a *conformal transformation* $\Lambda(x)$ acting on the D-dimensional metric tensor $g_{\mu\nu}$ such that

$$g_{\mu\nu}(\mathbf{x}) \to g'_{\mu\nu}(\mathbf{x}') = \Lambda(\mathbf{x}) g_{\mu\nu}(\mathbf{x}) \ , \tag{D.1}$$

[1] The imaginary-time formalism relies on the connection between proper time, τ, and Euclidean time, t, via the Wick rotation $t = i\tau$ which translates the Euclidean signature to a Lorentz (Minkowskian) signature and vice versa.

[2] Local scale invariance and conformal invariance is often used interchangeably in theoretical physics, although the statement that a theory is invariant under conformal transformations is stronger than the statement that a theory is scale-invariant. In fact, the latter does not in general imply conformal invariance as shown by Polchinski in 1988 [108]. By assuming the theory to be local and unitary, Polchinski managed to show that 1+1-dimensional scale invariance implies conformal invariance. However, in higher dimensions and without imposing unitarity and locality the implication has not yet been shown [109].

[3] This aspect is investigated in detail in Appendix C.

with $\Lambda(\mathbf{x})$ being a conformal factor which locally scales the metric.[4] Clearly, the Poincaré (Lorentz-symmetry+translations) group is a subgroup of the conformal group with $\Lambda(\mathbf{x}) = 1$. Using the metric tensor, we may form the line element, ds^2, according to

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu \ , \tag{D.2}$$

which transforms under a local infinitesimal coordinate transformation $x_\mu \to x'_\mu = x_\mu + \epsilon_\mu(\mathbf{x})$ in the following fashion:

$$ds^2 \to ds^2 - (\partial_\mu \epsilon_\nu + \partial_\nu \epsilon_\mu) dx^\mu dx^\nu \ , \tag{D.3}$$

since

$$g'_{\mu\nu} = \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} g_{\alpha\beta} = (\delta^\alpha_\mu - \partial_\mu \epsilon^\alpha)(\delta^\beta_\mu - \partial_\nu \epsilon^\beta) g_{\alpha\beta} = g_{\mu\nu} - \partial_\mu \epsilon_\nu - \partial_\nu \epsilon_\mu \ . \tag{D.4}$$

For the transformation to be conformal we therefore , by comparison with (D.2),

$$\partial_\mu \epsilon_\nu + \partial_\nu \epsilon_\mu = f(\mathbf{x}) g_{\mu\nu} \ , \tag{D.5}$$

where $f(\mathbf{x})$ is easily obtained by taking the trace of both sides:

$$g^{\mu\nu} \partial_\mu \epsilon_\nu + g^{\mu\nu} \partial_\nu \epsilon_\mu = f(\mathbf{x}) g^{\mu\nu} g_{\mu\nu} \Rightarrow f(\mathbf{x}) = \frac{2}{D} \partial_\mu \epsilon^\mu \ . \tag{D.6}$$

Now, it turns out that $f(\mathbf{x})$ or more precisely the form of $\epsilon_\mu(\mathbf{x})$ is highly dependent on the spacetime dimension, D. For $D = 1$ no constraints at all are put on $f(\mathbf{x})$, and thus any smooth transformation is conformal in one spacetime dimension. With some simple manipulations one can show that the infinitesimal, ϵ_μ can be written as [81]

$$\epsilon_\mu = a_\mu + b_{\mu\nu} x^\nu + c_{\mu\nu\rho} x^\nu x^\rho \ , c_{\mu\nu\rho} = c_{\nu\rho\mu} \ , \tag{D.7}$$

for dimensions $D \geq 3$, pointing to the fact that a_μ amounts to a translation, $b_{\mu\nu}$ to an infinitesimal scale transformation, and $c_{\mu\nu\rho}$ to a *special conformal transformation* (SCT).[5] The latter is, as the name suggests, special and can be realized as an inversion, followed by a translation and an additional inversion. See [81] for further details. The corresponding finite transformations can be summarized as

$$\begin{aligned}
\text{(translation) } x'^\mu &= x^\mu + a^\mu \ , \\
\text{(dilation/scaling) } x'^\mu &= \alpha x^\mu \ , \\
\text{(rotation) } x'^\mu &= M^\mu{}_\nu x^\nu \ , \\
\text{(SCT) } x'^\mu &= \frac{x^\mu - b^\mu \mathbf{x}^2}{1 - \mathbf{b} \cdot \mathbf{x} + b^2 \mathbf{x}^2} \ .
\end{aligned}$$

A consequence of this result is that the conformal group is finite-dimensional for $D > 2$. $D = 2$ dimensions is a special case which requires extra attention. In particular, it

[4] The transformation is very similar to regular (differentiable) coordinate transformations where $g_{\alpha\beta} = \frac{\partial x^\alpha}{\partial x'^\mu} \frac{\partial x^\beta}{\partial x'^\nu} g_{\alpha\beta}$. In fact, conformal transformations form a subgroup of such diffeomorphisms with the word "conformal" referring to the fact that they preserve angles between two vectors.

