Weyl semimetals: Euler structures and disorder

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Abstract

We extended the idea of Euler structures and the Euler chain representation of Weyl semimetals within the framework of disordered free fermions to all ten symmetry classes. Euler structures are very useful in understanding the global topology of a Weyl semimetal and provide additional topological information besides the local invariant given by the Weyl charge. This additional information is encoded in the Euler chain and defines the Euler chain representation of a WSM. They also show a deep connection to surface Fermi arcs which are a direct experimental evidence of Weyl points. Moreover, we work out the effects of symmetries on the presence of Weyl points and corresponding Euler chains. In a second part we study the effects of disorder on Weyl points and try to derive a field theoretic description for Weyl semimetals. We use the methods of superbosonization and non-abelian bosonization to gain some insights to what a bosonic field theory of a WSM should look like. A three dimensional model of stacked two dimensional networks is constructed and we show that it describes a WSM phase. Further analysis of the model leads to a proposal of a potential field theory for the model.

Kurzzusammenfassung

Wir haben die Idee der Euler-Strukturen und die Euler-Kettendarstellung der Weyl-Halbmetalle im Rahmen ungeordneter freier Fermionen auf alle zehn Symmetrieklassen ausgedehnt. Euler-Strukturen sind sehr nützlich für das Verständnis der globalen Topologie eines Weyl-Halbmetalls und liefern neben der lokalen Invariante, die durch die Weyl-Ladung gegeben ist, zusätzliche topologische Informationen. Diese zusätzlichen Informationen sind in der Euler-Kette kodiert und definieren die Euler-Kettendarstellung eines Weyl Halbmetalls. Weiterhin hat die Euler-Kette eine tiefe Verbindung zu Fermi-Bögen auf der Oberfläche, welche ein direkter experimenteller Nachweis für Weyl-Punkte sind. Darüber hinaus arbeiten wir den Effekt von Symmetrien auf das Vorhandensein von Weyl-Punkten und entsprechenden Euler-Ketten heraus.

In einem zweiten Teil untersuchen wir die Auswirkungen von Unordnung auf Weyl-Punkte und versuchen, eine feldtheoretische Beschreibung für Weyl-Halbmetalle abzuleiten. Wir verwenden die Methoden der Superbosonisierung und der nicht-abelschen Bosonisierung, um zu einem besseren Verständnis, wie eine bosonische Feldtheorie eines Weyl Halbmetalls aussehen sollte, zu gelangen. Es wird ein dreidimensionales Modell gestapelter zweidimensionaler Netzwerke konstruiert und wir zeigen, dass es eine Weyl Halbmetall-Phase beschreibt. Die weitere Analyse des Modells führt zu einem Vorschlag einer potentiellen Feldtheorie für das Modell.

Contents

1	Introduction	1
2	Mathematical preliminaries 2.1 Homotopy theory 2.2 Homology theory 2.2.1 The Hurewicz theorem 2.2.2 Cohomology groups 2.2.3 Relative (co-)homology 2.3 Obstruction theory 2.4 Vector bundles and vector fields 2.4.1 Vector bundles 2.4.2 Vector fields	3 3 7 10 11 12 12 16 16 18
3	Weyl semimetals 3.1 Many-body framework 3.2 Symmetries 3.3 Lattice model and translational invariance 3.4 Dirac materials 3.4.1 Dirac and Weyl points	19 19 22 23 27 28
4	Euler chain representation of Weyl semimetals and Weyl superconductors 4.1 Euler structures - abstract definition 4.2 Euler chain representation of Weyl semimetals and superconductors 4.2.1 Weyl semimetals 4.2.2 Weyl semimetals 4.2.3 Fermi arcs 4.3 Summary and discussion	33 34 40 42 50 56 57
5	Disordered Weyl semimetals 5.1 Introduction 5.2 General setting 5.2.1 Supersymmetry 5.2.2 Model - details and disorder average 5.3 Gradient expansion 5.4 Cumulant expansion 5.5 Stacked network model 5.5.1 Chalker-Coddington Model	59 59 59 61 63 66 70 70

Contents

5.6	Stacked Chalker-Coddington model	73
	5.6.1 The 3D model	73
5.7	Discussion and Outlook	83

1 Introduction

The story of topology and condensed matter probably begins with the discovery of the quantum Hall effect [21] in 1980. The introduction of topology into the topic of condensed matter systems led to a revisit of band theory in insulators and superconductors and the idea of a *topological insulator* was born. The quantum Hall effect was the first example of such a novel phase of matter. Soon afterwards many more topological phases were found and also the introduction of symmetries led to some new predictions.

All of this then culminated in the attempt to provide a classification of topological phases. In [19] algebraic methods alongside K-theory were used to derive a pattern among topological insulators and superconductors, the periodic table of topological insulators and superconductors. Soon after that different approaches derived similar results in different settings [32],[1]. Moreover, the connection between the topological nature of the bulk and states on the surface, the so-called bulk-boundary correspondence, was shown in [1] with some tools from non-commutative K-theory.

The success of topological considerations in the framework of topological insulators and superconductors stimulated the search for similar phenomena in other fields. The extension from insulators and superconductors to semimetals and metals was the logical next step and anticipated for example in [13],[23] and later established theoretically and experimentally in [7],[30],[31],[28].

Since, unlike insulators and superconductors, semimetals and metals do not have an energy gap at the Fermi energy in their spectrum topology has to be studied in a different way in that case. One of the most prominent topological invariant that can be defined on the Fermi surface is for example the flux of Berry curvature through the Fermi surface. A particular interesting feature of a topological semimetal is the presence of *Fermi arcs* on the surface. Fermi arcs were for example also used to verify the topological phase in TaAs in [30].

In this thesis we introduce some tools from topology that can be used to understand semimetals. We will be focusing on a certain class of semimetals, *Weyl semimetals*. A Weyl semimetal gets its name from the spectrum of low-energy excitations. The points where the band gap closes can be understood to be sources and sinks of Berry curvature. Due to the spectrum in the vicinity of these points they are called *Weyl points* and they are the main subject of study throughout this work.

In recent years Weyl points and Weyl semimetals became a research topic of much interest as they are a prime example of a topological semimetal.

This thesis comprises two main parts and is organized in the following way. The first

1 Introduction

chapter gives a short overview and introduction to important tools from topology. It does not contain any physics and can as well be skipped and returned to if needed.

An introduction to the framework used to describe semimetals is given in the second chapter. It also introduces symmetries and their action in the presented framework. Moreover, Weyl points and some basic properties are considered.

In the third chapter we define *Euler structures* and the *Euler chain representation* of a Weyl semimetal. Furthermore, we show in what sense these tools capture and describe the topology of Weyl semimetals. Then we include symmetries to the picture and work through the ten symmetry classes to understand Euler structures in the presence of symmetries. In the end we give a short discussion on the connection of Euler chains to Fermi arcs.

In the second part we are concerned with Weyl semimetals in the presence of disorder. We set out from a quite general model and try to derive a field theoretic description of it. To achieve this we follow three different approaches with various success. In the end we discuss the success and issues of all three approaches and give an outlook to open questions.

The goal of this chapter is twofold. On the one hand, it lays the mathematical foundations for this work and introduce various tools from different fields in mathematics that are used in the remainder; on the other hand, it introduces notation and terminology used throughout this work. It is not supposed to contain a full introduction to these topics, but rather a brief introduction of the relevant aspects. This includes basic definitions and notations as well as some examples. For more general and more extensive discussions on the introduced topics, there will be references to the respective literature given.

The tools introduced here range from the fields of homotopy theory and homology theory over obstruction theory to vector bundles and vector fields. Each of which will be discussed in a separate section. The application to physical situations will not be part of this introductory chapter, but instead will be given in detail in the following chapters.

2.1 Homotopy theory

Homotopy theory provides a vast collection of tools that have a useful application in physics. We will begin with the very basics of homotopy theory: the definition of homotopy, homotopy groups and as a more specific example the homotopy groups of spheres, as they are quite important and will come up frequently.

The main ingredients for homotopy theory are topological spaces and the notion of continuity. Therefore, all spaces and maps mentioned in this introduction are, unless stated otherwise, considered to be at least topological spaces and continuous maps.

Homotopies. Let us begin with the definition of a homotopy:

Definition 1. Let X and Y be two topological spaces and $f_0, f_1 : X \to Y$ two continuous maps. Then a homotopy F is a continuous map $F : X \times [0,1] \to Y$, such that $F|_{X \times \{0\}} \equiv f_0$ and $F|_{X \times \{1\}} \equiv f_1$.

The two maps f_0 and f_1 are said to be *homotopic* if there exists such a homotopy. We write $f_0 \simeq f_1$.

Next, we define equivalence classes of maps $f : X \to Y$ with the equivalence relation being a homotopy. Since this idea of forming equivalence classes will be used frequently throughout this work, we give a brief definition of an equivalence relation.

Definition 2. A binary relation \sim is called *equivalence relation* if it fulfills the following three properties for any three objects a, b, c:

- reflexive a ∼ a,
- symmetric $a \sim b \Leftrightarrow b \sim a$,
- transitive $a \sim b$ and $b \sim c \Rightarrow a \sim c$.

These three properties can easily be observed for homotopic maps. We immediately see that f is homotopic to itself, that $f \simeq g$ is equivalent to $g \simeq f$ and finally that if $f \simeq g$ and $g \simeq h$ then also $f \simeq h$, simply by concatenating two homotopies. Taking these properties together shows that the relation of being homotopic defines an equivalence relation. And we call the resulting equivalence class $[f] := \{g : X \to Y | f \simeq g\}$ the homotopy class of f. We denote the set of all homotopy classes of maps from X to Y by [X, Y].

In the category of topological spaces with morphisms being continuous maps, isomorphisms are called *homeomorphisms*. A homeomorphism between two spaces X, Y is a continuous function f that has a continuous inverse g.

However, there is a slightly weaker relation for two topological spaces based on the notion of a homotopy. Two spaces X and Y are said to be *homotopic equivalent* if there exist two maps $f: X \to Y$ and $g: Y \to X$, such that $f \circ g \simeq \operatorname{Id}_Y$ and $g \circ f \simeq \operatorname{Id}_X$.

We can easily see that this is a slightly weaker relation than being homeomorphic, i.e. every homeomorphism is a homotopy equivalence, but not every homotopy equivalence is a homeomorphism.

To give a specific example which also plays an important role in the remainder, we consider the homeomorphism between the sphere and the quotient of the disc(square) and its boundary. The explicit map will not be given here, we instead give a sketch of the intuitive idea behind the homeomorphism (see fig.2.1). In the remainder we use all three representations of the d-dimensional sphere

$$S^d \simeq D^d / \partial D^d \simeq I^d / \partial I^d$$
.

The definition of homotopy groups in the following section requires to extend the definition of a homotopy to pairs (X, A) of a topological space and a subspace. Consider pairs (X, A) and (Y, B) with $A \subseteq X$ and $B \subseteq Y$, a map $f : (X, A) \to (Y, b)$ is a map $f : X \to Y$ with the property that $f(A) \subseteq B$. In the definition of homotopy groups the subspace will be just a distinguished point, called *base point*, $x_0 \in X$.

A map $f: (X, x_0) \to (Y, y_0)$ is map $f: X \to Y$, such that $f(x_0) = y_0$ and a homotopy F between two such maps is called *base point preserving* if $F(x_0, t) = y_0$ for all $t \in [0, 1]$. More generally, a homotopy between two maps $f_0, f_1: (X, A) \to (Y, B)$ respects the subset structure and $F(A, t) \subseteq B \ \forall t \in I$.

We denote the set of equivalence classes of maps $f : (X, x_0) \to (Y, y_0)$ with the equivalence relation given by base point preserving homotopies by $[(X, x_0), (Y, y_0)]$.



Figure 2.1: Sketch of the idea behind the homeomorphism between S^d and $D^d/\partial D^d$. The blue point and the orange circle are mapped to the north and south pole of the sphere, respectively.

Homotopy groups. With the definitions of equivalence classes from the previous section we now want to distinguish a special set of equivalence classes, the so called *homotopy group*. As the name suggests, a well-defined group structure can be given to this set. The homotopy group will be associated to a space with base point (X, x_0) and it turns out to be very useful tool in topology. Some applications will be discussed here as examples. Throughout this work, more applications will become apparent.

Definition 3. Let (X, x_0) be a topological space with base point x_0 . The homotopy group $\pi_d(X, x_0)$ is defined as

$$\pi_d(X, x_0) := [(S^d, s_0), (X, x_0)].$$

This defines the homotopy group as a set. Furthermore, we can define a group structure for $\pi_d(X, x_0)$. This will be done in the following in detail.

Remark 1. The base point x_0 will often be dropped from the notation since it can easily be shown that the homotopy group does not depend on either base point s_0 or x_0 . However, it is important to choose one and use the base point preserving property of homotopies. Which specific base point is chosen does not matter.

The group structure of $\pi_d(X)$ can probably best be understood in the representation of $S^d \simeq I^d / \partial I^d$. Set I = [0, 1] and consider two maps $f, g: (I^d / \partial I^d, \mathfrak{o}) \to (X, x_0)$. Their product is then defined by the concatenation along any one of the coordinates:

$$(f*g)(x_1,\ldots,x_d) := \begin{cases} f(2x_1,\ldots,x_n) & \text{for } 0 \le x_1 \le 1/2\\ g(2x_1-1,\ldots,x_n) & \text{for } 1/2 \le x_1 \le 1 \end{cases}$$
(2.1)

This definition descends to the level of homotopy classes and defines a group multiplication on $\pi_d(X)$. For a formal proof of this statement see for example [14].

This multiplication turns out to be abelian for higher homotopy groups $d \ge 2$, for d = 1, however, this is not the case. The first homotopy group $\pi_1(X)$, also known as the *fundamental group*, is the space of based loops in X and the multiplication is given by concatenation of loops, which is not abelian in general.

Figure 2.2 should give an idea of how the group structure looks in dimensions $d \leq 2$ and why it is abelian.



Figure 2.2: Series of homotopies between f * g and g * f which suggests that the group multiplication really is abelian for dimension $d \ge 2$.

Homotopy groups of spheres. Homotopy groups are a great tool to understand the topology of a space X and one of the central tasks in homotopy theory is to compute the homotopy groups of spheres $\pi_d(S^n)$. While this question is not very rich for $d \leq n$ it becomes more interesting for d > n. The more important case for this work, however, is $d \leq n$, or more precisely d = n since $\pi_d(S^n) = 0$ for 0 < d < n and $\pi_n(S^n) \simeq \mathbb{Z}$.

The simplest case n = 1 is very intuitive and serves as a good example. So for $\pi_1(S^1)$ we are looking for the homotopy classes of maps from $S^1 \to S^1$. These can be understood quite intuitively since each one can be characterized by the number of times the circle gets wrapped around another circle. The key observation for this visualization is that the identity map is not homotopic to the constant map to the base point. This shows that $\pi_1(S^1)$ is generated by the homotopy class $[\mathrm{id}_{S^1}]$ and thus $\pi_1(S^1) = \mathbb{Z}$. The argument for the higher dimensional spheres is the same and each $\pi_n(S^n) = \mathbb{Z}$ is generated by the homotopy class of the identity map.

Given a map $f: S^d \to S^d$, the integer defined by the homotopy class $[f] \in \pi_d(S^d)$ is called the *mapping degree* deg(f) of f. In the case d = 1 this is sometimes called *winding number* as well.

2.2 Homology theory

The theory introduced in this section, homology theory, and its dual theory are very important tools in topology and have a wide range of applications in theoretical physics. There are various different versions of homology theory. We will focus on the definition and discussion of singular homology here and roughly follow the introduction of Hatcher in [14] (Sec. 2.1). However, all different versions are based on the general concept of a *chain complex*. We begin with the very basics and general definitions for homology groups, which are the same for all different versions of homology theory. It will also be come clear how there can be different versions of homology theories arising from the same basic idea. In the next sections the notions of *cohomology* and relative (co)homology are introduced.

Definition 4. A chain complex is a sequence of abelian groups A_0, A_1, A_2, \ldots connected by homomorphisms $\partial_n : A_n \to A_{n-1}$, such that $\partial_{n-1} \circ \partial_n = 0$ for all n. It may be written in the form

$$\cdot \leftarrow A_0 \xleftarrow{\partial_1} A_1 \xleftarrow{\partial_2} A_2 \xleftarrow{\partial_3} A_3 \leftarrow \dots$$

We will also write (A_i, ∂_i) in short.

Elements in the kernel of ∂ are called *cycles* (or closed elements) and elements in the image of ∂ are called *boundaries* (or exact elements). By definition every exact element is closed, i.e. $\operatorname{im}(\partial_{n+1}) \subseteq \operatorname{ker}(\partial_n)$. And with that the homology group $H_n(A_i, \partial_i)$ of a chain complex is defined as

$$H_n(A_i, \partial_i) := \ker(\partial_n) / \operatorname{im}(\partial_{n+1}).$$
 (2.2)

Note that H_n is always a well defined group since we started by considering abelian groups A_i .

As stated above, the notion of a chain complex can be defined for different objects A_i and this gives rise to different notions of homology.

We take this opportunity to mention the somewhat related notion of an *exact sequence*, which is frequently used in algebraic topology. Consider a sequence of groups A_i (not

necessarily abelian) and group homomorphism $f_i: A_i \to A_{i+1}$. Such a sequence is called exact if for all i

$$im(f_i) = ker(f_{i+1}).$$
 (2.3)

Note that this definition can be made for other algebraic structures as long as kernel and cokernel make sense.

Exact sequences have a wide range of application in algebraic topology and they . More details will be discussed when needed and we leave it with the general introduction at this point.

Now, to introduce the notion of singular homology, we start with the basic building blocks:

Definition 5. The standard *n*-simplex is defined as the set

$$\Delta^{n} := \{(t_0, \dots, t_n) \in \mathbb{R}^{n+1} \mid \sum_{i} t_i = i \text{ and } t_i > 0 \,\forall i\}.$$
(2.4)

Note that the ordering of indices determines an orientation on the edges according to increasing indices.

The (n-1)-simplex Δ_i^{n-1} obtained by omitting the *i*-th vertex of Δ^n is a face of Δ^n and is (canonically) isomorphic to Δ^{n-1} . The boundary $\partial \Delta^n$ of Δ^n is given by the union of all n-1 faces and the open *n*-simplex $\mathring{\Delta}^n$ is $\Delta^n - \partial \Delta^n$.

A singular n-simplex in a topological space X is a continuous map $\sigma : \Delta^n \to X$. Let $C_n(X)$ be the free abelian group with the singular n-simplices in X as a basis. An element of $C_n(X)$ is called (singular) n-chain and is a finite formal sum $\sum_i n_i \sigma_i$ with $n_i \in \mathbb{Z}$ and $\sigma_i : \Delta^n \to X$. The boundary map $\partial_n : C_n(X) \to C_{n-1}(X)$ is defined in the following way:

$$\partial_n : C_n(X) \to C_{n-1}(X)$$

 $\sigma \mapsto \partial_n(\sigma) = \sum_{i=0}^n (-1)^i \sigma|_{\Delta_i^{n-1}}$

This definition implies the canonical isomorphism $\Delta_i^{n-1} \simeq \Delta^{n-1}$ mentioned before, so that $\sigma|_{\Delta^{n-1}}$ is indeed a singular (n-1) simplex.

Lemma 1. The composition of two boundary maps $\partial_{n-1} \circ \partial_n : C_n(X) \to C_{n-2}(X)$ is zero.

Proof. Consider $\sigma \in C_n(X)$. Then

$$\partial_n(\sigma) = \sum_{i=0}^n (-1)^i \sigma|_{\Delta_i^{n-1}}$$

8



Figure 2.3: Sketch of the standard 1-simplex and the standard 2-simplex.

and

$$(\partial_{n-1} \circ \partial_n)(\sigma) = \sum_{j < i}^n (-1)^j \sigma|_{\Delta_{ji}^{n-1}} + \sum_{j > i}^n (-1)^j (-1)^{j-1} \sigma|_{\Delta_{ij}^{n-1}} = 0.$$

These two sums cancel since exchanging i and j in the second sum gives the negative of the first sum. $\qedsymbol{\square}$

This Lemma tells us that the singular chains $C_n(X)$ with the boundary map ∂ define a chain complex and we can define the homology group $H_n^{sing}(X)$ of that chain complex.

Remark 2. The standard *n*-simplex Δ^n is homeomorph to the *n*-disk D^n and its boundary to S^{n-1} . We mention this here, as it might be sometimes more intuitive to consider maps $D^n \to X$, and furthermore a (singular) *n*-chain is often written as a linear combination of maps $c_i : D^n \to X$ in the following sections.

Example. Let us discuss a simple example at this point. Consider the three dimensional space $X = \mathbb{R}^3 \setminus \{0\}$ with the origin removed. Now, in order to compute the homology group $H_n^{\text{sing}}(X)$, we need to find a closed (singular) *n*-chain, which is not the boundary of a singular (n + 1)-chain in X.

For n = 1 this is not possible, given any closed 1-chain we find a 2-chain, such that its boundary is the considered 1-chain. For n = 3 this is trivial as well, since there are no 4-chains in $\mathbb{R}^3 \setminus \{0\}$, but there also is no closed 3-chain and therefore $H_3^{sing}(X) = 0 =$

$H_1^{\text{sing}}(X).$

But for n = 2 things are a little more interesting. There exists a closed 2-chain, which is not the boundary of a 3-chain, namely the 2-chain, which contains the origin on the inside. To be more precise, consider the boundary of the 3-simplex that is located in $\mathbb{R}^3 \setminus \{0\}$ such that the origin is on the inside of the tetrahedron. Now, even though you can think of this 2-chain as the boundary of a 3-chain, this 3-chain is not a valid 3-chain in X and this 2-chain generates the homology group $H_2^{sing}(X) = \mathbb{Z}$.

One might even go further and show that $X \simeq S^2$ and see that we have just computed the homology groups of the 2-sphere – even though we did not worry to much about the details here and a proof of this fact would need a more careful discussion.

An example of a topological invariant based on homology that will be important later on, is the so called *Euler characteristic* of a topological Space X.

Definition 6. Let X be a d-dimensional topological space and $b_n := \operatorname{rank}(H_n(X))$ the so called *n*-th Betti number. Then is the Euler characteristic $\chi(X)$ defined as the alternating sum

$$\chi(X) := \sum_{i=0}^d (-1)^i b_i$$

The homology group of a topological space measures topological information in a similar way as the homotopy group, but it is often much easier to compute. This comes with a price, as the homotopy group is the finer tool and can detect information, that the homology group can not detect. The most famous example for this would be the Hopf map $S^3 \to S^2$. But we will not go into more detail here. Nonetheless, the next theorem states a connection between homology and homotopy groups of a space X.

2.2.1 The Hurewicz theorem

The *Hurewicz theorem* is one of the central results in algebraic topology and builds a connection between homotopy theory and homology theory. We will only state the theorem and refer for example to Hatcher [14] for a proof of the statement.

Theorem 2. Let X be a topological space. Then there exists a group homomorphism for every $k \in \mathbb{N}$

$$h_*: \pi_k(X) \to H_k(X)$$
.

Now, let n be another positive integer and if X is path connected and $\pi_k(X) = 0$ for all k < n then h_* is an isomorphism for all $k \leq n$ (for $n \geq 2$ and the abelianization for n = 1.

We do not go into more detail on this topic as it is not of importance for this work, but it still worth to mention the established connection between the two topics introduced before.

2.2.2 Cohomology groups

Cohomology groups are another different invariant that can be assigned to a topological space and are closely related to homology groups. As it was the case for homology there exist various different versions of cohomology. Even more as for homology. As the name suggests, some of them can be obtained from a homology theory by dualizing. We will start with the basic idea and the general definition of *cochain complex* (very similar to chain complexes).

Definition 7. A cochain complex is a sequence of abelian groups A_0, A_1, A_2, \ldots connected by homomorphisms $d_n : A_n \to A_{n-1}$, such that $d_{n+1} \circ d_n = 0$ for all n. It may be written in the form

$$\cdots \to A_0 \xrightarrow{d_0} A_1 \xrightarrow{d_1} A_2 \xrightarrow{d_2} A_3 \to \dots$$

Elements in the kernel of d are called *cocycles* (or closed elements) and elements in the image of d are called *coboundaries* (or exact elements). By definition every exact element is closed, i.e. $\operatorname{im}(d_n) \subseteq \operatorname{ker}(d_{n+1})$. And with that the cohomology group H^n of a cochain complex is defined as

$$H^n := \ker(d_n) / \operatorname{im}(d_{n-1}).$$
 (2.5)

As it was the case for a chain complex, the notion of a cochain complex can be defined for different objects and gives rise to the different notions of cohomology.

Example. A first example of this is the cochain complex of differential forms on a manifold M with the exterior derivative $d: \Omega^n(M) \to \Omega^{n+1}(M)$. The cohomology associated to this cochain complex is usually called *deRham cohomology* $H^n_{dR}(M)$.

For any chain complex there exists a cochain complex, obtained by dualizing. That means replacing every group A_i by its dual group $A_i^* := \text{Hom}(A_i, R)$, for a fixed abelian group R, and every homomorphism ∂_i by the dual homomorphism

$$d_{i-1}: A_{i-1}^* \to A_i^*,$$
$$f \mapsto f \circ \partial$$

Singular cohomology. Starting from *n*-chains $(C_n(X), \partial)$, a singular cochain can be defined as $C^n(X; R) := \text{Hom}(C_n(X), R)$. The coboundary operator d is then defined as the dual of the boundary operator ∂ and the cohomology group as

$$H^n_{\text{sing}}(X; R) := \ker(d_n) / \operatorname{im}(d_{n-1}).$$
 (2.6)

We usually work with the coefficients being $R = \mathbb{Z}$. However, in the section on obstruction theory, the obstruction cochain will be constructed as a cochain with coefficients in some homotopy group $\pi_k(Y)$. In that case one needs to have the restriction $k \geq 2$ for the homotopy group to be abelian.

2.2.3 Relative (co-)homology

There also is a relative version of homology. Consider a pair (X, A) with $A \subseteq X$. Since chains in A are obviously also chains in X, we have that $C_n(A)$ is a subgroup of $C_n(X)$ and therefore define

$$C_n(X, A) := C_n(X)/C_n(A).$$
 (2.7)

The boundary operator ∂ descends to a map $\partial : C_n(X, A) \to C_{n-1}(X, A)$ and is still a well defined boundary map. The homology group of this chain complex is then defined as

$$H_n^{\text{sing}}(X, A) := \ker(\partial|_{C_n(X, A)}) / \operatorname{im}(\partial|_{C_{n+1}(X, A)}).$$
(2.8)

With the definition of $C_n(X, A)$ (2.7) there is an intuitive way to picture representatives of elements in $H_n^{\text{sing}}(X, A)$ as chains c in X whose boundary ∂c lies in A. This means elements in $C_n(X, A)$ do not need to be closed, but their boundary needs to be in $C_{n-1}(A)$.

The relative version of cohomology can be introduced in a similar way as before by dualizing the relative homology. And even for cohomologies, such as deRham cohomology, which are not obtained by dualizing, a relative version can usually be defined. For more details on the relative version of deRham cohomology consider for example Bott and Tu [4], chapter 1.6.

