Symmetry and topology of nodal semimetals

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Publication Date:
2017

Permanent Link:
https://doi.org/10.3929/ethz-b-000216959

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Symmetry and Topology of Nodal Semimetals

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Diss. ETH No. 24453
Symmetry and topology of nodal semimetals

A thesis submitted to attain the degree of
DOCTOR OF SCIENCES of ETH ZÜRICH
(Dr. sc. ETH Zürich)

presented by
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2017
Space is big. Really big. You just won't believe how vastly, hugely, mind-bogglingly big it is. I mean, you may think it’s a long way down the road to the chemist, but that’s just peanuts to space.

Douglas Adams
(in The Hitchhiker’s Guide to the Galaxy)

[...] there is an alternative formulation of the many-body problem, i.e. how many bodies are required before we have a problem? [...] for those interested in exact solutions, this can be answered by a look at history. In eighteenth-century Newtonian mechanics, the three-body problem was insoluble. With the birth of general relativity around 1910, and quantum electrodynamics around 1930, the two- and one-body problems became insoluble. And within modern quantum field theory, the problem of zero bodies (vacuum) is insoluble. So, if we are out after exact solutions, no bodies at all is already too many!

Richard D. Mattuck
(in A Guide to Feynman Diagrams in the Many-Body Problem)

Getting an education was a bit like a communicable sexual disease. It made you unsuitable for a lot of jobs and then you had the urge to pass it on.

Terry Pratchett
(in Discworld #20 – Hogfather)
THE SUBJECT matter of this thesis is the appearance of various nodal semimetals in crystalline solids. The valence and the conduction bands of such materials touch at points or along lines in momentum space, and their chemical potential is adjusted to the energy of this touching. As a consequence, these materials have a vanishing or a very small density of states at the Fermi level, while not being characterized by an energy gap in the bulk excitation spectrum. This places nodal semimetals at the fine borderline between metals and insulators. In this work, we investigate the role of space group symmetries in enabling such band touchings, the so-called nodes, and the way they are protected by the topology of the electron wave functions, their so-called topological invariants.

The most famous example of a nodal semimetal is certainly graphene. In this two-dimensional material, a pair of bands disperses linearly around a touching point. As a consequence, electrons in graphene can be described by the massless Dirac equation borrowed from high-energy physics. This analogy is manifested in various transport signatures, for example in the absence of back-scattering on a certain type of barrier, known as Klein tunnelling. More recently, three-dimensional cousins of graphene called Weyl semimetals have been theoretically proposed in 2011 and experimentally observed in TaAs crystals in 2015. These materials allow for a condensed matter realization of another effect originally considered in high-energy physics, the chiral anomaly, which is responsible for an increase of conductivity if parallel magnetic field is applied to a sample. Weyl semimetals also exhibit unusual surface states, which have the form of open-ended Fermi arcs connecting the projections of bulk Weyl points inside the surface Brillouin zone. Soon after the proposal of Weyl semimetals, a plethora of other three-dimensional nodal
semimetals with more intricately structured nodes have been identified and studied.

This thesis is a collection of three projects concerning nodal semimetals and related gapless materials. In the first project, we focus on Weyl semimetals. Our strategy to realize this phase is to start with a three-dimensional band structure which contains Dirac points at time-reversal invariant momenta on the Brillouin zone boundary. Such a situation arises for example in certain pyrochlore iridates due to the non-symmetric character of their space group. We consider a tight-binding description of such materials which incorporates the leading coupling of the electrons to an elastic degree of freedom, and show that such a model may exhibit a lattice instability at low temperatures. We present detailed group-theoretical arguments to explain why such a lattice distortion alters the band structure from Dirac semimetal through Weyl semimetal to an insulator. We numerically investigate the phase diagram of this model and find that for a certain range of parameters it exhibits an exotic reentrant behaviour when a symmetry-broken phase can be reached from a symmetric phase at both higher and lower temperatures. We further observe that the connectivity of the surface Fermi arcs can be changed by tuning the model parameters. We call this phenomenon a Weyl-Lifshitz transition, and we suggest a way for its detection using quantum oscillation experiments.

The second project is concerned with nodal line semimetals. Such materials are associated with nearly-flat surface bands, which were predicted to trigger various magnetic or superconducting surface instabilities. After briefly reviewing the previously known realizations of nodal lines, we show that space group symmetry imposes their existence in spin-orbit coupled materials with a glide plane and no centre of inversion. Furthermore, this species of nodal lines occurs automatically at the Fermi level provided that a few simple criteria are met. We study the relation of such nodal lines to the usual massless Dirac spectrum, and use this to explain their peculiar Landau levels which exhibit a direction-selective chiral anomaly. We further show that similar systems with a pair of glide planes lead to a band touching along two connected loops, which in the extended momentum space look like an infinite chain. We thereby call such materials nodal-chain metals. We show that such a phase might be realized in an existing compound IrF$_4$. We use group theory and Wilson operators to explain the complex nature of its surface states.
Finally, in the last project we attempt at more generality. We consider band structures of centrosymmetric systems, and classify them according to their global symmetries (i.e. time-reversal symmetry, particle-hole symmetry and chiral symmetry) into ten groups which we call centrosymmetric extensions of the Atland-Zirnbauer classes. We use homotopy theory to show that some of these classes exhibit nodes characterized by a pair of topological charges. As a consequence, such nodes reach the very high degree of stability similar to that of Weyl points: A continuous evolution of the underlying Hamiltonian can freely move such nodes throughout the Brillouin zone, but the only way to get rid of them is a pairwise annihilation. We remark that no further crystalline symmetries beyond the spatial inversion are necessary for the appearance of such nodes. We describe this property as robustness. We find that robust nodes appear in four out of the ten centrosymmetric extensions, which are relevant for both semimetallic and superconducting systems. For example, we predict a qualitatively new species of nodal lines of singlet superconducting gap in certain topologically non-trivial Fermi surfaces. As another example, exotic nodal surfaces were very recently identified in certain time-reversal breaking multiorbital superconductors. We develop a simple tight-binding model and provide a geometric interpretation of the pair of charges for all four species of doubly charged nodes possible in three spatial dimensions. We indicate how these concepts generalize to higher spatial dimensions.

The thesis contains an additional chapter in the beginning, which provides an introduction into topological aspects of band structures. Furthermore, two mathematical appendices are included at the very end, one concerning irreducible representations of non-symmorphic space groups, and the other containing the derivations of the classifying spaces of the individual Atland-Zirnbauer classes. We conclude with some closing remarks, containing both comments on certain unresolved issues touched upon in the text as well as possible future directions.
Zusammenfassung


ten auf Verallgemeinerungen dieser Konzepte in höheren Raumdimensionen hin.

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Introduction

This brief preface provides a very broad historical overview of the topics that meet together in our work. The topics are organized chronologically as they became relevant for condensed matter physics. After getting acquainted with the leading actors, we outline the contents of the individual chapters.

Symmetry

Symmetry plays a central role in physics [1]. It brings beauty to the world around us, and simplifies its mathematical description. While some symmetries correspond to simple transformations of space and time [2], other describe more abstract internal degrees of freedom like particle spins and gauge fields [3]. But symmetries also constrain the possible dynamics of a system. Breaking of a symmetry facilitates phenomena that would not be possible otherwise [4]. After all, there is not much symmetry left in a typical living organism, and it would certainly be wrong to conclude that this makes it less interesting to understand!

In condensed matter systems, the amount of symmetry becomes a knob that one can turn and observe the consequences. Cool down a drop of mercury, and it breaks translational and rotational symmetries – becoming a solid in the process. Cool it down even more, and it breaks gauge symmetry – turning into a superconductor [5]. In a step-like fashion, crystalline solids allow us to try various combinations of symmetries and observe the consequences. The notion of symmetry is deeply integrated in the mathematical framework of condensed matter physics.

It has long been recognized that whenever two phases of matter have different symmetry, they cannot be smoothly evolved into one another
Introduction

without hitting a phase transition [6]. On the other hand, such a restriction is usually absent for phases with the \textit{same} symmetry. The most familiar example is offered by the three common phases of water. While the liquid phase has continuous rotational and translational symmetry, the solid phase only preserves a discrete subset of them. As a consequence, the two phases are separated by a transition line in the parameter space. On the other hand, the gaseous and the liquid phase possess the same symmetry, and one can indeed connect the two without hitting a phase transition simply by circumventing the critical point.

Another important phenomenon associated with symmetry breaking is the appearance of new particles. Microscopically, phase transitions correspond to a rearrangement of the constituent “building blocks” – electrons and ions in the case of condensed matter systems. This rearrangement modifies the effective low-energy degrees of freedom, which manifest themselves experimentally as new species of particles. In the example of water alluded to above, breaking of the translational symmetry leads to the appearance of transverse phonons in the solid phase. Note that these new particles can be very different from the constituent matter: Although crystalline solids are composed entirely of fermionic electrons and nucleons, phonons always come out bosonic.

Topology

A whole new chapter of condensed matter physics was opened with the experimental discovery of quantum Hall effect [7]. Consequent theoretical studies [8, 9] revealed that this phenomenon has a topological origin. Topological considerations had not been foreign to condensed matter physics, for example they had been extensively used in the study of order parameter defects [10]. But the quantum Hall state was different, because here topology entered the description of the ordered ground state \textit{per se}. A decade ago, the study of topological aspects of condensed matter systems underwent a second revolution with the theoretical proposal [11, 12] and the consequent experimental discovery [13, 14] of topological insulators.

These breakthrough discoveries revealed that a phase of matter \textit{with a gap in the bulk excitation spectrum} is characterized not only by its symmetry, but also by certain topological quantities called \textit{topological invariants}. Whenever two phases of matter differ in their symmetry or in their
Introduction

Topological invariants, they cannot be evolved into one another without hitting a phase transition. This supplements the discussion of the previous section with the notion of *topological phase transitions* – transitions in which the symmetry is preserved but a topological invariant is changed. In such transitions, the gap in the bulk excitation spectrum temporarily closes, i.e. they are realized via a metallic state.

Today, the notion of ground state topology forms an established part of condensed matter physics [15–19]. Similar to the case of symmetry breaking phase transitions, topological phase transitions are also associated with the (dis)appearance of particles in the low-energy degrees of freedom. These are either boundary states which evade the phenomenon of Anderson localization [20, 21], or qualitatively new bulk states, often of unusual non-Abelian fractional character [22]. In the latter case we speak of *topological order* [23], and examples include phases like fractional quantum Hall states [24, 25] and quantum spin liquids [26]. Both species of topologically enabled states have promising applications in quantum computation [27, 28]. In this thesis we will be concerned only with weakly interacting topological systems which *do not* exhibit the more exotic topological order.

**Nodal semimetals**

The above definition of topological invariants and of topological phase transitions is applicable only to insulating systems. However, certain topological properties can also be ascribed to *gapless* band structures like that of *nodal semimetals*. In such systems, several bands can touch each other at a point, line or surface in momentum space, and such a *node* may be protected by some quantity of topological nature. The situation is in a way reminiscent of the knotted shoelaces on the thesis cover. Nodes can also appear in superconducting phases where they tie the Bogolyubov-de-Gennes bands.

Band structure nodes can be perceived as particles living in momentum space. They can be moved around using continuous evolutions of the underlying Hamiltonian, they can meet and annihilate in pairs, or they can split into other species of nodes or even spontaneously disappear if the symmetry of the system is changed. In gapless systems, topological invariants are not attributed to the overall band structure, but to the individual nodes. Because of the particle-like interpretation in
momentum space, we often call these invariants as topological charges.