[5] The constraints for conformal invariance must be independent of x^μ. Therefore, each term in ϵ_μ can be considered individually.

turns out that (D.5) can be rewritten in such a way that the components of ϵ_μ obey the Cauchy-Riemann equations of complex analysis, thereby forcing the conformal transformations in two dimensions to include an analytic function $\epsilon(z)$ and an anti-analytic function $\bar{\epsilon}(\bar{z})$ with $z = v\tau - ix$ and $\bar{z} = v\tau + ix$, τ being the proper time, $\tau = it$, x the position coordinate and v the Fermi velocity. The complex coordinates z and $\bar{z}$ are often used in the language of conformal field theory and deserves to be specified (along with its derivative correspondence) below:

$$z = v\tau - ix \ , \partial_z = -\frac{i}{2}(\frac{1}{v}\partial_t - \partial_x) \ , \tag{D.8}$$

$$\bar{z} = v\tau + ix \ , \partial_z = -\frac{i}{2}(\frac{1}{v}\partial_t + \partial_x) \ . \tag{D.9}$$

Since $\epsilon(z)$ and $\bar{\epsilon}(\bar{z})$ are arbitrary analytic functions it follows that the group of conformal transformations in $D = 2$ has to be infinite-dimensional, in contrast to CFTs in $D \geq 3$. In other words, the conformal group is the set of all analytic mappings. In our new coordinates z and $\bar{z}$ we may express the line element as

$$ds^2 = dzd\bar{z} \ , \tag{D.10}$$

and an infinitesimal conformal transformation $z \to f(z) = z + \epsilon(z)$ (similarly for $\bar{z}$) results in the line element transforming as

$$ds^2 = dzd\bar{z} \to \frac{\partial f}{\partial z}\frac{\partial f}{\partial \bar{z}} dzd\bar{z} \ . \tag{D.11}$$

Now, for the conformal group to be a proper group the analytic mappings have to be invertible and the whole complex plane (including infinity) has to be mapped to itself. The transformations which perform this trick are referred to as *global* conformal transformations. If we consider $f(z)$ as such a mapping it must not have any *essential* singularities or branch points. However, it may have poles, enabling us to write

$$f(z) = \frac{P(z)}{Q(z)} \ . \tag{D.12}$$

Since we want $f(z)$ to be a well-defined invertible mapping it is moreover crucial that $P(z)$ does not have distinct zeros. The same reasoning applies for the function $Q(z)$ in the denominator in the sense that the inverse image of infinity has to be well-defined. This means that $f(z)$ must be a rational polynomial with $P(z)$ and $Q(z)$ being linear polynomials in z:

$$f(z) = \frac{az + b}{cz + d} \ , \ , a, b, c, d \in \mathbf{C} \tag{D.13}$$

with the additional constraint that the determinant $ad - bc$ is non-zero (due to invertibility). This transformation is also referred to as a *projective conformal transformation* or a Möbius transformation.

D.2 Central Charge in Conformal Field Theory

In Chapter 5 we established that the central charge c , along with the winding number ν, completely characterize the topological phases of the symmetry class BDI. For instance, the critical Majorana chain is said to be described by a low-energy conformal field theory with $c = \frac{1}{2}$. In this section, we therefore give a generic background on how the concept of central charge arises in conformal field theory and how it relates to fermionic and bosonic systems respectively. The discussion follows closely that of the standard literature, “the yellow book”, by Di Fransesco, Mathieu, and Sénechal but the calculations are made somewhat more explicit [81]. We will consider the bosonic case and the fermionic case separately, although the latter is of more use to us.

D.2.1 Free (massless) bosons

Consider the (conformal) action of a massless bosonic field φ:

$$\mathcal{S} = \frac{g}{2}\int d^2x \partial_\mu\varphi\partial^\mu\varphi \ , \tag{D.14}$$

where g is a coupling constant. From the action we may derive the scalar propagator by inserting the function $A(\vec{x},\vec{y}) = -g\delta^{(2)}(\vec{x}-\vec{y})\partial_x^2$ according to:

$$\mathcal{S} = \frac{1}{2}\int d^2xd^2y\varphi(\vec{x})A(\vec{x},\vec{y})\varphi(\vec{y}) \ . \tag{D.15}$$

Then, the propagator $K(\vec{x},\vec{y})$ is given by

$$K(\vec{x},\vec{y}) = A^{-1}(\vec{x},\vec{y}) \Rightarrow -g\partial_x^2 K(\vec{x},\vec{y}) = \delta^{(2)}(\vec{x}-\vec{y}) \ . \tag{D.16}$$

By demanding translational invariance we have $K(\vec{x},\vec{y}) = K(|\vec{x}-\vec{y}|)$ and therefore it seems reasonable to introduce $r = |\vec{x}-\vec{y}|$. Let us then integrate the equation over the disk D with radius r:

$$-2\pi g\int_0^r d\rho\rho(\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho K'(\rho))) = -2\pi g r K'(r) = 1 \ , \tag{D.17}$$

where we expressed the second derivative in cylindrical coordinates. Now, the propagator is easily evaluated by integration:

$$K(r) = -\frac{1}{2\pi g}\log(r) + \text{const} \ , \tag{D.18}$$

or equivalently

$$K(x-y) = -\frac{1}{4\pi g}\log(x-y)^2 + \text{const} = \langle\varphi(x)\varphi(y)\rangle \ , \tag{D.19}$$

and $\langle\varphi(x)\varphi(y)\rangle$ denotes the two-point correlation function. For later, we would like to express the correlation function in terms of complex variables $z, \bar{z}$ and $w, \bar{w}$:

$$\langle\varphi(z,\bar{z})\varphi(w,\bar{w})\rangle = -\frac{1}{4\pi g}\bigg(\log(z-w) + \log(\bar{z}-\bar{w})\bigg) + \text{const} \ . \tag{D.20}$$