With the definition of relative *n*-chains $C_n(X, A)$ (2.7) comes a (short) exact sequence

$$0 \to C_n(A) \xrightarrow{i} C_n(X) \xrightarrow{p} C_n(X, A) \to 0, \qquad (2.9)$$

with the inclusion $i : C_n(A) \hookrightarrow C_n(X)$ and the projection on equivalence classes $p: C_n(X) \to C_n(X)/C_n(A)$.

This is indeed an exact sequence. To see this, note that the inclusion is injective and therefore ker(i) = 0. The projection p is surjective which proves the exactness at $C_n(X, A)$. The missing part is to show that ker(p) = im(i) which is clear from the definition of $C_n(X, A) = C_n(X)/C_n(A)$.

2.3 Obstruction theory

Obstruction theory does not play a major role in the remainder of this work, but it is, however, quite a useful tool to prove, for example, the existence of a homotopy. It is necessary to give a brief introduction to CW complexes for the definition of obstruction theory due to Eilenberg [12]. Nonetheless, CW complexes are an interesting topic on their own and they have many applications in algebraic topology. After the definition of CW complexes and an example of the torus as CW complex, the notion of cellular homology is introduced and followed by the basic idea of obstruction theory in terms of an extension problem. **CW complexes.** A CW complex X is often defined by an inductive construction process. This is quite instructive and gives a good intuitive understanding of CW complexes and therefore it is presented here. The idea is to build up a space X with cells of increasing dimension. Vice versa, one could think of this as the decomposition of a space X into cells.

Let us begin with a set of 0-cells X_0 . We call it the *0-skeleton* of a space X.

Now, we continue with one dimensional cells and attach any number of 1-cells via continuous maps $f_i: \partial D^1 \to X_0$ to obtain the 1-skeleton X_1 . In other words, we can think of this as the process of "gluing" 1-cells $c \simeq D^1 = [0, 1]$ into the 0-skeleton by assigning to each endpoint of the 1-cell one point in X_0 via the maps f_i . If both endpoints are mapped to the same point $x \in X_0$ the result is homeomorphic to the circle S^1 based at the point x. In general on could say that the 1-skeleton is a graph.

Next, we obtain the 2-skeleton by attaching 2-cells to the 1-skeleton, again via continuous maps $f_i: \partial D^2 \to X_1$.

By continuing in this way, we obtain an *n*-dimensional space $X_0 \subset X_1 \subset \cdots \subset X_n$, which we call a (finite dimensional) *CW complex*. This process can even continue infinitely to define an infinite-dimensional CW complex as the direct limit of the *n*-skeleta.

The name CW complex refers to the topology defined for such a space, where C stands for *closure finite* and W for weak topology. The technical details are not of importance here and can, alongside an introduction and further examples, be found for example in [14].

Example. One example of a CW complex that plays a central role in this work is the torus \mathbb{T}^d . To consider a tangible example let us set d = 2. The construction works similarly for all dimensions d.

The 0-skeleton of the 2-torus is just a single point $\{x_0\} = X_0$. The 1-skeleton consists of two 1-cells attached to X_0 by the continuous map $f: S^0 \to X_0$ which maps both points of S^0 to $x_0 \in X_0$. Finally, one 2-cell is attached via a continuous map $f: S^1 \to X_1$. The attaching map f can best be understood visually in figure 2.4. The gluing map f maps the boundary of the disc D^2 to the boundary of the square in the left figure of fig. 2.4. And since the boundary is build out of two 1-cells, it would first follow the blue 1-cell, then the orange 1-cell, then the blue 1-cell, but in reverse direction and finally the orange 1-cell also in reverse direction. In this fashion the interior of the square represents the two cell of the CW structure of the torus. In the right figure of fig.2.4 the torus is shown in its usual representation (embedded in \mathbb{R}^3).

Cellular homology. Given a CW complex we can define a chain complex associated to it. To this chain complex we can define the homology in the usual way and this is called *cellular homology*. The definition of this chain complex makes use of the construction of the *n*-skeleton from the (n - 1)-skeleton and it turns out that cellular homology groups



Figure 2.4: CW structure of the torus. The green dot represents the 0-skeleton, the two 1-cells are shown in orange and blue (in the left figure two opposite edges are identified) and the 2-cell is given by the interior of the square.

are quite easy to compute. To demonstrate this, the example of the torus comes up again and its homology groups are computed in this context. For a somewhat more detailed discussion of this topic consider again for example the book of Hatcher [14]

Let X be a CW-complex and consider the short exact sequence associated to the relative chain group $C_n(X_n, X_{n-1})$:

$$0 \to C_n(X_{n-1}) \xrightarrow{i} C_n(X_n) \xrightarrow{p} C_n(X_n, X_{n-1}) \to 0.$$
(2.10)

To any short exact sequence of chain complexes $C_*(X_n)$ there exists a long exact sequence in homology, if *i* and *p* are chain maps, i.e. commute with with the boundary operator:

$$\cdots \to H_k(X_{n-1}) \to H_k(X_n) \to H_k(X_n, X_{n-1}) \to H_{k-1}(X_{n-1}) \to H_{k-1}(X_n) \to \dots$$
(2.11)

Arranging parts of the long exact sequences for the pairs (X_{n+1}, X_n) , (X_n, X_{n-1}) and (X_{n-1}, X_{n-2}) in the correct way lets us define the *cellular chain complex*

$$\dots \to H_{n+1}(X_{n+1}, X_n) \to H_n(X_n, X_{n-1}) \to H_{n-1}(X_{n-1}, X_{n-2}) \to \dots$$
 (2.12)

The concatenation of two maps is zero, because it contains two successive maps in one of the long exact sequences. Therefore, it is indeed a chain complex and the homology groups of this chain complex are called *cellular homology groups* $H_n^{CW}(X)$. In fact the following theorem holds.

Theorem 3. Let X be a CW-complex. Then the homology groups $H_n(X) = H_n^{CW}(X)$ for all n.

Note, that if X has k n-cells, then $H_n(X_n, X_{n-1})$ is a free abelian group generated by k elements and therefore also $H^{CW}(X)$ is generated by at most k elements. Also, since elements in $H_n(X_n, X_{n-1})$ are equivalence classes of n-cells in X_n it often becomes fairly easy to explicitly compute the cellular homology groups as many CW complexes of interest have only finite skeleta. This becomes more clear in the following example.

Before we return to the example of the torus, there is another interesting fact for CW complexes worth mentioning here: The Euler characteristic of a CW-complex can be defined as the alternating sum $\chi(X) = k_0 - k_1 + k_2 - k_3 + \ldots$, where k_n is the number of *n*-cells in the complex. This is not really a definition, but it can be deduced from the previous definition of the Euler characteristic.

Example. Consider again the example of a torus, but this time the 3-torus $\mathbb{T}^3 = S^1 \times S^1 \times S^1$. Its CW structure is given by one 0-cell, three 1-cells, three 2-cells and one 3-cell. The cellular chain complex is thus of the form

$$0 \to \mathbb{Z} \to \mathbb{Z}^3 \to \mathbb{Z}^3 \to \mathbb{Z} \to 0.$$

It turns out that all three maps in this chain complex are the zero map and the homology groups of the torus are therefore given by $H_i(\mathbb{T}^3) = \mathbb{Z}$, for i = 0, 3 and $H_i(\mathbb{T}^3) = \mathbb{Z}^3$, for i = 1, 2.

Recall the definition of the Euler characteristic from the previous section: $\chi(X) = \sum_i (-1)^i b_i$. Now, that we have computed the homology groups of the three torus, we can as well compute the Euler characteristic of the three-torus as $\chi(\mathbb{T}^3) = 1 - 3 + 3 - 1 = 0$. As it turns out this is true for any dimension and $\chi(\mathbb{T}^d) = 0$ for all d.

We want to take the opportunity at this point to introduce a notion which will be important for later. A subtorus of a torus \mathbb{T}^d is a (d-1)-dimensional torus $\mathbb{T}^{d-1} \subset \mathbb{T}^d$. In case of d = 3, consider a parametrization

$$(0, 2\pi)^3 \to \mathbb{T}^3 = S^1 \times S^1 \times S^1$$
$$(\theta_1, \theta_2, \theta_3) \mapsto (e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}).$$

Then a subtorus can for example be obtained by fixing one of the angles. For later purposes we call a subtorus, where θ_1 is fixed, a 23-subtorus (or a *yz*-torus). Analogously for the *zx*- and *xy*-subtori.

Extension problem. The basic question we seek to answer is wether a continuous map f, defined on a subset $A \subset X$, can be extended to a continuous map \tilde{f} on all of X with $\tilde{f}|_A \equiv f$ or not. If X and A are CW complexes, we can first look at the simpler case,

where f is defined on the *n*-skeleton and the question can be if it can be extended over the (n+1)-skeleton. In other words, we are looking for an inductive process of extending f over the *n*-skeleta of X.

Assume that $f: X_n \to Y$ is a continuous map defined on the *n*-skeleton of *X*. The (n+1)-skeleton X_{n+1} is constructed from X_n by attaching some (n+1)-cells to it via continuous maps $\varphi_i: (D^{n+1}, S^n) \to (X_{n+1}, X_n)$ $(i = 1, \ldots, k)$. Note, that $f \circ \varphi_i : S^n \to Y$ and $[f \circ \varphi_i] \in [S^n, Y] = \pi_n(Y)$ is a collection of elements of the *n*-th homotopy group of *Y*. Therefore, one can define a (n+1)-cochain by assigning to each (n+1)-cell the homotopy class of the map defined on its boundary. This defines an (n+1)-cochain $\theta^{n+1}(f)$ with values in $\pi_n(Y)$, so $\theta^{n+1}(f) \in C^{n+1}(X;\pi_n(Y))$. In fact, if $\theta^{n+1}(f)$ is defined this way, the following Lemma holds.

Lemma 4. Let $f : X_n \to Y$ be a continuous map defined on the n-skeleton of X. Then the above defined cochain $\theta^{n+1}(f)$ is a cocyle, i.e. $\delta\theta^{n+1}(f) = 0$.

Returning to the question in the beginning, assume that $f : A \to Y$ is defined on a subset $A \subset X$. We can follow the inductive process from above, but in the definition of $\theta^{n+1}(f)$ we define it to be 0 on (n+1)-cells in $C_{n+1}(A)$, since f is already defined on A. This way $\theta^{n+1}(f)$ defines a cocyle in the relative cohomology group $H^{n+1}(X, A; \pi_n(Y))$.

With this the main theorem of obstruction theory can be formulated:

Theorem 5. Let (X, A) be relative CW complex. Let $f : X_n \to Y$ be continuous map. Then the cellular cocycle $\theta(f) \in C^{n+1}(X, A; \pi_n(Y))$ which vanishes if and only if f extends to a map $X_{n+1} \to Y$. If and only if $[\theta(f)] \in H^{n+1}(X, A; \pi_n(Y))$ vanishes, there exists a map g with $g|_{X_{n-1}} = f|_{X_{n-1}}$ and homotopic to f on X_n such that g extends over X_{n+1} .

2.4 Vector bundles and vector fields

Vector bundles and vector fields are the key ingredients in the Euler chain representation of a Weyl semimetal. Therefore, we give a brief introduction to the topic and the basic definition for the concepts that will be discussed in the main chapter of this work. Vector bundles in general play a very important role in many areas of theoretical physics and give a good mathematical description of various physical phenomena. The introduction here is for the purpose of this work and is probably not a sufficient basis for all physics literature. There are various mathematical and also physics textbooks on this topic that give a more detailed introduction see for example [4] or [15].

2.4.1 Vector bundles

We start with a slightly more general definition of vector bundles, even though we will only consider vector bundles over manifolds. **Definition 8.** Let M and E be topological spaces. A vector bundle (E, M, π) is given by a base space M, the total space E and the continuous surjection $\pi : E \to M$ (projection) and the condition that for every $p \in M$ the fiber $\pi^{-1}(p)$ has the structure of a finite dimensional real (or complex) vector space. Furthermore, there exist an open neighborhood U for every p, a natural number k and a homomorphism $\phi : U \times \mathbb{R}^k \to \pi^{-1}(U)$, such that

- $\pi \circ \phi(p, v) = x \quad \forall v \in \mathbb{R}^k$
- $v \mapsto \phi(p, v)$ is a linear isomorphism for all $p \in M$.

The open set U and the map ϕ are called a *local trivialization* (U, ϕ) .

Given two charts (U_i, ϕ_i) and (U_i, ϕ_i) there is a linear isomorphism for every $p \in U_i \cap U_i$

$$g_{ji}(p) := \phi_j \circ \phi_i^{-1}|_p : \mathbb{R}^k \to \mathbb{R}^k,$$

Which is called *transition function*. Note, that these transition functions have the property

$$g_{ii} \equiv 1, \quad g_{ij} \circ g_{jk} = g_{ik} \,. \tag{2.13}$$

Given two vector bundles (E_1, M_1, π_1) and (E_2, M_2, π_2) a morphism between two vector bundles is a pair of maps $f: E_1 \to E_2$ and $g: M_1 \to M_2$, such that $\pi_2 \circ f = g \circ \pi_1$ and that for every $p \in M_1$ the map $\pi_1^{-1}(p) \to \pi_2^{-1}(g(p))$ induced by f is a linear map of vector spaces.



Next, we introduce two operations on vector bundles, the *Whitney sum* (or direct sum) and the *tensor product* of two vector bundles. For that let (E_1, M, π_1) and (E_2, M, π_2) be two vector bundles over M.

A prominent example of a vector bundle is the tangent bundle TM of a manifold M. This bundle is defined as the collection of all tangent spaces T_pM at all $p \in M$ and it is usually one of the first examples one encounters.

Definition 9. Let (E, M, π) be a vector bundle. A (global) section of a vector bundle is a map $s: M \to E$ such that $(\pi \circ s)(p) = p$, for all $p \in M$.

The set of all (global) sections of a vector bundle is denoted by $\Gamma(E)$. This set contains at least one section, the zero section.

Remark 3. In the case of a (more general) fiber bundle there does not need to exist a global section. It makes sense to define the notion of local section in this case.

2.4.2 Vector fields

Returning to the previous example of the tangent bundle of a manifold TM, a section $\mathbf{v} \in \Gamma(TM)$ associates a tangent vector $\mathbf{v}(p)$ to every point $p \in M$, so sections in $\Gamma(TM)$ are (tangent) vector fields on M.

There are many results on vector fields on a manifold M. The most important results for this work will be stated here.

Definition 10. Let $\mathbf{v} \in \Gamma(TM)$ be a vector field with an isolated zero at $p \in M$. The *index* of \mathbf{v} at p index_p(\mathbf{v}) is defined to be the degree of the map

$$S_p^{d-1} \to S^{d-1}, \quad x \mapsto \frac{\mathbf{v}(x)}{|v(x)|},$$

where S_p^{d-1} is the boundary ∂D_p of a small ball centered around $p \in M$, such that $\mathbf{v}(x) \neq 0 \,\forall x \in D_p \setminus p$.

There is a famous theorem which relates the index of vector field on M to the Euler characteristic of M.

Theorem 6. (*Poincaré-Hopf*). Let M be a compact differentiable manifold. Let $\mathbf{v} \in \Gamma(TM)$ be a vector field on M with isolated zeroes. Then

$$\sum_{i} index_{p_i}(\mathbf{v}) = \chi(M) \,,$$

where the sum is over all isolated zeroes and $\chi(M)$ is the Euler characteristic of M.

3 Weyl semimetals

This chapter gives an introduction to the topic of Weyl semimetals and Weyl superconductors and sets the stage for the main part of this work. We introduce the setting which is used in the classification of disordered fermion systems with a quadratic Hamiltonian. Even though the framework and classification addresses disordered fermions, disorder is not introduced explicitly in this first part of this work. In the second part, disorder will play a more prominent role and it will be introduced accordingly there. But even if disorder is not explicitly considered in this first part, it is always considered as an important part of physical systems and should be kept in mind.

The introduction to the general setting is split into three parts, first the step from the single-particle Hilbert space to the many body Fock space is done. Next, the notion of symmetry and symmetry groups and their action in the many body framework are introduced. The third part then explicitly introduces the translation group of the lattice and consequences for translationally invariant systems, since we will assume translational invariance throughout this first part.

This chapter then closes with a short overview over so called Dirac materials, which are materials where the low energy excitations are Dirac or Weyl fermions. Furthermore, the notion of Dirac and Weyl points are introduced and a few remarks on their basic properties are made.

3.1 Many-body framework

The systems under consideration are semimetals and superconductors and they consist of a vast number of interacting particles (of the order $10^{10} - 10^{25}$). The theory of manybody quantum mechanics introduces a formalism to treat such systems in a satisfactory way. As was already mentioned we will focus on quadratic Hamiltonians and thus we are only considering interactions described by mean-field theory and neglecting all further contributions. In the Physics literature and more specific in the context of insulators, semimetals and superconductors this is known as the Hartree-Fock-Bogoliubov approximation.

Another central ingredient is the symmetry group G. Symmetries play a very important role in all areas of physics and they obviously are very important for the idea of a symmetry classification. Dyson's threefold way [10] is a very famous result of a symmetry classification for free fermions and the extension done by Heinzner, Huckleberry and Zirnbauer [16] is inspired by Dyson's original approach. Besides the general frameork, the symmetry group G and its action will be part of this introduction and the overall framework. The introduction given here is somewhat based on [16] since the framework is similar, it is however still very useful to give a detailed overview of the basic definitions

3 Weyl semimetals

here, as some specifics and details of the framework are different.

The first important step to extend the setting introduced in Dyson's threefold way [10] is the passing from single-particle quantum mechanics to the framework of manybody quantum mechanics. This usually goes under the name of second quantization. Here, we want to lay out the mathematical foundation of this procedure in a concise way.

Our starting point is the single-particle Hilbert space V with Hermitian scalar product $\langle \cdot, \cdot \rangle_V$. For simplicity only finite-dimensional vector spaces $V = \mathbb{C}^N$ will be considered here. The Hermitian structure defines an isomorphism between V and its dual space V^* , which is given by $\phi : V \to V^*$, $v \mapsto \langle v, \cdot \rangle_V$ (also known as Frechet-Riesz isomorphism). Furthermore, it determines a unitary group U(V), which is the group of \mathbb{C} -linear operators g satisfying $\langle v, w \rangle = \langle g(v), g(w) \rangle$ for all $v, w \in V$.

Remark 4. The finite-dimensional Hermitian vector space and its unitary group are two ingredients for Dyson's threefold way [10] – the missing ingredient is an anti-unitary transformation such as time-reversal. There are more details on that in the section on symmetry classification later on.

Now, let us pass from the single-particle setting V to the fermionic Fock space $\bigwedge(V)$ of many-body quantum mechanics. The Fock space is graded by the particle number $\bigwedge(V) = \bigoplus_n \bigwedge^n(V)$ and the *n*-particle subspace $\bigwedge^n(V)$ carries an induced Hermitian structure, given by

$$\langle v_1 \wedge \dots \wedge v_n, w_1 \wedge \dots \wedge w_n \rangle := \operatorname{Det} \begin{pmatrix} \langle v_1, w_1 \rangle & \cdots & \langle v_1, w_n \rangle \\ \vdots & \ddots & \vdots \\ \langle v_n, w_1 \rangle & \cdots & \langle v_n, w_n \rangle \end{pmatrix}$$

With this, the fermionic Fock space itself has the structure of a Hilbert space.

There are two important operations on the Fock space: exterior multiplication by $v \in V$

$$\varepsilon(v): \bigwedge^{n}(V) \to \bigwedge^{n+1}(V)$$

and contraction by $\varphi \in V^*$

$$\iota(\varphi): \bigwedge\nolimits^n(V) \to \bigwedge\nolimits^{n-1}(V)$$

with the physical interpretation of creating and annihilating a particle. Let $\{e_i\}_{i=1,\dots,N}$ be a basis of V and $\{f_i\}_{i=1,\dots,N}$ be the dual basis of V^* with $f_i(e_j) = \delta_{ij}$ then the standard physics notation is to write $c_i^{\dagger} := \varepsilon(e_i)$ for creation operators and $c_i := \iota(f_i)$ for annihilation operators. Some algebra reveals that these operators satisfy the so called *Canonical Anti-commutation Relations* (or CAR for short)

$$c_i^{\dagger} c_j^{\dagger} + c_j^{\dagger} c_i^{\dagger} = 0 = c_i c_j + c_j c_i , \quad c_i^{\dagger} c_j + c_j c_i^{\dagger} = \delta_{ij} .$$
 (3.1)

3.1 Many-body framework

These relations are in fact the representation of the underlying Clifford algebra relations of the Clifford algebra Cl(W, B) of the vector space $W := V \oplus V^*$ with the symmetric bilinear form

$$\{v + \varphi, v' + \varphi'\} = \varphi'(v) + \varphi(v').$$
(3.2)

This representation of the Clifford algebra $Cl(W, \{,\})$ on the Fock space $\bigwedge(V)$ defined above is called *Spinor representation*. The vector space $W = V \oplus V^*$ in this context is often known as the *Nambu space*, or the space of *field operators* ψ .

Besides the symmetric bilinear form $\{\cdot, \cdot\}$ there is another important structure on W, which is the real structure γ . A real structure (\mathbb{C} -antilinear involution) on W is determined by the Hermitian scalar product $\langle \cdot, \cdot \rangle_V$ on V

$$\gamma: W \to W, v + \varphi \mapsto \phi^{-1}\varphi + \phi v.$$
 (3.3)

In physics language the space $W_{\mathbb{R}} := \text{fix}_W(\gamma)$ is usually called the space of *Majorana* fields. It is the real vector space spanned by the Majorana operators $e_k + f_k$ and $ie_k - if_k$.

Each of these to structures induces an action on the linear transformations $L \in$ End(W). For γ this is given by

$$L \mapsto \gamma \circ L \circ \gamma$$
,

which defines an anti-linear involution on End(W). And we can define a linear antiinvolution $L \mapsto L^T$ called *transposition* and defined through the relation

$$\{\psi, L^T\psi'\} = \{L\psi, \psi'\}, \ \forall \psi, \psi' \in W.$$

Using these two structures, we can define a Hermitian structure on the the Nambu space $\langle \cdot, \cdot \rangle_W$. Let $w, w' \in W$, then

$$\langle w, w' \rangle := \{\gamma w, w'\}$$

defines a natural Hermitian scalar product on W.

The reason to introduce the Nambu space is to simplify the process of classification. The classification according to the tenfold way is guided by the question "what is the structure of the set of *one-body* time evolutions of $\bigwedge(V)$ which commute with a given *G*-action?"[33]. Therefore, we are interested in one-body, or quadratic (in the creation and annihilation operators), self-adjoint Hamiltonians *H*:

$$H = \frac{1}{2} \sum_{lm} Y_{lm} (c_l^{\dagger} c_m - c_m c_l^{\dagger}) + \frac{1}{2} \sum_{lm} Z_{lm} c_l^{\dagger} c_m^{\dagger} + \bar{Z}_{lm} c_m c_l \,.$$
(3.4)

It makes much more sense to consider the anti-hermitian operators iH instead of H. This might seem like a trivial modification, but unlike hermitian operators the anti-hermitian operators are closed under the commutator and Hamiltonians iH of the form (3.4) form the Lie algebra $\operatorname{Cl}_2(W_{\mathbb{R}})$ of skew-symmetrized elements of degree 2. This can easily be verified as $W_{\mathbb{R}}$ is spanned by Majorana operators $c_k + c_k^{\dagger}$ and $ic_k - ic_k^{\dagger}$ and a general

3 Weyl semimetals

skew-symmetrized product of two elements $X, Y \in W_{\mathbb{R}} \subset \operatorname{Cl}(W_{\mathbb{R}})$ can be written in the form *iH* with *H* as in eq.(3.4). Exponentiating this Lie algebra gives the Spin group $\operatorname{Spin}(W_{\mathbb{R}})$ and therefore time evolutions $U = e^{-iHt/\hbar}$ are elements in $\operatorname{Spin}(W_{\mathbb{R}})$.

The isomorphism of the Lie algebras $\operatorname{Cl}_2(W_{\mathbb{R}}) \simeq \mathfrak{so}(W_{\mathbb{R}})$ exponentiates to a mapping on the level of Lie groups ρ : $\operatorname{Spin}(W_{\mathbb{R}}) \to \operatorname{SO}(W_{\mathbb{R}})$, given by $\rho(g)v = gvg^{-1}$ for $v \in W_{\mathbb{R}}$. This mapping, however, is not an isomorphism, but is a 2:1 cover, i.e. $\rho(-g) = \rho(g)$. Nonetheless it is a representation of $\operatorname{Spin}(W_{\mathbb{R}})$ on the real vector space $W_{\mathbb{R}}$, which can be extended to a representation on W by \mathbb{C} -linearity. This fact allows us to study representations of $\operatorname{Spin}(W_{\mathbb{R}})$ on the Nambu space W instead of the full Fock space $\Lambda(V)$.

3.2 Symmetries

Symmetries play an important role in the understanding of physical systems and they are the fundamental building blocks of the classification of disordered fermions in the so called tenfold way. This approach as well as the name are based on Dyson's original threefold way. Now, we want to understand how the symmetries are introduced into the many-particle framework established in the previous section and thus build the setting for the tenfold classification.

We already mentioned the unitary group U(V) determined by the Hermitian structure of our Hilbert space V. Now, let G_0 be the group of unitary symmetries. That means there is some group G_0 which acts on V by unitary operators $\rho_V(g) \in U(V)$ (we will simply write $\rho_V(g) \cong g$). Since the group action is defined on V we equip the Nambu space W with the induced G_0 -representation. That means that V is equipped with the given representation and for $f \in V^*$ and $g \in G_0$

$$(g^{-1})^t \varphi = \varphi \circ g^{-1} \,. \tag{3.5}$$

The group G_0 is a normal subgroup of a larger group, the full symmetry group G. The group G contains G_0 as a subgroup and, furthermore, elements g_T which act as antiunitary operators $T: W \to W$. These are referred to as distinguished "time-reversal" symmetries. In fact, modulo G_0 there exist at most two such distinguished operators and they satisfy $T^2 = \pm 1$.

Every element in the set of anti-unitary elements in the full symmetry group can be written as the right multiplication of a distinguished element, here one of the time reversal operators T, with an element of G_0 and we can write the enlarged symmetry group as $G_0 \cup TG_0$.

Thus far we introduced the setting of Dyson's threefold way. However, the Fock space structure allows us to define another anti-unitary operator, that of particle-hole conjugation C, and extend the setting of Dyson

Let Ω be a generator of $\bigwedge^N(V)$ with $N = \dim(V)$ and normalization $\langle \Omega, \Omega \rangle = 1$. Then the *particle-hole conjugation* is the anti-unitary operator $C : \bigwedge^n(V) \to \bigwedge^{N-n}(V)$ defined 3.3 Lattice model and translational invariance

by the relation

$$C\psi) \wedge \psi' = \langle \psi, \psi' \rangle \,\Omega \,.$$

A simple calculation shows that for a *T*-invariant choice of Ω , which we can always do, the two operators *C* and *T* commute, CT = TC, and also that Cg = gC for all $g \in G_0$ under the assumption that the vacuum and the fully occupied state are invariant under G_0 .

Now, we can enlarge the symmetry group even further by allowing a twisted version of particle hole conjugation. This twist can be achieved by an unitary operator $S \in U(V)$, such that $S^2 = \text{Id}$, $S\Omega = \Omega$ and $SG_0S^{-1} = G_0$. A twisted particle-hole conjugation then refers to the operator $\tilde{C} := SC = CS$. Note, that with the conditions on S we also have $\tilde{C}G_0\tilde{C}^{-1} = G_0$ and $\tilde{C}T = T\tilde{C}$.