The low-energy bulk degrees of freedom of such system often exhibit unusual spectra like Weyl fermions [29] or loop fermions [30]. Nodal semimetals have also been found to facilitate anomalous transport features like the negative longitudinal magnetoresistance [31, 32], or non-local response to applied electromagnetic fields [33]. They are also associated with new species of surface states.

**Organization of the thesis**

The presented thesis lies at the confluence of the three topics summarized above. The text is structured in the following way: In chapter I we review the tools used to study topology of band structures in weakly interacting crystalline solids. Apart from serving as a reference for subsequent chapters, the author also felt compelled to provide his own perspective of this quickly developing field. The vast majority of the information presented in this chapter nevertheless deals with established results, and we include references pointing the reader to the original articles. This chapter is purposefully ignorant of the chronology in which the presented results were first derived.

In chapter II we focus on 3D semimetals exhibiting nodal points, i.e. Weyl semimetals [29] and Dirac semimetals [34, 35]. These materials are prominently associated with surface Fermi arcs [29] and phenomena emanating from chiral anomaly [31, 32]. After a brief general introduction, we elaborate on our work [36] which considers the appearance of the Weyl semimetallic phase in elastic pyrochlore iridates. Here, we use group theoretical arguments to describe how a symmetry protected Dirac point splits into multiple Weyl points upon a spontaneous inversion-breaking lattice distortion. We also investigate how such a topological transition manifests itself in the surface states. Finally, we introduce here the notion of a Weyl-Lifshitz transition, in which the surface Fermi arcs reconnect when model parameters are varied. This section is supplemented with a mathematical appendix located at the end of the thesis.

Afterwards, in chapter III we turn our attention to nodal line (semi-)metals [30]. After briefly reviewing the properties and symmetry classification of such systems, we focus on findings of our work [37]. Here, we distinguish two species of nodal loops in the presence of spin-orbit cou-
pling, which we dub accidental and non-symmorphic. The latter appear in non-centrosymmetric systems with a glide plane, and we argue that it is associated with an unusual direction-selective chiral anomaly. Additionally, we show that in certain space groups with two mutually perpendicular glide plains, a pair of non-symmorphic nodal loops touch, forming a chain-like structure in the extended momentum space. We also discuss the associated topological characteristics. This work was greatly complemented with first-principle calculations performed by Dr. Quan-Sheng Wu from the computational physics group.

Finally, in chapter IV we take a step back and develop a classification of nodes protected solely by global symmetries (i.e. particle-hole, time-reversal and chiral) together with inversion symmetry. It has recently been noticed that certain nodes of such systems can be characterized with a pair of topological charges rather than just a single one [38, 39]. Following our work [40], we present here a modified version of the Atland-Zirnbauer classification [41] better suited for centrosymmetric systems. We find that in 3D, doubly charged nodes appear in four out of the ten symmetry classes. One of them includes a novel type of singlet superconductors appearing in nodal line metals. We develop a simple tight-binding model and discuss the meaning of the pair of topological charges for all four cases, and we indicate how the concept of multiply charged nodes generalizes to higher spatial dimensions.
This chapter introduces the notion of topological invariants as well as of certain related and useful quantities like Berry connection and Wilson loop operators. As mentioned in the introduction, this chapter contains only a few original results, and mostly serves as a reference for the methods applied in subsequent chapters. The author took this as an opportunity to lay out his own way of perceiving the growing body of knowledge about topological band structures.

The chapter is divided into three sections. The first section focuses on time-reversal symmetry (TRS) breaking two-dimensional (2D) insulators which are characterized by a $\mathbb{Z}$-valued topological invariant called the (first) Chern number. We begin with a simple half-filled two-band model which enables a clear geometric interpretation of the invariant, and then we generalize the discussion to a general model using the notions of Berry phase and Berry curvature. We also squeeze in a discussion of the $(\pm 1)^{2s}$ phase acquired by spin-s particles upon a $2\pi$-rotation, since it can be understood in the same context. Such a visualization is useful in the study of certain nodal lines in chapter III.

In the second section we switch to time-reversal symmetric systems. We show that TRS enforces the Chern number to be trivial. However, a new $\mathbb{Z}_2$ invariant is enabled in spin-orbit coupled systems, which is related to quantum spin Hall effect. We first explain this charge using the original Pfaffian formulation, and then switch towards the more enlightening Wilson loop formulation. The advantage of the latter approach is that it allows one to formulate both the Chern number and the $\mathbb{Z}_2$ in-
variant in a unified fashion. This section also includes some comments about the misleading features of the Pfaffian approach, and about the geometric interpretation of the Pfaffian invariant in 3D systems.

Finally, in the last section we briefly present the tenfold way classification of topological insulators and superconductors without extraneous explanations. This section serves as a starting point for the discussion of multiply charged nodes in centrosymmetric systems in chapter IV.

I.1 Chern insulators

I.1.1 The simplest model

Consider a non-interacting two-dimensional model with two bands. The Hamiltonian $\mathcal{H}(k)$ of such a system is a Hermitian $2 \times 2$ matrix function of momentum $k$ that can be decomposed as

$$\mathcal{H}(k) = h_0(k) \mathbb{1}_\sigma + h(k) \cdot \sigma$$

(I.1)

where $h_{0,x,y,z}(k)$ are real-valued continuous functions of momentum $k = (k_x, k_y)$, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices$^1$ and $\mathbb{1}_\sigma$ is the identity matrix. The spectrum of such a Hamiltonian is easily found$^2$ to be

$$\varepsilon_{1,2}(k) = h_0(k) \pm |h(k)|.$$  

(I.3)

A half-filled model described by Hamiltonian (I.1) can be insulating only if the two bands are non-degenerate throughout the entire Brillouin zone (BZ), thus requiring $\forall k \in \text{BZ} : |h(k)| > 0$. Under such circumstances it is natural to define a mapping from BZ (which is topologically

---

$^1$At this point, we are not interested in the microscopic origin of the two-level degree of freedom associated with every Bravais vector $\mathbf{R}$ in real space.

$^2$Due to the anticommutation relation $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$, the square of the Hamiltonian is

$$\mathcal{H}^2(k) = \left(h_0^2(k) + h^2(k)\right) \mathbb{1}_\sigma.$$  

(I.2a)

Eigenvalues (I.3) follow from the pair of conditions

$$\text{tr} \mathcal{H}(k) = \varepsilon_1(k) + \varepsilon_2(k) = 2h_0(k)$$  (I.2b)

$$\text{tr} \mathcal{H}^2(k) = \varepsilon_1^2(k) + \varepsilon_2^2(k) = 2h_0^2(k) + 2h^2(k)$$  (I.2c)

where we used that $\text{tr} \sigma_i = 0$. 

---
I.1. Chern insulators

Figure I.1: Folding of 2D Brillouin zone. (a) Momentum space is periodic with respect to reciprocal lattice vectors \( g_1, g_2 \). The tile enclosed by \( g_1, g_2 \) is the first Brillouin zone (BZ), and the corners A, B, C and D correspond to the same \( k \) point. (b) Due to the periodicity, we identify points \( k \sim k + n_1 g_1 + n_2 g_2 \) with \( n_{1,2} \in \mathbb{Z} \). The outcome of such orbifolding is a square with identified opposite edges, as indicated by arrows. (c) Identification of the horizontal edges makes up a cylinder and, (d), identification of the vertical edges then produces a torus \( T^2 \). For a system with \( D \) spatial dimensions, one can similarly argue that \( \mathbb{R}^D / \mathbb{Z}^D \cong T^D \) [42].

equivalent to a torus \( T^2 \), see Fig. I.1) to a unit sphere \( S^2 \)

\[
 f : \quad T^2 \quad \rightarrow \quad S^2 \\
 k \quad \mapsto \quad n(k) = \frac{h(k)}{\|h(k)\}}. 
\] (I.4)

A small patch of size \( dk_x dk_y \) located at \( k \in T^2 \) will map onto a small patch on \( S^2 \) covering an (oriented) solid angle

\[
 d\omega = \left[ n(k + dk_x \epsilon_x) - n(k) \right] \times \left[ n(k + dk_y \epsilon_y) - n(k) \right] \\
 = \left[ (\partial_x n) \times (\partial_y n) \right] dk_x dk_y + O(dk^3) 
\] (I.5)

where \( \epsilon_i \) is a unit vector in direction \( k_i \) and \( \partial_i = \partial / \partial k_i \). The crucial observation is that since \( T^2 \) does not have a boundary, neither does its image on \( S^2 \). As a consequence, the (oriented) solid angle \( \omega \) covered by the entire BZ on \( S^2 \) must be an integer multiple of \( 4\pi \) (the area of the unit sphere), and therefore

\[
 c = \frac{1}{4\pi} \oint_{BZ} dk_x dk_y \left[ (\partial_x n) \times (\partial_y n) \right] \in \mathbb{Z}. 
\] (I.6)

The value of \( c \) corresponds to the number of times BZ wraps around the sphere [9]. It is called the (first) Chern number, and it is our first example of a topological invariant.

Clearly, \( c \) cannot be changed using only continuous deformations of \( n(k) \). Instead, its change requires “punching a hole” in the torus and
Chapter I. Topological invariants

Figure I.2: Topological transitions in a simple Chern insulator model. The arrows show $n(k)$ of Eq. (I.4) for the model defined by Eqs. (I.1) and (I.7) and the indicated values of parameter $m$. The colour of the arrows depends on the $z$-component of the arrows. For $m = -3$ (+3) all the arrows point nearly downward (upward), corresponding to the vicinity of the south (north) pole of $S^2$. No wrapping takes place and therefore $c = 0$. On the other hand, for $m = -1$ (+1), unit vectors $n(k)$ cover all of the sphere once. Taking into account the orientation of the covering, we find that the Chern number is $c = +1$ ($-1$).

pulling the sphere through the opening. At the level of model (I.1), this corresponds to setting $h = 0$ at some momentum $k_0$, such that the mapping (I.4) becomes undefined at $k_0$. According to Eq. (I.3), this corresponds to leaving the insulating state. We thus conclude that a change of the Chern number (I.6) is not possible without entering a metallic state.

To make these observations more palpable, we consider a specific model on a square lattice\(^3\) with lattice constant $a = 1$, for which

\[
h_0(k) = 0 \quad \text{and} \quad h(k) = \nu \left( \sin k_x, \sin k_y, m - \cos k_x - \cos k_y \right) ^\top \quad (I.7)
\]

where $m$ is a tunable parameter and $\nu > 0$ has the dimension of velocity.

\(^3\)This is half of the time-reversal symmetric model introduced in Ref. [43].
As one continuously increases the value of this parameter from large negative to large positive values, gap closings occur on three occasions:

- For $m = -2$ at a single point $k = (\pi, \pi)^\top$.
- For $m = 0$ at two points $k \in \{(\pi, 0)^\top, (0, \pi)^\top\}$.
- For $m = +2$ at a single point $k = (0, 0)^\top$.

These three points separate four topological regions. We plot the field $n(k)$ for $m \in \{-3, -1, 1, 3\}$ in Fig I.2. We see that while for $m = \pm 3$ the mappings do not wrap around the sphere (such that $c = 0$), they wrap around the sphere once for $m = \pm 1$ (such that $|c| = 1$). A more careful analysis shows that $c = +1$ for $m = -1$, while $c = -1$ for $m = +1$.