We focus on the holomorphic field $\partial_z \varphi = \partial \varphi$ and then

$$\langle \partial_z \varphi(z,w) \partial_w \varphi(z,w) \rangle = -\frac{1}{4\pi g} \partial_z \left(\frac{-1}{(z-w)} \right) = -\frac{1}{4\pi g} \frac{1}{(z-w)^2} = \langle \partial\varphi(z) \partial\varphi(w) \rangle \ . \tag{D.21}$$

The following is also referred to as the *operator product expansion* (OPE) of the operator $\partial\varphi$:

$$\langle \partial\varphi(z) \partial\varphi(w) \rangle \sim -\frac{1}{4\pi g} \frac{1}{(z-w)^2} \ , \tag{D.22}$$

where the $\sim$ refers to the fact that there may be more terms in the expansion which are regular as $z \to w$.

Next, we turn our attention to the energy-momentum tensor for the free bosonic (massless) theory:[6]

$$T_{\mu\nu} = g(\partial_\mu \varphi \partial_\nu \varphi - \frac{1}{2} \eta_{\mu\nu} \partial_\rho \varphi \partial^\rho \varphi) \ . \tag{D.23}$$

In the quantized theory of conformally invariant scalar bosons the stress-tensor is given (in terms of the complex coordinate z introduced in (D.9)) by:

$$T(z) = -2\pi T_{zz} = -2\pi g : \partial\varphi \partial\varphi : \ , \tag{D.24}$$

where : : denotes normal ordering, required to make the vacuum expectation value of the stress-energy tensor finite – actually equal to zero since we are dealing with a free theory. The normal ordering product can also be interpreted as

$$: \partial\varphi\partial\varphi := \lim_{z \to w} (\partial\varphi(z)\partial\varphi(w) - \langle \partial\varphi(z)\partial\varphi(w) \rangle) \ . \tag{D.25}$$

Let us now evaluate the OPE of $T(z)$ with $\partial\varphi(w)$:

$$T(z)\partial\varphi(w) = -2\pi g : \partial\varphi(z)\partial\varphi(z) : \partial\varphi(w) \ . \tag{D.26}$$

To get further, we have to invoke *Wick's theorem* for four bosonic fields ϕ_1, ϕ_2, ϕ_3 and ϕ_4:

$$\mathcal{T}(: \phi_1\phi_2\phi_3\phi_4 :) =: \phi_1\phi_2\phi_3\phi_4 : + \text{ all possible contractions} \ , \tag{D.27}$$

where $\mathcal{T}(...)$ is the *time-ordering operator*. In particular, in our case we get[7]

$$: \partial\varphi(z)\partial\varphi(z) : \partial\varphi(w) \sim: \partial\varphi(z)\partial\varphi(z) : \partial\varphi(w) + : \partial\varphi(z)\partial\varphi(z) : \partial\varphi(w) \ ,$$

and since

$$: \phi_1\phi_2 : \ = \langle \phi_1\phi_2 \rangle \ , \tag{D.28}$$

we must have (using (D.22))

$$T(z)\partial\varphi(w) \sim -2\pi g \left(-\frac{1}{(4\pi g)(z-w)^2} - \frac{1}{(4\pi g)(z-w)^2} \right) \partial\varphi(z) = \frac{\partial\varphi(z)}{(z-w)^2} \ . \tag{D.29}$$

[6]Recall that $T^{\mu\nu}$ can be calculated due to Noether as $T^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} - g^{\mu\nu}\mathcal{L}$.

[7]Applying the time-ordering operator on two operators ϕ_1 and ϕ_2 gives $\mathcal{T}(\phi_1\phi_2) =: \phi_1\phi_2 : + \langle \phi_1\phi_2 \rangle$. However, the expectation values are dropped in our calculations.

Moreover, we may expand $\varphi(z)$ around w such that $\varphi(z) \approx \varphi(w) + (z-w)\partial_w \varphi(w)$ and therefore

$$T(z)\partial\varphi(w) \sim \frac{\partial_w \varphi(w)}{(z-w)^2} + \frac{\partial_w^2 \varphi(w)}{(z-w)} \ , \tag{D.30}$$

and we conclude that $\partial\varphi(w)$ is a *primary* field with conformal (scaling) dimension $h = 1$.[8] Now, let us instead consider the OPE of the energy-momentum tensor $T(z)$ with itself. We follow the recipe:

$$\begin{aligned}
T(z)T(w) &= 4\pi^2 g^2 : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : \\
&\sim 4\pi^2 g^2 \Big(: \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : + : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : \\
&\qquad + : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : + : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : \\
&\qquad + : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : + : \partial\varphi(z)\partial\varphi(z) :: \partial\varphi(w)\partial\varphi(w) : \Big) \\
&= 4\pi^2 g^2 \left(\frac{2}{(4\pi g)^2 (z-w)^4} - \frac{4 : \partial\varphi(z)\partial\varphi(w) :}{4\pi g (z-w)^2} \right) \\
&= \frac{1/2}{(z-w)^4} - \frac{4\pi g : \partial\varphi(z)\partial\varphi(w) :}{(z-w)^2} \\
&\sim \frac{1/2}{(z-w)^4} - \frac{4\pi g : \partial_w\varphi(w)\partial_w\varphi(w) :}{(z-w)^2} - \frac{4\pi g : \partial_w^2\varphi(w)\partial_w\varphi(w) :}{(z-w)} \\
&= \frac{1/2}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial_w T(w)}{(z-w)} \ ,
\end{aligned}$$