This lets us now write the full symmetry group G as $G = G_0 \cup TG_0 \cup \tilde{C}G_0 \cup T\tilde{C}G_0$, with $T\tilde{C} = \tilde{C}T$, and we call it a minimal extension of Dyson's setting.

Now, since we want to work on the space of field operators W, we need to understand how \tilde{C} acts on W. For G_0 and T this is clear from eq.(3.5), but for \tilde{C} it takes a little bit more effort. Let $\psi \in \bigwedge^n(V)$ and $\psi' \in \bigwedge^{n+1}(V)$ and c_k, c_k^{\dagger} annihilation and creation operators for some state k. We want to know what the particle-hole conjugate $\tilde{C}c_k^{\dagger}\tilde{C}^{-1}$ of c_k^{\dagger} is. Therefore, we do the following calculation

$$\begin{split} & (\tilde{C}c_k^{\dagger}\psi) \wedge \psi' = \langle Sc_k^{\dagger}\psi, \psi' \rangle \Omega = \langle S\psi, Sc_k S^{-1}\psi' \rangle \Omega \\ & = (\tilde{C}\psi) \wedge (Sc_k S^{-1})\psi' = (-1)^{N-n+1} (Sc_k S^{-1}\tilde{C}\psi) \wedge \psi' \,. \end{split}$$

Thus we see that $\tilde{C}c_k^{\dagger}\tilde{C}^{-1} = \pm Sc_kS^{-1} \in V^*$, where the sign alternates with the particle number.

Remark 5. Note that for the untwisted particle-hole conjugation this is nothing else than the Frechet-Riesz isomorphism $\phi: V \to V^*$ and the full particle-hole symmetry \tilde{C} is equivalent to γ .

3.3 Lattice model and translational invariance

In this section the model used to describe the physical systems under consideration is presented. The more general setting that was laid out in the previous sections will become more specific.

We assume there is periodic lattice in d spatial dimensions, which describes the real systems, for example the position of atoms in a crystal, in some approximation. The lattice spacing is assumed to be uniform and, unless explicitly stated otherwise, we assume it to be normalized to 1. Mathematically this lattice can be described by \mathbb{Z}^d . To begin again with the single particle-picture, we associate a Hilbert space \mathbb{C}^n , which

describes a number n of complex degrees of freedom, to every point in the lattice. In the tight binding model this leads to the single-particle Hilbert space $V = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^n$. For

3 Weyl semimetals

the following considerations it might be useful to fix a basis for V. We write $|\mathbf{x}, l\rangle \in V$ as the basis elements, where l labels some orthonormal basis of \mathbb{C}^n and \mathbf{x} labels the series with a 1 at the position $\mathbf{x} \in \mathbb{Z}^d$ and 0 anywhere else.

First, we want to introduce the translation operator $t_{\mathbf{y}}$, which is a unitary operator defined as

$$t_{\mathbf{y}}|\mathbf{x},l\rangle := |\mathbf{x}+\mathbf{y},l\rangle$$
.

For the majority of the remainder we will assume that translations by \mathbb{Z}^d are a symmetry, i.e. that the Hamiltonian commutes with $t_{\mathbf{y}}$ for all $\mathbf{y} \in \mathbb{Z}^d$. In the setting of the tenfold way, that means that $\mathbb{Z}^d \subset G_0$ is a subgroup of the unitary symmetries. A translation invariant Hamiltonian will be of the general form

$$H \left| \mathbf{x}, l \right\rangle = \sum_{\mathbf{y}, m} h_{ml}(\mathbf{y}) \left| \mathbf{x} + \mathbf{y}, m \right\rangle,$$

with a matrix $h(\mathbf{y}) : \mathbb{C}^n \to \mathbb{C}^n$.

From quantum mechanics we know, that we can find a simultaneous eigenbasis of all t_y and the Hamiltonian defined in terms of the Fourier transform

$$|\mathbf{k},l\rangle := rac{1}{\sqrt{2\pi V}} \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x},l\rangle$$

Here **k** is an element of the *d*-dimensional torus \mathbb{T}^d and we introduced a volume *V* in order to make $\{|\mathbf{k}, l\rangle\}$ into an orthonormal basis. As a quick check, we can compute

$$t_{\mathbf{y}}|\mathbf{k},l\rangle = \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x}+\mathbf{y},l\rangle = e^{-i\mathbf{k}\cdot\mathbf{y}} |\mathbf{k},l\rangle.$$
(3.6)

And furthermore, H has to leave the eigenspaces of $t_{\mathbf{y}}$ invariant

$$\begin{split} H|\mathbf{k},l\rangle &= \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{x},\mathbf{y},m} e^{i\mathbf{k}\cdot\mathbf{x}} h_{ml}(\mathbf{y}) \, |\mathbf{x}+\mathbf{y},m\rangle \\ &= \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{x},\mathbf{y},m} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} h_{ml}(\mathbf{y}) \, |\mathbf{x},m\rangle \\ &= \sum_{m} \tilde{h}_{ml}(\mathbf{k}) \, |\mathbf{k},m\rangle \,, \end{split}$$

with $\tilde{h}_{ml}(\mathbf{k}) := \frac{1}{\sqrt{2\pi}} \sum_{\mathbf{y}} e^{-i\mathbf{k}\cdot\mathbf{y}} h_{ml}(\mathbf{y})$. This form of the Hamiltonian is often known as the *Bloch Hamiltonian* and we will write $\tilde{h}(\mathbf{k})$ simply as $h(\mathbf{k})$, as it should be clear from the context. This also means that the Hilbert space V decomposes into the eigenspaces $V_{\mathbf{k}}$ corresponding to the eigenvalue $e^{-i\mathbf{k}\cdot\mathbf{y}}$ of the translation operator $t_{\mathbf{y}}$

$$V = \bigoplus_{\mathbf{k}} V_{\mathbf{k}}$$

3.3 Lattice model and translational invariance

Now, adapting this procedure to the Nambu space $W = V \oplus V^*$, recall the action of the translation operator t_y on the dual space V^* is given by $(t_y^{-1})^t$. With this in mind, the construction of an eigenbasis of the translation operator on the Nambu space works in a similar fashion

$$|\mathbf{k},l\rangle + \langle -\mathbf{k},m| := \frac{1}{\sqrt{2\pi V}} \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x},l\rangle + e^{-i\mathbf{k}\cdot\mathbf{x}} \langle \mathbf{x},m| \,.$$

With a calculation similar to (3.6) it is relatively easy to check that this defines an eigenstate of the translation operator with the eigenvalue $e^{-i\mathbf{k}\cdot\mathbf{y}}$.

Following the arguments on the single-particle level, the Nambu space has a decomposition into eigenspaces with eigenvalue $e^{-i\mathbf{k}\cdot\mathbf{y}}$ as well

$$W = \bigoplus_{\mathbf{k}} W_{\mathbf{k}} = \bigoplus_{\mathbf{k}} V_{\mathbf{k}} \oplus V_{-\mathbf{k}}^*.$$

With the Nambu space in momentum representation established, we can take quick look back to the structures introduced in the previous section and give more details on their specific forms in this context.

Let $c_l^{\dagger}(\mathbf{k})$ be the operator that creates a particle in the state $|\mathbf{k}, l\rangle \in V_{\mathbf{k}}$ and $c_l(\mathbf{k})$ the corresponding annihilation operator. With these we can write a field operator $\psi \in W_{\mathbf{k}}$ as

$$\psi = \sum_{l} u_l c_l^{\dagger}(\mathbf{k}) + v_l c_l(-\mathbf{k}) \,.$$

The action of the real structure γ is now given by

$$\begin{split} \gamma : W_{\mathbf{k}} &\to W_{-\mathbf{k}} \\ \sum_{l} u_{l} c_{l}^{\dagger}(\mathbf{k}) + v_{l} c_{l}(-\mathbf{k}) \mapsto \sum_{l} \bar{u}_{l} c_{l}(\mathbf{k}) + \bar{v}_{l} c_{l}^{\dagger}(-\mathbf{k}) \,. \end{split}$$

On the other hand we have the CAR bracket $\{\cdot, \cdot\} : W_{\mathbf{k}} \otimes W_{-\mathbf{k}} \to \mathbb{C}$, which is defined by the anti-commutator of two field operators ψ and ψ' . As we have seen before, if we take these two structures together, we obtain a Hermitian scalar product on $W_{\mathbf{k}}$.

A general one-body Hamiltonian in this setting will be of the form

$$H(\mathbf{k}) = \frac{1}{2} \sum_{l,m} Y_{lm}(\mathbf{k}) \left(c_l^{\dagger}(\mathbf{k}) c_m(\mathbf{k}) - c_m(\mathbf{k}) c_l^{\dagger}(\mathbf{k}) \right)$$
(3.7)

$$+\frac{1}{2}\sum_{l,m}Z_{lm}c_l^{\dagger}(\mathbf{k})c_m^{\dagger}(-\mathbf{k}) + \bar{Z}_{lm}c_m(-\mathbf{k})c_l(\mathbf{k}).$$
(3.8)

Note, that the form of the Hamiltonian is restricted by the condition that it commutes with translations, which in their momentum space representation look like:

$$t_{\mathbf{y}} = \int_{\mathbb{T}} d^d k \sum_{l} e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{y}} c_l^{\dagger}(\mathbf{k}) c_l(\mathbf{k}) \,.$$

25

3 Weyl semimetals

From a physical perspective this condition seems reasonable, since translational invariance is associated to momentum conservation and the momentum can only be conserved if the terms in (3.8) which create/annihilate pairs of electrons create/annihilate electrons with opposite momenta.

Similar to the Bloch Hamiltonian, there is an endomorphism $H_{BdG}(\mathbf{k}) : W_{\mathbf{k}} \to W_{\mathbf{k}}$, called the Bogoliubov – de Gennes Hamiltonian, associated to the quadratic Hamiltonian (3.8). Let

$$\left(\mathbf{c}^{\dagger}(\mathbf{k})\,,\,\mathbf{c}(-\mathbf{k})\right):=\psi^{\dagger}(\mathbf{k})\in W_{\mathbf{k}}^{*} \text{ and } \left(\begin{array}{c}\mathbf{c}(\mathbf{k})\\\mathbf{c}^{\dagger}(-\mathbf{k})\end{array}\right):=\psi(\mathbf{k})\in W_{\mathbf{k}}$$

denote field operators in $W_{\mathbf{k}}$, then $H(\mathbf{k})$ can be written as

$$H(\mathbf{k}) = \psi^{\dagger}(\mathbf{k}) \cdot \begin{pmatrix} \frac{1}{2}h(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^{\dagger}(\mathbf{k}) & -\frac{1}{2}h(-\mathbf{k})^{t} \end{pmatrix} \cdot \psi(\mathbf{k}) =: \psi^{\dagger}(\mathbf{k}) \cdot H_{BdG}(\psi(\mathbf{k})) .$$
(3.9)

The notation for H_{BdG} here adopted the standard notation from physics and wrote Δ for the off-diagonal terms. These off-diagonal terms Δ allow for the description of superconductors in mean-field theory and denote the superconducting gap in BCS theory. Due to the CAR the relation $\Delta(\mathbf{k}) = -\Delta(-\mathbf{k})^T$ holds.

If we consider translations to be a symmetry, the group of unitary symmetries G_0 contains at least the group of translations as a subgroup in all cases. However, as demonstrated in the previous section, the Hamiltonian becomes block-diagonal and everything decomposes over the momentum space. This can actually be thought of as a general reduction procedure, which will not be explained in more detail here, but can be found for example in [16].

Since translations are symmetries, all other symmetries in G need to commute with translations $t_{\mathbf{y}}$. This holds for all elements $g \in G$ and since there can be unitary and anti-unitary symmetries in G this implies for any $v \in V$

$$t_{\mathbf{y}} \, g(v) = g \, t_{\mathbf{y}}(v) = g \, e^{-\mathrm{i} \mathbf{k} \cdot \mathbf{y}} \, v = \left\{ \begin{array}{ll} e^{-\mathrm{i} \mathbf{k} \cdot \mathbf{y}} \, gv & \text{for } g \text{ unitary} \\ e^{\mathrm{i} \mathbf{k} \cdot \mathbf{y}} \, gv & \text{for } g \text{ anti-unitary} \end{array} \right.$$

That means that a unitary symmetry maps $g|_{W_{\mathbf{k}}} : W_{\mathbf{k}} \to W_{\mathbf{k}}$, whereas an anti-unitary symmetry maps $g|_{W_{\mathbf{k}}} : W_{\mathbf{k}} \to W_{-\mathbf{k}}$.

Besides translations, there are more symmetries which define the ten symmetry classes. These are the unitary symmetries of charge conservation $U(1)_Q$ and spin rotations $SU(2)_{spin}$ defining G_0 and the anti-unitary symmetries of time-reversal T and (twisted) particle-hole conjugation \tilde{C} . All of these generate the full symmetry group G.

In the grand scheme of topological insulators and superconductors there exists a sequence of introducing these symmetries systematically and build up the ten symmetry classes one by one. The starting point of this so-called Kitaev sequence is symmetry class D with no symmetry at all. Followed by class DIII, which has a time-reversal symmetry

T. The next class in this sequence is class AII, which has a time-reversal symmetry T and a charge conservation symmetry Q and so on. The names of these symmetry classes derive from the fact that the set of time evolution operators $e^{-iHt/\hbar}$ commuting with the respective symmetries defines an irreducible classical symmetric space of compact type and their respective label in Cartans classification [8] gives the name for the symmetry class.

We do not follows this sequence in a strict sense here, but we divide the ten classes into two subclasses. In this case it makes sense to distinguish between Weyl semimetals and Weyl superconductors, or speaking in terms of the mathematical model, distinguish between systems with particle number conservation and systems without.

Particle number conservation goes along with charge conservation and the unitary symmetry is represented by the operator $e^{i\theta Q} \in U(1)$. It is generated by the charge operator Q and acts on $W_{\mathbf{k}}$ by

$$e^{\mathrm{i}\theta Q}: \quad v + \varphi \mapsto e^{\mathrm{i}\theta} \, v + e^{-\mathrm{i}\theta} \, \varphi$$

e

We can use the fact that commuting with $e^{i\theta Q}$ is equivalent to commuting with Q which acts as +1 on $V_{\mathbf{k}}$ and as -1 on $V_{-\mathbf{k}}$.

The general form of the Hamiltonian is given in (3.8) and its matrix representation is

$$H = \left(\begin{array}{cc} Y & Z \\ Z^{\dagger} & -Y^t \end{array}\right) \,.$$

In order for a Hamiltonian to commute with the action of Q it must be of the form

$$H = \left(\begin{array}{cc} Y & 0\\ 0 & -Y^t \end{array}\right) \tag{3.10}$$

and it is sufficient to consider Y.

For systems without charge conservation (Weyl superconductors) the form of the general Hamiltonian is not constraint, but we adapt the notation to connect to common physics literature and replace Z by Δ as it is usually written in the mean field theory of superconductivity (compare to (3.9)).

There will be a detailed discussion on systems in all of the ten symmetry classes in the next chapter and concrete realizations of the symmetries and the conditions they put on the Hamiltonian will be discussed there.

3.4 Dirac materials

The framework introduced in this chapter is quite general. It describes fermion systems within the approximation of one-body Hamiltonians. It hosts, for example, topological insulators as well as superconductors in the mean field approximation.

In the study of topological properties of insulators and superconductors without disorder the vector bundle structure of the translational invariant Nambu space W_k is very

3 Weyl semimetals

essential. Ground states can be identified as sub-vector bundles of the so called Bloch bundle $W \to M$. However, if we want to include (Weyl) semimetals in the discussion, we are out of luck. This is due to the fact, that the vector bundle description relies very much on the existence of an energy gap. In an insulator the *Fermi energy* μ defines a clear distinction between energy levels above μ (conduction states) and energy levels below μ (valence states). This is what makes the system insulating towards perturbations smaller than the energy gap and thus gives insulators their name. Moreover, the gap between valence and conduction states allows for a mathematically rigorous description by vector bundles.

A semimetal describes a system without such an insulating energy gap, but with a small number of states close to the Fermi energy. In fact, the systems studied in this work have a certain spectrum of low energy states close to the Fermi energy; these excitations are described by the Weyl equation. In an idealization we assume that there is a band crossing exactly at the Fermi energy μ .

Since the vector bundle description does not work in the case of semimetals, there are a lot of different questions that need further inspection: What are the effects of such isolated band crossings in general? Is there a good mathematical model to describe such a system in a similar way as for insulators and superconductors? Does such a model allow for a topological classification of Weyl semimetals?

These are some very basic questions that ask for a good mathematical model for such systems. Even though there are already many questions with regard to such band crossings and their properties answered, there is not really any systematic approach to understand them. To be able to take some steps towards answers to some of these questions, this section gives a more detailed introduction to the topic of Weyl semimetals.

We will focus on a very prominent example of such band crossings, the so called *Dirac* nodes. *Dirac materials* or *Dirac matter* is a term describing such materials, which exhibit such Dirac nodes in their low-energy spectrum. They can have different origin, but since the low-energy excitations are similar in these materials, many of their properties are similar as well. And since the linear dispersion close to the Dirac nodes is qualitatively different from the quadratic dispersion in conventional metals and semiconductors, they form a unique class of materials. They are also not restricted to metals and semimetals, but also a superconductor can have Dirac nodes in its energy spectrum.

The Name Dirac node comes from the fact that these low-energy excitations can be described by the Dirac equation

$$\hbar \frac{\partial}{\partial t} \psi = D \,\psi = \left(c \,\boldsymbol{\alpha} \cdot \mathbf{p} + \beta \,mc^2\right) \,\psi \tag{3.11}$$

and these fermionic excitations are often called Dirac fermions.

3.4.1 Dirac and Weyl points

We assume that the band gap closes only at finitely many (isolated) points, but remains everywhere else. This assumption is fairly reasonable and it is a good place to start. So, we assume that at a single Dirac node two energy bands overlap precisely at the Fermi energy. Or in other words: Unlike in a metal, where the Fermi energy lies *in* one of the bands, for a semimetal the Fermi energy still lies between two bands, but the two bands closest to the Fermi energy may have an overlap at finitely many, isolated points.

We will begin here with some local considerations in the vicinity of such points and continue with some basic properties of these.

Weyl points. Consider the most simple case of only two energy bands (or as an approximation, only the two bands closest to the Fermi energy can be considered). This situation can be described by a (2×2) Hamiltonian of the form

$$H(\mathbf{k}) = h_0(\mathbf{k}) \,\mathbb{1} + \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma} = \begin{pmatrix} h_0 + h_z & h_x - \mathrm{i} \, h_y \\ h_x + \mathrm{i} \, h_y & h_0 - h_z \end{pmatrix}.$$
(3.12)

The two eigenvalues of this Hamiltonian are then given by

$$E_{\pm}(\mathbf{k}) = h_0(\mathbf{k}) \pm \sqrt{h_x^2(\mathbf{k}) + h_y^2(\mathbf{k}) + h_z^2(\mathbf{k})}$$

That means the band gap closes at points where $h_x^2 + h_y^2 + h_z^2 = 0$. In the vicinity of such a point the Hamiltonian has the form of the massless Weyl Hamiltonian $H \approx v_F \mathbf{k} \cdot \boldsymbol{\sigma}$ and such a point is therefore called *Weyl point*. The term $h_0 \mathbb{1}$ only shifts the band crossing in energy, and since we are looking for band crossings close to (or at) the Fermi level, it will not be important for further considerations.

In 1929 von Neumann and Wigner considered general systems as in (3.12) and deduced that in the absence of symmetries all three parameters h_i have to be tuned to obtain a (2×2) matrix with the same eigenvalue twice. Without further reducing the parameters this can only be expected in three spatial dimensions. From these considerations it also becomes clear why a single Weyl point should be stable to small perturbations of the Hamiltonian, because a perturbation proportional to 1 only shifts the Weyl point in energy and any other perturbation (proportional to σ) only shifts it in momentum space. There is also a topological argument that a Weyl point is stable under small perturbations. If we consider a Weyl point at an isolated k_0 there is a small neighborhood of $k_0 \in U \subset M$ where the energy gap is finite and therefore the vector bundle well defined. By choosing a sphere around k_0 in such a way that the energy gap is finite for all $k \in S_{k_0}$ we can define a vector bundle $E \to S_{k_0}^2$. Now, the *Chern number* determines wether that bundle is trivial or not and we call the Chern number of that vector bundle the *Weyl charge* $q(k_0)$ of the Weyl point at k_0 .

A more physically motivated view of this would be in terms of the Berry curvature. The singular points in the band structure can be thought of as sources and sinks of Berry curvature, which is closely related to the Chern number. Another interesting viewpoint might be that the Berry curvature of the energy bands behaves like a magnetic field, but with the possibility of monopoles (Weyl nodes).

3 Weyl semimetals

In a similar approach, the Weyl charge can be defined as the index of the vector field describing the Hamiltonian in the vicinity of k_0 . In detail this works as follows: Consider a vector field **h** on the 3D Brilluoin zone M parameterizing a two-band Hamiltonian as in eq (3.12). As mentioned above, Weyl points occur at zeroes of the vector field. So, let $\mathbf{h}(\mathbf{k}_0) = 0$ for $\mathbf{k}_0 \in M$ and choose a sphere $S^2_{\mathbf{k}_0}$ surrounding \mathbf{k}_0 , but not enclosing any other zeroes of **h**. Since **h** is non-zero on all of $S^2_{\mathbf{k}_0}$ we can define the map

$$S^2_{\mathbf{k}_0} \to S^2 ,$$

 $\mathbf{k} \mapsto \frac{\mathbf{h}(\mathbf{k})}{|\mathbf{h}(k)|}$

The degree of this map is an integer and defines the Weyl charge associated to the Weyl point at k_0 . The Weyl charge of the Weyl point at k = 0 of 3.12 is the degree of the identity map, which is +1. If the Weyl charge is zero, the gap can be opened and a transformation to an insulating system is possible. However, if the Weyl charge is non-zero, there does not exist such a transformation and the Weyl node is protected against small perturbations.

Besides these local considerations, there is also a global statement on the topology of these Weyl nodes. They can only occur with a total charge of zero. This was first formulated by Nielsen and Ninomyia [24] in the context of lattice gauge theory and originally it was formulated as a no-go theorem.

In the vector field description it is known as the statement of the Poincaré -Hopf theorem, which relates the Euler-characteristic of a manifold with the total index of a tangent vector field with isolated zeroes. And because the Euler-characteristic of the torus is zero, that means that only vector fields with total index equal to zero are possible on the momentum torus.

Remark 6. The Poincaré -Hopf theorem for vector fields v on a manifold M relates the index of a vector field to the Euler characteristic of the manifold

$$\sum_{i} \text{IND}_{v}(x_{i}) = \chi(M) \,. \tag{3.13}$$

Since the vector field parameterizing the Hamiltonian is a vector field on the torus (and $\chi(\mathbb{T}) = 0$), only zeroes with a total index of 0 can appear. The argument by Nielsen and Ninomiya [24] to prove their no-go theorem, which says that Weyl fermions can only come in pairs with an opposite handedness (in our terms: Weyl charge) is based on the Poincaré-Hopf theorem, or on some analog statement in algebraic topology.

Now, if a Hamiltonian commutes with a given symmetry group, there are some constraints on the form of the Hamiltonian and therefore there will be constraints on the Weyl points in such systems. The symmetry of time-reversal will be of most interest here, as the discussion of time-reversal and inversion symmetry are very general and
are usually the symmetries discussed in the literature. There will be more detailed discussions on the interaction of the different symmetries and Weyl points in the following chapter, however, this is more dependent on the specific framework used in that chapter. The effect of time-reversal and inversion can be discussed on more general grounds and we will see in the following chapter, that the discussion here is still valid.

Consider a Weyl point at k_0 , then the Hamiltonian describing the bands close to that Weyl point $k \approx k_0$ is

$$H(k) \approx \pm v_F (\mathbf{k} - \mathbf{k}_0) \cdot \boldsymbol{\sigma}$$
,

where the sign depends on the Weyl charge of the Weyl point. Now, under the operation of time-reversal, $T = i\sigma_y \circ K$ could be a concrete realization, the momentum and also σ reverses sign: $k \mapsto -k$ and $\sigma \mapsto -\sigma$. In the vicinity of the Weyl point this means

$$H(k) \mapsto H(-k) \approx \pm v_F (-\mathbf{k} - \mathbf{k}_0) \cdot (-\boldsymbol{\sigma}) = \pm v_F (\mathbf{k} + \mathbf{k}_0) \cdot \boldsymbol{\sigma}$$

We see, that time-reversal symmetry implies, that for every Weyl point at k_0 , there is a Weyl point at $-k_0$ with the same Weyl charge. This means that there have to be two more Weyl points with the opposite Weyl charges due to the Poincaré-Hopf, or the Nielsen-Ninomiya theorem. So in total, there is a minimum of four Weyl points if the system is time-reversal symmetric.

The reasoning for inversion symmetry is very similar. But under inversion it is only the momentum which reverses the sign $k \mapsto -k$ and $\sigma \mapsto \sigma$. Therefore, for every Weyl point at k_0 there is a Weyl point at $-k_0$ but the Weyl charge is opposite, $q(k_0) = -q(-k_0)$. If a system has time-reversal **and** inversion symmetry, then by the above argument, for a Weyl point at k_0 there has to be a Weyl point with opposite Weyl charge by inversion symmetry and a Weyl point with the same Weyl charge by time-reversal symmetry. This cannot both be true, thus there cannot be any Weyl points in systems with time-reversal

and inversion symmetry.

Dirac points. From the relativistic Dirac theory we know, that the massless Dirac equation can be decomposed into two equations, the so-called Weyl equations with opposite chirality. Something similar can happen here. Consider the situation of four energy bands and a Hamiltonian of the form (written in a (2×2) -block decomposition):

$$H = \left(\begin{array}{cc} v_F \, \mathbf{k} \cdot \boldsymbol{\sigma} & m \\ m & -v_F \, \mathbf{k} \cdot \boldsymbol{\sigma} \end{array}\right) \,.$$

The energy eigenvalues of this Hamiltonian are $E_{\pm} = \pm \sqrt{v_F^2 |\mathbf{k}|^2 + m^2}$, which reveals that there are two doubly degenerate bands and a band gap of the order 2m. If m goes to 0, the band gap closes at $\mathbf{k} = 0$ and there is a so called *Dirac point*, a crossing of four bands. A closer inspection of the Hamiltonian in a basis of Weyl fermions reveals, that there are two Weyl fermions present a $\mathbf{k} = 0$ and they are of opposite chirality. If $m \neq 0$ it couples the two Weyl fermions and opens up the gap. There are many more ways to

3 Weyl semimetals

introduce a perturbation of the Dirac point (m = 0) which splits it into two Weyl points. This can be achieved for example with a perturbation of the form $m \mathbb{1}_2 \otimes \sigma_z$:

$$H = \begin{pmatrix} v_F \mathbf{k} \cdot \sigma + m\sigma_z & 0\\ 0 & -v_F \mathbf{k} \cdot \sigma + m\sigma_z \end{pmatrix}.$$

The energy eigenvalues of this Hamiltonian are then given by

$$E_{\pm} = \pm v_F \sqrt{k_x^2 + k_y^2 + (m \pm k_z)^2}$$

and we see that there are two Weyl points at $k_0 = (0, 0, \pm m)$.