We conclude the discussion of the simple model by showing that such topological phase transitions are associated with the appearance or disappearance of an edge mode. For simplicity, we focus on the transition of model (I.7) at $m = -2$. Assuming $m$ very close to the critical value, we expand $m = -2 + \delta m$. Then we can approximate the spectrum in the vicinity of the BZ corner using a Taylor expansion as

$$h((\pi, \pi) + \delta k) = v(-\delta k_x, -\delta k_y, \delta m). \quad (I.8)$$

We consider a horizontal edge modelled with $\delta m(y) = \delta m f(y)$ where $f(y)$ smoothly interpolates between $-1$ for $y \to -\infty$ and $+1$ for $y \to +\infty$ [16]. The loss of translational invariance in $y$-direction means that we have to replace eigenvalue $\delta k_y$ by operator $-i \partial_y$, but the $\delta k_x$ quantum number remains well defined. Then the resulting effective Hamiltonian describing the low-energy physics becomes

$$\mathcal{H}(\delta k_x, y) = v \begin{pmatrix} \delta m f(y) & -\delta k_x + \partial_y \\ -\delta k_x - \partial_y & -\delta m f(y) \end{pmatrix}, \quad (I.9)$$

and seemingly has a pair of low-energy solutions

$$\psi_{k_x, \pm}(x, y) = e^{i\delta k_x x} e^{\pm \delta m \int_0^y f(y') dy'} \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix} \text{ with } \epsilon_{k_x, \pm} = \pm v k_x. \quad (I.10)$$

for every $k_x$. These two solutions propagate along the edge with velocity $\partial \epsilon_{k_x, \mp} / \partial k_x = \pm v$, i.e. in opposite directions. However, only one of the two solutions is normalizable and therefore physical. More specifically, for $\delta m > 0$ ($\delta m < 0$) only the $\psi_-$ ($\psi_+$) is present, which corresponds
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Figure I.3: Edge modes of a Chern insulator. (a) Hamiltonian (I.9) for $\delta m > 0$ has one edge mode propagating to the left, while (b) for $\delta m < 0$ it has one edge mode propagating to the right. (c) The previous two situations can be understood as the top and bottom edge of a small Chern insulator island located within a trivial insulator, such that the edge mode moves around the island in the clockwise direction. Note that the relative phase between the upper and lower component of $\psi(k_x)$ in Eq. (I.10) changes from negative on the top edge to positive on the bottom edge. It can be shown [44] that the relative phase depends on the local slope $\phi$ of the boundary (defined with zero indicated by the arrow) as $\psi_\downarrow / \psi_\uparrow = e^{i\phi}$.

to an edge mode propagating to the left (right). The two situation are clarified in Fig. I.3.

In the same spirit, every crossing of a topological phase transition creates a new edge mode propagating in one direction or the other. However, a pair of counter-propagating modes can gap out. We illustrate this in Fig. I.4 where three right-propagating modes meet one mode propagating in the opposite direction. Since there is no symmetry involved, these modes all belong to the same irreducible representation and can hybridize. After including the hybridization, only $3 - 1 = 2$ right-propagating edge modes remain.

I.1.2 Wilson loop operator and Berry phase

The formulation of the Chern number $c$ developed in the previous subsection is not very useful in practice because it only applies to half-filled two-band models. In order to generalize this concept to a system with $n$ occupied and $\ell$ unoccupied bands, it is convenient to switch to the language of Wilson loops and Berry phases.

Consider the adiabatic evolution of an occupied state $|u^\beta(k_{in.})\rangle$ at some initial momentum $k_{in.}$ along path $\gamma \subset \text{BZ}$ to a final momentum
Figure I.4: **Interaction of counter-propagating edge modes.** We consider here a simple model with three right-propagating and one left-propagating edge modes. The solid background indicates the bulk spectrum projected into the edge Brillouin zone. Since all edge modes belong to the same irreducible representation (there is no symmetry assumed), any crossing can in principle hybridize as indicated in the right illustration. As a result, only $3 - 1 = 2$ right-propagating modes remain, which corresponds to Chern number $|c| = 2$.

$k_{\text{fin.}}$ with occupied states $|u^a(k_{\text{fin.}})\rangle$. This process can be understood as a parallel transport, i.e. we choose a set of momenta $\{k_i\}_{i=1}^{N} \subset \gamma$ and keep projecting the current state onto the set of occupied state at the next momentum using projector operators

$$P(k_i) = \sum_{a=1}^{n} |u^a(k_i)\rangle\langle u^a(k_i)| \quad \iff \quad P(k_i) = U(k_i)U^\dagger(k_i).$$

where $U(k_i)$ is an $(n + \ell) \times n$ matrix which has columns corresponding to the occupied states at $k_i$. The amplitude to propagate the initial state to the final one can be expressed as

$$W^{a\beta}(\gamma) = \lim_{N \to \infty} \langle u^a(k_{\text{fin.}}) | \left[ \prod_{\{k_i\}_{i=1}^{N} \subset \gamma} P(k_i) \right] | u^\beta(k_{\text{in.}}) \rangle$$

where the horizontal bar in $\prod$ indicates path-ordering. The expression above contains a series of scalar products

$$\langle u^a(k) | u^b(k - \text{d}k) \rangle = \langle u^a(k) | \left( |u^b(k)\rangle - \text{d}k \cdot \nabla_k |u^b(k)\rangle + O(\text{d}k^2) \right)$$

$$\approx \delta^{ab} - \text{d}k \cdot \langle u^a(k) | \nabla_k |u^b(k)\rangle$$

$$\approx \exp \left[ -\text{d}k \cdot \langle u^a(k) | \nabla_k |u^b(k)\rangle \right]$$

$$\equiv \exp \left[ -\text{d}k \cdot \mathcal{A}^{ab}(k) \right].$$

(I.13)
where we include minus sign before $dk$ at the second state because it corresponds to moving backwards along $\gamma$. Vector $A^{ab}$ is called the Berry connection and will be discussed more carefully in the next subsection.

If we plug expression (I.13) back to Eq. (I.12), we can write the result using a path-ordered exponential $\exp$ as

$$W(\gamma) = \lim_{N \to \infty} \prod_{i=1}^{N} (1 - dk \cdot A(k)) \equiv \exp \left[ - \int dk \cdot A(k) \right] \quad (I.14)$$

where $W$ is now understood as a matrix of transition amplitudes between all occupied states at $k_{\text{in}}$ and all occupied states at $k_{\text{fin}}$. We will call such a quantity as a Wilson operator.

The problem with Wilson operator in Eq. (I.14) is that it depends on gauge. Mixing the occupied states with a matrix $X(k_i) \in U(n)$ such that

$$\tilde{U}(k_i) = U(k_i)X(k_i)$$

leads to

$$\tilde{P}(k_i) = \tilde{U}(k_i)\tilde{U}^\dagger(k_i) = U(k_i)X(k_i)X^\dagger(k_i)U^\dagger(k_i) = P(k_i) \quad (I.15)$$

i.e. the projector operators in Eq. (I.12) are unaffected. However, the gauge transformation matrix does not cancel for the end-points of $\gamma$, hence

$$\tilde{W}(\gamma) = X(k_{\text{fin.}})W(\gamma)X^\dagger(k_{\text{in.}}). \quad (I.17)$$

The problem is removed if $k_{\text{fin.}} = k_{\text{in.}}$, such that $\gamma$ is a closed loop. Then $W(\gamma)$ becomes a gauge invariant quantity called Wilson loop operator. This allows us to define a gauge invariant quantity

$$\varphi_B(\gamma) = -i \log \det W(\gamma) \quad (I.18)$$

called Berry phase. It corresponds to the complex phase acquired by the occupied states along a closed path $\gamma$. Clearly, $W(\gamma)$ is a unitary matrix with a $U(1)$ determinant, and the “$-i \log$” part extracts its complex phase. Since determinant is insensitive to the path-ordering in Eq. (I.14),
we can simplify
\[
\varphi_B(\gamma) = -i \lim_{N \to \infty} \log \left[ \prod_{\{k_i\}_{i=1}^N \subset \gamma} \det (1-dk \cdot A(k)) \right]
\]
\[
= -i \lim_{N \to \infty} \sum_{\{k_i\}_{i=1}^N \subset \gamma} \log \left( 1 - dk \cdot \text{tr} A(k) + O(dk)^2 \right)
\]
\[
= +i \lim_{N \to \infty} \sum_{\{k_i\}_{i=1}^N \subset \gamma} dk \cdot \text{tr} A(k) = i \oint dk \cdot \text{tr} A(k) \quad (I.19)
\]
where in the second line we used \(\log(\prod_i x_i) = \sum_i \log x_i\) and the identity
\[
\det(1 + \epsilon M) = 1 + \epsilon \text{tr} M + O(\epsilon^2) \quad (I.20)
\]
where \(M\) is any matrix and \(\epsilon\) is an infinitesimally small positive number.

In the last line we used Taylor approximation of the logarithmic function and assumed the \(N \to \infty\) limit.

I.1.3 Berry connection and Berry curvature

Before presenting the generalization of Chern number (I.6) in the next subsection, we provide here an alternative description of Berry phase defined in Eq. (I.18). Recall from Eq. (I.13) that in \(D\) spatial dimensions, Berry connection \(A(k)\) of a system with \(n\) occupied and \(\ell\) unoccupied bands is a \(D\)-component vector of \(n \times n\) matrices\(^4\) defined as [47, 48]
\[
A_i^{ab}(k) = \langle u^a(k) | \partial_i | u^b(k) \rangle = (U^*)^{aa}(k) \partial_i U^{ab}(k) \quad (I.22)
\]
where \(a, b\) are among the \(n\) occupied bands, and \(|u_a(k)\rangle\) are the cell-periodic parts of the Bloch wave functions at \(k\),
\[
|\psi^a(k)\rangle = e^{ik \cdot r} |u^a(k)\rangle. \quad (I.23)
\]

\(^4\) Using the language of differential geometry, we are in fact encountering a \(U(n)\) fiber bundle with the Brillouin zone \(\text{BZ} \cong T^D\) as the base manifold. The Berry connection
\[
A = U^\dagger dU, \quad (I.21)
\]
where \(d\) is the exterior derivative, endows the bundle with the notion of parallel transport [45]. Berry connection is then a 1-form usually called the gauge potential [46]. Since the metric on BZ is flat (Euclidean), we do not distinguish between lower and upper indices and instead place them to our convenience.
We can write definition (I.22) equivalently as
\[ \mathcal{A} = U^\dagger \nabla U. \] (I.24)

The gauge transformation (I.15) transforms the Berry connection into\(^5\)
\[ \tilde{A}_i = \mathcal{X}^\dagger A_i \mathcal{X} + \mathcal{X}^\dagger \partial_i \mathcal{X} \] (I.26)
where we suppressed the momentum arguments for brevity.

The second term in Eq. (I.26) can be understood as a gradient. To see this, note that matrix \( \mathcal{X} \) is invertible and can therefore be locally written as a matrix exponential
\[ \mathcal{X}(k) = e^{\mathcal{X}(k)} \] (I.27a)
where \( \mathcal{X} \in u(n) \) is an element of the Lie algebra of skew-Hermitian matrices. Then it becomes clear that
\[ \partial_i \mathcal{X} = \mathcal{X} \partial_i \mathcal{X} \Rightarrow \mathcal{X}^\dagger \partial_i \mathcal{X} = \partial_i \mathcal{X}. \] (I.27b)

Berry phase (I.19) after the gauge transformation becomes
\[ \bar{\phi}_B = i \oint_{\gamma} dk_i \text{tr} \tilde{A}_i(k) \]
\[ = i \oint_{\gamma} dk_i \text{tr} \left( \mathcal{X}^\dagger A_i \mathcal{X} \right) + i \oint_{\gamma} dk_i \partial_i \text{tr} \mathcal{X}. \] (I.28)

Using the cyclic property of trace we see that the first integral reproduces \( \phi_B \) before the gauge transformation.

The second term in Eq. (I.28) is an integral of a gradient on a closed path, and its nature depends on whether the integration path \( \gamma \) is contractible or not. If it is contractible, then the initial and final value of the integrand \( \text{tr} \mathcal{X}(k) \) coincide and the term vanishes.