where the first term is due to the double contractions and the second term is due to the four single contractions. Note that we also expanded $\varphi(z)$ in the last step. The first term is special. It has no dependence on $T(z)$ and therefore it can not be a primary. In fact, the term is really a conformal anomaly. The factor $\frac{1}{2}$ in the nominator is important and is related to the central charge as we will see. However, first let us first perform the analogous analysis for the fermionic case.

D.2.2 Free Majorana fermions

Now, we consider the action of a free (massless) fermionic theory. This is slightly trickier since we have to deal with two-component spinors $\Psi = (\psi, \bar{\psi})$ and Dirac matrices, which increases the dimensionality of the problem. The action reads

$$\mathcal{S} = \frac{g}{2} \int d^2x \Psi^\dagger \gamma^2 \gamma^\mu \partial_\mu \Psi \ , \tag{D.31}$$

where the Dirac matrices are precisely the Pauli matrices in two dimensions, i.e.

$$\gamma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \gamma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \ . \tag{D.32}$$

[8] In general we may have $T(z)\mathcal{O} \sim \frac{h\mathcal{O}}{(z-w)^2} + ...$, where h is the scaling dimension. If $\mathcal{O}$ appear (without any derivatives acting on it) in the right-hand side, $\mathcal{O}$ is referred to as a primary field.

Then, by performing the matrix product we may write the action as

$$\mathcal{S} = g \int d^2z(\bar{\psi}\partial_z\bar{\psi} + \psi\partial_{\bar{z}}\psi) \ , \tag{D.33}$$

with $\partial_z = \partial_0 - i\partial_1$. Note the striking resemblance between this action and the action obtained in (5.42) (set $g = v_F$ and take only one copy). Clearly, the equations of motion for ψ and $\bar{\psi}$ are independent and given by

$$\partial_z\bar{\psi} = 0 \ ,$$
$$\partial_{\bar{z}}\psi = 0 \ ,$$

where the first equation implies that $\bar{\psi}$ is a chiral and holomorphic field and ψ is an anti-chiral and anti-holomorphic field. Now, it is in order to calculate the propagators for the fermionic fields. We carry out the same procedure as in the bosonic case and introduce

$$A(x,y) = g\delta(x^\mu - y^\mu)\gamma^2\gamma^\mu\partial_\mu \ , \tag{D.34}$$

such that

$$\mathcal{S} = \frac{g}{2}\int d^2xd^2y\Psi^\dagger A(x,y)\Psi \ , \tag{D.35}$$

from which we find the Feynman propagators[9]

$$\langle\psi(z)\psi(w)\rangle \sim \frac{1}{2\pi g}\frac{1}{z-w} \ ,$$
$$\langle\bar{\psi}(z)\bar{\psi}(w)\rangle \sim \frac{1}{2\pi g}\frac{1}{\bar{z}-\bar{w}} \ ,$$
$$\langle\bar{\psi}(z)\psi(w)\rangle = 0 \ .$$

Note that the anti-symmetry between fermionic operators is manifest in these expressions. Swapping $\psi(z)$ and $\psi(w)$ induces a minus sign in the propagator, which is consistent with $\{\psi(z),\psi(w)\} = 0$. Moreover, the stress tensor is (due to Noether):

$$T(z) = -\pi g : \psi\partial\psi : \ , \tag{D.36}$$

where $\partial = \partial_z$ as before. Continuing to the operator product expansion of $T(z)$ and $\psi(w)$ we have:

$$\begin{aligned}
T(z)\psi(w) &= -\pi g : \psi(z)\partial\psi(z) : \psi(w) \\
&\sim -\pi g\Big(: \psi(z)\partial\psi(z) : \psi(w) + : \psi(z)\partial\psi(z) : \psi(w)\Big) \\
&= -\pi g\Big(-\frac{\partial\psi(z)}{2\pi g(z-w)} - \frac{\psi(z)}{2\pi g(z-w)^2}\Big) \\
&= \frac{\partial\psi(z)}{2(z-w)} + \frac{\psi(z)}{2(z-w)^2} \\
&\sim \frac{\partial_w\psi(w)}{2(z-w)} + \frac{\psi(w) + (z-w)\partial_w\psi(w)}{2(z-w)^2} \\
&= \frac{\psi(w)}{2(z-w)^2} + \frac{\partial_w\psi(w)}{(z-w)} \ ,
\end{aligned}$$

[9] This seems reasonable. Since $A(x,y)$ is linear in derivatives we should expect a factor $(z-w)$ in the denominator rather than $(z-w)^2$, we had in the bosonic case.

that is $\psi(w)$ is a primary field with $h = \frac{1}{2}$. Note that we had to be careful about signs since the ψ fields anti-commute. An analogous calculation shows that the same holds for $\bar{\psi}$. Now, it remains to do the OPE for $T(z)$ with itself:

$$T(z)T(w) = \pi^2 g^2 : \psi(z)\partial_z\psi(z) :: \psi(w)\partial_w\psi(w) : \ .$$