In the case where m = 0 is forced by a symmetry (for example time-reversal) the Dirac node is topologically stable. This can, however, only happen at *time-reversal invariant momenta (TRIM)*.

In the following chapters a more detailed discussion about Weyl semimetals in the different symmetry classes is given. Moreover, there are many more examples of vector fields describing Weyl semimetals and how Weyl nodes appear in the band structure in the these classes.

Disorder will then be a major agent in the final chapter of this work. There we present a few considerations on three dimensional Weyl semimetal with disorder and we explore some routes towards a field theoretic description of such systems.

In recent years Dirac materials became a very interesting and active field in condensed matter theory. The most characteristic feature of these materials, i.e. Weyl points, are usually studied with the focus on local considerations close to the node. Moreover, nodes are studied in specific cases and concrete examples. There seems to be no good mathematical description or systematic approach as there exists for the case of topological insulators (TI) and superconductors (TS). Even more so, there is no attempt to use symmetries as a guiding principle in a classification scheme in the studies of Weyl semimetals. This is probably due to the fact that the theory of topological insulators and superconductors relies very much on the existence of an energy gap to model TI's and TS's as a vector bundle or equivalently the classifying map. Therefore, the situation in a Weyl semimetal (WSM) is strikingly different, since (at least) two energy bands have to overlap at the Fermi energy for the low-energy excitations to be described by the Dirac equation.

Therefore, if one would begin in the framework of topological insulators and start with a vector bundle description, there is no way to introduce these band crossing anywhere, because at that point the vector bundle would not be well-defined. It is still possible to make some sense out of this description, this is however more of a local study of these nodes. One can for example define the vector bundle everywhere in the momentum space $M \setminus W$ away from the Weyl points W. And one would find that on a sphere surrounding a Weyl point (in a 3d momentum space) the vector bundle has a non-trivial Chern number corresponding to the *Weyl charge* of the Weyl point. So, one can still obtain some topological information from this description of a WSM, but since a Weyl point in this model is a discontinuity it is not easy to work with. For example: Consider a second WSM which simply has its Weyl point located at a slightly different momentum. It is not obvious how to relate these two WSMs even though the physics should not be that different.

The power of topological studies in insulators and superconductors allowed to avoid these difficulties, because topological invariants do not change under continuous transformation, which from a physics standpoint is quite reasonable.

In this chapter an approach to understanding the topology of WSMs is presented, which tries to avoid a treatment of Weyl points as a discontinuity of the model. So that it is possible to perform continuous transformations on a WSM and use tools from topology. The idea used here was first introduced by Mathai and Thiang [22]. The mathematical concepts, however, go back to Turaev in 1990 [27]. It is based on the

notion of vector fields where a Weyl point will correspond to a zero of a vector field.

The essence of the idea is summarized in the remainder of this introduction while the details will be presented in the following sections. Essentially, we consider Hamiltonians of the form

$$H = \mathbf{h} \cdot \boldsymbol{\sigma}$$
, (4.1)

with a vector field **h** and Pauli matrices $\boldsymbol{\sigma}$. We call such a Hamiltonian a *Dirac type Hamiltonian*. This allows us to consider Hamiltonians of a more general form than introduced in the previous section on Dirac materials, as the local description of Weyl points by the Dirac equation will be replaced by a global description by a vector field. Close to a Weyl point the Hamiltonian will have the form of the usual Dirac/Weyl Hamiltonian (up to linear order). Moreover, this includes a certain class of topological insulators and superconductors as well.

Nevertheless, this approach still follows Dyson's guiding principle, as these Hamiltonians are considered to commute with a given symmetry group G. Therefore, they can be divided into the ten different symmetry classes known from the framework of topological insulators and superconductors.

The introduction of symmetries will put some constraints on the Hamiltonian, which will in turn translate to constraints on the vector field parameterizing the Hamiltonian. Furthermore, symmetries will also put constraints on the existence of Weyl points and their corresponding Weyl charges. Besides these symmetries, also the Poincaré-Hopf theorem gives a relation between the Weyl points with their Weyl charge and the Euler number of the base manifold (in our case the torus).

4.1 Euler structures - abstract definition

The goal of this section is to give an introduction of Euler structures for vector fields on manifolds. Euler structures were first introduced in the context of vector fields by Turaev [27] in 1990. The introduction in this section follows an article by Mathai and Thiang [22], who first used this idea in the context of Weyl semimetals, and a comprehensive introduction to Euler structures given by Burghelea and Haller [6]. This section will focus on the mathematical definition of Euler structures starting from a vector field on a manifold. How these ideas can be used in the analysis of WSMs and WSCs will be the content of the next section.

Let M be a closed connected manifold of dimension d with Euler characteristic $\chi(M) = 0$ and let \mathbf{h} be a vector field on M with a finite number of isolated zeros. Denote the zero set of \mathbf{h} by $W_{\mathbf{h}}$ and define the singular zero-chain $\mathcal{W}_{\mathbf{h}} := \sum_{w \in W_{\mathbf{h}}} \text{IND}_{\mathbf{h}}(w)w$. This zero-chain is called the chain of *local charges* and the index_w(\mathbf{h}) $\in \mathbb{Z}$ is the local charge at $w \in W$.

Definition 11. Let $\mathcal{W}_{\mathbf{h}}$ be a 0-chain in M whose coefficients sum to zero. Then an *Euler chain* is a 1-chain $l \in C_1(M, \mathbb{Z})$ such that $\partial l = \mathcal{W}_{\mathbf{h}}$. An Euler chain l defines

a relative homology class $[l] \in H_1(M, W; \mathbb{Z})$ where W is the set of points that $\mathcal{W}_{\mathbf{h}}$ is defined on. Let $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}}) \subset H_1(M, W; \mathbb{Z})$ denote the subset of relative homology classes of 1-chains in M whose boundary is $\mathcal{W}_{\mathbf{h}}$.



Figure 4.1: Two examples of Euler chains for two different 0-chains W.

Remark 7. All definitions can be adjusted to the case of non-zero Euler characteristic. In this case we add a term $\chi(M) x_0$ to $\mathcal{W}_{\mathbf{h}}$ with some fixed base point $x_0 \in M$. But since we are interested in a physical application and the torus is the only manifold considered, the treatment will follow the assumption $\chi(M) = 0$.

Note, that the set of all Euler chains a priori does not have a group structure, since the sum of two Euler chains is not an Euler chain. This can easily be verified, as the boundary of the sum of two different Euler chains is twice the 0-chain $\mathcal{W}_{\mathbf{h}}$. We can nonetheless define an action of the group $H_1(M)$ on $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ by

$$H_1(M) \times \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}}) \to \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$$
$$([\sigma], [l]) \mapsto [\sigma] + [l] := [\sigma + l]$$

1

It is easy to check that this defines a free and transitive action, i.e. for any two elements $[l], [l'] \in \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ there exists an element $[\sigma] \in H_1(M)$, such that $[\sigma] + [l] = [l']$, and if $[\sigma] + [l] = [l]$ holds, then $[\sigma]$ has to be equal to the identity element (the constant loop). In this sense $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ is a coset of $H_1(M)$ in $H_1(M, W)$.

Another way to think about this is to consider the exact sequence associated to the relative homology group $H_1(M, W)$:

$$0 = H_1(W) \to H_1(M) \to H_1(M, W) \to H_0(W) \to H_0(M) \to \cdots$$

$$(4.2)$$

At first we note that $H_1(W) = 0$ since W only consists of points and therefore there are no non-trivial 1-chains on W.

This leads to the next observation, namely, that the first map $H_1(M) \to H_1(M, W)$ has to be injective due to the exactness of the sequence. That means, we can identify $H_1(M)$ as a subgroup of $H_1(M, W)$. This fact is easily understood since the boundary of an element in $H_1(M)$ is zero and hence it is contained in W.

So, let [l] be any element in $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$. Then we can write $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ as the coset $H_1(M) + [l] \subset H_1(M, W)$. In particular this means that the difference of [l] and $[l'] \in \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ is an element of $H_1(M)$; see for an example fig4.2.



Figure 4.2: Two different Euler chains $(l_0 \text{ and } l_1)$ for the same 0-chain W. The difference $l_1 - l_0$ is a closed loop, which represents an element in the first homology group $H_1(M)$.

The pair $(\mathbf{h}, [l])$ of a vector field \mathbf{h} on M and an associated Euler chain $[l] \in \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}})$ is called *Euler structure* of M.

The goal of the following paragraph is to introduce an equivalence relation for these Euler structures; the so-called non-degenerate homotopy. This is not only needed to define the set of Euler structures of a manifold M but it also gives a way to understand how pairs of zeroes can be created and annihilated.

Definition 12. Let $\mathbf{h}_0, \mathbf{h}_1$ be two smooth vector fields. And let p^*TM be the pullback of the tangent bundle $TM \to M$ under the projection $p : [0,1] \times M \to M$. A nondegenerate homotopy \mathbf{f} between \mathbf{h}_0 and \mathbf{h}_1 is a section transverse to the zero section of p^*TM , which restricts to \mathbf{h}_0 on $\{0\} \times M$ and to \mathbf{h}_1 on $\{1\} \times M$.

A definition like this might arise the question how to find such a non-degenerate homotopy, or at least, if there exists one. To answer this question we can use the tools from obstruction theory and ask wether a section \mathbf{f} , coinciding with \mathbf{h}_0 on $\{0\} \times M$ and with \mathbf{h}_1 on $\{1\} \times M$, can be extended over all of $[0, 1] \times M$.

To see that there always exists such a homotopy over the torus, we need the fact that the tangent bundle of \mathbb{T}^d is trivial. Such a manifold with trivial tangent bundle is called *parallelizable* and the following is true for all parallelizable manifolds: Any function $\mathbf{h}: M \to \mathbb{R}^d$ defines a vector field on M. With this we are now in a position to apply the tool from obstruction theory and deduce the existence of such a homotopy.

Let us assume that M has a CW structure and is parallelizable. Then $[0,1] \times M$ has a canonical CW structure given by the product of cells and the usual CW structure of [0,1] with two 0-cells and one 1-cell. Now, the obstruction in (n+1)-dimensions is an element of $H^{n+1}([0,1] \times M, \partial[0,1] \times M; \pi_n(\mathbb{R}^d))$, where $\pi_n(\mathbb{R}^d) = 0$. Therefore, all obstruction classes vanish and there exists an extension \mathbf{f} of \mathbf{h}_0 and \mathbf{h}_1 over all of $[0,1] \times M$. And even though this extension might not be transverse to the zero section, it is possible to perturb \mathbf{f} in such a way that the result will be transverse.

We can make use of a non-degenerate homotopy \mathbf{f} to define a map between Euler structures associated to two vector fields \mathbf{h}_0 and \mathbf{h}_1 . Moreover, this homotopy allows for the movement of zeroes of vector fields as well as the creation and annihilation of pairs of zeroes with equal and opposite charges in a continuous way. Note that when a pair of charges is created/annihilated the transversality of the intermediate vector field \mathbf{f}_t and the zero set fails. However, the full section \mathbf{f} is still transverse to the zero set of p^*TM and by the transversality theorem the zero set $\mathcal{W}_{\mathbf{f}}$ of \mathbf{f} is a 1-dimensional submanifold in $[0, 1] \times M$ with boundary $\mathcal{W}_{\mathbf{h}_1}^{(1)} - \mathcal{W}_{\mathbf{h}_0}^{(0)}$.

Now, for some $[l_0] \in \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_0})$ the 1 chain $\mathcal{W}_{\mathbf{f}} + l_0$ is a 1-cycle in the relative homology group $H_1([0, 1] \times M, \{1\} \times M)$ and since $H_1([0, 1] \times M, \{1\} \times M) = 0$ there exists a 2-chain Σ whose boundary relative to $\{1\} \times M$ is $\mathcal{W}_{\mathbf{f}} + l_0$. Then we set $l_1 := \mathcal{W}_{\mathbf{f}} + l_0 - \partial \Sigma$. From this definition follows that $\partial l_1 = \mathcal{W}_{\mathbf{h}_1}$ and $[l_1] \in \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_1})$. The assignment

$$\phi_{10}: \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_0}) \to \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_1})$$
$$[l_0] \mapsto [l_1]$$

is well defined and does not depend on the choice of the homotopy \mathbf{f} , the 2-chain Σ or the representative of $[l_0]$.



Figure 4.3: Sketch of a non-degenerate homotopy \mathbf{f} with the homotopy parameter increasing from left to right. The zero set $\mathcal{W}_{\mathbf{f}}$ (orange) has as boundary the difference of the two Euler chains $l_1 - l_0$ and together they form the boundary of Σ (blue).

To summarize: For every vector field **h** the set of Euler chains is a coset of $H_1(M)$ and for two vector fields \mathbf{h}_0 and \mathbf{h}_1 there is a map ϕ_{10} with the properties $\phi_{11} = \text{id}$ and $\phi_{32} \circ \phi_{21} = \phi_{31}$.

These properties are easily verified: *i*) A vector field **h** is homotopic to itself by the trivial homotopy $\mathbf{f}_t \equiv \mathbf{h}$. Therefore, for any 1-chain $l_0 \in C_1(M, W)$ we can choose $\Sigma = [0, 1] \times l_0$ and then $\partial \Sigma = [0, 1] \times \partial l_0 + \partial [0, 1] \times l_0$. And finally $l_1 := [0, 1] \times W + l_0 - ([0, 1] \times W + \{0\} \times l_0 - \{1\} \times l_0) = \{1\} \times l_0$. We therefore can write $\phi_{11} = \mathrm{id}$. *ii*) Let \mathbf{h}_i with i = 1, 2, 3 be three vector fields on M and \mathbf{f}_t and \mathbf{g}_t be two homotopies with $\mathbf{f}_0 = \mathbf{h}_1$, $\mathbf{f}_1 = \mathbf{g}_0 = \mathbf{h}_2$ and $\mathbf{g}_1 = \mathbf{h}_3$. Then we know that

$$\mathbf{H}_t = \begin{cases} \mathbf{f}_t & \text{for } t \in \left[0, \frac{1}{2}\right] \\ \mathbf{g}_t & \text{for } t \in \left[\frac{1}{2}, 1\right] \end{cases}$$

defines a homotopy between \mathbf{h}_1 and \mathbf{h}_3 . Using this fact one can easily see that $\phi_{32} \circ \phi_{21} = \phi_{31}$.

These properties allow us to associate a vector field \mathbf{h} with a fixed Euler chain by choosing a reference vector field \mathbf{h}_{ref} . In our case the reference \mathbf{h}_{ref} can be for example the constant vector field along one of the torus cycles. Since the constant vector field has no zeroes, it has no associated Euler chain. Following the construction above, we then define the Euler chain l for \mathbf{h} by a homotopy between \mathbf{h}_{ref} and \mathbf{h} .

There is an intuitive way to understand the Euler chain associated to \mathbf{h} in this way. Starting from the constant vector field with no zeroes, the Euler chain traces out the history of creation of two zeroes with opposite charges.

Adopting this picture, we can think about the following process: Start from the constant vector field with no zeroes. Then create two zeroes with opposite charges, move them along a non-trivial loop and finally annihilate them again. This leaves the final vector field with no zeroes. Even though the final vector field does not have any zeroes, it has a non-trivial "winding".

That means the notion of a non-degenerate homotopy describes a continuous way to deform one vector field to another and it allows for the continuous movement of zeroes as well as creation and annihilation of two zeroes with opposite charges. If the two vector fields \mathbf{h}_1 and \mathbf{h}_2 have the same zero chains $\mathcal{W}_{\mathbf{h}_1} = \mathcal{W}_{\mathbf{h}_2}$, then $\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_1}) \equiv \mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_2})$ and the endomorphism $\phi_{21} \in \operatorname{End}(\mathfrak{Eul}(M, \mathcal{W}_{\mathbf{h}_1}))$ gives the homological change in the Euler chains l_1 and l_2 under the non-degenerate homotopy \mathbf{f} taking \mathbf{h}_1 to \mathbf{h}_2 .

If \mathbf{h}_1 and \mathbf{h}_2 have different zero chains, then a homotopy \mathbf{f} taking \mathbf{h}_1 to \mathbf{h}_2 defines the map ϕ_{21} and allows us to identify the pairs $(\mathbf{h}_1, [l_1])$ and $(\mathbf{h}_2, \phi_{21}([l_1]))$. Due to the properties of ϕ_{ij} this defines an equivalence relation and we can form equivalence classes $[\mathbf{h}, [l]]$ and define the following.

Definition 13. Let **h** be a vector field on M with a finite set of non-degenerate zeroes and $[l] \in \mathfrak{Gul}(M, \mathcal{W}_{\mathbf{h}})$ an Euler chain of **h**. Then the pair $(\mathbf{h}, [l])$ is called an *Euler* structure of M.

Two Euler structures $(\mathbf{h}_1, [l_1])$ and $(\mathbf{h}_2, [l_2])$ are said to be equivalent if there exists a non-degenerate homotopy \mathbf{f} between \mathbf{h}_1 and \mathbf{h}_2 and $[l_2] = \phi_{21}([l_1])$. We denote the equivalence classes by $[\mathbf{h}, l]$ and the set of equivalence classes of Euler structures of Mby $\mathfrak{Eul}(M)$.

When Turaev first introduced the idea of Euler structures, he used a different notion of equivalence for vector fields, which nonetheless results in the same equivalence classes. Moreover, he proved an interesting relation between vector fields and Euler structures of M, which is particular interesting in the case of $\chi(M) = 0$. The relation for this special case, which is also the case of our interest, and his definition of the equivalence relation are briefly presented in this final paragraph

Let $\mathfrak{X}_0(M)$ denote the set of non-singular vector fields on M – vector fields with no zeroes. If $\chi(M) = 0$ and d > 2, one can show that the map $\pi_0(\mathfrak{X}_0(M)) \to \mathfrak{Eul}(M)$, $\mathbf{h} \mapsto [\mathbf{h}, 0]$ is surjective (see Burghelea and Haller [6]). Furthermore, this map is even injective if a slightly different equivalence relation on the set of non-singular vector fields is used.

Definition 14. Two smooth non-singular vector fields \mathbf{h}_1 and \mathbf{h}_2 on M are said to be homologous iff for some open ball $D \subset M$ the vector fields \mathbf{h}_1 and \mathbf{h}_2 are homotopic on $M \setminus D$ in the class of non-singular vector fields on $M \setminus D$. Denote the set of equivalence classes by $\mathfrak{vect}(M)$.

With this equivalence relation one can show that the above mapping $\mathbf{h} \mapsto [\mathbf{h}, 0]$ is bijective. For a proof of this, we refer for example to the article by Burghelea and Haller [6]).

4.2 Euler chain representation of Weyl semimetals and superconductors

This section introduces the previously defined Euler structures in the context of Weyl semimetals and superconductors. However, considering the ten symmetry classes in the framework, it is not immediately obvious that Hamiltonians in all of the ten classes can be parameterized by a vector field on M. In the remainder of this section we will discuss the cases for which it is possible and how the introduction of Euler structures gives some new insights into the topology of WSMs/WSCs in these symmetry classes.

Consider a Hamiltonian realizing one of the ten symmetry classes (labeled by s = 0, ..., 7 for the eight real classes and just A and AIII for the two complex classes) that is parameterized by a vector field **h** on M in the following way.

Definition 15. The vector field **h** describes a normal insulating or superconducting state if it is non-vanishing. If **h** has a set of isolated zeroes $W_{\mathbf{h}}$, it describes a Weyl semimetal or Weyl superconductor and we call $W_{\mathbf{h}}$ the set of *Weyl points* of **h**. To each Weyl point $w \in W_{\mathbf{h}}$ we associate an integer, the *Weyl charge* $q(w) = \text{IND}_{\mathbf{h}}(w)$.

From this data we can define the 0-chain $\mathcal{W}_{\mathbf{h}} = \sum_{w \in W_{\mathbf{h}}} \text{IND}_{\mathbf{h}}(w) w \in C_0(M)$ and the one chain $l \in C_1(M)$ such that $\partial l = \mathcal{W}_{\mathbf{h}}$.

Next, we want to assign an Euler structure to a given semimetal Hamiltonian/vector field. In order to do this in a well-defined way, a choice of a reference vector field \mathbf{h}_{ref} has to be made. In this context it makes sense to choose a representative of the trivial insulating class, for example the constant vector field along one of the torus cycles. Note that the reference vector field \mathbf{h}_{ref}^{*} has to be chosen for every symmetry class separately (as it has to fulfill the symmetry constraints). We will see that it will not always be possible to choose a **non-vanishing** vector field that fulfills the symmetry constraints, as for example time-reversal symmetry forces the vector field to have zeroes at the TRIM. Therefore, there will be a short discussion on the reference vector field in each paragraph.

Choosing the trivial insulator as reference leads to an interesting interpretation of Euler chains. In this case Euler chains can be thought of as the "history of creation" of two Weyl points as was discussed in the previous section: A non-degenerate homotopy

between \mathbf{h}_{ref} and \mathbf{h} has a zero set, that indicates how Weyl point are created and continuously moved apart.

We will close this section with a few more general remarks on Euler structures and how to understand them as topological invariants. The next section will then deal with more specific discussions on WSMs and WSCs in all symmetry classes and what the set of Euler structures is in all cases.

Euler structures and topological invariants. The chains $W_{\mathbf{h}}$ and l describe different topological invariants that can be associated to a Weyl semimetal/superconductor. The 0-chain $W_{\mathbf{h}}$ describes the local charges of Weyl points, while the Euler chain l contains some global topological information. Probably the best way to view these topological invariants and how they are connected is by looking at the long exact sequence associated to the relative homology group $H_1(M, W_{\mathbf{h}})$:

$$\dots \to 0 = H_1(W_{\mathbf{h}}) \to H_1(M) \to H_1(M, W_{\mathbf{h}}) \to H_0(W_{\mathbf{h}}) \to H_0(M) \to \dots$$
(4.3)

Here the homology group $H_0(M)$ contains the local charge information $\mathcal{W}_{\mathbf{h}}$ while the Euler chain l is an element in $H_1(M, \mathcal{W}_{\mathbf{h}})$. As mentioned before, the total sum of all charges q has to be zero and therefore the set of possible Weyl charges is equal to the equivalence class of zero element in $H_0(M)$. In that sense $\mathcal{W}_{\mathbf{h}}$ contains only local information, namely the integer given by $\pi_2(S^2)$ defined in the neighborhood of each Weyl point. If this integer is zero, it is possible to open the band gap without changing the topology and the Weyl point can be gaped out. On the other hand, if the Weyl charge is non-zero, it is still not sufficient to distinguish different Weyl semimetals, as there can be different Euler chains associated to a single 0-chain $\mathcal{W}_{\mathbf{h}}$; see fig. 4.2.

There exists a long exact sequence, dual to the on in (4.3). In their article Mathai and Thiang call it the *cohomological semimetal MV (Mayer-Vietoris) sequence*:

$$\dots 0 \to H^{d-1}(M) \to H^{d-1}(M \setminus W_{\mathbf{h}}) \to H^{d-1}(S_{W_{\mathbf{h}}}) \to H^{d}(M) \to 0.$$

$$(4.4)$$

This is the Mayer-Vietoris sequence for the two open set $M \setminus W_{\mathbf{h}}$ and $D_{W_{\mathbf{h}}}$, where $D_{W_{\mathbf{h}}}$ is a disjoint union of open discs, where each disc contains one Weyl point $w \in W_{\mathbf{h}}$ and $S_{W_{\mathbf{h}}}$ is the disjoint union of boundaries of $D_{W_{\mathbf{h}}}$.

The interpretation of this long exact sequence is very similar to the interpretation of (4.3). Here $H^d(M)$ is the group of total charge and as mentioned above and the dual of the 0-chain $\mathcal{W}_{\mathbf{h}}$ is the zero element in $H^d(M)$. The group $H^{d-1}(S_{W_{\mathbf{h}}}) = \bigoplus_{w \in W_{\mathbf{h}}} H^{d-1}(S_w)$ contains the local charge information of the Weyl points at w and the map $\Sigma : H^{d-1}(S_{W_{\mathbf{h}}}) \to H^d(M)$ is the sum of the local charges. Therefore, a Weyl semimetal defines an element in the kernel ker Σ . The group $H^{d-1}(M)$ contains the Poincaré-dual of Euler chains l. Moreover, from the theory of topological insulators and superconductors we know that (d-1)-dimensional weak invariants are elements in

 $H^{d-1}(M)$. For example for class A in d = 3 these invariants are two dimensional Chern invariants $c_{ij}(m) \in H^2(M)$, defined on two dimensional submanifolds $S \subset M$ (usually 2D subtori in \mathbb{T}^3).

This gives us another way to view the Euler chain in terms of weak topological invariants $H^2(M)$ given as Chern classes on subtori $\mathbb{T}^2 \subset \mathbb{T}^3$. Starting from the trivial insulator, all (weak and strong) invariants are zero. Now, creating a pair of Weyl points with opposite charges at some point in the momentum space and moving them slightly apart, changes the weak invariants between the two Weyl points.

To make this statement more precise, consider a closed 2-dimensional surface $S \subset M$ away from the two Weyl points. Integrating the Berry curvature of the associated vector bundle (which is well-defined on $M \setminus W$) over S yields an integer. This integer is zero if the surface S does not enclose any Weyl point – or both Weyl Points, which is actually the same situation due to the periodicity of M. If S encloses only one of the Weyl points the integral is equal to the Weyl charge $\pm q$ associated to the Weyl point. On the other hand integrating the Berry curvature over one of the 2-dimensional subtori gives the 2DChern numbers associated to the weak invariants.

Returning to the previous thought: If we move the two Weyl points further apart along one of the torus cycles until they are close to each other again and then annihilate them, leaves the whole system in a topologically different state. Previously we called this a "winding". Now we can understand how the final state is topologically different from before, as a change in one of the weak invariants (the one, which is Poincaré dual to the resulting 1-cycle) has occurred. However, if the two Weyl points are moved back along the way they were created and annihilated again, the system will be in the same state as before.

4.2.1 Weyl semimetals

We begin with the assumption of a band structure in such way, that we can simplify the situation and just consider the two closest bands to the Fermi energy. This assumption is justified if we consider a band structure in which the two closest bands are somewhat separated from the rest of the bands, meaning that if the band gap closes at isolated points, the overlap is between the two bands closest to the Fermi energy and there is no additional overlap of other bands.

Under this assumption we arrive at a description of Weyl semimetals in terms of a Hamiltonian H of the form (3.12) if we just describe the behavior of the two relevant bands. The eigenenergies of such a Hamiltonian are given by

$$E_{\pm}(k) = h_0(k) \pm \sqrt{h_1^2(k) + h_2^2(k) + h_3^2(k)} \,. \tag{4.5}$$

The energy offset h_0 can be neglected, because it does not have any influence on the eigenstates and the band gap of H. Therefore, we are only interested in the three components h_i . In a three dimensional system we can think of these three parameters as

a vector field \mathbf{h} on the momentum space M. This is always the case, because the tangent bundle of the torus \mathbb{T} is trivial and any triple of well-defined and smooth functions defines a vector field on M. However, there is a requirement on the three parameters wether the defined vector field is a reasonable choice or not. This is due to the fact, that we would like to associate Weyl points in the band structure to zeroes of the vector field. This requirement is definitely fulfilled in the case of a Dirac-type Hamiltonian as in eq (4.1). It might be the case though that the Hamiltonian is not precisely of this form, but there is still a reasonable vector field parameterizing the Hamiltonian in the required way. Such a case can easily be included into this framework. We will nonetheless focus on the case of a Dirac-type Hamiltonian.