On the other hand, if path \( \gamma \) is not contractible (for example if \( \gamma \) winds around BZ), only the initial and the final value of \( \mathcal{X}(k) \) are guaranteed to coincide, but not their logarithms \( \bar{\mathcal{X}}(k) = \log \mathcal{X}(k) \) which may differ by a logarithm of the identity matrix \( 1_n \). Using the identity
\[ \text{tr} \log \mathcal{M} = \log \det \mathcal{M} \] (I.29)

\(^5\)In the language of differential forms,
\[ \tilde{A} = \mathcal{X}^{-1} A \mathcal{X} + \mathcal{X}^{-1} d \mathcal{X}. \] (I.25)

The \( U(n) \) character of the fiber bundle mentioned in footnote (4) relates to \( \mathcal{X} \in U(n) \).
which is valid for any invertible square matrix $M$, we find that

$$\tilde{\varphi}_B - \varphi_B = i \oint_{\gamma} dk_i \partial_i \log X(k) = i \text{tr} \log \frac{X|_{\text{fin.}}}{X|_{\text{in.}}}$$

$$= i \text{tr} \log 1_n = i \log \det 1_n = 2\pi n$$

(I.30)

where $n \in \mathbb{Z}$, meaning that on non-contractible loops the Berry phase is well-defined only modulo $2\pi$.

Berry phase can be conveniently expressed using *Berry curvature*

$$F_{ij} = \partial_i A_j - \partial_j A_i + [A_i, A_j]$$

(I.32)

where the square brackets denote matrix commutator, and we left out the momentum arguments and band indices for brevity. Clearly, Berry curvature is skew-symmetric, $F_{ji} = -F_{ij}$. It can be shown that thanks to the commutator in Eq. (I.32) the Berry curvature transforms *covariantly* under gauge transformation (I.15), i.e.

$$\tilde{F} = X^\dagger F X.$$  

(I.34)

---

6 Using the language of differential geometry, $F$ is a 2-form called the *gauge field strength* and is obtained simply as

$$F = dA + A \wedge A$$

(I.31)

where the “wedge” $\wedge$ is the exterior product.

7 The proof of this statement is more compact in the language of differential forms. Inserting Eq. (I.25) into Eq. (I.31) gives

$$\tilde{F} = d\tilde{A} + \tilde{A} \wedge \tilde{A}$$

$$= d(\chi^{-1} A \chi + \chi^{-1} d\chi) + (\chi^{-1} A \chi + \chi^{-1} d\chi) \wedge (\chi^{-1} A \chi + \chi^{-1} d\chi)$$

$$= (d\chi^{-1}) \wedge A \chi + \chi^{-1} (dA) \chi - \chi^{-1} A \chi \wedge d\chi + (d\chi^{-1}) \wedge (d\chi)$$

(I.33a)

$$+ \chi^{-1} A \chi \wedge \chi^{-1} A \chi \wedge d\chi + (\chi^{-1} d\chi) \wedge (\chi^{-1} A \chi) \wedge (\chi^{-1} d\chi)$$

where we dropped term $\chi^{-1} dd \chi$ because $dd = 0$. It further follows from $1 = \chi^{-1} \chi$ that $(d\chi^{-1}) \chi = -\chi^{-1} d\chi$, and the red minus sign in Eq. (I.33a) follows from the graded Leibniz rule for exterior derivative $d$. Consequently, most of terms in Eq. (I.33a) cancel each other in pairs according to the indicated colouring, and only the black ones survive, thus leading to

$$\tilde{F} = \chi^{-1} (dA + A \wedge A) \chi = \chi^{-1} F \chi.$$  

(I.33b)
On the other hand, the linearity and the cyclic property of trace imply
\[
\text{tr } F_{ij} = \text{tr} (\partial_i A_i - \partial_j A_i) + \text{tr} (A_i A_j) - \text{tr} (A_j A_i) \\
= \partial_i \text{tr } A_j - \partial_j \text{tr } A_i = \sum_{a=1}^{n} \left( \partial_i A_{ja} - \partial_j A_{ia} \right) .
\] (I.35)

For a contractible loop $\gamma = \partial D$ (where $\partial$ is the boundary operator and $D$ a 2D domain), we can apply Stokes theorem to find

\[
\varphi_B = i \int_{\partial D} \text{tr } A_i = i \sum_{i<j}^{D} \int_{\partial D} dk_i dk_j \left( \partial_i \text{tr } A_j - \partial_j \text{tr } A_i \right) \\
= i \sum_{i<j}^{D} \int_{\partial D} dk_i dk_j \text{tr } F_{ij}
\] (I.37)

where we only sum over $i < j$ to prevent double counting. Clearly, the cyclic property of trace together with relation (I.34) guarantee the gauge invariance of $\varphi_B$. This also follows from the gauge invariance of Wilson loop operator $W(\gamma)$ and from Eq. (I.18) of the previous subsection.

Notice that, the off-diagonal terms of $A(k)$ cancel out after performing the trace in Eq. (I.35). In the case of non-degenerate bands, this allows us to decompose the Berry curvature $F(k)$ into the contributions of the individual bands,

\[
\text{tr } F_{ij} = \sum_{a=1}^{n} F_{ij}^a \quad \text{with} \quad F_{ij}^a = \langle \partial_i u^a | \partial_j u^a \rangle - (i \leftrightarrow j) .
\] (I.38)

We conclude this subsection by deriving an alternative expression for the single-band Berry curvature. This expression is particularly useful for the analysis of spin rotations. It should be noted that an identical expression has also been derived by Thouless et al. in Ref. [9] when analysing the Hall conductance in QHE states. We first expand

\[
\langle \partial_i u^a | \partial_j u^a \rangle - (i \leftrightarrow j) = \sum_{b \neq a} \langle \partial_i u^a | u^b \rangle \langle u^b | \partial_j u^a \rangle - (i \leftrightarrow j)
\] (I.39)

---

\footnote{The differential geometry analogue of these equations is remarkably simple, namely}

\[
\varphi_B = i \int_{\partial D} A = i \int_{D} dA = i \int_{D} F .
\] (I.36)
where \( \sum_b |u^b \rangle \langle u^b| = 1 \) sums over all states, but \( b = a \) is dropped from the summation because it cancels upon antisymmetrization in indices \( i, j \) by the virtue of

\[
\delta^{ab} = \langle u^a | u^b \rangle \quad \Rightarrow \quad \langle \partial_i u^a | u^b \rangle = -\langle u^a | \partial_i u^b \rangle. \quad \text{(I.40)}
\]

Furthermore, for \( b \neq a : 0 = \langle u^a | \mathcal{H} | u^b \rangle \) from which it follows that

\[
\langle u^a | (\partial_i \mathcal{H}) | u^b \rangle = -\langle \partial_i u^a | \mathcal{H} | u^b \rangle = -\epsilon^b \langle \partial_i u^a | u^b \rangle - \epsilon^a \langle u^a | \partial_i u^b \rangle
\]

\[
\Rightarrow \quad (\epsilon^a - \epsilon^b) \langle \partial_i u^a | u^b \rangle \quad \text{(I.41)}
\]

which upon inserting to Eq. (I.39) leads to

\[
F^a_{ij} = \sum_{b \neq a} \frac{\langle u^a | (\partial_i \mathcal{H}) | u^b \rangle \langle u^b | (\partial_j \mathcal{H}) | u^a \rangle - (i \leftrightarrow j)}{(\epsilon^a - \epsilon^b)^2} \quad \text{(I.42)}
\]

Note that expression (I.42) is antisymmetric under exchanging \((a \leftrightarrow b)\). This implies that \( \sum_a F^a_{ij} = 0 \) vanishes identically, i.e. the Chern number of a complete band structure of any Hamiltonian is trivial.\(^9\)

### I.1.4 Berry curvature in low-dimensional systems

Let us apply the very general discussion of the previous subsection to systems with low number of spatial dimensions, namely 1D, 2D and 3D.

In \( D = 1 \) the language of \( \mathcal{F} \) does not actually exist.\(^10\) In fact, the only interesting closed path in a 1D BZ corresponds to increasing \( k \) from

\[^9\] Let us derive here the same conclusion for the case of degenerate bands when the decomposition (I.38) does not apply. Taking all bands into account, \( U \in U(n + \ell) \) becomes a square matrix which can be expressed as \( e^{\mathcal{X}_U} \) where \( \mathcal{X}_U \in u(n + \ell) \) is a skew-Hermitian matrix. Then the Berry connection

\[
\mathcal{A} = U^\dagger \nabla U = e^{-\mathcal{X}_U} e^{\mathcal{X}_U} \nabla \mathcal{X} = \nabla \mathcal{X}
\]

becomes a gradient of \( \mathcal{X}(k) \). Consequently, it follows from Eq. (I.35) that

\[
\text{tr} \mathcal{F}_y = \sum_{a=1}^{n+\ell} (\partial_i \partial_j \mathcal{X}^{aa} - \partial_j \partial_i \mathcal{X}^{aa}) = 0. \quad \text{(I.44)}
\]

\[^{10}\] It is not possible to choose two linearly independent directions \( i \) and \( j \) in definition (I.32). At the level of differential geometry, recall that \( p \)-forms correspond to completely antisymmetric tensors of rank \( p \). The space of \( p \)-forms with \( p > D \) is non-existent. For \( 0 \leq p \leq D \) the space has \( \binom{D}{p} = \frac{D!}{p!(D-p)!} \) dimensions.
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\[-\pi/a \text{ to } \pi/a. \text{ The result}

\[\varphi_{Zak} = i \int_{-\pi/a}^{+\pi/a} dk \text{ tr } A(k) \mod 2\pi \quad (I.45)\]

is usually called the Zak Phase [49]. It is quantized to \(\varphi_{Zak} \in \{0, \pi\}\) in the presence of certain crystalline symmetries as we show in Subsec. I.2.3. Zak phase also turns out to be a useful construction in more-dimensional systems as is discussed in Subsec. I.2.5. We will encounter Zak phase in multiple places throughout the thesis, especially in chapter III.

For \(D = 2\) with coordinates \(x\) and \(y\), there is just one independent component of Berry curvature, \(\mathcal{F}_{xy} = -\mathcal{F}_{yx}\). This implies that Berry curvature behaves as a scalar, and Berry phase can be expressed as

\[\varphi_B = i \iint_D d{k_x} d{k_y} \text{ tr } \mathcal{F}_{xy}. \quad (I.46)\]

An important application of Eq. (I.46) corresponds to choosing \(D = \text{BZ}\). In fact, this choice leads to the generalization of Chern number (I.6) to an arbitrary gapped band structure.

However, as BZ is not a contractible manifold, one cannot apply Stokes theorem (I.37) directly. Especially, \(\text{BZ} \cong \mathbb{T}^2\) does not have a boundary (\(\partial \text{BZ} = \emptyset\) is an empty set), such Eq. (I.37) would suggest \(\varphi_B \propto \oint_{\emptyset} = 0\) always vanishes, which is not true! Instead, one should imagine cutting BZ back into the parallelogram of Fig. I.1(a) which \(\text{is}\) contractible and \(\text{has}\) a boundary. We decompose the boundary into four segments AB, BC, CD and DA as indicated in Fig. I.1(a). Then

\[\varphi_B(\text{BZ}) = \varphi_B(\text{AB}) + \varphi_B(\text{BC}) + \varphi_B(\text{CD}) + \varphi_B(\text{DA}) \quad (I.47a)\]

Each of these four segments forms a closed non-contractible loop, meaning that by Eq. (I.30) the corresponding Berry phase is only well-defined modulo \(2\pi\). On the other hand, paths AB and CD correspond to the same path with opposite orientation, therefore

\[\varphi_B(\text{CD}) = -\varphi_B(\text{AB}) \mod 2\pi \quad (I.47b)\]

such that the sum of their contributions is 0 modulo \(2\pi\). An analogous conclusion is found for the vertical edges BC and DA. Inserting these relations to Eq. (I.47a) leads to

\[\varphi_B(\text{BZ}) = 0 \mod 2\pi, \quad (I.47c)\]
meaning that it equals to an integer multiple of $2\pi$.