We have to be *very* careful about signs when expanding the Wick product:[10]

$$\begin{aligned}
: \psi(z)\partial_z\psi(z) :: \psi(w)\partial_w\psi(w) : \sim & : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : \\
& + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : \\
& + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : \\
= & - : \psi(z)\psi(w) :: \partial\psi(z)\partial\psi(w) : + : \psi(z)\partial\psi(w) : \partial\psi(z)\psi(w) : \\
& - : \psi(z)\psi(w) :: \partial\psi(z)\partial\psi(w) : + : \psi(z)\partial\psi(z) :: \psi(w)\partial\psi(w) : \\
& + : \psi(z)\partial\psi(w) :: \partial\psi(z)\psi(w) : - : \psi(z)\partial\psi(z) :: \partial\psi(w)\psi(w) : \\
= & \frac{2}{(2\pi g)^2(z-w)^4} - \frac{1}{(2\pi g)^2(z-w)^4} \\
& - \frac{: \partial\psi(z)\partial\psi(w) :}{2\pi g(z-w)} - \frac{: \psi(z)\partial\psi(w) :}{2\pi g(z-w)^2} \\
& + \frac{: \partial\psi(z)\psi(w) :}{2\pi g(z-w)^2} + \frac{2 : \psi(z)\psi(w) :}{2\pi g(z-w)^3} \\
\sim & \frac{1/4}{\pi^2 g^2(z-w)^4} - \frac{: \partial\psi(w)\partial\psi(w) :}{2\pi g(z-w)} - \frac{: \psi(w)\partial\psi(w) :}{2\pi g(z-w)^2} \\
& - \frac{: \partial\psi(w)\partial\psi(w) :}{2\pi g(z-w)} + \frac{: \partial\psi(w)\psi(w) :}{2\pi g(z-w)^2} + \frac{: \partial^2\psi(w)\psi(w) :}{2\pi g(z-w)} \\
& + \frac{2 : \psi(w)\psi(w) :}{2\pi g(z-w)^3} + \frac{2 : \partial\psi(w)\psi(w) :}{2\pi g(z-w)^2} + \frac{: \partial^2\psi(w)\psi(w) :}{2\pi g(z-w)} \\
= & \frac{1/4}{\pi^2 g^2(z-w)^4} - \frac{2 : \psi(w)\partial\psi(w) :}{\pi g(z-w)^2} \\
& \underbrace{- \frac{\partial\psi(w)\partial\psi(w)}{\pi g(z-w)} - \frac{: \psi(w)\partial^2\psi(w) :}{\pi g(z-w)}}_{=\partial_w T(w)/(\pi^2 g^2(z-w))} + \frac{: \psi(w)\psi(w) :}{\pi g(z-w)^3} \\
= & \frac{1/4}{\pi^2 g^2(z-w)^4} + \frac{2T(w)}{\pi^2 g^2(z-w)^2} + \frac{\partial T(w)}{\pi^2 g^2(z-w)} + \underbrace{\frac{: \psi(w)\psi(w) :}{\pi g(z-w)^3}}_{=0\ ,\{\psi(w),\psi(w)\}=0} \ .
\end{aligned}$$

To conclude, we obtain the OPE

$$T(z)T(w) \sim \frac{1/4}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial T(w)}{(z-w)} \ . \qquad \text{(D.37)}$$

[10] To tidy up the calculation we have abbreviated both ∂_z and ∂_w by ∂. Obviously, whenever ∂ is acting on $\psi(w)$ it is a derivative with respect to w and similarly for $\psi(z)$.

Note that the factor $\frac{1}{4}$ in front of the first term is different from the bosonic expression ($\frac{1}{2}$). We may therefore conclude that

$$T(z)T(w) \sim \frac{c/2}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial T(w)}{(z-w)} \,, \tag{D.38}$$

where c is the *central charge*. In particular, we thus find that $c = +1$ for free (massless) bosons and $c = +\frac{1}{2}$ for free (Majorana) fermions. The central charge is considered a conformal anomaly which softly[11] breaks conformal symmetry.

D.3 The c-theorem

The c-theorem was proven by Zamolodchikov in 1986 and relates the central charge in CFT to the renormalization group (RG) flow[12] [110]. Given a conformal field theory one can find a positive function $C(g_i, \mu)$ depending on the coupling constants g_i and the energy scale μ which has the properties

- $C(g_i, \mu)$ decreases monotonically under the RG flow
- All fixed points of the RG flow are specified by fixe-point couplings, g^*, such that the function $C(g^*, \mu) = c$ is constant.

[11]The soft breaking of symmeries refer to the fact that only the low-energy behavior of the physical gets affected, while at high energies the physics are unchanged.

[12]In the context of quantum field theory, a renormalization group flow is induced when a conformal field theory, $\mathrm{CFT}_{\mathrm{UV}}$, gets perturbed by an operator such that its degrees of freedom get distorted leading to a new theory, $\mathrm{CFT}_{\mathrm{IR}}$, at long distances. More simply put, the RG flow describes a curve which parameters in the theory follow as the energy is lowered.