If we now assume that the Hamiltonian is of Dirac-type, and the vector field **h** vanishes for some value of $k = k_0$, the eigenspaces for E_+ and E_- are degenerated and the band gap closes at k_0 . This describes a Weyl point and we define the Weyl charge q at the Weyl point k_0 as before as the index of the vector field at k_0 .

In the remainder of this chapter symmetries are introduced and all ten symmetry classes will be discussed. We will introduce symmetries in a certain sequence which will roughly follow the Kitaev sequence. However, there was already one change mentioned, as systems with charge conservation and without charge conservation are grouped together. We begin with the classes of Weyl semimetals, i.e. with systems that have charge conservation as a symmetry. After that also Weyl superconductors will be discussed. Recall, that translations are always considered a symmetry in this section.

Class A. The first class is the complex symmetry class A. A Hamiltonian in class A has only one symmetry, namely that of charge conservation. Therefore, the (reduced) group of symmetries is just the unitary group

$$G \equiv G_0 = U(1)_Q$$

As already mentioned the group $U(1)_Q$ acts as $e^{i\theta Q}$ with the generator

$$Q = \left(\begin{array}{cc} -\mathbb{1}_n & 0\\ 0 & \mathbb{1}_n \end{array}\right) \,.$$

Now, a Hamiltonian in this symmetry class has to commute with Q and hence is of the form $H = \text{diag}(Y, -Y^t)$. Since we are only focusing on the two bands closest to the Fermi energy, we set n = 2. Thus we write the Hamiltonian with $Y(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma}$ for some vector field $\mathbf{h}(k)$ on $M = \mathbb{T}^3$. Both of the two non-zero blocks in H are parameterized by the same vector field \mathbf{h} and the vector field \mathbf{h} does not need to fulfill any further symmetry constraints.

Remark 8. The framework that was introduced earlier, is quite general and with the introduction of the space of field operators W the single-particle Hilbert space was basically doubled. This is necessary to describe superconductors in the mean field approximation, but for insulators/semimetals it is not. This fact can be seen in the form

of the Hamiltonian $H = \text{diag}(Y, -Y^t)$. It just adds another copy of Y and it is sufficient to just consider Y instead of H. One could think, that there are now four energy bands for H, but this is not true. The rewriting of the single-particle Hamiltonian Y in the form of H does not create any new energy bands.

Since there are no symmetry constraints on \mathbf{h} we know from the Poincaré-Hopf theorem that any vector field on M has to have a total index of zero. This means Weyl points $w_i \in \mathbf{W}_{\mathbf{h}}$ can occur with a minimum number two and the sum over all Weyl charges $\sum_{w_i \in \mathbf{W}_{\mathbf{h}}} q(w_i) = 0$ has to vanish while each individual Weyl charge can be any integer $q(w_i) \in \mathbb{Z}$. Let the number of Weyl points be $r \in \mathbb{N}_0$, $r \geq 0$ and $r \neq 1$. Then the invariant given by the Weyl charges at these r Weyl points is a collection of r integers, but because the Weyl charge of the r-th Weyl point has to equal the (negative) sum of first (r-1) Weyl points are r-1 independent integers and therefore an element in \mathbb{Z}^{r-1} . The set of Euler chains l in d = 3 is given by $\mathbb{Z}^3 \cong H_1(M)$. To obtain the a 1:1 correspondence the reference frame $\mathbf{h}_{\text{ref}}^A$ has to be chosen. In this symmetry class this can be chosen as the constant vector field along one of the torus cycles.

At this point we can revisit the connection between Euler chains and the weak 2D invariants of topological insulators. As already mentioned, due to the existence of Weyl points (or any band touchings in general) the 3D topological invariants are not defined for semimetals. However, lower dimensional weak invariants can still be defined on a 2D surface away from the Weyl points. For topological insulators in class A these weak invariants are 2D Chern numbers c_{ij} $(i, j = x, y, z, i \neq j)$, where c_{ij} is defined on an ij-subtorus. For semimetals they can be defined on subtori away of $M \setminus W_h$.

Consider the simplest case with two Weyl points (as for example in fig. 4.4). With an Euler chain connecting these two Weyl points. Now, the Chern number, computed on a 2D surface, which intersects with the Euler chain of the two Weyl points, is non-trivial. On the other hand, Chern numbers computed on a surface, which does not intersect with the Euler chain, is zero. An analogy of this can be seen in fig. 4.4. The figure shows an exemplary vector field for a Weyl semimetal in class A on the xz-subtorus. It shows two Weyl points and their connecting Euler chain.

The analog of the 2D Chern number is the winding number of the vector field along a non-trivial cycle. Following a cycle, which does not cross the Euler chain, the vector field has a winding number of zero. On the other hand, following the vector field along a cycle, which does cross the Euler chain, it has a winding number of 1.

The situation in 3D is very similar with winding numbers replaced by Chern numbers. The Chern number on a surface jumps by the Weyl charge of the Weyl point when the surface crosses a Weyl point.

One of the most prominent examples of such a system in the current literature is the Weyl semimetal phase in a topological insulator multilayer structure. This was first introduced by Burkov and Balents [7] as a simple realization of a 3D Weyl semimetal. The case for an insulating vector field **h** describing a topological insulator in class A was for example studied in a paper by Kennedy [18]. In his paper he discussed the special

situation of insulators with only two energy bands as this is different form the general situation in systems with many bands. Also more details on the weak topological invariants corresponding to $H_1(M) \cong H^2(M)$ can be found there. Note that the situation is slightly different, as it is not possible to define a truly 3D invariant if the vector field has a zero. However, the discussion on the 2D invariants applies to our case as well and corresponds to the set of Euler chains $H_1(M) \simeq \mathbb{Z}^3$.

The idea of Burkov and Balents in [7] is to build up a 3D system by the stacking of 2D topological insulators and normal insulators. The Hamiltonian describing such a multilayer heterostructure consisting of layers of topological insulators and normal insulators can be written as

$$\mathcal{H} = \sum_{\mathbf{k},i,j} v_F \tau^z (\mathbf{e}_z \times \boldsymbol{\sigma}) \cdot \mathbf{k} \delta_{i,j} + m \sigma_z \delta_{i,j} + \Delta_S \tau^x \delta_{i,j} + \frac{1}{2} \Delta_D \tau^+ \delta_{i,j+1} + \frac{1}{2} \Delta_D \tau^- \delta_{i,j-1}.$$
(4.6)

The two surface states of the top and bottom surface of a topological insulator layer are labeled by *i* and *j* and Pauli matrices σ act on the spin degrees of freedom while Pauli matrices τ act on the top/bottom pseudospin degree of freedom. The tunneling between the surfaces of the *same* layer and *different* layers is described by Δ_S and Δ_D . Block-diagonalization of this Hamiltonian leads to

$$\mathcal{H}_{\pm} = v_F \left(\mathbf{e}_z \times \boldsymbol{\sigma} \right) \cdot \mathbf{k} + \left[m \pm \Delta(k_z) \right] \sigma_z$$

with $\Delta(k_z) = \sqrt{\Delta_s^2 + \Delta_D^2 + 2\Delta_s\Delta_D \cos(k_zd)}$. In this case there are four energy bands and a Dirac semimetal phase (m = 0) appears if the ratio of the two tunneling amplitudes $\frac{\Delta_s}{\Delta_D} = \pm 1$ with a Dirac point at $k = (0, 0, \pi/d)$. The explicit breaking of time reversal invariance due to a magnetic term proportional to m, leads to a separation of the two Weyl points, which are forming the Dirac point at $k_z = \pi/d$, into the bulk along the k_z axis and yields a stable Weyl semimetal phase with two Weyl points.

Two of the four bands do not have zeroes (described by \mathcal{H}_+), the other two bands, however, host the Weyl points and the Hamiltonian \mathcal{H}_- describing these two bands is of the form $\mathcal{H}_- = \mathbf{h} \cdot \boldsymbol{\sigma}$ with $\mathbf{h}(k) = (v_F k_y, v_F k_x, (m - \Delta(k_z)))$ a vector field in class A. A slice of the vector field \mathbf{h} in the xz-plane is plotted in fig 4.4.

Class AIII. The second complex symmetry class AIII has an anti-unitary (twisted) particle-hole symmetry \tilde{C} besides charge conservation $U(1)_Q$. The full symmetry group is thus given by

$$G = G_0 \cup \tilde{C}G_0 \,,$$

with $G_0 = U(1)_Q$.

We know that \tilde{C} induces an anti-unitary involution $V \leftrightarrow V^*$ on W and "twisting" refers to an operator $S = S^{\dagger} = S^{-1} : V_k \to V_k$ with transpose $S^t : V_k^* \to V_k^*$. We can define a representation of \tilde{C} on W which is given by the operator $\tilde{C} : W_k \to W_{-k}$:

$$\tilde{C} = K \circ \begin{pmatrix} 0 & S \\ S^t & 0 \end{pmatrix}.$$
(4.7)

4 Euler chain representation of Weyl semimetals and Weyl superconductors



Figure 4.4: A 2D exemplary vector field in the xz-plane in class A. This example resembles the prime example given by Burkov and Balents in a multilayer structure [7]. The Euler chain (blue arrow) connecting the two Weyl points indicates that the two Weyl Points are created at $k_z = \pi$ and are separated along k_z into the bulk.

This is, however, not the full story, because this representation of \tilde{C} has to anti-commute with the matrix representation of H. This can be most easily understood for the case with no twisting S = 1. The particle-hole conjugation is then equal to the operation of Hermitian conjugation $\gamma : W_k \to W_{-k}$. We also know that H does commute with the Hermitian conjugation γ , which is due to the canonical anti-commutation relations for the second quantized Hamiltonian. However, if we write H as a matrix as in eq (3.9) and also $\tilde{C} = \gamma$ as in eq(4.7) for S = 1, we do not account for the CAR and therefore the relation $H\gamma = \gamma H$ on the level of operators on W translates to the matrix representation as

$$\sigma_x H \sigma_x = -H \,,$$

with \bar{H} standing for the operation of complex conjugation. This relation is often stated as particle-hole symmetry in the literature, even though it is simply a constraint resulting from the CAR and the chosen matrix representations.

For the situation at hand this means that untwisted particle-hole conjugation is actually not a meaningful symmetry. To obtain a meaningful symmetry we need to introduce a non-trivial S. The exact form of such a non-trivial twisting obviously depends on the situation at hand. It could be given for example as a sub-lattice symmetry or something similar, but its exact form is not too important. We can for example just make a choice of basis, where for n = 1 the twisting S takes the form $S = \sigma_z$. For $H = \mathbf{h} \cdot \boldsymbol{\sigma}$ the symmetry relation then reads

$$\sigma_z \left(h_x(k)\sigma_x - h_y(k)\sigma_y + h_z(k)\sigma_z \right) \sigma_z = -\mathbf{h}(-k)\boldsymbol{\sigma} \,,$$

where the sign of σ_y on the left hand side is reversed due to complex conjugation. And thus we deduce the following relation for h:

$$h_x(k) = h_x(-k), \quad h_y(k) = -h_y(-k), \quad h_z(k) = -h_z(-k).$$
 (4.8)

Assuming this symmetry and considering that **h** vanishes at some $k_0 \in M$ it follows that **h** also vanishes at $-k_0$ and the Weyl charge at $-k_0$ is opposite to the Weyl charge at k_0 , so $q(k_0) = -q(-k_0)$. A possible reference vector field in this class would be the constant vector field along the k_x -cycle. The constant vector fields along the k_y - or the k_z -cycle would not fulfill the symmetry constraint (4.8).

The Weyl charge at a single Weyl point is $q \in \mathbb{Z}$. Note, that Weyl points always come in pairs at opposite momenta. Hence, let the number of Weyl points be 2r, $r \in \mathbb{N}_0$. The invariant associated to the Weyl charges is then given by \mathbb{N}^r as we can only consider the Weyl points with positive Weyl charge.

The group of Euler chains is again given by $\mathbb{Z}^3 \cong H_1(M)$. An example for vector field in class AIII can be seen in fig. 4.5.



Figure 4.5: (a) Plot of an exemplary vector field on the Fermi sphere. A Weyl point with Weyl charge +1 can be seen on the left hemisphere. In figure (b) a slice of the same vector field in the z = 0 plane is shown. The corresponding Weyl point with charge +1 is the one on the left. The Weyl point on the right is the corresponding partner at opposite k and with the opposite Weyl charge.

Class AII. The first real symmetry class AII is the class of time-reversal symmetric systems with charge conservation. The unitary symmetry group G_0 is still given by $U(1)_Q$ and additionally there is the anti-unitary time-reversal symmetry T with $T^2 = -1$. The full symmetry group is then given by

$$G = G_0 \cup TG_0$$
.

As before, the Hamiltonian H is of the form (3.10), but now the vector field **h** parameterizing H has to be time reversal symmetric. To make this more precise, consider a concrete realization of the time-reversal operator $T = K \circ i\sigma_y \otimes 1$, with complex conjugation K. A choice like that can always be made, by a choice of basis vectors that come in Kramers pairs. Now, if we assume that H and T commute,

$$\begin{pmatrix} \mathrm{i}\sigma_y & 0\\ 0 & \mathrm{i}\sigma_y \end{pmatrix} \begin{pmatrix} \mathbf{h}(k)\boldsymbol{\sigma} & 0\\ 0 & -(\mathbf{h}(-k)\boldsymbol{\sigma})^T \end{pmatrix} \begin{pmatrix} -\mathrm{i}\sigma_y & 0\\ 0 & -\mathrm{i}\sigma_y \end{pmatrix} = \begin{pmatrix} \mathbf{h}(-k)\boldsymbol{\sigma} & 0\\ 0 & -(\mathbf{h}(k)\boldsymbol{\sigma})^T \end{pmatrix},$$

we get to the constraint for h:

$$\mathbf{h}(k) = -\mathbf{h}(-k)\,.\tag{4.9}$$

This has some implications on possible Weyl points. First, we notice that the vector field vanishes at the time-reversal invariant momenta (TRIM), where k = -k. These zeroes are, however, fixed by time-reversal symmetry and can not be moved or lifted from these points. Second, if we consider a Weyl point at $k = k_0$, then from (4.9) we get that there is a second Weyl point at $-k_0$. Computing the Weyl charge $q(k_0)$ and $q(-k_0)$, we find that the Weyl charges are equal $q(k_0) = q(-k_0)$. And since the total Weyl charge has to be zero, this means that there have to be two more Weyl points with the opposite charges and hence there has to be a minimum of four Weyl points.

Note, that one of the differences to the situation in the previous paragraph (class AIII) is that the vector field is zero at the TRIM $(k_0 = -k_0)$. Another difference is the interaction of Euler chains and strong topological invariants of topological insulators in this symmetry class.

Thiang, Sato and Gomi [25] worked out this interaction of Euler structures and Fu-Kane-Mele invariants of 3D time-reversal-invariant topological insulators in time-reversalinvariant Weyl semimetals (T-WSMs). The interaction is similar to the interaction between Euler chains and weak topological invariants in previous discussions, but for a more detailed discussion consider the original article [25].

Class CII. The real symmetry class CII has the unitary symmetry group $G_0 = U(1)_Q$ and two anti-unitary symmetries. The time reversal symmetry T with $T^2 = -1$ as in class AII and, further, particle-hole conjugation \tilde{C} with $\tilde{C}^2 = +1$. All this leaves the full symmetry group to be

$$G = G_0 \cup TG_0 \cup CG_0 \cup CTG_0.$$

The action of T, \tilde{C} and Q were introduced before and their action constraints the form of the Hamiltonian H and therefore the form of the vector field **h**. As seen for class AIII the particle-hole symmetry constraints **h** to be of the form (4.8). Time-reversal symmetry

constraints the vector field to be of the form (4.9). Combining these two relations one obtains the following constraint:

$$h_x(k) \equiv 0, \ h_y(k) = -h_y(-k), \ h_z(k) = -h_z(-k).$$

Since there are only two components of the vector field non-zero, it is not a reasonable vector field on M and it makes more sense to consider a two dimensional system. In that case the relation is very much like the relation for time-reversal symmetric systems. A good reference vector field for this class in two dimensions might be $\mathbf{h}_{\mathrm{ref}}^{\mathrm{CII}}(k_x,k_y) = (\sin(k_x),\sin(k_y))$ (see fig 4.6.a).

A two dimensional vector field in class CII is then very similar to a time-reversal symmetric vector field in 3D. Weyl points can only occur with a minimum number of four, since for every Weyl point at k_0 , there is a partner Weyl point at $-k_0$ with the same Weyl charge.



Figure 4.6: Plots of two 2D vector fields in class CII. Figure a) shows a possible reference vector field, where the vector field needs to vanish at the TRIM. In figure b) a vector field for a Weyl semimetal with Weyl points away from the TRIM is shown.

Class *BDI*. Symmetry class *BDI* is usually the last one in the sequence of topological insulators and superconductors and therefore has the largest total symmetry group. As before the group of unitary symmetries consists of the $U(1)_Q$ charge conservation group and the $SU(2)_{spin}$ spin-rotation group, $G_0 = U(1)_Q \times SU(2)_{spin}$. The full symmetry

group is then given by

$$G = G_0 \cup TG_0 \cup CG_0 \cup CTG_0,$$

which is similar to class CII, but with a larger group of unitary symmetries. The constraints put on a vector field parameterizing a Hamiltonian realizing this symmetry class are

$$h_x(k) \equiv 0, \ h_y(k) \equiv 0, \ h_z(k) = -h_z(-k).$$

Now, this is not a reasonable vector field in three dimensions, but the system could be considered in one spatial dimension.

The situation in one dimension is quite restricted. The vector field needs to vanish at TRIM $(k = 0, \pi)$ and the situation is mirrored for $k \mapsto -k$. Resulting in the fact that such a system is already uniquely described by its number of Weyl points $4r \in 4\mathbb{N}_0$ which come in groups of 4.

Remark 9. There might be a possible way to realize this symmetry class in a superconductor with an odd time reversal symmetry. Where "odd" refers to the fact that T would need to square to +1 instead of -1. This is connected to the periodicity of eight in the framework of topological insulators and superconductors, which relates the symmetry classes for s = 7 and s = -1. Therefore, this could be thought of constructing class s = -1 from class s = 0 by going in the opposite direction.

4.2.2 Weyl superconductors

Similar to Weyl semimetals a Weyl superconductor is a system in the class of a topological superconductor, where the band gap closes at isolated points. However, it is not immediately clear which of these systems can be parameterized by vector fields. As the particle number (and with it the total charge) is no longer conserved in superconductors and the general form of the Hamiltonian in the Bogoliubov-deGennes (BdG) formalism is given by

$$H = \frac{1}{2} \sum_{k} \left(c_{k,l}^{\dagger}, c_{-k,l} \right) \begin{pmatrix} h' & \Delta \\ -\Delta^* & -h'^T \end{pmatrix} \begin{pmatrix} c_{k,l} \\ c_{-k,l}^{\dagger} \end{pmatrix}.$$
(4.10)

The $2n \times 2n$ matrix \mathcal{H} associated to such a Hamiltonian can usually not be described by three real components and therefore is not in general parameterized by a vector field. There are, however, cases where it is still possible and we consider these cases in the remainder of this section.

Class *D*. The real symmetry class *D* is the usual starting point in the Kitaev sequence of topological insulators and superconductors as it is the class with no symmetries (besides translations). The full symmetry group is therefore given by $G = G_0 = \{e\}$. A realization of this symmetry class is given by a general Hamiltonian of the form (4.10).

Consider the special case of spinless or, equivalently, fully spin-polarized fermions. In this case the Hamiltonian is given by a 2×2 -matrix (n = 1) of the form

$$\mathcal{H}(k) = \varepsilon(k)\sigma_z + \Delta_x(k)\sigma_x + \Delta_y(k)\sigma_y, \qquad (4.11)$$

with $\Delta =: \Delta_x + i\Delta_y$.

This Hamiltonian already has the form of the Weyl Hamiltonian with a vector field given by $\mathbf{h}(k) = (\Delta_x(k), \Delta_y(k), \varepsilon(k))$. The eigenenergies are given by $E_{\pm} = \pm \sqrt{\varepsilon^2 + |\Delta|^2}$ and Weyl nodes can appear as zeroes of the vector field \mathbf{h} . Even though there are no constraints due to symmetries, the CAR still put some constraints on this Hamiltonian. First, the normal-state dispersion $\varepsilon(k)$ needs to be symmetric $\varepsilon(-k) = \varepsilon(k)$ and second the superconducting order parameter Δ needs to be anti-symmetric $\Delta(-k) = -\Delta(k)$. For a vector field of this form we can derive the following properties concerning possible

Weyl points. Consider a Weyl point at k_0 , i.e. $\mathbf{h}(k_0) = 0$, then there has to be a second Weyl point at $-k_0$ with the opposite Weyl charge $q(k_0) = -q(-k_0)$. Therefore, Weyl points can only occur in pairs. A possible reference vector field in this class could be of the form $\mathbf{h}_{ref}^D(k) = (\sin(k_x), \sin(k_y), 1)$. The vector field is constant in z-direction, while being anti-symmetric in the x- and y-direction. Note, that $h_x \equiv 0 \equiv h_y$ would also be a choice which is anti-symmetric in x and y, but the vector field would no longer parametrize a superconductor since $\Delta \equiv 0$.

These considerations lead to the topological classification of Weyl superconductors in class D to be $\mathbb{Z}^3 \oplus \mathbb{Z}^r$, where $2r \in \mathbb{N}$ is the number of Weyl points in M. The \mathbb{Z}^3 factor describes the possible Euler chains in this symmetry class $\mathbb{Z}^3 = H_1(M)$, which can be obtained from the Euler chain which connects the two partners of a pair and then acting with $H_1(M)$ on it.

Let us consider an explicit example in this class. The Anderson-Brinkman-Morel (ABM) state [3], which is believed to occur in the A-phase of superfluid ³He, is one of such examples. It is a state of a three dimensional superfluid of fermions with a $(p_x \pm ip_y)$ -wave pairing. The Hamiltonian describing the low energy physics of the ABM state is given by

$$\mathcal{H}(k) = \varepsilon(k)\sigma_z + \frac{\Delta_0}{k_F}(k_x\sigma_x + k_y\sigma_y), \qquad (4.12)$$

with the Fermi momentum k_F and the amplitude of the superconducting order parameter Δ_0 . The two eigenvalues of this Hamiltonian are

$$E_{\pm}(k) = \pm \sqrt{\varepsilon^2(k) + \frac{\Delta_0^2}{k_F^2}(k_x^2 + k_y^2)}.$$

We see that this spectrum has two Weyl points at $w_{\pm} = (0, 0, \pm k_F) \in M$.

In figure 4.7 a vector field of the type (4.12) is plotted on the fermi sphere. There are two Weyl points, one on the north and the other one on the south pole of the sphere. In figure b) we can see a plot of the (projection of the) vector field in the xz-plane. The two

Weyl nodes are shown with their respective Weyl charge an the Euler chain connecting the two Weyl points. The situation is similar to the one shown in fig 4.4. However, there is still a significant difference between the two vector fields, as one can for example see by the fact, that the difference of the respective Euler chains is a representative of a non-trivial element in $H_1(M)$.

Another feature that can be mentioned again at this point is the fact of the non trivial winding number of the vector field (in the 2D figure of fig 4.7.b) along a cycle which intersects with the Euler chain.



(a) Vector field plotted on the Fermi sphere.



Figure 4.7: Vector field of the ABM state. In (a) the vector field is plotted on the Fermi sphere S_F^2 in the BZ. It vanishes on the north and on the south pole of S_F^2 . In (b) a slice of the vector field at y = 0 is shown. The two Weyl points and their Weyl charge are indicated. The light blue 1-chain is the Euler chain associated to the two Weyl points (with the reference vector field being h_{ref}^D).

Class C. Symmetry class C can be realized in superconductors with only spin-rotational symmetry of the group $SU(2)_{spin}$. The requirement that the Hamiltonian commutes with the three generators of spin rotations J_i (i = x, y, z) allows us to reduce the Hamiltonian to a $(4n \times 4n)$ -matrix of the form

$$\mathcal{H} = \begin{pmatrix} a & 0 & 0 & b \\ 0 & a & -b & 0 \\ 0 & -c & -a^T & 0 \\ c & 0 & 0 & -a^T \end{pmatrix} .$$
(4.13)

Furthermore, this decomposes into two commuting $(2n \times 2n)$ -blocks corresponding to a spin-singlet state and it is sufficient to consider one of them. The BdG-Hamiltonian to

consider in this symmetry class then is of the form

$$\mathcal{H}(k) = \begin{pmatrix} \varepsilon(k) & \Delta(k) \\ \Delta^*(k) & -\varepsilon(k) \end{pmatrix}.$$
(4.14)

Note, that the CAR again constrain the form of ε and Δ . In this case both of these terms have to be symmetric: $\varepsilon(-k) = \varepsilon(k)$ and $\Delta(-k) = \Delta(k)$.

The situation is again very similar to the one in class D. We can define the vector field $\mathbf{h}(k) = (\Delta_x, \Delta_y, \varepsilon)$ and the constraint is given by $\mathbf{h}(k) = \mathbf{h}(-k)$. This leads to the fact that every Weyl point at k_0 has a partner Weyl point at $-k_0$ with opposite charge. This is equivalent to the situation in class D. The Weyl charge can be any integer $q \in \mathbb{Z}$ and for a total number 2r of Weyl points there are r independent Weyl charges which leads to a \mathbb{Z}^r invariant. The group of Euler chains is again given by $\mathbb{Z}^3 = H_1(M)$. A reference vector field in this class could be the constant vector field $\mathbf{h}_{\text{ref}}^{C}(k) = (1, 1, 1)$.

Note, that by the same argument as before, the constant vector field along only one of the cycle directions is not a good choice, as it does not parametrize a superconducting Hamiltonian.

The prime example in this class is a spin-singlet superconductor. To give a concrete example of this, consider the chiral $(d_{x^2-y^2} \pm id_{xy})$ -wave state. The low energy physics of this is described by the Hamiltonian

$$\mathcal{H}(k) = \varepsilon(k)\sigma_z + \frac{\Delta_0}{k_F^2} \left[(k_x^2 - k_y^2)\sigma_x + 2k_x k_y \sigma_y \right] \,. \tag{4.15}$$

An exemplary vector field of this type is shown in figure 4.8. There are two Weyl points, one at the north pole and one at the south pole of the Fermi sphere. The Weyl charges of these two Weyl points are ± 2 , which can be seen in the right figure of 4.8. The two dimensional weak invariants of a superconductor in class C are also Chern numbers. In the example given here, these invariants are even integers and therefore the Weyl charge also should be an even integer indicating the jump of the weak invariants between two Weyl charges. This can also be seen in the right of fig.4.8. The two slices show the profile of zeroes with an index of ± 2 .

Class CI. The third symmetry class is commonly realized in superconductors is class CI, which have spin-rotation and time-reversal symmetry. The group of unitary symmetries is therefore $G_0 = SU(2)_{\text{spin}}$ and the group of all symmetries is

$$G = G_0 \cup TG_0$$
.