We now show that the integer

$$c = \frac{i}{2\pi} \int_{\text{BZ}} dk_x dk_y \text{tr} \mathcal{F}_{xy} \in \mathbb{Z} \quad \text{(I.48)}$$

is a natural generalization of the Chern number (I.6) to a system with an arbitrary number of occupied and unoccupied bands. To achieve this, we show that both methods give the same result for the half-filled two-band model (I.1). Decomposing $h = h(\sin \theta_h \cos \phi_h, \sin \theta_h \sin \phi_h, \cos \theta_h)$ in spherical coordinates, the occupied state is

$$|u^{\text{occ.}}\rangle = \begin{pmatrix} -\sin \frac{\theta_h}{2} \\ \text{e}^{i\phi_h} \cos \frac{\theta_h}{2} \end{pmatrix} \quad \text{(I.49)}$$

which leads to Berry connection and Berry curvature

$$i \in \{x, y\} : A_i = i \cos^2 \frac{\theta_h}{2} (\partial_i \phi_h) \quad \text{(I.50)}$$

$$\mathcal{F}_{xy} = -\frac{i}{2} \sin \theta_h (\partial_x \theta_h)(\partial_y \phi_h). \quad \text{(I.51)}$$

The integrand in Eq. (I.46) becomes

$$\text{id} k_x \text{d} k_y \mathcal{F}_{xy} = \frac{1}{2} \sin \theta_h \text{d} \theta_h \text{d} \phi_h. \quad \text{(I.52)}$$

Up to a multiplicative factor, this is precisely the small solid angle as in Eq. (I.5). This completes the proof of equivalence.

Finally for $D = 3$ the Berry curvature contains three independent components $\mathcal{F}_{xy}, \mathcal{F}_{yz}$ and $\mathcal{F}_{zx}$. This allows us to interpret $\mathcal{F}$ as a vector\footnote{The chosen gauge has a singularity at $\theta_h = 0$. An alternative gauge is obtained by multiplying (I.49) by $\text{e}^{-i\phi_h}$, which moves the singularity to $\theta_h = \pi$. The two gauge choices lead to different Berry connection $A$, but the same Berry curvature $\mathcal{F}$, as explained in Subsec. I.1.3 [50].} through the mapping\footnote{More precisely as a pseudo\textit{vector} (or an axial\textit{ vector}) because it is unaffected by spatial inversion, as we show in Subsec. I.2.2}

$$\Omega_i = \frac{i}{2} \epsilon_{ijk} \mathcal{F}_{jk} \quad \text{(I.53)}$$

where $\epsilon_{ijk}$ is the Levi-Civita symbol. Inserting (I.31) into Eq. (I.53) leads to a form

$$\Omega = i \nabla \times A + i A \times A \quad \text{(I.54)}$$

\footnote{In the language of differential forms, $\Omega = i \star \mathcal{F}$ where $\star$ is the Hodge dual operator.}
where both $\mathbf{A}$ and $\Omega$ are three-component vectors (with matrix entries).

Following the discussion around Eq. (I.38), for non-degenerate bands we are allowed to drop the second term in Eq. (I.54) and decompose the first term into contributions of individual bands as $\text{tr} \Omega = \sum_{a=1}^n \Omega^a$ with

$$\Omega^a = \nabla \times A^a \quad \Rightarrow \quad \nabla \cdot \Omega^a = 0 \quad \text{(I.55a)}$$

where $A^a$ is a single-band Berry connection, componentwise

$$A^a_i(k) = i \langle u^a(k) | \partial_i | u^a(k) \rangle \quad \text{and} \quad \Omega^a_i = -\epsilon_{ijk} \partial_j A^a_k. \quad \text{(I.55b)}$$

The dual form of expression (I.42) becomes

$$\Omega^a = i \sum_{b \neq a} \frac{\langle u^a | (\nabla \mathcal{H}) | u^b \rangle \times \langle u^b | (\nabla \mathcal{H}) | u^a \rangle}{(\epsilon^a - \epsilon^b)^2}. \quad \text{(I.55c)}$$

$I.1.5$ Spin rotations

We conclude this section by showing that the $(\pm 1)^{2s}$ phase obtained by spin-$s$ particles upon a $2\pi$-rotation can be understood as a Berry phase effect [18, Sec. 2.4]. These considerations are relevant for the understanding of time-reversal operator in the next section, as well as for the Berry phase quantization in certain nodal line semimetals in chapter III.

Consider the Hamiltonian of a spin-$s$ particle in magnetic field $\mathbf{B}$,

$$\mathcal{H}(\mathbf{B}) = g \mathbf{B} \cdot \mathbf{J}^s \quad \text{(I.56)}$$

where $\mathbf{J}^s = (J_x^s, J_y^s, J_z^s)$ are spin-$s$ rotation matrices fulfilling $[J_i^s, J_j^s] = i\epsilon_{ijk} J_k^s$, $\mathbf{B} = (B_x, B_y, B_z)$ is magnetic field, and $g$ is a multiplicative factor. As is well-known from the theory of angular momentum, Hamiltonian (I.56) has $2s + 1$ eigenstates $|m\rangle$ with energies $\epsilon^m = g B m$ where

---

14 In subsequent chapters we will encounter a similar Hamiltonian for Weyl semimetals where $\mathbf{B}$ is replaced by momentum $\mathbf{k}$.

15 Recall that one typically adopts the eigenbasis of $J_x^s$, which consists of states $J_x^s |m\rangle = m |m\rangle$ with $2s + 1$ integers $-s \leq m \leq s$. Natural ordering of the basis then leads to $J_x^s = \text{diag} \{-s, -s+1, \ldots, s-1, s\}$. One then constructs matrices $J_\pm^s = J_x^s \pm iJ_y^s$. It follows from the commutation relations that $[J_+^s, J_-^s] = \pm J_z^s$, which further entail $J_\pm^s |m\rangle = \hat{c}_\pm^s m |m\rangle$ where $\hat{c}_\pm^s m$ are scalar factors. A more careful analysis regarding the boundedness of the operators shows [51] that $|\hat{c}_\pm^s m|^2 = s(s+1) - m(m \pm 1)$. The phases of vectors $|m\rangle$ are then chosen such that $\hat{c}_\pm^s m$ are positive real, such that matrix elements $\langle J_\pm^s | m\rangle = (m |J_\pm^s | m\rangle$ are also real. Consequently, $J_\pm^s = (J_+ + J_-)/2$ is real, while $J_y^s = (J_+ - J_-)/2i$ is imaginary.
I.1. Chern insulators

$m \in \{-s, -s + 1, \ldots, s - 1, s\}$ and $B = \|B\|$. We will determine the Berry phase (I.55c) inside the parameter space $B$. Clearly, $\nabla_B \mathcal{H} = g J^s$. We see that factors $g^2$ in the numerator and denominator cancel out, such that

$$\Omega^m = i \sum_{m' \neq m} \frac{\langle m|J^s|m'\rangle \times \langle m'|J^s|m\rangle}{B^2(m-m')^2}. \tag{I.58a}$$

Now we want to analyze the matrix elements $\langle m|J^s|m'\rangle$. At this stage it is convenient to rotate the coordinates of the vector space such that $\tilde{J}_z^s$ is parallel to $B$ while $\tilde{J}_x^s$ and $\tilde{J}_y^s$ are perpendicular to it. Then $B \cdot J^s = B\tilde{J}_z^s$ implies that states $|m\rangle$ are the eigenstates of $\tilde{J}_z^s$. We denote the rotated Berry curvature as $\tilde{\Omega}^m$.

Since $\tilde{J}_z^s$ is diagonal, $m' \neq m$ summands do not contribute to the result and we pay attention only to the $\tilde{J}_x^s$ and $\tilde{J}_y^s$ terms. These lead to only non-vanishing component

$$\tilde{\Omega}_z^m = i \sum_{m' \neq m} \frac{\langle m|\tilde{J}_x^s|m'\rangle \langle m'|\tilde{J}_y^s|m\rangle - (x \leftrightarrow y)}{B^2(m-m')^2}. \tag{I.58b}$$

According to footnote Eqs. (I.57), only $m' = m \pm 1$ give non-vanishing matrix elements, therefore

$$\tilde{\Omega}_z^m = \frac{i}{B^2} \sum_{m' = m \pm 1} \left[ \langle m|\tilde{J}_x^s|m'\rangle \langle m'|\tilde{J}_y^s|m\rangle - (x \leftrightarrow y) \right]. \tag{I.58c}$$

After inserting here expressions (I.57) and carefully going through the algebra, one finds $\tilde{\Omega}_z^m = -m/B^2$. Rotating back to the original coordinate basis leads to

$$\Omega^m = -m \frac{B}{B^3}. \tag{I.58d}$$

One possibility to rotate a spin by $2\pi$ is to slowly rotate magnetic field $B$ by $2\pi$ in the $x, y$-plane. This corresponds to a closed loop $\gamma$ in the parameter space which is associated with a Berry phase. This loop is contractible, i.e. $\gamma = \delta D$. A convenient choice of $D$ corresponds to a

This also means that the only non-vanishing matrix elements of $J^s_x$ and $J^s_y$ are

$$\langle m \pm 1|J^s_x|m\rangle = \frac{1}{2} \sqrt{s(s+1) - m(m \pm 1)} \tag{I.57a}$$

$$\langle m \pm 1|J^s_y|m\rangle = \pm \frac{1}{2i} \sqrt{s(s+1) - m(m \pm 1)}. \tag{I.57b}$$
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half-sphere that has $\gamma$ as its “equator”. Since this surface has area $2\pi B^2$ and a constant Berry flow density $-m/B^2$, the acquired Berry phase is

$$\varphi_B = -2\pi m.$$  \hfill (I.59)

Since $m$ is (half-)integer for (half-)integer $s$, the phase acquired upon $2\pi$-rotation is

$$e^{i\varphi_B} = (-1)^{2s} = \left\{ \begin{array}{ll} +1 & \text{for integer spins} \\ -1 & \text{for half-integer spins} \end{array} \right.$$  \hfill (I.60)

as we wanted to show.

### I.2 Time-reversal symmetric insulators

#### I.2.1 Time-reversal operator

According to the Wigner theorem [52], every symmetry of a quantum system is expressed either as a unitary or as an antiunitary operator on the Hilbert space. Time-reversal symmetry $T$ corresponds to the latter case. To see this, consider evolving state $|\psi\rangle$ according to two scenarios:

1. Evolve the state from $t = 0$ to $t = t_{\text{fin.}}$, then reverse $t_{\text{fin.}} \rightarrow -t_{\text{fin.}}$ by applying $T$.