E

Connecting Topological Phases within the BDI Class

In our discussion in section 5.4 in Chapter 5 we argued that the meromorphic function $f(z)$ can be tuned to the canonical form

$$f(z) = \pm(z^{2c} \pm 1)z^{\nu} \tag{E.1}$$

without breaking translational symmetry. Previously, we have noted that the topological invariant ν can not change unless a phase transition is induced. However, models with different signs in $f(z)$ can still be connected without causing a bulk transition. Due to the one-to-one correspondence between $f(z)$ and the Hamiltonian we may thus connect Hamiltonians $H = \pm(H_{2c+\nu} \pm H_{\nu})$ with different overall signs and intermediate signs. Define the unitary transformation

$$U(\theta) = \exp(\frac{\theta}{2}\sum_n \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}) \ , \tag{E.2}$$

which can be rewritten by making use of the Taylor expansion of the exponential and the Majorana algebra

$$\begin{aligned}
\exp(\frac{\theta}{2}\sum_n \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}) = \prod_n \sum_k (\frac{\theta}{2}\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n})^k/k! &= \prod_n 1 + \frac{\theta}{2}\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n} + (\frac{\theta}{2})^2\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}\frac{1}{2!} \\
&+ \quad (\frac{\theta}{2})^3(\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n})^3\frac{1}{3!} + ... \\
&= \prod_n 1 - (\frac{\theta}{2})^2\frac{1}{2!} + ...\tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}(\frac{\theta}{2} - (\frac{\theta}{2})^3\frac{1}{3!} + ...) \\
&= \prod_n \cos(\frac{\theta}{2}) + \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}\sin(\frac{\theta}{2}) \ ,
\end{aligned}$$

that is

$$U(\theta) = \prod_n \cos(\frac{\theta}{2}) + \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}\sin(\frac{\theta}{2}) \ . \tag{E.3}$$

We will need to perform the transform $U(\pi)H_{\alpha}U^{\dagger}(\pi)$, with

$$U(\pi) = \prod_n \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n} \ . \tag{E.4}$$

This is since

$$U(\pi)H_{\alpha}U^{\dagger}(\pi) = -H_{\alpha} \ , \tag{E.5}$$

i.e. Hamiltonians with different overall signs can be connected. Let us prove this identity. Written out in its entirety we have

$$
\begin{aligned}
U(\pi)H_\alpha U^\dagger(\pi) &= \frac{i}{2}\prod_n \tilde{\gamma}_{2n-1}\tilde{\gamma}_{2n}\sum_k \tilde{\gamma}_k\gamma_{k+\alpha}\prod_i \tilde{\gamma}_{2n}\tilde{\gamma}_{2n-1} \\
&= \frac{i}{2}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N}\tilde{\gamma}_k\gamma_{k+\alpha}\tilde{\gamma}_{2N}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1 \\
&= \frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N}\tilde{\gamma}_k\tilde{\gamma}_{2N}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= \frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N}(2\delta_{2N,k}-\tilde{\gamma}_{2N}\tilde{\gamma}_k)\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= i(-1)^{2N}\tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{2N+\alpha} \\
&\quad -\frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N}\tilde{\gamma}_{2N}\tilde{\gamma}_k\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= i(-1)^{4N-1}\underbrace{\tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-1}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1}_{=1}\tilde{\gamma}_{2N}\gamma_{2N+\alpha} \\
&\quad -\frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-1}\tilde{\gamma}_k\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= i(-1)^{4N-1}\underbrace{\tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-1}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1}_{=1}\tilde{\gamma}_{2N}\gamma_{2N+\alpha} \\
&\quad -\frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-1}(2\delta_{2N-1,k}-\tilde{\gamma}_{2N-1}\tilde{\gamma}_k)\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= i(-1)^{4N-1}\underbrace{\tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-1}\tilde{\gamma}_{2N-1}\cdot\ldots\cdot\tilde{\gamma}_2\tilde{\gamma}_1}_{=1}\tilde{\gamma}_{2N}\gamma_{2N+\alpha} \\
&\quad -i(-1)^{4N-2}\sum_k \underbrace{\tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-2}\cdot\tilde{\gamma}_{2N-2}\cdots\cdot\tilde{\gamma}_2\tilde{\gamma}_1}_{=1}\tilde{\gamma}_{2N-1}\gamma_{2N-1+\alpha} \\
&\quad +\frac{i}{2}(-1)^{2N}\sum_k \tilde{\gamma}_1\tilde{\gamma}_2\cdot\ldots\cdot\tilde{\gamma}_{2N-2}\tilde{\gamma}_k\cdot\tilde{\gamma}_{2N-2}\cdots\cdot\tilde{\gamma}_2\tilde{\gamma}_1\gamma_{k+\alpha} \\
&= i(-1)^{4N-1}\left(\tilde{\gamma}_{2N}\gamma_{2N+\alpha}+\tilde{\gamma}_{2N-1}\gamma_{2N-1+\alpha}+\ldots+\right) \\
&\quad +\frac{i}{2}\sum_k \tilde{\gamma}_k\gamma_{k+\alpha} \\
&= -i\sum_k \tilde{\gamma}_k\gamma_{k+\alpha}+\frac{i}{2}\sum_k \tilde{\gamma}_k\gamma_{k+\alpha} = -\frac{i}{2}\sum_k \tilde{\gamma}_k\gamma_{k+\alpha} = -H_\alpha\ ,
\end{aligned}
$$

which we set out to prove. Note that we had to use the anti-commutator relations $\{\tilde{\gamma}_i,\tilde{\gamma}_j\}=2\delta_{i,j}$ and $\{\tilde{\gamma}_i,\gamma_j\}=0$ repetetively to arrive at the result. A similar, although perhaps a more technical calculation, can be performed to change the intermediate sign in $\pm(H_\nu+H_{2c+\nu})$. See [18] for details.