As before, we can reduce the Hamiltonian \mathcal{H} to the form (4.13) with the use of spinrotational symmetry. Considering the situation n = 1, time-reversal symmetry T requires c and b to be real numbers and hermiticity requires c = b. This leads to a

4 Euler chain representation of Weyl semimetals and Weyl superconductors



(a) Vector field plotted on the Fermi sphere. (b) Slice of the Vector field at $k_z = \pm k_F$.

Figure 4.8: Plot of an exemplary vector field in class C. In (a) the vector field is plotted on the Fermi sphere in the BZ. (b) shows two slices of the vector at $\pm k_F$. The Weyl charge of the two Weyl points is ± 2 which can be seen from the behavior of the vector field close to the Weyl points.

reduction of the matrix to a (2×2) -matrix of the form

$$\mathcal{H} = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}, \tag{4.16}$$

with $a, b \in \mathbb{R}$.

This constraints the vector field to be of the form

$$h_x(k) = h_x(-k), \ h_y(k) \equiv 0, \ h_z(k) = h_z(-k).$$

Again, this is not a good vector field on the three-dimensional torus. However, considering this as a vector field on the two-dimensional torus, Euler structures can be used to understand the topology of WSM in this case. An example of such a vector field is plotted fig.4.9. A reference vector field in this class is for example the constant vector field $\mathbf{h}_{cf}^{CI}(k) = (1,0,1)$.

In the example it is already visible that Weyl points come with a minimum number of 4. This is due to the fact that for every Weyl point at k_0 there is a partner Weyl point at $-k_0$ with the same Weyl charge. Therefore, in order to add up to a total Weyl charge of zero, there has to be another pair of Weyl points with the opposite Weyl charge. However, a fundamental difference to time-reversal symmetric WSMs is that the vector field does not need to vanish at the TRIM. The set of Euler chains is again $\mathbb{Z}^3 = H_1(M)$, where Euler chains need to come in pairs. Let 2r be the number of Weyl points $(r \in \mathbb{N}_0, r \neq 1)$, then the local invariant associated to the Weyl points is given by \mathbb{Z}^{r-1} .



Figure 4.9: Plot of a vector field for class *C*I. Weyl points opposite to each other have the same Weyl charge and a minimum of four Weyl points is required. The difference to a time reversal symmetric vector field can also be seen, as the symmetry constraint in this class does not force the vector field to vanish at the TRIM.

Class *D***III.** Symmetry class *D*III is discussed somewhat separately in this final paragraph since it is not clear in what sense superconductors in this symmetry class can be parameterized by a vector field in a general sense. Systems realizing class *D*III only have time-reversal symmetry. This is not enough to reduce the number of parameters to three. Nevertheless, there might be systems which can be parameterized by a vector field and Euler structures can be used to understand the topology of these Weyl Superconductors.

From the considerations in all the other classes, we can already say, that due to timereversal symmetry, a Weyl point at k_0 has a partner Weyl point at $-k_0$ with the same Weyl charge. Therefore, the minimum number of Weyl points for systems in class *D*III is four. Further analysis of any specific model is, however, necessary to give a more detailed discussion about Euler structures in class *D*III.

4.2.3 Fermi arcs

A particularly interesting feature of Euler chains is their direct connection to the so called Fermi arcs. Fermi arcs are well known in the study of Weyl semimetals, as they are directly observable in experiments and give a direct indication of the existence of Weyl points in the bulk. They can be observed on the surface of Weyl semimetals and are usually measured with angle-resolved-photoemission-spectroscopy (ARPES).

The first experimental discovery of these Fermi arcs was on the surface of tantalum arsenide (TaAs) [30]. The group around Xu et al. used ARPES to measure the surface states as well as the Weyl points in the bulk and therefore successfully identified TaAs as a Weyl semimetal.

The measurement done with ARPES allows to directly measure the dispersion relation of the electrons on the surface. The idea is based on the photoelectric effect. Photoemission is generated by the illumination with X-rays or with ultraviolet light (ARUPS). The valence electrons emitted from the surface by the photoelectric effect are detected and measured at different angles. Measuring the energy of the emitted electron as well as the angle allows to determine the dispersion relation of these surface electrons. Thus, in the case of Weyl semimetals ARPES provides a direct indication of zero modes on the surface. A picture of the experimental results can be found for example in [30].

We want to provide a somewhat qualitative argument why the Euler chain of a WSM is connected to the surface Fermi arcs measured in an experiment. From the theory of topological insulators and superconductors we know, that a topologically non-trivial state admits zero modes on its surface. Fermi arcs are a direct result of this in the case of a semimetal with at least two Weyl points in the bulk.

Consider two Weyl points in the bulk of the Brillouin zone, which are separated along the z-direction. Then there will be zero modes in the spectrum of the surfaces, not orthogonal to the separation of the two Weyl points. Or in other words: The Fermi arcs connect the projection of the Weyl points on the respective surface.

If the projection of the two Weyl point coincides, there will be no zero mode on that surface. In the example of a separation along the z-axis, this would be the case on a xy-surface. The existence of these zero modes on any other surface is due to the fact that the system is topologically non-trivial between the two Weyl nodes while trivial outside. The surface states therefore do only exists between the projection of two such Weyl points.

Recalling the definition of the Euler chain associated to a set of Weyl points and the discussion on the reference vector field \mathbf{h}_{ref} corresponding to some trivial class, these were done in such a way, that the Euler chain (or its projection on some surface) corresponds precisely to Fermi arcs. Recall, that weak topological invariants were only non-trivial between the two Weyl points. Or following the more mathematical argument made in the previous discussion for class A: The integral of the Berry curvature over a 2D closed surface depends only on the total Weyl charge enclosed in the surface and its value is proportional to the total Weyl charge.

We conclude that the measurement of Fermi arcs is not only a good indication on the existence of Weyl points, but it also already gives some information on the topology of the respective WSM. Moreover, the deep connection between Euler chains and their experimental counterparts make the study of Euler structures more interesting and valuable.

4.3 Summary and discussion

We set out motivated by the idea to find a classification scheme for Weyl semimetals and Weyl superconductors. Due to the fact that the vector bundle is not defined at the Weyl points it is obvious that a new mathematical model was needed. In [22] the authors introduced vector fields and Euler structures to describe Weyl semimetals in class A and in a seminal paper [25] also class AII. The idea of introducing vector fields as a description of the band structure avoids the issue of discontinuity, as Weyl points are described by zeroes of the vector field. This allows to describe the band structure of such systems in a mathematically well-defined way. Movement, creation and annihilation of Weyl points can then also be described in a continuous way. Moreover, this approach furnished the definition of a global topological invariant, which extends the locally defined Weyl charges.

We laid out a general framework for semimetals and superconductors and introduced Euler structures in all symmetry classes. Moreover, we discussed possible topological invariants in form of Euler chains and how the action of the symmetry group constraints them. From a physical point of view, these Euler chains or better their projection onto the surface corresponds directly to experimentally observed Fermi arcs. These surface states play an important role in the experimental verification of Weyl semimetals [30] and the notion of Euler structures provides some theoretical insights into their structure.

Another interesting aspect of Euler structures is the interaction of Euler chains with the topological invariants of insulators and superconductors – weak and strong. This is particularly interesting in the case where time-reversal symmetry is present, as was discussed in [25].

However, even though the introduction of Euler structures allowed us to discuss all symmetry classes of Weyl semimetals and superconductors in a general framework, the approach has its limitations. Probably the most striking limitation is that not all WSMs and WSCs can be parametrized by vector fields and therefore can not be described by Euler structures. Inspired by the initial success of the vector field description, we were looking for a generalization which would not depend on a vector field, but still was able to describe Weyl points continuously. The idea of co-Euler structures, in a sense dual to Euler structures, was already mentioned in [22] and [6]. This seemed like a promising notion that would allow for a generalization, but it turned out that it is not so easy to generalize as similar restrictions as for vector fields hold. Also some other ideas based on differential forms on the Bloch bundle were not fruitful and the question

if a generalization of Euler structures is possible is left open.

Another drawback of the Euler chain representation of WSMs and WSCs is the absence of disorder. The effects of disorder would break translational invariance and thus can not be included. Of course disorder effects are anticipated to play a significant role in general condensed matter systems and therefore should be included in a good model. As already mentioned, the second part of this work is concerned with the effects of disorder and will bring some more insights into the effects of disorder in a Weyl semimetal.

5 Disordered Weyl semimetals

5.1 Introduction

In the second part of this thesis we want to work towards a better understanding of the effects of disorder on Weyl points. Since disorder was not the main focus of the first part and was only considered in the background but not truly implemented into the model, we take a different route here. Disorder is quite an important factor in a more realistic model for condensed matter systems such as semimetals, insulators or superconductors. For this reason we want to include disorder in our mathematical description. However, as was already mentioned before, this is not possible in the previously used framework. We therefore now turn to a different approach which allows us to introduce different models of disorder and study its effects.

We begin with a short introduction to the setting and give a few details on the mathematical framework. After a short discussion of the model, we continue with the analysis and perform the disorder average over all possible disorder configurations. In order to work with the result of the disorder average there are different methods which can be used. We will present three approaches to work with the disorder averaged result and discuss advantages and problems of them. In the end we propose a potential result which is strongly indicated by presented calculations.

5.2 General setting

In order to deal with disorder effects, quantum field theoretical methods have proven valuable in many different occasions. We will specifically make use of the so-called *supersymmetric* method. The idea of supersymmetry is to introduce bosonic and fermionic degrees of freedom simultaneously which has some advantages over introducing only one kind. For more details on supersymmetry we refer to one of the many textbooks on the topic. In the context of condensed matter quantum field theory the book by Efetov [11] is for example a good reference and we will use his approach in this part.

The method of supersymmetry is particularly useful when we perform the disorder average and will be the starting point for all three approaches presented in the remainder.

5.2.1 Supersymmetry

We begin with the introduction of the so called Wegner-Efetov method of supersymmetry, as for example described in the book "Supersymmetry in Disorder and Chaos" by K. Efetov [11]. There will be only a very brief introduction to the basic definitions and the notation for the remainder. For a more detailed introduction consider for example

5 Disordered Weyl semimetals

[11]. The key idea is to introduce supervectors and supermatrices and express physical quantities as integrals over supervectors. This makes it possible to perform the step of disorder averaging and then continue with further calculations. Let us introduce a supervector ψ as

$$\psi = \left(\begin{array}{c} \chi \\ S \end{array} \right) \, , \label{eq:phi}$$

with a vector χ of p Grassmann variables and S a vector of q complex numbers. We also introduce the Hermitian conjugation

$$\bar{\psi} = \left(\chi_1^* \dots \chi_p^* S_1^* \cdots S_q^*\right) ,$$

where S_i^* is the complex conjugate of S_i and χ_j , χ_j^* are independent Grassmann variables.

A supermatrix is a linear transformation F of supervectors and is of the form

$$F = \left(\begin{array}{cc} a & \sigma \\ \tau & b \end{array}\right) \,,$$

where a and b are $p \times p$ and $q \times q$ square matrices with complex entries and σ and τ are $p \times q$ and $q \times p$ rectangular matrices with Grassmann variables. There are analogues of the conventional trace and determinant of a matrix for the super case:

STr
$$F = \text{Tr } a - \text{Tr } b$$
,
SDet $F = \text{Det} (a - \sigma b^{-1} \tau) \text{ Det} b^{-1}$

The analog relation to the non super case, Tr $\ln A = \ln \text{Det } A$, also holds here: $\ln \text{SDet } F = \text{STr } \ln F$.

Furthermore, we introduce the Berezin superintegral form

$$D\bar{\psi}D\psi := \frac{1}{(2\pi)^p} d\bar{S}dS \partial_{\bar{\chi}}\partial_{\chi}, \quad d\bar{S}dS = \prod_{l=1}^q 2 d\operatorname{Re}(S^l) d\operatorname{Im}(S^l) \quad \partial_{\bar{\chi}}\partial_{\chi} = \prod_{m=1}^p \frac{\partial^2}{\partial\chi^{m*}\partial\chi^m}$$

At last we introduce the matrix Λ , which distinguishes between advanced and retarded sector. We denote the number of retarded bosons by q_+ and the number of advanced bosons by q_- (with $q_+ + q_- = q$). Then Λ is the diagonal matrix

$$\Lambda = \operatorname{diag}\left(\mathbb{1}_p, \mathbb{1}_{q_+}, -\mathbb{1}_{q_-}\right) \,.$$

There is no need to introduce an additional minus sign in the fermion-fermion sector as it can be absorbed in the definition of χ and we do not want to introduce an unnecessary sign here.

Now, let us state the two key results which justify the introduction of supervectors:

$$\int \exp\left(-\bar{\psi}F\psi\right) \, D\bar{\psi}D\psi = \text{SDet } F \,, \tag{5.1}$$

$$\frac{\int \psi_i \psi_j^* \exp\left(-\psi F\psi\right) \ D\psi D\psi}{\operatorname{SDet} F} = (F^{-1})_{ij} \,. \tag{5.2}$$

The most important point of this is that the denominator in (5.2) is absent when used for calculations in quantum field theory due to the fact that F is chosen to be unity in the supersymmetry space. Another way to understand this is that the factors DetA and Det⁻¹A, usually appearing in such calculations, cancel each other out in the supersymmetric method since we introduce fermionic variables alongside bosonic ones.

This leads to the generating functional

$$Z = \int D\psi D\bar{\psi} \exp\left(\int d^3x \operatorname{STr}\left(\bar{\psi}\,\mathrm{i}(H-E)\,\psi - \varepsilon\,\bar{\psi}\Lambda\psi\right)\right)\,,\tag{5.3}$$

with Λ distinguishing retarded and advanced sector, energy E and $\varepsilon = 0_+$. The name generating functional comes from the fact, that it is used to compute correlation functions of the Greens function $G^{R/A} = (H - E \pm i \varepsilon)^{-1}$.

5.2.2 Model - details and disorder average

We begin with the Hamiltonian describing the low-energy spectrum of two Weyl nodes with opposite charges ± 1

$$H = \sum_{l} (\sigma^{l} \otimes \tau_{3}) (-\mathrm{i}\partial_{l} - A_{l}) + (\sigma^{l} \otimes \mathbb{1}_{2}) b_{l} + V = H_{0} + H_{\mathrm{dis}}, \qquad (5.4)$$

where σ are Pauli matrices in spinor space, τ_3 distinguishes the two Weyl nodes and 2b separates the two nodes in momentum space. The vector and scalar potential **A** and V are two possible ways of introducing disorder to the model and their components are meant to be random numbers.

As a starting point, we begin by considering only a Gaussian distributed scalar potential and no vector potential $\mathbf{A} = 0$. Also, we are interested in the system at Fermi energy $E_F = 0$.

We introduce supersymmetric integration variables ψ corresponding to the Wegner-Efetov supersymmetry method. Supersymmetric integration variables in that case can be written as variables with two indices s, r, where r goes over the super(replica) degrees of freedom while s goes over the spinor degrees of freedom of the model Hamiltonian. The advantage of the introduction of these supersymmetric variables becomes evident when performing the disorder average. We assume a Gaussian distribution for V

$$\langle V \rangle = 0$$
, $\langle V(x)V(y) \rangle = \beta^2 \delta(x-y)$.

5 Disordered Weyl semimetals

Then the disorder averaged generating functional $\langle Z \rangle$ is

$$\int d^3x \, D\psi D\bar{\psi} \, e^{-\frac{1}{2\beta^2} V^2(x)} \exp\left(\int d^3x \operatorname{STr} \bar{\psi} \, \mathrm{i} H_0 \psi - \varepsilon \bar{\psi} \Lambda \psi + \mathrm{i} \, V(x) \bar{\psi} \psi\right) \,,$$
$$= \int D\psi D\bar{\psi} \exp\left(\int d^3x \operatorname{STr} \bar{\psi} \, \mathrm{i} H_0 \psi - \varepsilon \bar{\psi} \Lambda \psi - \frac{\beta^2}{2} (\bar{\psi} \psi)^2\right) \,.$$

Recalling the spinor structure of the variables ψ , the disorder contribution

$$\frac{\beta^2}{2} \int d^3x (\bar{\psi}\psi)^2$$

can also be written as an *inter* node and an *intra* node interaction, but we do not go into more details on that here.

The usual way to continue at this point, is to decouple the quartic interaction by a supermatrix field B. The introduction of B makes use of an integral identity similar to the Fourier transformation of a normal distribution; for historical reasons this is usually known as a *Hubbard-Stratonovich transformation* in physics literature:

$$e^{-\frac{\beta^2}{2}(\bar{\psi}\psi)^2} = \int dB \, e^{-\frac{1}{2}B^2 - i\beta \, B \, (\bar{\psi}\psi)}$$

Applying this identity to our situation at hand yields an extended generating functional $Z[\psi, \bar{\psi}, B]$

$$\int D\psi D\bar{\psi} \, DB \exp\left(\int d^3x \operatorname{STr} \bar{\psi}(\mathrm{i}H_0 - \varepsilon \Lambda - \mathrm{i}\beta B)\psi - \frac{1}{2}B^2\right)$$

and after integrating out the fermionic fields $\psi, \bar{\psi}$ we obtain the effective action

$$S_{\text{eff}} = \int d^3x \, \frac{1}{2} B^2 - \ln \, \text{SDet}(\Lambda \varepsilon - iH_0 + i\beta B) \tag{5.5}$$

Remark 10. A word of caution might be needed at this point: Even though the Hubbard-Stratonovich transformation is based on an exact integral identity, the result is only valid for small disorder strength β due to the highly oscillatory nature of the result for strong interactions.

A saddle point analysis gives a mean field solution with the diagonal ansatz $B = i\kappa\Lambda$ similar to the result of the self consistent Born approximation (SCBA). We note that this solution is not unique, but in fact there is a full manifold of saddle point solutions, since the action is invariant under the supersymmetry group G = U(r, r|2r). Furthermore, we note that there is a subgroup $K \subset G$ of elements which commute with Λ and thus the manifold of solutions is generated by fluctuations $T \in G/K$.

The strategy following this point will be to start from the manifold of saddle point solutions $M = i\frac{m}{\beta}T\Lambda T^{-1}$, with $T \in U(r, r|2r)$ and m some constant, written in this form to simplify the notation in the following section, where we want to expand the effective action in terms of gradients of T.

5.3 Gradient expansion

To make the notation and calculations a little simpler, we use the fact that the model has a symmetry Lie supergroup U(r, r|2r). Therefore, we can focus on the non-compact boson-boson sector U(r, r), where Λ can be written as Σ_3 , distinguishing between the advanced and retarded sector. To return to the general setting we can then use the supersymmetry of the model to infer the full action.

Before we begin with the expansion of the functional determinant, we want to bring the expression in a form that will make the computations easier. First, we make a similarity transformation

$$\begin{aligned} &\operatorname{Det}\left(\sum_{l}\sigma^{l}(\tau_{3}\partial_{l}+\mathrm{i}b_{l})+\mathrm{i}m\,T\Sigma_{3}T^{-1}\right)\\ &=\operatorname{Det}\left(T^{-1}\left(\sum_{l}\sigma^{l}(\tau_{3}\partial_{l}+\mathrm{i}b_{l})+\mathrm{i}m\,T\Sigma_{3}T^{-1}\right)T\right)\\ &=\operatorname{Det}\left(\sum_{l}\sigma^{l}(\tau_{3}(\partial_{l}+A_{l})+\mathrm{i}b_{l})+m\Sigma_{3}\right)\,,\end{aligned}$$

with $A_l = T^{-1} \partial_l T$. Next, in order to simplify the following computation even further we also multiply the operator under the determinant with Σ_3 and define the generalized Dirac operator

$$D := (\sigma^{\mu} \otimes \mathbb{1}_2 \otimes \Sigma_3)((\partial_{\mu} \otimes \mathbb{1}_2 + \mathrm{i}b_{\mu} \otimes \tau_3) \otimes \mathbb{1}_{2r|2r} + \mathbb{1}_4 \otimes A_{\mu}) + m.$$
(5.6)

In short we write

$$D = \Sigma_3 \sigma^{\mu} (\partial_{\mu} \pm i b_{\mu} + A_{\mu}) + m \, .$$

The goal is to expand the functional determinant $\text{Det}^{-1}D$ in powers of the gradient of T. However, the determinant needs some way of regularization first due to some UV divergencies. The method of choice here is the *heat-kernel-regularization* or *zetafunction-regularization*.

For that we use the fact that we can rewrite $\text{Det}^{-1}D$ as

$$\mathrm{Det}^{-1}D = \exp\left(-\frac{1}{2}\mathrm{ln} \ \mathrm{Det}(DD^*) + \frac{1}{2}\mathrm{ln} \ \mathrm{Det}(D^{-1}D^*)\right) = e^{-S_R + S_I}$$

and apply the heat-kernel regularization to the first part:

$$S_R = \frac{1}{2} \int_{\varepsilon}^{\infty} \frac{d\tau}{\tau} \operatorname{Tr} \, e^{-\tau DD^*} = \int_{\varepsilon}^{\infty} \frac{d\tau}{\tau} \int d^3x \int \frac{d^3k}{(2\pi)^3} \operatorname{Tr}(e^{-ikx}e^{-\tau DD^*}e^{ikx}) \,.$$
(5.7)

On the right hand side we already explicitly expressed the trace over position space in terms of the two integrals. The latter expression is the one we are looking to expand in gradients of T with the intention of extracting the singular part for the limit of the UV

5 Disordered Weyl semimetals

regularization parameter $\varepsilon \to 0$.

The first step is to simplify the integrand and for that we begin with the hermitian conjugate of ${\cal D}$

$$D^* = -\Sigma_3 \sigma^\mu (\partial_\mu \pm \mathrm{i} b_\mu + A_\mu) + m$$

This follows from the fact that $A_{\mu} \in \text{Lie } U(r, r)$ and therefore $A_{\mu}^* = -\Sigma_3 A_{\mu} \Sigma_3$. With this we can now simplify the expression $DD^* = -(\sigma^{\mu} \nabla_{\mu}^s)^2 + m^2$ with $\nabla_{\mu}^s = \Sigma_3 (\partial_{\mu} + sib_{\mu} + A_{\mu})$ and $s = \pm 1$. Using the commutation relations of the Pauli matrices and ∇_{μ}^s and introducing the notation

$$2A_{\mu}^{-} := A_{\mu} - \Sigma_3 A_{\mu} \Sigma_3$$

for the part of A_{μ} that anti-commutes with Σ_3 , we simplify the expression for the momentum shifted operator Tr $e^{-ikx}DD^*e^{ikx}$:

$$e^{-\tau k^2} \sum_{s=\pm 1} \text{Tr}((\partial^{\mu} + A^{\mu} + sib^{\mu})(\partial_{\mu} + A_{\mu} + sib_{\mu} + 2ik_{\mu})$$
(5.8)

$$-2A_{\nu}^{-}\sigma^{\nu}\sigma^{\mu}(\partial_{\mu}+A_{\mu}+i(s\,b_{\mu}+k_{\mu}))).$$
(5.9)

Here the sum over s comes from the fact that the 4×4 -matrix is block diagonal with the only difference between the two blocks being the sign of the momentum shift **b**. We also took a factor of $e^{-\tau k^2}$ out of the trace to compute the k-integral in (5.7). The integral therefore has the form of a Gaussian integral with zero mean and variance $1/2\tau$.

Next, we want to expand this integrand in τ and express the effective action in terms of gradients A_{μ} .

As stated above, the k-integral only allows for terms which are even in k_{μ} to contribute, since $\langle k_{\mu} \rangle = 0$ and every quadratic term contributes $\langle k_{\mu} k_{\nu} \rangle = \delta_{\mu\nu}/2\tau$.

With this, a short computation shows that the contributions from the first term (5.8) cancel each other.

The second term (5.9) has a contribution and the expansion is as follows

$$\sum_{s} \left(2 - 4\tau (\operatorname{Tr} A_{\mu}^{-}(A^{\mu} + \operatorname{sib}^{\mu}) + 2\tau^{2} (A_{\nu}^{-}\sigma^{\nu}\sigma^{\mu}(\partial_{\mu} + A_{\mu} + \operatorname{sib}_{\mu} + \operatorname{i} k_{\mu}))^{2}\right)$$

Up to linear order in τ the contributions are

$$4 - 8\tau \operatorname{Tr} A^{-}_{\mu} A^{\mu} + 4\tau \operatorname{Tr} A^{-}_{\mu} A^{\mu} + \mathcal{O}(\tau^{2}).$$

The second order contributions read

$$\sum_{s} 2\tau^2 (A_\nu^- \sigma^\nu \sigma^\mu (\partial_\mu + A_\mu + sib_\mu)^2 \,.$$

We note that only even terms in b contribute due to the factor s in front of b and the consequence that odd terms cancel each other in the sum. Moreover, we are more

interested in contributions quadratic in A and ∂ , hence we only look at the second term containing two factors of b:

$$-4\tau^2 \text{Tr}(A_{\nu}^{-}\sigma^{\nu}\sigma^{\mu}b_{\mu})^2 = -16\tau^2 \text{Tr}(A_3^{-}A^3) b^2 + 8\tau^2 \text{Tr}A_{\mu}^{-}A^{\mu} b^2.$$

Following this, we take a look at the contributions from the mixed terms (of order τ^2). Terms with a quadratic term in k contribute to $\mathcal{O}(\tau)$:

$$\sum_{s} 2\tau^2 (\partial^\mu + A^\mu + s \mathbf{i} b^\mu) k_\mu (A^-_\nu \sigma^\nu \sigma^\lambda k_\lambda) = 8\tau \mathrm{Tr} A^\mu A^-_\mu$$

The contribution of \mathbf{b} cancels and the first term has a factor of two, because the contribution is symmetric. The rest of the second order contribution is then given by

$$-\sum_{s}\tau^{2}(\partial^{\mu}+A^{\mu}+\mathrm{si}b^{\mu})(\partial_{\mu}+A_{\mu}+\mathrm{si}b_{\mu})(A^{-}_{\nu}\sigma^{\nu}\sigma^{\mu}(\partial_{\mu}+A_{\mu}+\mathrm{si}b_{\mu})\,,$$

where we can now again look at the terms quadratic in A, ∂ :

$$\begin{split} \sum_{s} &\tau^2 (2b^{\mu}(\partial_{\mu} + A_{\mu})(A^-_{\nu}\sigma^{\nu}\sigma^{\lambda}b_{\lambda}) + b^{\mu}b_{\mu}A^-_{\nu}\sigma^{\nu}\sigma^{\lambda}A_{\lambda}) \,, \\ &= 8b^2\tau^2 \mathrm{Tr}A^{\nu}A^-_{\nu} + 4b^2\tau^2 \mathrm{Tr}A^-_{\mu}A^{\mu} \,. \end{split}$$

Collecting all of the terms, we arrive at

$$4 + \tau (4 \text{Tr} A_{\mu}^{-} A^{\mu} + \tau^{2} (20b^{2} \text{Tr} A_{\mu}^{-} A^{\mu} - 16b^{2} \text{Tr} A_{3}^{-} A^{3}) + \mathcal{O}(\tau^{2}).$$
 (5.10)

The effective action can now be written in terms of A_{μ} and the leading order reads

$$\begin{split} S_{\text{eff}} = & \frac{1}{2} \int_{\varepsilon}^{\infty} \frac{d\tau}{\tau} e^{-m^2 \tau} \int \frac{d^3k}{(2\pi)^3} e^{-k^2 \tau} 4 \left(1 + \tau \operatorname{Tr} \, A_{\mu}^- A^{\mu} + \mathcal{O}(\tau^2) \right) \,, \\ = & \frac{1}{4\sqrt{\pi^3}} \int_{\varepsilon}^{\infty} \frac{d\tau}{\tau^{5/2}} e^{-m^2 \tau} (1 + \tau \operatorname{Tr} \, (A_{\mu}^- A^{\mu} + \mathcal{O}(\tau^2)) \,. \end{split}$$

And for small τ the integral has the expected singularity

$$S_{\text{eff}} = \frac{1}{2\sqrt{\pi^3}} \left(\varepsilon^{-3/2} + \varepsilon^{-1/2} \operatorname{Tr} \left(A_{\mu}^{-} A^{\mu} \right) + \dots \right) \,.$$

Note that $\text{Tr}A_{\mu}^{-}A^{\mu} = \frac{1}{4} \text{Tr}[\Sigma_3, A_{\mu}]^2$ is equal to the known diffusive term

$$\frac{1}{4}\operatorname{Tr}[\Sigma_3,A_\mu]^2 = \frac{1}{4}\operatorname{Tr}(\partial_\mu M)^2\,,$$

with $M = i\frac{m}{\beta}T\Sigma_3T^{-1}$ as before.