2. Apply $T$ at $t = 0$ and then backward propagate the state from $t = 0$ to $t = -t_{\text{fin.}}$.

Obviously, these two procedures should result in the same state $|\psi'\rangle$ provided that the system respects time-reversal symmetry, i.e. when $T\mathcal{H} - \mathcal{H}T = [T, \mathcal{H}] = 0$. The explicit description of the two scenarios above leads to

$$Te^{-i\mathcal{H}t}|\psi\rangle = |\psi'\rangle = e^{+i\mathcal{H}t}T|\psi\rangle.$$  \hfill (I.61)

Then self-consistency requires antilinearity

$$Ti = -iT,$$  \hfill (I.62)

which means that $T$ is antiunitary. Alternatively, one may define time-reversal symmetry by requiring the physically clear properties $T\mathcal{H}T^{-1} = \mathcal{H}$. 


\[ \hat{x} \text{ and } T \hat{\rho}_x T^{-1} = -\hat{\rho}_x. \] However, if the commutation relation \([\hat{x}, \hat{\rho}_x] = i\) is to be preserved under \(T\), then antilinearity (I.62) is necessary again.

An antiunitary operator can be expressed as a product of a unitary operator and the operator of complex conjugation \(K\), i.e.

\[ T = u_T K \] (I.63)

For a spinless particle, the wave function does not have any integral structure and therefore \(T = K\). On the other hand, for a particle with a spin-s degree of freedom \((2s \in \mathbb{Z}_0^+)\), we require the time-reversal operator to invert the angular momentum, i.e. \(i \in \{x, y, z\} : T J^s_i T^{-1} = -J^s_i\).

The standard choice fulfilling these criteria is

\[ T = e^{-i\pi J^s_y} K \equiv u_T^s K \] (I.64)

To understand this solution, recall from footnote (15) that \(J^s_y\) is imaginary, meaning that it commutes with \(u_T^s\) but anticommutes with \(K\). The other two components \(J^s_x\) and \(J^s_y\) are real and commute with \(K\), but \(u_T^s\) corresponds to a \(\pi\)-rotation around \(y\)-axis which inverts the sign of the \(x\) and \(z\) coordinates. This completes the explanation of (I.64). We remark that for \(s = \frac{1}{2}\) the exponentiation with \(J^1/2_y = \frac{1}{2}\sigma_y\) (i.e. half the second Pauli matrix) leads to

\[ T = -i\sigma_y K \] (I.65)

which is frequently used throughout the thesis. We will sometimes ignore the minus sign, which corresponds to \(T\) defined with a \(\pi\)-rotation around \(y\)-axis in the opposite direction.

Furthermore, \(iJ^s_y\) is real such that the exponential \(u_T^s\) is also real and thus commutes with \(K\). The square of \(T\) therefore equals

\[ T^2 = (u_T^s)^2 = e^{-i2\pi J^s_y} = (-1)^{2s} \] (I.66)

where in the last step we recognized that this is just the \(2\pi\)-rotation analysed in Subsec. I.1.5.

Let us analyse result (I.66) more carefully. Let us assume that \(T\) has an eigenstate \(|\psi_1\rangle\), i.e. \(T |\psi_1\rangle = c |\psi_1\rangle\) with some \(c \in \mathbb{C}\). Then by the antilinearity

\[ T^2 |\psi_1\rangle = |c|^2 |\psi_1\rangle. \] (I.67)

For integer spins \(s\) this implies \(|c|^2 = 1\). If we write \(c = e^{i\varphi_c}\), then \(e^{i\varphi_c/2} |\psi_1\rangle\) is an eigenstate of \(T\) with eigenvalue 1.
On the other hand, for half-integer spin the Eq. (I.67) does not have a solution for any \( c \), because that would require negative absolute value. However, the same equation implies that every state \( |\psi_1\rangle \) is an eigenstate of the square \( T^2 \) with eigenvalue \(-1\). This suggests, that every state \( |\psi_1\rangle \) is associated with a different state \( |\psi_2\rangle = T|\psi_1\rangle \) such that the two are exchanged under time-reversal. This is the well-known Kramers theorem [53].

### I.2.2 Berry curvature of time-reversal symmetric bands

In this subsection we investigate the implication of time-reversal symmetry on the Chern number of a system. Consider two momenta \( k \neq -k \) and their small non-overlapping neighbourhoods. Then it is possible to find a gauge\(^{16}\) such that

\[
|u^a(-k)\rangle = |Tu^a(k)\rangle. \tag{I.70}
\]

Following the definition in Eq. (I.22), we derive

\[
\mathcal{A}_{i}^{ab}(-k) = \frac{1}{dk} \left[ \langle u^a(-k)|u^b(-k + dk\epsilon_i)\rangle - \langle u^a(-k)|u^b(-k)\rangle \right] \\
= \frac{1}{dk} \left[ \langle Tu^a(k)|Tu^b(k - dk\epsilon_i)\rangle - \delta^{ab} \right] \\
= \frac{1}{dk} \left[ \langle u^b(k - dk\epsilon_i)|u^a(k)\rangle - \delta^{ab} \right] = \ldots \tag{I.71}
\]

where in the last line we used that for an antiunitary operator \( \mathcal{A} \)

\[
\langle \mathcal{A}\psi_1|\mathcal{A}\psi_2 \rangle = \langle \psi_1|\psi_2 \rangle^* = \langle \psi_2|\psi_1 \rangle. \tag{I.72}
\]

\(^{16}\) This is possible for any value of spin. However, the inverse transformation \( |u^a(k)\rangle = \pm |Tu^a(-k)\rangle \) then depends on the sign of \( T^2 \).

\(^{17}\) To avoid confusion, we denote the action of antiunitary operators as \( |\mathcal{A}\psi\rangle \) rather than \( \mathcal{A}|\psi\rangle \). The second notation would lead to a problem within bra-ket expressions. While for a unitary operator \( U \)

\[
\langle U^{-1}\psi_1|\psi_2 \rangle = \langle \psi_1|U\psi_2 \rangle = \langle \psi_1|U\psi_2 \rangle \tag{I.68}
\]

the “sandwiched” operator can be thought of as acting in either direction, the same is not true for an antiunitary operator \( \mathcal{A} \) when

\[
\langle \mathcal{A}^{-1}\psi_1|\psi_2 \rangle \neq \langle \psi_2|\mathcal{A}^{-1}\psi_1 \rangle^* = \langle \psi_1|\mathcal{A}\psi_2 \rangle. \tag{I.69}
\]
Then using Eq. (I.40) and the definition of Berry connection once again

\[ \frac{d}{dk} \left[ \delta_{ab} - dk \langle \partial_i u^b(k) | u^a(k) \rangle - \delta_{ab} \right] \]

\[ = - \langle \partial_i u^b(k) | u^a(k) \rangle = \langle u^b(k) | \partial_i u^a(k) \rangle = A_{i}^{ba}(k) \quad (I.73) \]

i.e. \( \mathcal{A}(-k) = \mathcal{A}^\top(k) \) in the chosen gauge (I.70) where \( ^\top \) is matrix transpose in the two band indices. But we are really after the gauge-invariant relation between Berry curvatures \( \mathcal{F}_{ij}(k) \) and \( \mathcal{F}_{ij}(-k) \). We do this piecewise. First note that

\[ \partial_i \mathcal{A}_j(-k) = \frac{1}{dk} \left[ \mathcal{A}_j(-k + dke_i) - \mathcal{A}_j(-k) \right] \]

\[ = \frac{1}{dk} \left[ \mathcal{A}_j^\top(k - dke_i) - \mathcal{A}_j^\top(k) \right] = - \partial_i \mathcal{A}_j^\top(k) \quad (I.74a) \]

and further that

\[ \mathcal{A}_i(-k) \mathcal{A}_j(-k) = \mathcal{A}_i^\top(k) \mathcal{A}_j^\top(k) = [\mathcal{A}_j(k) \mathcal{A}_i(k)]^\top \quad (I.74b) \]

Inserting Eqs. (I.74a) and (I.74b) reveals that in time-reversal symmetric systems

\[ \mathcal{F}_{ij}(-k) = - \mathcal{F}_{ij}^\top(k) \quad \Rightarrow \quad \text{tr} \mathcal{F}_{ij}(-k) = - \text{tr} \mathcal{F}_{ij}(k) \quad (I.75) \]

meaning that the net Berry curvature is antisymmetric in \( k \). As a consequence, the Chern number (I.48) of a time-reversal symmetric system equals zero, because the contributions to the integral from momenta \( k \) and \(-k\) cancel out. In other words, a Chern insulator is not possible in a time-reversal symmetric system.

Before moving on, note that we may similarly consider the symmetry of Berry curvature in the presence of spatial inversion symmetry \( \mathcal{I} \). The necessary arguments are analogous to Eqs. (I.70) to (I.75) with the important difference that \( \mathcal{I} \) is a unitary operator, and a generic unitary rotation \( \mathcal{U} \) preserves scalar products,

\[ \langle \mathcal{U}\psi_1 | \mathcal{U}\psi_2 \rangle = \langle \psi_1 | \psi_2 \rangle. \quad (I.76) \]

As a consequence, in a gauge with \( |u^a(-k)\rangle = \mathcal{I}|u^a(k)\rangle \) we find Berry connection \( \mathcal{A}(-k) = - \mathcal{A}(k) \) and Berry curvature

\[ \mathcal{F}_{ij}(k) = \mathcal{F}_{ij}(-k) \quad \Rightarrow \quad \text{tr} \mathcal{F}_{ij}(-k) = \text{tr} \mathcal{F}_{ij}(k) \quad (I.77) \]
meaning that the dual $\Omega$ of Eq. (I.53) transforms as a pseudovector as we already remarked in footnote (12). In systems with both $T$ and $I$, Eqs. (I.75) and (I.77) force Berry curvature to vanish identically, and BZ is said to be flat.

### I.2.3 Wilson loop operator of 1D systems

We mentioned in Subsec. I.1.4 that in one spatial dimension there is only one interesting closed loop in $k$-space, namely the 1D BZ itself. In the present subsection we derive important results for the Wilson operator along this loop for a system respecting time-reversal symmetry $T$ or spatial inversion $I$ for systems with $s = \frac{1}{2}$. The first of these results plays a central role in understanding the $\mathbb{Z}_2$ invariant of topological insulators in Subsec. I.2.6.

Recall from Subsec. I.1.2 that the (edge-to-edge) Wilson operator along the 1D BZ, denoted $\mathcal{W}(-\pi \to +\pi) \equiv \mathcal{W}_{\text{BZ}}$, corresponds to

$$
\mathcal{W}_{\text{BZ}} = \lim_{N \to \infty} U^\dagger(+\pi) \left[ \prod_{\{k_i\}_{i=1}^N \subset \text{BZ}} U(k_i)U^\dagger(k_i) \right] U(-\pi). \quad (I.78)
$$

Because of TRS, the occupied states $U(k_i)$ at $k_i$ are related to occupied states $U(-k_i)$ at $-k_i$, namely

$$
U(k_i) = [TU(-k_i)]\mathcal{B}(k_i) \quad (I.79a)
$$

where $[TU(-k_i)]$ correctly spans the basis of occupied states at $k_i$ and $\mathcal{B}(k_i) \in U(n)$ is a gauge transformation to the correct set of eigenstates (i.e. the sewing matrix). Applying time-reversal twice constrains

$$
U(k_i) = \{TU(k_i)]\mathcal{B}(-k_i)\}\mathcal{B}(k_i)
= T^2U(k_i)\mathcal{B}^*(-k_i)\mathcal{B}(k_i) \Rightarrow \mathcal{B}^*(-k_i)\mathcal{B}(k_i) = -\mathbb{1}. \quad (I.79b)
$$

which will come to play in the end of our analysis. Plugging rela-
I.2. Time-reversal symmetric insulators

\[ \mathcal{W}_{\text{BZ}} = \lim_{N \to \infty} B(\pi)[T U(-\pi)]^\dagger \]

\[ \cdot \prod_{\{k_i\}_{i=1}^N \subset \text{BZ}} [T U(-k_i)] B(k_i) B^\dagger(k_i) [T U(-k_i)]^\dagger \cdot [T U(\pi)] B(-\pi) \]

\[ = \lim_{N \to \infty} B(\pi) \cdot \prod_{\{k_i\}_{i=1}^N \subset \text{BZ}} [U^\dagger(-k_i)] U(-k_i) \cdot U(\pi) \cdot \ast \cdot B(-\pi) \]

\[ = B(\pi)^\dagger \mathcal{W}_{\text{BZ}}^\dagger B(\pi) \]  \hspace{1cm} (I.80)

where in the second equation mark we used relation (I.72) valid for antiunitary operators, and in the last line we realized that \(B^\dagger(\pi) \equiv B(\pi)\) and we identified the original Wilson operator in the centre of the expression. Note that because of Eq. (I.79b),

\[ B^\ast(\pi) B(\pi) = -1. \]  \hspace{1cm} (I.81)

The Wilson operator \(\mathcal{W}_{\text{BZ}} \in \text{U}(n)\) describes a unitary rotation among the occupied states, and as such has eigenvalues lying along the unit circle in complex plane. An important result that we are about to derive is that for a TRS-preserving system, eigenvalues of \(\mathcal{W}_{\text{BZ}}\) come in \textit{pairs} [54].