F

Generalized Kitaev Hamiltonian by Zhao and Wang

In this appendix we will provide details on how to perform an inverse Fourier transformation of the Zhao/Wang BdG Hamiltonian in (6.1) to express the model in real space. Note that the result obtained differs from that of Zhao-Wang [93]. Starting with the Bloch Hamiltonian and using $\Psi_k^\dagger = (a_{k\uparrow}^\dagger, a_{k\downarrow}^\dagger, a_{-k\downarrow}, -a_{-k\uparrow})$ (and similarly for Ψ_k) and expanding the tensor products we get

$$
\begin{aligned}
H_{\mathrm{ZW}}^{\mathrm{CII}} &= \sum_k (a_{k\uparrow}^\dagger, a_{k\downarrow}^\dagger, a_{-k\downarrow}, -a_{-k\uparrow}) H_{\mathrm{ZW}(k)} \begin{pmatrix} a_{k\uparrow} \\ a_{k\downarrow} \\ a_{-k\downarrow}^\dagger \\ -a_{-k\uparrow}^\dagger \end{pmatrix} \\
&= \sum_k (a_{k\uparrow}^\dagger, a_{k\downarrow}^\dagger, a_{-k\downarrow}, -a_{-k\uparrow}) \Bigg((t\cos k - \mu) \begin{pmatrix} a_{k\downarrow} \\ a_{k\uparrow} \\ -a_{-k\uparrow}^\dagger \\ a_{-k\downarrow}^\dagger \end{pmatrix} - i\Delta \sin k \begin{pmatrix} -a_{-k\downarrow}^\dagger \\ -a_{-k\uparrow}^\dagger \\ a_{k\uparrow} \\ -a_{k\downarrow} \end{pmatrix} \Bigg) \\
&= \sum_k \Bigg((t\cos k - \mu)\Big(a_{k\uparrow}^\dagger a_{k\downarrow} + a_{k\downarrow}^\dagger a_{k\uparrow} - a_{-k\uparrow} a_{-k\downarrow}^\dagger - a_{-k\downarrow} a_{-k\uparrow}^\dagger \Big) \\
&\qquad - i\Delta \sin k \Big(a_{-k\downarrow} a_{k\uparrow} + a_{-k\uparrow} a_{k\downarrow} - a_{k\downarrow}^\dagger a_{-k\uparrow}^\dagger - a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger \Big) \Bigg) \ .
\end{aligned}
$$

Next, we write the Hamiltonian in real space by making use of the discrete (inverse) Fourier transform:

$$
a_{ks} = \frac{1}{\sqrt{N}} \sum_j \mathrm{e}^{-ijk} a_{js} \ , \tag{F.1}
$$

with $s = \uparrow, \downarrow$. Note that the inverse transform of a_{-ks} only changes the sign of the argument in the exponential in (F.1). Then, treating the first term in (**??**) gives us

$$\begin{aligned}
&\sum_k \Bigg((t\cos k - \mu)\Big(a^\dagger_{k\uparrow}a_{k\downarrow} + a^\dagger_{k\downarrow}a_{k\uparrow} - a_{-k\uparrow}a^\dagger_{-k\downarrow} - a_{-k\downarrow}a^\dagger_{-k\uparrow}\Big) \\
&= \frac{1}{N}\sum_k\sum_{j,j'} \frac{t}{2}(\mathrm{e}^{i(j-j'+1)k} + \mathrm{e}^{i(j-j'-1)k})\Big(a^\dagger_{j\uparrow}a_{j'\downarrow} - a_{j\uparrow}a^\dagger_{j'\downarrow} + (\uparrow\leftrightarrow\downarrow)\Big) \\
&\qquad - \mu\mathrm{e}^{i(j-j')k}(a^\dagger_{j\uparrow}a_{j'\downarrow} - a_{j\uparrow}a^\dagger_{j'\downarrow} + (\uparrow\leftrightarrow\downarrow)) \\
&= \sum_{j,j'}\frac{t}{2}(\delta_{j+1,j'} + \delta_{j-1,j'})\Big(a^\dagger_{j\uparrow}a_{j'\downarrow} - a_{j\uparrow}a^\dagger_{j'\downarrow} + (\uparrow\leftrightarrow\downarrow)\Big) - \mu\delta_{j,j'}(a^\dagger_{j\uparrow}a_{j'\downarrow} - a_{j\uparrow}a^\dagger_{j'\downarrow} + (\uparrow\leftrightarrow\downarrow)) \\
&= \sum_j t\Big(a^\dagger_{j\uparrow}a_{j+1\downarrow} + a^\dagger_{j\downarrow}a_{j+1\uparrow} + a^\dagger_{j+1\uparrow}a_{j\downarrow} + a^\dagger_{j+1\downarrow}a_{j\uparrow}\Big) - 2\mu(a^\dagger_{j\uparrow}a_{j\downarrow} + a^\dagger_{j\downarrow}a_{j\uparrow}) \\
&= \sum_j t\hat{a}^\dagger_{j+1}\sigma_x\hat{a}_j - \mu\hat{a}^\dagger_j\sigma_x\hat{a}_j + \text{h.c.}\ ,
\end{aligned}$$