Even though we expected a diffusive term, this result cannot be the complete answer. Since the heat-kernel regularization only works for a hermitian operator, we applied it to $1/2\ln \text{Det}DD^*$, which only captures the absolute value of the determinant while the

5 Disordered Weyl semimetals

angular information is lost in that case. Unfortunately, we do not have a solution for this issue right now.

In the article [2] a similar analysis is done, but the method of regularization in that work differs from the heat-kernel regularization we used here.

Due to the unsatisfactory result and the concerns about validity of the Hubbard-Stratonovich transformation, we follow a different appraach in the next chapter. The method of superbosonization is often used in the case where the Hubbard-Stratonovich transformation fails as it still works for strong disorder.

5.4 Cumulant expansion

Another common approach to define a bosonic field theory based on the supersymmetry method is the so-called superbosonization method introduced in [5]. For this approach we again begin with the model Hamiltonian (5.4) with a random vector potential **A** and a random scalar potential V. After performing the disorder average as in the previous section, the disorder part of the Hamiltonian can be written in terms of gauge invariant expressions $\sum_{s} \bar{\psi}_{s}^{r} \psi_{r'}^{s}$. At this point the superbosonization method rewrites such an expression in terms of a supermatrix field $M_{r'}^{r} := \sum_{s} \bar{\psi}_{s}^{r} \psi_{r'}^{s}$. Based on these ideas we study the model Hamiltonian with two opposite Weyl nodes in the remainder of this section.

We begin the analysis with the disorder part of the Hamiltonian (5.4). The effects of disorder are described by a random vector potential **A** and a random scalar potential $V =: A_0$, which we both assume as random variables with a Gaussian distribution $\langle A_{\mu} \rangle = 0, \langle A_{\mu}(x)A_{\nu}(y) \rangle = \beta^2 \delta_{\mu\nu} \delta(x-y)$, with $\mu = 0, \ldots 3$.

The disorder average of the generating functional Z can be done as before and we obtain

$$\begin{split} \langle Z \rangle &= \left\langle \exp\left(-\mathrm{i} \int d^3 x \operatorname{STr} \, \bar{\psi} \sum_{\mu} (\sigma^{\mu} \otimes \tau_3) A_{\mu} \psi\right) \right\rangle \\ &= \exp\left(-\frac{\beta^2}{2} \int d^3 x \sum_{\mu} (\operatorname{STr} \bar{\psi} (\sigma^{\mu} \otimes \tau_3) \psi)^2\right), \end{split}$$

where we used the convetion $\sigma^0 = \mathbb{1}_2$. Using the identity

$$\sum_{\mu} (\sigma_{\mu})^{s}_{\ t} (\sigma_{\mu})^{s'}_{\ t'} = 2 \delta^{s}_{t'} \delta^{s'}_{t} \,,$$

the disorder average can further be evaluated to

$$\langle Z \rangle = e^{-\beta^2 \int d^3x \operatorname{STr} M^2},$$
 (5.11)

with the definition of the superbosonization field $M_{r'}^r := \sum_s \bar{\psi}_s^r \psi_{r'}^s$, or $\Leftrightarrow \psi \otimes \bar{\psi} = M$. The supermatrix M can be understood in terms of its four different blocks, where M_{BB}
is positive Hermitian matrix, M_{FF} is a unitary matrix and M_{BF}, M_{FB} are matrices of Grassmann variables.

Remark 11. Note that we avoided the decoupling of the disorder term with the Hubbard-Stratonovich transformation, which was problematic in the limit of strong disorder. Therefore, it is better to work with the superbosonization field M.

In the second step we would like to express the kinetic term of the Hamiltonian (5.4) in terms of the superbosonization field M. It is, however, not immediately clear how this can be done. Here we use a trick that is based on the observation that the expression $M = \sum_s \bar{\psi}_s^r \psi_{r'}^s$ is invariant under transformations $\psi \mapsto u\psi, \bar{\psi} \mapsto \bar{\psi}u^{-1}$ with $u \in U(4)$. In order to make use of such local gauge transformations, we average over all possible gauge transformations and derive an effective action by expanding the average in terms of cumulants. After taking the average over all gauge transformations, the result will have a gauge invariant form and the superbosonization method can be applied to these expressions.

In order for this trick to work, we need the model to be defined on a discrete lattice with lattice constant a. With this the discrete kinetic term of (5.4) becomes

with the discrete differential operator $a \partial_l = \partial_l(x, y)$.

If we now use the local gauge transformation $u(x) \in U(4)$ and average over U(4), we obtain the following generating functional

$$\begin{split} \langle Z \rangle &= \int D\psi D\bar{\psi} \exp \int d^3x \operatorname{STr} \left(-\varepsilon \Lambda M - \beta^2 M^2 \right) \cdot e^{-F[M]}, \\ -F[M] &= \ln \left\langle \exp a^2 \sum_{x,y} \operatorname{STr} \bar{\psi}(x) u^{-1}(x) (\sigma^l \otimes \tau_3) \partial_l(x,y) u(y) \psi(y) \right. \\ &+ a \bar{\psi}(x) u^{-1}(x) b_\mu(\sigma^\mu \otimes \mathbb{1}_2) u(x) \psi(x) \left. \right\rangle_{U(4)}. \end{split}$$

We expand the last term F[M] in cumulants and then perform the integrals in the unitary group. For the integrals in the unitary group we use the Haar measure and the following integral property

$$\int_{U(N)} du \, u^s_{\ t}(x) (u^{-1})^{s'}_{\ t'}(y) = \frac{1}{N} \, \delta_{xy} \delta^s_{t'} \delta^{s'}_t \,. \tag{5.12}$$

From the properties of integrals in the unitary group it is immediately clear that the first order term vanishes. However, we are more interested in the second order and the third order term and we will derive them here.

The second order term will be of the form (summation over twice occurring indices is understood)

$$\frac{1}{2} \left\langle \left(a^2 \sum_{x \neq y} \bar{\psi}^r_s(x) u^{-1}(x)^s_{s'} (\sigma^l \otimes \tau_3)^{s'}_{t'} \partial_l(x,y) u(y)^{t'}_t \psi^t_r(y) + a \bar{\psi}(x) u^{-1}(x) b_\mu (\sigma^\mu \otimes \mathbb{1}_2) u(x) \psi(x) \right)^2 \right\rangle_{U(4)}.$$
(5.13)

With (5.12), the identity $\bar{\psi}_s^r A_t^s \psi_r^t = \text{STr}(\psi \otimes \bar{\psi}) A$ and a change of variables $(\psi \otimes \bar{\psi}) \mapsto M$ the first term becomes

$$\frac{a^4}{32} \sum_{x \neq y} \operatorname{STr} M(x) M(y) \operatorname{Tr} \sum_{k,l} (\sigma^k \otimes \tau_3) (\sigma^l \otimes \tau_3) \partial_k(x, y) \partial_l(y, x) \,.$$

And with the properties of Pauli matrices σ we can further simplify the expression to

$$\frac{a^4}{8}\operatorname{STr}\,M(x)\,M(y)\,\sum_{k=1}^3\partial_k(x,y)\partial_k(y,x)\,.$$
(5.14)

The second term in (5.13) reads

$$\frac{b_\mu b^\mu}{8} \operatorname{STr} \, M(x)^2 \, .$$

Since the fields in the second term are taken at the same position while the fields in the first term are taken at different positions, mixed terms between the two contributions vanishes.

In the final step, we can now complete the expression (5.14) to the square of the gradient of M by the addition of a small diagonal term $\frac{1}{4}\int d^3x \operatorname{STr} M^2$

$$\begin{split} &\frac{a^4}{8} \sum_{k=1}^3 \sum_{x \neq y} \text{STr} \ M(x) \ \partial_k(x, y) \ M(y) \ \partial_k(y, x) \ + \text{diagonal term} \\ &= \frac{a^4}{4} \sum_{k=1}^3 \sum_x \text{STr} \ M(x) \ \partial_k(x, x + e_k) \ M(x + e_k) \ \partial(x + e_k, x) \ + \text{diag.} \\ &= \frac{a^4}{8} \sum_x \sum_{k=1}^3 \text{STr} \ \left(M(x)^2 - 2M(x)M(x + e_k) + M(x + e_k)^2 \right) \\ &= \frac{a^4}{8} \sum_x \sum_{k=1}^3 \text{STr} \ \left(M(x + e_k) - M(x) \right)^2 \approx \frac{a^3}{8} \int d^3x \sum_{k=1}^3 \text{STr} \ (\partial_k M)^2 \ , \end{split}$$

And with this the effective action $\langle Z \rangle$ takes the form

$$\int dM \exp \int d^3x \operatorname{Str}\left(-\varepsilon \Lambda M + \frac{4}{a^3} \ln M - \beta^2 M^2 + (\hbar v_F)^2 \frac{a^3}{8} \sum_k \operatorname{STr}(\partial_k M)^2 + (\hbar v_F)^2 a^6 \frac{b^2}{8} M^2\right), \quad (5.15)$$

68

where we changed the integration variable to ${\cal M}$ and the change of the Berezin integration measure

$$\prod_r \prod_{s=1}^4 d\psi_{r'}^s d\psi_s^r = \mathrm{SDet}^4(M) \prod_{r,r'} dM_{r'}^r \,,$$

appears as $\ln M$ in the effective action.

Now, the third order term is expected to be of importance to the field theory as it would break the chiral symmetry, which is expected for a field theory describing two Weyl points with opposite chirality.

Turning now to the third order term

$$\frac{1}{6} \left\langle \left(a^2 \sum_{x \neq y} \bar{\psi}_s^r(x) u^{-1}(x)_{s'}^{s} (\sigma^l \otimes \tau_3)_{t'}^{s'} \partial_l(x,y) u(y)_t^{t'} \psi_r^t(y) \right)^3 \right\rangle_{U(4)}$$

we look for non-zero contributions. We dropped the second term, proportional to the separation of the Weyl points b, because there is no non-zero contribution from this term. The cross terms vanish by the same argument as before and the cubic term of the pauli matrices and the vector **b** vanishes.

Similar to the result above, we find

$$\frac{a^{6}}{384}\operatorname{STr} M(x)M(y)M(z)\operatorname{Tr}\left((\sigma^{k}\otimes\tau_{3})\partial_{k}(x,y)(\sigma^{l}\otimes\tau_{3})\partial_{l}(y,z)(\sigma^{m}\otimes\tau_{3})\partial_{m}(z,x)\right).$$

This term vanishes, because the two contributions comming from the two Weyl nodes (distinguished by τ_3) cancel each other. However, we can as well take a look at the individual contributions

$$\frac{1}{48} \operatorname{STr} M(x)M(y)M(z) \operatorname{Tr} \left(\sigma^k \partial_k(x,y) \sigma^l \partial_l(y,z) \sigma^m \partial_m(z,x) \right) = \frac{i}{24} \varepsilon^{klm} \operatorname{STr} \partial_k(z,x) M(x) \partial_l(x,y) M(y) \partial_m(y,z) M(z) .$$

Unfortunately, this term also vanishes. One can understand that this term vanishes by the fact, that the difference vectors between the three positions x, y, z actually lie in a plane (defined by x, y, z) and therefore this contribution vanishes due to the ε -tensor.

We set out from a discrete Hamiltonian with two Weyl nodes in the presence of disorder in form of a random vector potential and a random scalar potential. After the disorder average we applied the method of superbosonization to obtain an effective action (5.15)in terms of the supermatrix field M. The result is still unsatisfactory, since it has a chiral symmetry, which is expected to be broken for an action with two opposite Weyl nodes.

5.5 Stacked network model

In this section a 3D network model based on the well-known *Chalker-Coddington model* is introduced. The idea is to start with stack of 2D network models and introduce an interaction between neighboring layers. We derive the Hamiltonian of the network model and see that for a certain choice of scattering between the layers the Hamiltonian describes to Weyl nodes. This idea is inspired by similar considerations in the study of Weyl semimetals, where Burkov and Balents show that a system of stacked topological insulators and normal insulators hosts a WSM phase [7].

We begin with a short reminder of the 2D Chalker-Coddington model as it introduces many of the ideas for the 3D case in a nice way. Afterwards the model of the 3D stacked network is introduced and we derive the Hamiltonian of the 3D model in the clean case without disorder. In a final step we reintroduce (weak) disorder to the system and derive an effective Hamiltonian with a random vector potential and scalar potential.

After the introduction of the model, we use the explicit two dimensional structure of the layers and apply the method of non-abelian bosonization introduced by Witten [29] in 1984 to the layers. The crucial part then is to understand the coupling of neighboring layers in terms of the bosonic field theory.

5.5.1 Chalker-Coddington Model

The 2D Chalker-Coddington Model was introduced by Chalker and Coddington [9] to simulate the single-particle dynamics of the integer quantum Hall effect (IQHE) by a square lattice of directed links. It describes the physics of electrons in a two dimensional plane with uniform perpendicular magnetic field and a slowly varying random potential. Chalker and Coddington derive the details of the model by matching solutions of the Schrödinger equation in different regions along common boundaries. The solution in a certain Landau level along strip of an equipotential line can be fully described by an amplitude $Z \in \mathbb{C}$ [26]. These are modeled by links in the model. In regions where two strips come close to each other, quantum tunneling has to be considered and gives a relation between the amplitudes in each strip before and after the tunneling. This can be modeled by nodes, where each node has two incoming and two outgoing links attached to it. We will formulate such a process in terms of a unitary scattering matrix as introduced in [20], as opposed to the original formulation in [9] with a transfer matrix. The following section gives a more detailed introduction to the 2D Chalker-Coddington model and its relation to the 2D Dirac Hamiltonian.

Each link of the network carries a copy of the (link)-Hilbert space $\mathbb{C}_l \equiv \mathbb{C}$ and the total Hilbert space is given by $H = \bigoplus_l \mathbb{C}_l$. The dynamics of the network are described by the discrete time-evolution $U = U_r U_s$, which is composed of a random phase U_r and a non-random scattering process U_s . To define these operators consider a basis $\{|l\rangle\}$ of unit vectors $|l\rangle \in \mathbb{C}_l$ for H. The random phase operator acts diagonal $U_r|l\rangle = e^{\mathrm{i}\phi_l}|l\rangle$, with uniformly distributed and independent random phases ϕ_l .

To define U_s , denote by l_{\pm} the to links following l by a left turn (+) or a right turn (-).

5.5 Stacked network model

Then the scattering process is described by

$$U_s|l\rangle = e^{+i\pi/4} \sin(t_n) |l_+\rangle + e^{-i\pi/4} \cos(t_n) |l_-\rangle, \qquad (5.16)$$

where $t_n \in [0, \pi/2]$ defines the probability for a right/left turn at every node n. A full rotation, i.e. taking four times a left (right) turn, should amount to a factor of -1 due to the described particles being electrons with spin 1/2. This total factor of -1 can be distributed into four phases of $e^{\pm i\pi/4}$ for each left/right turn and highlights the invariance of the model under a rotation of an integer multiple of $\pi/2$.



Figure 5.1: Chalker-Coddington model in a quasi-1D strip geometry. In the case $t_n = 0$ (only left turns) the electrons circle around the elementary plaquettes as indicated by the orange arrows and the model is in the trivial insulator phase. For $t_n = \pi/2$ (only right turns) the blue arrows indicate the circulation of the electrons and the system is in the quantum Hall insulator phase with two boundary channels.

Making a particular choice of unit cell and cartesian coordinates, we arrive at a description of the scattering process by a scattering matrix $U: H \to H$ of the form

$$U = \left(\begin{array}{cc} 0 & M\\ N & 0 \end{array}\right),$$

where $N : \mathbb{C}_1 \oplus \mathbb{C}_3 \to \mathbb{C}_2 \oplus \mathbb{C}_4$ and $M : \mathbb{C}_2 \oplus \mathbb{C}_4 \to \mathbb{C}_1 \oplus \mathbb{C}_3$. Now, with eq. (5.16) we can

write down N and M explicitly

$$N = \begin{pmatrix} e^{-i\pi/4}\cos(t_n) & e^{i\pi/4}\sin(t_n)e^{i(k_x+k_y)} \\ e^{i\pi/4}\sin(t_n)e^{-i(k_x+k_y)} & e^{-i\pi/4}\cos(t_n) \end{pmatrix},$$
(5.17)

$$M = \begin{pmatrix} e^{i\pi/4} \sin(t_n) e^{i(k_y - k_x)} & e^{-i\pi/4} \cos(t_n) \\ e^{-i\pi/4} \cos(t_n) & e^{i\pi/4} \sin(t_n) e^{i(k_x - k_y)} \end{pmatrix}.$$
 (5.18)

The model becomes critical if the probability for a left turn and a right turn are equal, i.e. $\cos(t_n) = \sin(t_n) = 1/\sqrt{2}$, which is equivalent to $t_n = \pi/4$ for all nodes. In the remainder we will be mostly interested in the model at the critical point and, hence, replace $\sin(t_n)$ and $\cos(t_n)$ by $1/\sqrt{2}$.

The critical behavior can be shown by computing the localization length at that point and finding that it grows linearly. On the other hand, one can anticipate the critical behavior for symmetry reasons. For that consider a finite open strip of the network model, see fig 5.1. If $t_n = 0$ (only left turns), electrons circle around elementary squares in a clockwise rotation and thus are all strongly localized (orange squares in fig 5.1). However, if $t_n = \pi/2$ (only right turns), electrons circle around elementary squares analogously, but there appears a boundary state at the edge of the strip (blue squares and boundary in fig 5.1). The appearance of this boundary state indicates a transition from the normal insulating state to the quantum Hall insulator and therefore indicates the existence of a critical point somewhere between $t_n = 0$ and $t_n = \pi/2$, which for symmetry reasons should be at $t_n = \pi/4$.

Since we are mainly interested in the model at the critical point, we will assume $t_n = \pi/4$ in the remainder.

In order to decouple the two spinor spaces $\mathbb{C}_1 \oplus \mathbb{C}_3$ and $\mathbb{C}_2 \oplus \mathbb{C}_4$ we consider the two-step time evolution U^2 . Taking the square of the time evolution U, we obtain a block-diagonal matrix $U^2 = \text{diag}(MN, NM)$, where each of the blocks is an endomorphism of one of the two spinor spaces $MN \in \text{End}(\mathbb{C}_1 \oplus \mathbb{C}_3)$ and $NM \in \text{End}(\mathbb{C}_2 \oplus \mathbb{C}_4)$. Let us first take a look at MN. As a matter of fact, the other block NM is the same up to a rotation by $-\pi/2$ in the momentum space $\{k_x, k_y\}$.

$$MN = \frac{1}{2} \begin{pmatrix} e^{i(k_y - k_x)} + e^{-i(k_x + k_y)} & e^{ik_y} \left(e^{i\pi/2} e^{ik_y} + e^{-i\pi/2} e^{-ik_y} \right) \\ e^{-ik_y} \left(e^{-i\pi/2} e^{ik_y} + e^{i\pi/2} e^{-ik_y} \right) & e^{i(k_x - k_y)} + e^{i(k_x + k_y)} \end{pmatrix}$$
(5.19)

And from that we can see that at the critical point $MN = 1 - iH + O(k^2)$ with

$$H = \begin{pmatrix} k_x & -\mathrm{i}k_y \\ \mathrm{i}k_y & -k_x \end{pmatrix},\tag{5.20}$$

which can be brought into the form of the Dirac operator $H = k_x \sigma_x + k_y \sigma_y$ with the unitary transformation of the spinor basis

$$T = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & -1\\ 1 & 1 \end{array} \right).$$

5.6 Stacked Chalker-Coddington model

From the 2D Chalker-Coddington networks we no construct a 3D model in such a way that two neighboring layers have opposite link direction. We construct the model with the reversed link directions between two layers with the hindsight that we want to take the continuum limit in the stacking direction in the end and the reversed link direction will lead to a derivative in that limit. We show that the Hamiltonian obtained from this 3D model hosts a Dirac point at $\mathbf{k} = 0$ and by introducing a splitting in the pseudospin degree of freedom, this Dirac point can be split into two Weyl points separated along the stacking direction of the 2D network models.

All of this will be explained in more detail in the following sections. However, we begin with the introduction of the 3D model and follow with a more detailed analysis afterwards.

5.6.1 The 3D model

We begin with the details of the three dimensional model. The in-plane scattering process is the same as in the 2D model. So an incoming electron can scatter left and right in the same layer or in forward and backward direction in the neighboring layers above or below. We write again $\sin(t_n)$ and $\cos(t_n)$ for the amplitudes of a left and right turn, to resemble the 2D network in the limit of vanishing tunneling probability between two layers. We denote the amplitudes for a tunneling process between two layers a and b, where a is the amplitude for scattering inside the unit cell and b for scattering out of the unit cell.



Figure 5.2: Model of a 3D stacked Chalker-Coddignton model. (Left) Two layers of 2D Chalker Coddington networks with opposite link directions. The unit cell consists of four links in the lower layer – orange – and four links of the upper layer – blue. (Right) Top view of the stacked 2D layers. The numbers indicate a choice of a total of eight links in the unit cell, where the blue layer is on top of the orange layer.

There are two types of layers, A and B and we choose a unit cell consisting of four links in each layer (A, B), which makes eight links in total, see fig 5.2. Also we chose cartesian coordinates as indicated in fig 5.2.

The scattering at each node happens between four incoming and four outgoing links and U_s is described by a 4×4 unitary matrix. The in-plane scattering is just as in the 2D model, but there are two different scattering phases t_{n_A} and t_{n_B} for the two layers A and B. The scattering between two different layers is of the form $a e^{i(k_l+k_z/2)} + b e^{i(k_l-k_z/2)}$, where the center of the unit cell in k_z direction is chosen to be in between two layers. In order to keep unitarity we multiply with a normalization $\mathcal{N} = \sqrt{1 + 2(a^2 + b^2 + 2ab \cos(k_z))}$, which becomes 1 in the limit of $a, b \to 0$.

As we have seen in the 2D case, there are two types of scattering processes, one from the odd links to the even links and the second one from even links to odd links. A common way to write it down is with the block decomposition of $H = H_{\text{odd}} \oplus H_{\text{even}}$ into an even part $H_{\text{even}} = H_2 \oplus H_4 \oplus H_6 \oplus H_8$ and an odd part $H_{\text{odd}} = H_1 \oplus H_3 \oplus H_5 \oplus H_7$. In this decomposition the unitary time evolution U is given by

$$U = \frac{1}{\mathcal{N}} \left(\begin{array}{cc} 0 & M \\ N & 0 \end{array} \right) \,.$$

And as before we can decouple the even and odd part by considering the two-step time evolution U^2 .

Since the full (4×4) -matrices M and N would be too large to fully display here, we only show the off-diagonal blocks. The diagonal blocks are exactly the same as in the 2D network model (5.17) and (5.18), but with a rotation by $\pi/2$ in momentum space for one of the blocks, as the two layers are rotated with respect to each other. The off-diagonal blocks encode the scattering between two different layers and there are four (2×2) -blocks $N_{I,II} : \mathbb{C}_1 \oplus \mathbb{C}_3 \to \mathbb{C}_6 \oplus \mathbb{C}_8$, $N_{II,I} : \mathbb{C}_5 \oplus \mathbb{C}_7 \to \mathbb{C}_2 \oplus \mathbb{C}_4$, $M_{I,II} : \mathbb{C}_2 \oplus \mathbb{C}_4 \to \mathbb{C}_5 \oplus \mathbb{C}_7$ and $M_{II,I} : \mathbb{C}_6 \oplus \mathbb{C}_8 \to \mathbb{C}_1 \oplus \mathbb{C}_3$. Similar to the $e^{\pm i\pi/4}$ phases in (5.17), there is a phase $e^{\pm i\pi/2}$ for these four off-diagonal blocks. However, the phase is chosen in such a way, that the Hamiltonian at the critical point becomes a Dirac Hamiltonian with a Dirac point at $\mathbf{k} = 0$. The phase is picked up for the scattering process in forward direction one layer up or down. The four off-diagonal block matrices are then as follows (without normalization): 5.6 Stacked Chalker-Coddington model

$$\begin{split} N_{I,II} &= \begin{pmatrix} ae^{\mathrm{i}(-k_y + \frac{k_z}{2})} + be^{\mathrm{i}(-k_y - \frac{k_z}{2})} & e^{-\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(k_x + \frac{k_z}{2})} + be^{\mathrm{i}(k_x - \frac{k_z}{2})} \right) \\ e^{-\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(-k_x + \frac{k_z}{2})} + be^{\mathrm{i}(-k_x - \frac{k_z}{2})} \right) & ae^{\mathrm{i}(k_y + \frac{k_z}{2})} + be^{\mathrm{i}(k_y - \frac{k_z}{2})} \end{pmatrix} \\ N_{II,I} &= \begin{pmatrix} ae^{\mathrm{i}(k_y - \frac{k_z}{2})} + be^{\mathrm{i}(k_y + \frac{k_z}{2})} & e^{-\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(k_x - \frac{k_z}{2})} + be^{\mathrm{i}(k_x + \frac{k_z}{2})} \right) \\ e^{-\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(-k_x - \frac{k_z}{2})} + be^{\mathrm{i}(-k_x + \frac{k_z}{2})} \right) & ae^{\mathrm{i}(k_x - \frac{k_z}{2})} + be^{\mathrm{i}(-k_y + \frac{k_z}{2})} \end{pmatrix} \end{pmatrix} \\ M_{I,II} &= \begin{pmatrix} e^{\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(k_y + \frac{k_z}{2})} + be^{\mathrm{i}(k_x - \frac{k_z}{2})} \right) & ae^{\mathrm{i}(k_x + \frac{k_z}{2})} + be^{\mathrm{i}(-k_y - \frac{k_z}{2})} \\ ae^{\mathrm{i}(-k_x + \frac{k_z}{2})} + be^{\mathrm{i}(-k_x - \frac{k_z}{2})} & e^{\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(-k_y + \frac{k_z}{2})} + be^{\mathrm{i}(-k_y - \frac{k_z}{2})} \right) \end{pmatrix} \\ M_{II,II} &= \begin{pmatrix} -e^{\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(k_y - \frac{k_z}{2})} + be^{\mathrm{i}(k_x + \frac{k_z}{2})} \right) & -ae^{\mathrm{i}(-k_x - \frac{k_z}{2})} - be^{\mathrm{i}(-k_x + \frac{k_z}{2})} \\ -ae^{\mathrm{i}(k_x - \frac{k_z}{2})} - be^{\mathrm{i}(k_x + \frac{k_z}{2})} & -e^{\mathrm{i}\frac{\pi}{2}} \left(ae^{\mathrm{i}(-k_y - \frac{k_z}{2})} + be^{\mathrm{i}(-k_y + \frac{k_z}{2})} \right) \end{pmatrix} \\ \end{split}$$

This model becomes critical at $\mathbf{k} = 0$ for $t_{n_A} = t_{n_B} = \pi/4$ and a = -b.