To achieve our goal, assume that \(|\psi\rangle\) is an eigenvector of \(\mathcal{W}_{\text{BZ}}\) with eigenvalue \(e^{i\phi}\). First, the unitarity implies that

\[ \mathcal{W}_{\text{BZ}}^\dagger |\psi\rangle = \mathcal{W}_{\text{BZ}}^\dagger e^{-i\phi} \mathcal{W}_{\text{BZ}} |\psi\rangle = e^{-i\phi} |\psi\rangle \]  \hspace{1cm} (I.82a)

meaning that \(|\psi\rangle\) is also an eigenvector of \(\mathcal{W}_{\text{BZ}}^\dagger\) with the conjugate eigenvalue \(e^{-i\phi}\). But due to relation (I.80), \(B(\pi)^\ast |\psi\rangle^\ast\) is an eigenvector of \(\mathcal{W}_{\text{BZ}}\) with eigenvalue \(e^{i\phi}\) again, because

\[ \mathcal{W}_{\text{BZ}} B(\pi)^\ast |\psi\rangle^\ast \overset{(I.80)}{=} B(\pi)^\dagger \mathcal{W}_{\text{BZ}}^\dagger B(\pi) B(\pi)^\ast |\psi\rangle^\ast \overset{(I.81)}{=} -B(\pi)^\dagger \left( \mathcal{W}_{\text{BZ}}^\dagger |\psi\rangle \right)^\ast \]

\[ \overset{(I.82a)}{=} -B(\pi)^\dagger e^{i\phi} |\psi\rangle^\ast \overset{(I.81)}{=} e^{i\phi} B(\pi)^\ast |\psi\rangle^\ast. \]  \hspace{1cm} (I.82b)

Importantly, \(B(\pi)^\ast \mathcal{K}\) is an antiunitary operator squaring to \(-1\), similar to time-reversal operator \(T\). Consequently, the Kramers theorem implies that \(B(\pi)^\ast \mathcal{K} |\psi\rangle\) is linearly independent of \(|\psi\rangle\). To see this, we apply iden-
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ity (I.72) to derive

\[ \langle \psi | B^*_\pi K \psi \rangle = \langle B^*_\pi B^*_\pi \psi | B^*_\pi K \psi \rangle = \langle B^*_\pi B^*_\pi \psi | B^*_\pi K \psi \rangle \quad \text{(I.81)} \]

meaning that the two states are orthogonal. We have thus proved that eigenvalues of \( W_{\text{BZ}} \) of a TRS-preserving 1D system come in pairs.

There is a simple physical interpretation of this result related to the fact that eigenvalues \( e^{i \phi^a} \) of \( W_{\text{BZ}} \) of a 1D system are related to the positions \( \bar{x}^a \) of the centres of Wannier orbitals within a unit cell [49, 54, 55]. Specifically,

\[ \frac{\bar{x}^a}{a} = \frac{\phi^a}{2\pi} \mod 1 \quad (I.84) \]

where “a” is the unit cell dimension of the 1D system.

With this insight, the result about the eigenvalue degeneracies of Wilson loop operator \( W_{\text{BZ}} \) of TRS-preserving systems can then be understood using the Kramers theorem: Every Wannier orbital (located at \( \bar{x}^a \)) has a time-reversal related partner obtained by complex conjugation and flipping spin (thus also located at \( \bar{x}^a \)).

An analogous argumentation can be made for inversion symmetric systems. We repeat steps (I.79a) to (I.80) with

\[ U(k_i) = U(-k_i) \tilde{B}(k_i) \quad (I.85a) \]

\[ i \phi^a = - \int_{-\pi}^{\pi} dk |u^a(k)|^2 \partial_k |u^a(k)|. \quad (I.83a) \]

Recall that the cell-periodic part of Bloch wave functions can be expressed using the Wannier orbitals up to the normalization factor as [55]

\[ \langle x | u^a(k) \rangle \equiv \bar{u}^a_k(x) \propto \sum_R e^{-ik(x-R)} W^a(x-R) \quad (I.83b) \]

where \( R \) are the Bravais vectors and \( W^a(x-R) \) is the \( a \)th Wannier orbital corresponding to unit cell labelled by \( R \). Insertion of relation (I.83b) into Eq. (I.83a) after some massaging yields

\[ \phi^a = \frac{2\pi}{a} \int_{-\infty}^{+\infty} dx |W^a(x)|^2 x \equiv \frac{2\pi}{a} \bar{x}^a. \quad (I.83c) \]

The generalization to the case of degenerate bands is derived in Appendix D of Ref [56].

18 For non-degenerate bands, \( A(k) \) of a 1D system becomes diagonal such that we can drop the path-ordering in Eq. (I.12). The phases of eigenvalues of \( W_{\text{BZ}} \) are thus trivially

\[ i \phi^a = - \int_{-\pi}^{\pi} dk |u^a(k)|^2 \partial_k |u^a(k)|. \quad (I.83a) \]

Recall that the cell-periodic part of Bloch wave functions can be expressed using the Wannier orbitals up to the normalization factor as [55]

\[ \langle x | u^a(k) \rangle \equiv \bar{u}^a_k(x) \propto \sum_R e^{-ik(x-R)} W^a(x-R) \quad (I.83b) \]

where \( R \) are the Bravais vectors and \( W^a(x-R) \) is the \( a \)th Wannier orbital corresponding to unit cell labelled by \( R \). Insertion of relation (I.83b) into Eq. (I.83a) after some massaging yields

\[ \phi^a = \frac{2\pi}{a} \int_{-\infty}^{+\infty} dx |W^a(x)|^2 x \equiv \frac{2\pi}{a} \bar{x}^a. \quad (I.83c) \]

The generalization to the case of degenerate bands is derived in Appendix D of Ref [56].

19 In fact, the argument applies equally well to system with a mirror symmetric that related \( H(k) \) to \( H(-k) \). At the mathematical level, all one needs is a unitary operator which related the two Hamiltonians for all \( k \in BZ \).
where $\mathcal{I}$ is the unitary operator of spatial inversion, and the sewing matrix is constrained by self-consistency to fulfil\(^\text{20}\)

$$
\widetilde{B}(-k_i)\widetilde{B}(k_i) = 1 \quad \Rightarrow \quad \widetilde{B}^2 = 1.
$$

(I.85b)

One can derive that

$$
\mathcal{W}_{\text{BZ}} = \widetilde{B}^\dagger \mathcal{W}_{\text{BZ}}^\dagger \mathcal{B}.
$$

(I.86a)

It follows that if $|\psi\rangle$ is an eigenstate of $\mathcal{W}_{\text{BZ}}$ with eigenvalue $e^{i\varphi}$, then $\mathcal{B}^\dagger |\psi\rangle$ is an eigenstate with eigenvalue $e^{-i\varphi}$ because

$$
\mathcal{W}_{\text{BZ}} \mathcal{B}^\dagger |\psi\rangle \quad \overset{(I.86a)}{=} \quad \mathcal{B}^\dagger \mathcal{W}_{\text{BZ}} \mathcal{B} \mathcal{B}^\dagger |\psi\rangle \quad \overset{(I.82a)}{=} \quad e^{-i\varphi} \mathcal{B}^\dagger |\psi\rangle
$$

(I.86b)

However, since $\mathcal{B}$ squares to $+1$, Kramers theorem does not apply and the two states $|\psi\rangle$ and $\mathcal{B}^\dagger |\psi\rangle$ may be the same states, in which case $e^{i\varphi} = \pm 1$. Alternatively, the two states are different such that $\mathcal{W}_{\text{BZ}}$ has a pair of eigenvalues $(e^{i\varphi}, e^{-i\varphi})$.

This observation can be again interpreted using the relation between the $\mathcal{W}_{\text{BZ}}$ eigenvalues and the centres of Wannier orbitals. In an inversion symmetric system, an inversion symmetric Wannier orbital is either centred at a site ($\bar{x}^a = 0 \Rightarrow \varphi^a = 0$) or in the middle between neighbouring sites ($\bar{x}^a = a/2 \Rightarrow \varphi^a = \pi$). Alternatively, a Wannier orbital located at a generic $\bar{x}^a$ is mapped by inversion operator onto another Wannier orbital located at $-\bar{x}^a$ ($\Rightarrow e^{\pm i\varphi^a}$).

Result (I.86a) has another important implication, namely that $\det \mathcal{W}_{\text{BZ}}$ must be real. Consequently, inversion symmetry quantizes the Zak phase

$$
\varphi_{\text{Zak}} = -i \log \det \mathcal{W}_{\text{BZ}}
$$

(I.87)

to 0 and $\pi$ [49, 56, 57]. This is our first example of a topological crystalline invariant, i.e. an invariant which is only robust as long as certain crystalline symmetry is present [58–60]. The non-trivial situation with $\varphi_{\text{Zak}} = \pi$ is characterized by the presence of electronic states localized

\(^{20}\)The second equation has a simple physical interpretation. Inversion symmetry requires $\mathcal{T} \mathcal{H}(k_i) \mathcal{T}^\dagger = \mathcal{H}(-k_i)$, therefore $\mathcal{T} \mathcal{H}(\pi) - \mathcal{H}(\pi) \mathcal{T} = [\mathcal{T}, \mathcal{H}(\pi)] = 0$ and the two operators can be diagonalized simultaneously. Additionally, $\mathcal{I}^2 = 1$ because spatial inversion is just a permutation of real space positions unafflicting the integral spin degree of freedom, therefore the possible eigenvalues of $\mathcal{I}$ are only $\pm 1$. Consequently, $\mathcal{I} \mathcal{U}(\pi) = \mathcal{U}(\pi) \mathcal{M}$ where $\mathcal{M}$ is a diagonal matrix of $\pm 1$ inversion eigenvalues of states forming the columns of $\mathcal{U}(\pi)$. Comparing to Eq. (I.85a) we see that $\mathcal{B} = \mathcal{M}$ which clearly squares to $1$. 
at the system edges. Depending on whether such a state is occupied or unoccupied, the edge carries a fractional $\pm e/2$ charge \[61\]. Due to the absence of a particle-hole symmetry, these edge states are not bound to lie at zero energy \[57\] which also leads to a deviation from the exact $\pm e/2$ charge quantization.