where we introduced the operators $\hat{a}_j$ and $\hat{a}^\dagger_j$ with an implicit spin dependence such that $\hat{a}_j = (a_{j\uparrow}, a_{j\downarrow})$. Note that we here also assume that the parameters w, Δ and μ are real. Moving on to the next term we obtain

$$\begin{aligned}
&-\frac{\Delta}{2}\sum_k(\mathrm{e}^{ik} - \mathrm{e}^{-ik})\Big(a_{-k\downarrow}a_{k\uparrow} + a_{-k\uparrow}a_{k\downarrow} - a^\dagger_{k\downarrow}a^\dagger_{-k\uparrow} - a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow}\Big) \\
&= -\sum_k\frac{\Delta}{2N}\sum_{j,j'}(\mathrm{e}^{i(j-j'+1)k} - \mathrm{e}^{i(j-j'-1)k})\Big(a_{j\downarrow}a_{j'\uparrow} + a_{j\uparrow}a_{j'\downarrow} - a^\dagger_{j\downarrow}a^\dagger_{j'\uparrow} - a^\dagger_{j\uparrow}a^\dagger_{j'\downarrow}\Big) \\
&= -\frac{\Delta}{2}\sum_{j,j'}(\delta_{j+1,j'} - \delta_{j-1,j'})\Big(a_{j\downarrow}a_{j'\uparrow} + a_{j\uparrow}a_{j'\downarrow} - a^\dagger_{j\downarrow}a^\dagger_{j'\uparrow} - a^\dagger_{j\uparrow}a^\dagger_{j'\downarrow}\Big) \\
&= -\Delta\sum_j\Big(a^\dagger_{j+1\downarrow}a^\dagger_{j\uparrow} + a^\dagger_{j+1\uparrow}a^\dagger_{j\downarrow} + \text{h.c.}\Big) \\
&= -\Delta\sum_j(\hat{a}_{j+1}\sigma_1\hat{a}_j + \text{h.c.}\Big)\ .
\end{aligned}$$

To summarize we have

$$H^{\text{CII}}_{\text{ZW}} = \sum_j\Big(t\hat{a}^\dagger_{j+1}\sigma_x\hat{a}_j - \Delta\hat{a}_{j+1}\sigma_x\hat{a}_j - \mu\hat{a}^\dagger_j\sigma_x\hat{a}_j + \text{h.c.}\Big)\ . \tag{F.2}$$

In contrast to Zhao and Wang [93], the Pauli matrix σ_x is sandwiched between the fermionic ladder operators rather than the matrix $i\sigma_y$. By putting $\Delta = t$ and $\mu = 0$ and introducing Majorana operators we are able to make the MZMs apparent in the

Hamiltonian. To see how, let us first do some rewriting:

$$
\begin{aligned}
H^{\mathrm{CII}}_{\mathrm{Majorana}} &= \sum_j t\Big(\hat{a}^\dagger_{j+1}\sigma_1\hat{a}_j - \hat{a}_{j+1}\sigma_1\hat{a}_j + \mathrm{h.c.}\Big) \\
&= \sum_j t\Big(a^\dagger_{j\uparrow}a_{j+1\downarrow} + a^\dagger_{j\downarrow}a_{j+1\uparrow} + a^\dagger_{j+1\uparrow}a_{j\downarrow} + a^\dagger_{j+1\downarrow}a_{j\uparrow} \\
&\quad - a^\dagger_{j+1\downarrow}a^\dagger_{j\uparrow} - a^\dagger_{j+1\uparrow}a^\dagger_{j\downarrow} - a_{j\uparrow}a_{j+1\downarrow} - a_{j\downarrow}a_{j+1\uparrow}\Big) \\
&= \sum_j t\Big((a^\dagger_{j\uparrow} - a_{j\uparrow})(a_{j+1\downarrow} + a^\dagger_{j+1\downarrow}) + (a^\dagger_{j\downarrow} - a_{j\downarrow})(a_{j+1\uparrow} + a^\dagger_{j+1\uparrow})\Big) \\
&= -it\sum_j \Big(\tilde{\gamma}_{j\uparrow}\gamma_{j+1\downarrow} + \tilde{\gamma}_{j\downarrow}\gamma_{j+1\uparrow}\Big)\,,
\end{aligned}
$$

where $\tilde{\gamma}_{js} = i(a^\dagger_{js} - a_{js})$ and $\gamma_{js} = a^\dagger_{js} + a_{js}$. Thus, in terms of Majorana operators the Hamiltonian reads

$$
H^{\mathrm{CII}}_{\mathrm{Majorana}} = -it\sum_j \Big(\tilde{\gamma}_{j\uparrow}\gamma_{j+1\downarrow} + \tilde{\gamma}_{j\downarrow}\gamma_{j+1\uparrow}\Big)\,. \tag{F.3}
$$

From this Hamiltonian, we may easily read off the corresponding Majorana zero modes. There are two imaginary modes, $\tilde{\gamma}_{N\uparrow}, \tilde{\gamma}_{N,\downarrow}$ and two real modes, $\gamma_{1\uparrow}$, $\gamma_{1\downarrow}$.

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