Now, we can derive the Hamiltonian of this model as the linearized time evolution at the critical point. Hence, if we square the time evolution U^2 to decouple $H_{\rm odd}$ and $H_{\rm even}$, we get a block diagonal matrix and each one of the blocks is a (4×4) - matrix. Looking again at $MN: H_{\rm odd} \rightarrow H_{\rm odd}$, it can be written as $MN = 1 - iH + O(k^2)$ with

$$H = \begin{pmatrix} k_x & -ik_y & \frac{-1+i}{2}\alpha k_z & \frac{-1-i}{2}\alpha k_z \\ ik_y & -k_x & \frac{-1-i}{2}\alpha k_z & \frac{-1+i}{2}\alpha k_z \\ \frac{-1-i}{2}\alpha k_z & \frac{-1+i}{2}\alpha k_z & -k_y & -ik_x \\ \frac{-1+i}{2}\alpha k_z & \frac{-1-i}{2}\alpha k_z & ik_x & k_y \end{pmatrix},$$
(5.21)

with $\alpha = 2a$ introduced just to abbreviate the notation at this point. This can be brought into the known form of a Dirac operator by a unitary transformation

$$S = \frac{1}{2} \begin{pmatrix} 1 & -1 & \mathbf{i} & -\mathbf{i} \\ 1 & 1 & 1 & 1 \\ -1 & 1 & \mathbf{i} & -\mathbf{i} \\ 1 & 1 & -1 & -1 \end{pmatrix}.$$

With the transformation S this becomes

$$SHS^{\dagger} = v_F \mathbf{k} \cdot \boldsymbol{\sigma} \otimes \tau_3.$$
 (5.22)

Here v_F is the Fermi velocity and as already discussed, this Hamiltonian has the spectrum $E_{\pm} = \pm \sqrt{k_x^2 + k_y^2 + \alpha^2 k_z^2}$ with a Dirac point at $\mathbf{k} = 0$.

Since we are interested in the model for a Weyl semimetal, the goal now is to split this Dirac point into two Weyl points with opposite Weyl charge. This can for example be achieved by introducing a perturbation which breaks time-reversal symmetry. There are

several of such perturbations for this model. However, we can take inspiration from the two dimensional network model and introduce a difference in the right and left turning amplitudes $t_n \mapsto t_n + \frac{m}{2}$. Replacing $\cos(t_n)$ and $\sin(t_n)$ with $\cos(t_n + \frac{m}{2})$ and $\sin(t_n + \frac{m}{2})$ in the diagonal blocks of M and N leads to the perturbation of $M_{I,I}N_{I,I}$ (up to linear order of m):

$$\frac{1}{2} \begin{pmatrix} e^{i(k_y - k_x)} + e^{-i(k_x + k_y)} & ie^{ik_y} \left((1+m)e^{ik_y} - (1-m)e^{-ik_y} \right) \\ ie^{ik_y} \left((-1+m)e^{-ik_y} + (1+m)e^{ik_y} \right) & e^{i(k_x - k_y)} + e^{i(k_x + k_y)} \end{pmatrix}$$
(5.23)

The same is true for the lower right block of MN (up to a rotation by $\pi/2$ in momentum space) and in total we obtain

$$H = \begin{pmatrix} k_x & -ik_y - m & \frac{-1+i}{2}\alpha k_z & \frac{-1-i}{2}\alpha k_z \\ ik_y - m & -k_x & \frac{-1-i}{2}\alpha k_z & \frac{-1+i}{2}\alpha k_z \\ \frac{-1-i}{2}\alpha k_z & \frac{-1+i}{2}\alpha k_z & -k_y & -ik_x - m \\ \frac{-1+i}{2}\alpha k_z & \frac{-1-i}{2}\alpha k_z & ik_x - m & k_y \end{pmatrix} .$$
(5.24)

Following again the same transformations as for (5.21) we arrive at the Weyl Hamiltonian

$$H = v_F \mathbf{k} \cdot \boldsymbol{\sigma} \otimes \tau_3 - m\sigma_z \otimes \mathbb{1}_2, \qquad (5.25)$$

with energy eigenvalues $E_{\pm}^2 = k_x^2 + k_y^2 + (\alpha k_z \pm m)^2$. As we can now read off from eigenvalues, the Dirac point at k = 0 is now separated into two Weyl points at $k_x = k_y = 0$ and $k_z^0 = \pm \frac{m}{2a}$ and the separation of the two nodes along the z-axis is given by $\frac{m}{a}$.

Weak disorder. The above discussion is true for the case without disorder. But since we are interested in understanding the effects of disorder on a Weyl semimetal, we reintroduce it now. Recall, that disorder in this model is introduced through a random phase U_r , which is diagonal in the link space. Reinstating the unitary operator U_r into the full time evolution operator $U = U_r U_s$ we multiply U_s from the left with U_r

$$U_r U_s = \left(\begin{array}{cc} U_r^{\text{odd}} & 0\\ 0 & U_r^{\text{even}} \end{array}\right) \cdot \left(\begin{array}{cc} 0 & M\\ N & 0 \end{array}\right) \,,$$

where $U_r^{even} = \text{diag}(\phi_2, \phi_4, \phi_6, \phi_8)$ and $U_r^{\text{odd}} = \text{diag}(\phi_1, \phi_3, \phi_5, \phi_7)$. The upper left block of U^2 then becomes $U_r^{\text{odd}} M U_r^{\text{even}} N$.

As a first step it seems reasonable to begin with the case of weak disorder. In our model this means, that the random phases $e^{i\phi_l}$ are not uniformly distributed over the unit circle, but rather that they are close to unity. We assume that all of the phases are independent random variables with a Gaussian probability distribution. This is only an approximate statement, since the normal distribution is not defined on the circle. However, there exists close analogue of the normal distribution on the circle, the so

called *von Mises distribution*. In the limit of a small variance it resembles the usual normal distribution and we can assume that the phases ϕ_l are random variables with probability distribution functions

$$P(\phi_l) = \exp\left(-\frac{1}{2\beta^2}\phi_l^2\right) \,.$$

In this approximation the model can be rewritten as a Dirac Hamiltonian with a random vector potential, random scalar potential and mass term m – even though also a possible random variable, the random phases do not lead to a random mass term in this case. This was shown for the two dimensional Chalker-Coddington model in [17] and it can be done in a similar fashion for our 3D model. Therefore, we consider the upper left block of the two step time evolution operator $U_r^{\text{odd}}MU_r^{\text{even}}N$ and linearize the operator to extract the Hamiltonian.

We moreover assume a continuum approximation to be valid and replace the translation operators $T_i^{\pm}\psi(r) = \psi(r \pm \mathbf{e}_i)$ with

$$T_i^{\pm} \to 1 \pm \Delta_i \,\partial_i \,, \quad i = x, y, z \,,$$

with lattice constant Δ_i for each direction *i*.

Nonetheless, we keep in mind that we set out from a discrete network model on a lattice and, in fact, we will return to the discrete setting for the analysis of the kinetic term of the Hamiltonian. The notation of the continuum approximation helps to keep the notation concise and we can write the Hamiltonian as

$$H = \begin{pmatrix} m & -i\partial_{-} - A_{-}^{A} & 2a i\partial_{z} & 0\\ -i\partial_{+} - A_{+}^{A} & -m + \gamma & 0 & 2a i\partial_{z}\\ 2a i\partial_{z} & 0 & m & -(-i\partial_{-} - A_{-}^{B})\\ 0 & 2a i\partial_{z} & -(-i\partial_{+} - A_{+}^{B}) & -m - \gamma \end{pmatrix} + V, \quad (5.26)$$

where we furthermore introduced the notation $\partial_{\pm} = \partial_x \pm i \partial_y$ and equivalently for $A^j_{\pm} = A^j_x \pm i A^j_y$. The random variables \mathbf{A}, V and γ can be expressed in terms of the link phases in the unit cell as follows:

$$\begin{split} A_x^A &= \frac{\phi_1 - \phi_3}{2}, \quad A_y^A &= \frac{\phi_4 - \phi_2}{2}, \quad A_x^B &= \frac{\phi_6 - \phi_8}{2}, \quad A_y^B &= \frac{\phi_7 - \phi_5}{2} \\ A_0 &= V &= \frac{V_A + V_B}{2} = \frac{1}{4} \sum_{l=1}^8 \phi_l, \qquad \gamma = V_A - V_B \,. \end{split}$$

We assume these to be independent Gaussian variables with zero mean and variance $\langle A_{\mu}(x)A_{\nu}(y)\rangle = \beta^{2}\delta_{\mu\nu}\delta(x-y)$ and $\langle \gamma(x)\gamma(y)\rangle = (2\beta)^{2}\delta(x-y)$. These derive from the assumption above that the link phases ϕ_{l} are Gaussian variables with covariance β^{2} and zero mean.

In the first step we again use the supersymmetry method of Wegner and Efetov and use a supersymmetric generating functional Z for the above Hamiltonian. With the supersymmetric integration variables ψ we can then perform the disorder average. We denote the part of the Hamiltonian containing random variables by H_1 and the disorder average of that part of the generating function is given by

$$\left\langle \exp\left(\mathrm{i}\int d^{3}x\,\mathrm{STr}\,\bar{\psi}\,H_{1}\,\psi\right)\right\rangle$$
,

where H_1 is the disorder part of (5.26) and can be written as

$$H_1 = \begin{pmatrix} V & -A_x^A + iA_y^A & 0 & 0 \\ -A_x^A - iA_y^A & V + \gamma & 0 & 0 \\ 0 & 0 & V & A_x^B - iA_y^B \\ 0 & 0 & A_x^B + iA_y^B & V - \gamma \end{pmatrix}$$

Note, that the covariance of V and A_i is β^2 , while the covariance of γ is $(2\beta)^2$. Furthermore, the block structure of the Hamiltonian distinguishes between the two layers A and B, but the result after disorder averaging is identical for both blocks and the result can be written as the sum of those two terms. The two terms obtained after disorder averaging are of the form

$$\exp\left(-\frac{\beta^2}{2}\left(\int d^3x \operatorname{STr}\left(\bar{\psi}\psi\right)^2 + 2(\psi_{\downarrow}^*\psi_{\uparrow})(\psi_{\uparrow}^*\psi_{\downarrow}) + 4(\psi_{\downarrow}^*\psi_{\downarrow})^2\right)\right),\tag{5.27}$$

where the Hermitian scalar product in spinor space is understood in the first term.

After discussing the disorder average, we now turn to the free part of the generating functional:

$$Z = \exp i \sum_{j \in \mathbb{Z}} \int d^2 x \operatorname{STr} \bar{\psi} H_0 \psi \quad \text{with}$$
$$H_0 = \begin{pmatrix} m & -i\partial_- & 2ai\partial_z & 0\\ -i\partial_+ & -m & 0 & 2ai\partial_z\\ 2ai\partial_z & 0 & m & i\partial_-\\ 0 & 2ai\partial_z & i\partial_+ & -m \end{pmatrix}$$

Using the 2 × 2 block structure in spinor space, $\bar{\psi} = (\psi_{\uparrow}^{A^*}, \psi_{\downarrow}^{A^*}, \psi_{\uparrow}^{B^*}, \psi_{\downarrow}^{B^*})$, we can write out Z as

$$Z = \exp i \sum_{j} \int d^2 x \operatorname{STr} \left(\bar{\psi}^A H_0^A \psi^A + \bar{\psi}^B H_0^B \psi^B + 2ai \left(\bar{\psi}^A \partial_z \psi^B + \bar{\psi}^B \partial_z \psi^A \right) \right) , \quad (5.28)$$

with

$$H_0^j = \pm \begin{pmatrix} m & -\mathrm{i}\partial_- \\ -\mathrm{i}\partial_+ & -m \end{pmatrix}, \quad j = A, B.$$

78

Now, if we write the generating functional in this way, we see that we add the two diagonal blocks describing the free Hamiltonian in each layer A and B and some interaction part which couples the two neighboring layers. The goal of the next paragraph is to introduce a bosonization method for two dimensional systems introduced by Witten and apply this method to the 3D network model.

Non-abelian bosonization. The method of *non-abelian bosonization* in two dimensions was introduced by Witten in 1984 [29]. Witten's approach is based on an identification of conserved currents in the fermionic and in the bosonic theory. This way it derives a non-abelian bosonization formula in two dimensions and unfortunately it is restricted to the case of two dimensions. However, we can make use of the structure of our network model, which is stacking two dimensional networks to a 3D network. There is another slight adaption we have to make, since we are using supersymmetric integration variables.

We first give a short recap of Witten's approach for the to dimensional system and then discuss the application to the three dimensional model at hand. In another reference [34] a similar problem is considered. The discussion there is focused on the plateau transition of the integer quantum Hall effect and also derives the bosonic field theory for the 2D Chalker-Coddington network. One of the differences for example is that we only consider the case of weak disorder here.

As the two diagonal blocks are of equivalent form, let us first focus on one of the blocks

$$H^A = \begin{pmatrix} m & -\mathrm{i}\partial_- - A^A_- \\ -\mathrm{i}\partial_+ - A^A_+ & -m + \gamma \end{pmatrix} + V \,.$$

We introduce supersymmetric integration variables in the following way which slightly differs from the previous definition

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}, \quad \tilde{\psi} = \bar{\psi} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \psi_-^*, \psi_+^* \end{pmatrix}.$$

In his original work Witten considers fermions in 1+1 dimensions and uses light cone coordinates. In that case ψ_{-} refers to a right-moving fermion, while ψ_{+} refers to a left-moving fermion. This notation is usually adopted in the physics literature for example of the integer quantum Hall effect. In the scenario of the IQHE right and left moving refers to holomorphic and anti-holomorphic wave functions rather than left or right moving fermions, see for example [34]. This comes from the fact, that these wave functions fulfill the usual holomorphic/anti-holomorphic relation under the identification $\mathbb{R}^2 \simeq \mathbb{C}$.

We are not going to follow the full derivation of the bosonic field theory here, but rather state the identification rules and refer to the original article [29] for a more detailed

discussion. Let us begin with the free theory of the 2D Dirac fermion as considered by Witten

$$S_f[\tilde{\psi},\psi] = \int d^2x \; \tilde{\psi} \frac{1}{i} \begin{pmatrix} 0 & \partial_- \\ \partial_+ & 0 \end{pmatrix} \psi$$

The conserved currents in the fermionic theory translate to conserved currents in the bosonic theory for some bosonic supermatrix field M:

$$J_{\pm} = \psi_{\pm}^* \psi_{\pm} \leftrightarrow M^{-1} \partial_{\pm} M \,. \tag{5.29}$$

For the bosonic theory it turns out that the action is not the obvious one, but has an additional term, the so called *Wess-Zumino-Witten (WZW)-term*. One argument for the appearance of the WZW-term is that it is needed to give the same equations of motions for the bosonic theory as the fermionic theory does. With this the bosonic action then becomes

$$S_{WZW}^{m}[M] = \frac{\mathrm{i}m}{4\pi} \int d^{2}x \operatorname{STr} \left(M^{-1}(\partial_{-}M) \cdot M^{-1}(\partial_{+}M) \right) + \mathrm{i}m\Gamma[M],$$

$$\Gamma[M] = \frac{1}{12\pi} \int_{\Sigma} B, \quad dB = \operatorname{STr}(M^{-1}dM)^{\wedge 3}.$$
(5.30)

We wrote the action here in terms of ∂_{\pm} similar to the holomorphic and anti-holomorphic derivative, as for example in [34]. To translate this to the notation in [29] recall the definition of the exterior derivative $d = \partial + \bar{\partial} = 1/2(dw \partial_{-} + d\bar{w} \partial_{+}) = dx \partial_x + dy \partial_y$ with w := x + iy to abbreviate the notation. Here Σ is some Riemann surface bounding a three dimensional area on which the 3-form STr $(M^{-1}dM)^{\wedge 3}$ is defined. The constant m has to be an integer, which can be understood by the fact that the third homotopy group of the target manifold for M (in the fermion-fermion-sector the target is U(r)and $\pi_3(U(r)) = \mathbb{Z}$ for $r \geq 2$) is non-trivial and hence there exist topologically different choices for B which forces m to be integer valued. We further note that this integer, the so-called *level*, will be m = 1 in our case.

Moreover, we note that the additional term $\Gamma[M]$ is no longer parity invariant. Thus it will change its sign under a chirality transformation – such as reversing the link directions of the network model. Moreover, we observe that the expression of $\Gamma[M]$ contains a potential of a 3-form $B = d^{-1} \operatorname{STr} (M^{-1} dM)^{\wedge 3}$, where d^{-1} should be understood locally. And with these two considerations and the way the 3D model is constructed, we expect the field theory to contain a term proportional to $\operatorname{STr} (M^{-1} dM)^{\wedge 3}$.

Before we continue, we mention another identification rule. Witten argues that an expression like $\psi_{-}^{*}\psi_{+}$ in the fermionic theory should be identified with the bosonic supermatrix field M and analogously $\psi_{+}^{*}\psi_{-} \sim M^{-1}$. These are however not completely rigorous arguments, but more like strong suggestions as both expression are characterized by the same relations. Witten also argues further in favor of these identifications by their operator product expansions (OPE) and comparing the most singular parts of the fermionic and the bosonic fields. For the full discussion consider [29].

Transition to three dimensions. In order to use Witten's result in two dimensions, we begin with the scenario of completely decoupled layers of Chalker-Coddington networks. We assume the continuum limit to be already taken in the 2D layers and assume the non-abelian bosonization formula for the two different layers A and B as it was presented above. Instead of labeling the layers by A and B, we introduce an integer n, where even n represent layers of type B and odd n represent layers of type A. We also remind ourselves that the layers are stacked in the z-direction and therefore the z-coordinate is given by $z = n \cdot \Delta_z/2$ with Δ_z being the distance between two unit cells, i.e. the lattice constant in z direction.

Recall that the 3D model was constructed in such a way that neighboring layers have opposite link directions or opposite chirality. Up to this point that fact did not really matter. However, it should be noticed that besides the Wess-Zumino-Witten term $\Gamma[M]$ the rest of the action is invariant under the change of link directions.

Applying the non-abelian bosonization rules to the first two terms in (5.28) we obtain

$$S[M] = \sum_{n} \frac{\mathrm{i}}{4\pi} \int d^2 x \operatorname{STr} \left(M^{-1} (\partial_+ M_n) \cdot M^{-1} (\partial_- M_n) \right) + \mathrm{i} (-1)^n \Gamma[M] \,,$$

where we used the notation M_n for the bosonic field M in the layer n. Turning to the first term and taking the continuum limit we obtain

$$\begin{split} &\frac{\mathrm{i}}{4\pi}\sum_{n}\int d^{2}x\,\mathrm{STr}\left(M^{-1}(\partial_{+}M)\cdot M^{-1}(\partial_{-}M)\right)\\ &=&\frac{\mathrm{i}}{2\pi\Delta_{z}}\int d^{3}x\,\mathrm{STr}\left(M^{-1}(\partial_{+}M)\cdot M^{-1}(\partial_{-}M)\right) \end{split}$$

Now, the second term can be rewritten as a difference

$$i\sum_{n} \int d^{2}x \ (B_{2n} - B_{2n-1}) = i\frac{\Delta_{z}}{2} \sum_{n} \int d^{2}x \ \frac{B_{2n} - B_{2n-1}}{\Delta_{z}/2}$$
$$\approx \frac{i}{2} \int dB = \frac{i}{2} \int STr \left(M^{-1}dM\right)^{\wedge 3}.$$
(5.31)

We assumed a system without boundary in the xy-direction in order to write $\partial_z B dz = dB$. If the system has a boundary in xy-direction, we would need to subtract contributions from boundary terms in the full action.

Even though this already looks quite promising, we need to be cautious at this point. We assumed that we can write difference $B_n - B_{n-1}$ in the continuum limit as derivative. However, this relies on the fact that B or more precisely M_n varies only smoothly in z-direction. But there is so far no indication for that.

Recall, that we started from completely decoupled layers A and B. In order to justify the step in equation (5.31) we need a term which tells us that the difference $M_n - M_{n-1}$ is small and thus allows us to rewrite the finite difference as a differential.

In the search for such a term we turn to the coupling between two neighboring layers

$$2ai\sum_{n} \int d^{2}x \, \left(\bar{\psi}_{2n} \partial_{z} \, \psi_{2n-1} + \bar{\psi}_{2n+1} \partial_{z} \psi_{2n} \right) \,. \tag{5.32}$$

Unfortunately, Witten's non-abelian bosonization can not tell us what term in a bosonic field theory should be identified with a fermionic expression like this. Therefore, we look for inspiration in the analysis of the cumulant expansion. There we used the gauge invariance to average over all gauge transformations and expanded the result in cumulants up to second order. The kinetic part of the Hamiltonian considered in that expansion (5.4) is, up to a similarity transformation, the same as the one considered above.

We might therefore return to the discrete setting and look at the second order term of a cumulant expansion of (5.32). Due to the properties of the cumulant expansion, the method of superbosonization, which of course differs from non-abelian bosonization, was the preferred method to continue. So the question remains: In what sense can we compare the two results? An answer to this question and with it a glimmer of hope might come from the fact that such a cumulant expansion of the two dimensional (discrete) Dirac Hamiltonian would yield the "obvious" part of Witten's bosonic action. This treatment however does not lead to the WZW-term. This nonetheless suggests that we can assume the result of a cumulant expansion of (5.32) to appear in the bosonic field theory if translated properly.

Since the calculation and the result are very similar to the ones in the previous section, we only state the result. The cumulant expansion was done for the full Hamiltonian, not just the interaction term to make sure to not miss any contributions from mixed terms. As it turns out, all mixed terms vanish and the (second order) result for the interaction term is

$$\left\langle \left(2a \sum_{x,y} \left(\bar{\psi}_{2n} u^{-1} \partial_z(x,y) u \psi_{2n-1} + \bar{\psi}_{2n+1} u^{-1} \partial_z(x,y) u \psi_{2n} \right) \right)^2 \right\rangle_{U(2)} \\ = -\frac{a^2}{2} \sum_{x,y} \operatorname{STr} \left(\psi_s^{*r} \psi_r^{s}(2n) \psi_\tau^{*r'} \psi_r^{\tau}(2n-1) + \psi_s^{*r} \psi_r^{s}(2n+1) \psi_\tau^{*r'} \psi_r^{\tau}(2n) \right) .$$

Even though this result is in a form which usually suggests to proceed with the method of superbosonization, we can as well use Witten's identification rules $\sum_s \psi^{*s}_r \psi^{s}_r = M + M^{-1}$ to rewrite this expression in terms of the bosonic field M. It can be written as

$$\frac{a^2}{2} \sum_{x,y} \operatorname{STr} \left(M_{2n} - M_{2n-1}^{-1} \right) \left(M_{2n}^{-1} - M_{2n-1} \right) + \left(M_{2n} - M_{2n-1} \right) \left(M_{2n}^{-1} - M_{2n-1}^{-1} \right) + \left(M_{2n+1} - M_{2n}^{-1} \right) \left(M_{2n+1}^{-1} - M_{2n} \right) + \left(M_{2n+1} - M_{2n} \right) \left(M_{2n+1}^{-1} - M_{2n}^{-1} \right) - 8.$$
(5.33)

The two latter terms are the discrete versions of $\operatorname{STr} \partial_z M \cdot \partial_z M^{-1} = -\operatorname{STr} (M^{-1}\partial_z M)^2$, whereas the other two terms support the somewhat heuristic argument given before that

 ${\cal M}$ changes its parity between two neighboring layers.

Based on the results of the cumulant expansion (5.33) we therefore propose the free part of the field theory for our 3D network model to be

$$S[M] = \int d^3x \, \frac{\mathrm{i}}{2\pi\Delta} \mathrm{STr} \left(M^{-1}\partial_- M \cdot M^{-1}\partial_+ M \right) + \frac{\mathrm{i}a^2}{2\Delta} \mathrm{STr} \left((M^{-1}\partial_z M)^2 \right) + \frac{\mathrm{i}}{24\pi} \varepsilon^{klm} \mathrm{STr} (M^{-1}\partial_k M) (M^{-1}\partial_l M) (M^{-1}\partial_m M)$$
(5.34)

The disorder part for the field theory was derived above (5.27) and for the full action we need to add all contributions.

The arguments for the kinetic term of the action provided in this section are not mathematically rigorous and hence we can only make a proposal (5.34) for a bosonic field theory of a Weyl semimetal described by our network model. We nontheless presented some indications that support the proposal, but a rigorous proof of this statement is a task left open for future work.

5.7 Discussion and Outlook

In this second part of the thesis we presented a model for a Weyl semimetal in class A with disorder. We introduced disorder in terms of a random scalar potential and in form of a random vector potential with independent Gaussian probability distributions. With the introduction of supersymmetric integration variables we were able to average the model over all disorder configurations.

From the disorder averaged generating functional we then set out to continue our analysis. In a first attempt we introduced a Hubbard-Stratonovich field to decouple the interaction due to disorder which resulted in a manifold of saddle point solutions. After regularization we were able to derive a diffusive term from the regularized part of the effective action. Even though this could not be the full answer, we were not able to continue the analysis in a satisfactory way.

Therefore, we turned again to the disorder averaged generating functional and tried a different approach, superbosonization. In order to apply the method of superbosonization we used a trick based on the gauge invariance of superbosonization formulas. We discretized the continuum model and averaged over local gauge transformations. A subsequent expansion in cumulants can then be expressed in terms of a supermatrix field according to the rules of superbosonization. The result was more promising than our first attempt, but it could still not be the full answer. The lack of a parity dependent term is expected to appear in a field theory for a WSM since Weyl points are parity dependent, but the cumulant expansion did not reveal such a term.

Inspired by Witten's non-abelian bosonization result in two dimensions we tried a somewhat different approach. We developed a network model, build by stacking two dimensional Chalker-Coddington network in an appropriate way, which describes a WSM phase. This is in close resemblance with WSM phases in multilayer structures.

In this three dimensional network model we could make use of Witten's two dimensional results and propose a potential field theory for a three dimensional Weyl semimetal with disorder. However, we were not able to give a rigorous proof that it is the correct field theory.

In fact, this is certainly one point where future work can continue the analysis. Another point, which might be worth to follow up on, is the gradient expansion. As was pointed out, the regularization with a heat kernel did only work for the absolute value of the determinant, but not for the angular part. A closely related regularization scheme, the so-called *zeta-function regularization*, might help in that regard. This regularization is well-known in the studies of anomalies in quantum field theory and it might be worth to consider for our case. There is however still the issue of the Hubbard-Stratonovich transformation for strong disorder. This problem is avoided when the method of superbosonization is applied, so this might generally be the better way to proceed.

Even though we were not able to provide a rigorous result for disordered Weyl semimetals, we still gained some insights and maybe laid the foundations for an approach that turns out to be more successful.

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Köln, den 01. Juli 2020

Charles M. Guggenheim

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