**I.2.4 Quantum spin Hall insulators**

A possible way around the problem of vanishing Chern number in TRS-preserving systems is to consider a system that additionally preserves $s_z$ spin component. Then one may assume that our original model (I.1) corresponds to spin-up electrons, while the time-reversed image corresponds to spin-down electrons. For example, Hamiltonian

$$\mathcal{H}(k) = [h_0(k) \mathbb{1}_\tau + h(k) \cdot \tau] \otimes \sigma_z$$

(I.88)

where $\tau_i$ Pauli matrices correspond to an orbital and $\sigma_i$ to the spin degree of freedom, becomes time-reversal symmetric with $T = -i\sigma_y K$ when functions $h_{0,x,z}$ are odd and $h_y$ is even in $k$. Especially, the slightly modified version of (I.7) from Ref. [43]

$$h_0(k) = 0 \quad \text{and} \quad h(k) = (\sin k_y, m - \cos k_x - \cos k_y, \sin k_x)^	op$$

(I.89)

is compatible with time-reversal symmetry. The explicit presence of spin Pauli matrices in the Hamiltonian indicates that the hopping amplitudes have to be spin-dependent, which means that Hamiltonian (I.88) can only be realized in spin-orbit coupled systems.

Compatible with the discussion in Subsec. I.2.2, the total Chern number over the lower two bands is zero. However, the conservation of $s_z$ spin component allows us to define a spin Chern number

$$c_1^\uparrow = \frac{1}{2\pi} \oint_{\text{BZ}} dk_x dk_y \text{ tr } \mathcal{F}_{xy}^\uparrow(k) \in \mathbb{Z}.$$  (I.90)

where and $\mathcal{F}^\uparrow(k)$ [and the corresponding $\mathcal{A}^\uparrow(k)$] is defined analogous to Eqs. (I.22) and (I.32) but where we only collect the spin-up occupied bands. The spin Chern number of model (I.89) depends on $m$ in the same way as the (ordinary) Chern number of model (I.7). A system with spin Chern number $c_1^\uparrow$ develops $|c_1^\uparrow|$ spin-up edge modes moving around the sample in one direction, and the same number of spin-down edge modes moving in the opposite direction.
I.2. Time-reversal symmetric insulators

Figure I.5: Edge states of time-reversal symmetric insulators (a) A single pair of counter-propagating edge states of a TRS-preserving insulator need to cross at a TRIM. This crossing is protected by Kramers theorem and is therefore robust against all perturbations that respect TRS. On the other hand, (b), two pairs of edge modes lead to crossings at generic $k$-points. These are allowed to hybridize and thus open a gap in the edge excitation spectrum. This means that a situation with two pairs of edge modes is equivalent to a situation with no edge modes. The band crossings protected by Kramers theorem (indicated by arrows) do not affect the argument.

I.2.5 Pfaffian characterization of topological insulators

The problem with invariant (I.90) is that it ceases to be well-defined whenever the Hamiltonian (I.88) acquires terms proportional to $\sigma_x$ or $\sigma_y$ which break the spin-$s_z$ conservation. Then it is not possible to label the bands by their $s_z$ quantum number because they become a mixture of both. However, the breakthrough Refs. [11, 12] showed that $Z_2$ parity of the invariant continues to be well-defined.

The physical reason for the protection of a $Z_2$ invariant is not hard to understand and is related to Kramers theorem for half-integer spin: A single pair of counter-propagating edge modes has to cross at a time-reversal invariant momentum (TRIM) and the crossing is protected by TRS. Because of this degeneracy, there is no way of evolving the situation illustrated in Fig. I.5(a) into a situation without edge modes (unless we close the bulk gap). Therefore, a single pair of edge modes is robust, even if we keep including terms that violate the $s_z$ spin conservation.

On the other hand, two pairs of edge modes are not robust. As indicated in Fig. I.5(b), only the crossings occurring at a TRIM (indicated by arrows) are protected by Kramers theorem. The other two crossings occur at low-symmetry $k$-points and are allowed to hybridize. Therefore, a gap opens in the edge spectrum which allows us to remove all
Figure I.6: Understanding $\mathbb{Z}_2$ topological insulators using the Pfaffian invariant. (a) One pair of zeros of $\mathcal{P}(k) \in \mathbb{C}$ (red crosses) located at momenta $\pm k_0$ (indicated by thin straight arrows) is characterized by opposite phase windings (curly black arrows). The two points could in principle meet and annihilate at a TRIM $\Gamma$ (black dots), but TRS also enforces $|\mathcal{P}(\Gamma)| = 1$, rendering such a process impossible. Consequently, a single pair of zeros is robust. On the other hand, (b), two pairs of zeros can be brought together (wide arrows) and annihilated. This means that only the parity of the number of pairs of zeros is a topologically robust quantity, hence manifesting the $\mathbb{Z}_2$ classification of time-reversal symmetric insulators.

edge states with an adiabatic evolution without closing the bulk excitation gap. We thus conclude that two pairs of edge modes are equivalent to no edge modes, hence there is a $\mathbb{Z}_2$ topological classification.

Historically, the $\mathbb{Z}_2$ charge of topological insulators was first formulated using the matrix

$$
\mathcal{T}^{ab}(k) = \langle u^a(k) | T u^b(k) \rangle
$$

which can be easily shown to be antisymmetric [11, 62],

$$
\mathcal{T}^{ab}(k) = \langle u^a(k) | T u^b(k) \rangle = \langle T^2 u^b(k) | T u^a(k) \rangle = -\mathcal{T}^{ba}(k)
$$

and therefore has a well-defined Pfaffian $\mathcal{P}(k) = \text{Pf} \mathcal{T}(k)$. In the absence of additional symmetries, $\mathcal{P}(k)$ is a complex-valued function, meaning that two parameters (i.e. momenta) have to be tuned to obtain a zero. We say that the codimension of roots of $\mathcal{P}(k)$ is $\delta = 2$. Such a codimension argument implies that zeros of $\mathcal{P}(k)$ in two spatial dimensions generically occur at points.

A slight complication is that $\mathcal{P}(k)$ is not invariant under gauge transformation (I.15). This is seen from

$$
\tilde{\mathcal{T}}(k) = \mathcal{X}^\dagger(k) \mathcal{T}(k) \mathcal{X}^* \quad \Rightarrow \quad \tilde{\mathcal{P}}(k) = \mathcal{P}(k) \det \mathcal{X}^*(k)
$$
which is a $U(1)$ phase rotation. However, zeros of $\mathcal{P}(k)$ do not have a phase and are therefore gauge-invariant. Additionally, TRS implies that if $\mathcal{P}(k_0) = 0$ then also $\mathcal{P}(-k_0) = 0$. Finally, TRS also implies that at time-reversal invariant momenta (TRIMs) $k = \Gamma$, the matrix $T(\Gamma)$ takes a block-diagonal form

$$
T(\Gamma) = \bigoplus_{a} \begin{pmatrix}
0 & e^{i\varphi_a} \\
-e^{i\varphi_a} & 0
\end{pmatrix} \implies |\mathcal{P}(\Gamma)| = 1.
$$

This implies that a pair of TRS-related zeros of $\mathcal{P}(k)$ cannot meet and annihilate at a TRIM.

We show in Fig. I.6 that there are two possible scenarios, corresponding again to the $\mathbb{Z}_2$ invariant: Either there are no zeros of $\mathcal{P}(k)$ inside BZ, or there is precisely one pair of TRS-related zeros. Two pairs of zeros can be brought together and annihilated as shown in Fig. I.6(b), meaning that such a situation is equivalent to the trivial case. We conclude that only the parity of the number of pairs of zeros is a robust quantity.

Note that the same codimension argument implies that in 3D the zeros of $\mathcal{P}(k)$ occur along lines. Similar to the situation in 2D, these lines cannot pass through a TRIM, and have to be distributed symmetrically with respect to TRIMs. A careful analysis reveals that there are $16 = 2^4$ topologically inequivalent possibilities of distributing the lines of zeros which are compatible with these rules, and we list them in Fig. I.7. They can be described with four $\mathbb{Z}_2$ charges [63, 64]. One of them (the strong index $\nu_0$) corresponds to the parity of the number of lines of zero, while the other three [the weak indices $(\nu_x, \nu_y, \nu_z)$] describe the way the lines of zero cross the BZ boundary along the $(k_x, k_y, k_z)$-directions.\footnote{Note that the weak indices are absent in continuum models which expand BZ into $\mathbb{R}^D$ without a boundary, while the strong index survives such a procedure. The same dichotomy is predicted for the robustness against Anderson localization in the presence of disorder [64].}

Insulators with a non-trivial value of the strong index are associated with an odd number of surface Dirac\footnote{In the terminology of the subsequent chapters, we should actually call it \textit{surface Weyl cone} because of the absence of spin degeneracy of the surface bands. However, we stick here to the established terminology which ignores this subtlety.} cones located at TRIMs of the surface BZ.

The Pfaffian formulation of the $\mathbb{Z}_2$ invariant is modified in the pres-
I. Topological invariants

ence of spatial inversion symmetry $\mathcal{I}$. Then we find that

$$T(k) = U(k)^\dagger T U(k) = [T T I U(k)]^\dagger [T I U(k)]$$

$$= [T U(k) B(k)]^\dagger U(k) B(k) = B^\top(k) \left[ U^\dagger(k T U(k)) \right]^\dagger B(k)$$

$$= B^\top(k) T^\dagger(k) B(k) \quad (I.95)$$

where we used that the composed $\mathcal{IT}$ symmetry is antiunitary, that $[T, I] = 0$ mutually commute, and we introduced a sewing matrix $B(k)$. The Kramers theorem applying to $(\mathcal{IT})^2 = -\mathbb{1}$ allows us to locally find a gauge such that

$$B(k) = \bigoplus_{a=1}^{n/2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (I.96)$$

which has $\det B(k) = 1$. Then Eq. (I.95) implies that $\det T(k)$ is real, and the codimension of roots of $\mathcal{P}(k)$ becomes $\delta = 1$. Consequently, zeros of $\mathcal{P}(k)$ lie on lines in 2D and on surfaces in 3D systems. These lines or surfaces separate TRIMs with positive and negative inversion eigenvalues of the occupied bands and allow for an alternative expression for the strong index

$$(-1)^{v_0} = \prod_{k \in \text{TRIMs}} \left( \prod_{a=1}^{n} \delta_k^a \right) \quad (I.97)$$

where $\delta_k^a$ is inversion eigenvalue of state $|u^a(k)\rangle$. Similar expressions (where the first product goes only over TRIMs with $k_i = \pi/a$) also exist for weak indices $v_i$ [65].

Crystalline symmetries can constrain the possible values of these four topological indices. For example, in cubic lattices the symmetry enforces the three weak indices to take the same value [66]. Another example are 2D systems with a glide-plane symmetry which automatically have a non-trivial $\mathbb{Z}_2$ index in the case of $4n + 2$ occupied bands [37] as we discuss in chapter III. On the other hand, there are also multiple circumstances when a crystalline symmetry facilitates new species of topological invariants [59, 67–69].

We remark that the Pfaffian formulation of the $\mathbb{Z}_2$ invariant of TRS-preserving systems does not offer a particularly deep explanation of what is really going on. In fact, it becomes misleading if one tries to apply it to other symmetry classes. For example, in the absence of spin-orbit coupling (SOC) one can effectively drop the spin degree of freedom
Figure I.7: Topological phases of 3D time-reversal symmetric insulators

The blue box is the BZ with periodic boundaries, the black dots indicate TRIMs, and red lines correspond to zeros of $P(k)$. Each time-reversal symmetric insulator (in the absence of additional symmetries) has zeros of $P(k)$ which can be adiabatically evolved without closing the bulk gap into one of the sixteen plotted situations. Furthermore, the sixteen listed situations cannot be adiabatically evolved into one other. This indicates the presence of four $\mathbb{Z}_2$ indices. One of them (the strong index) describes the parity of the number of lines of zero (odd in the upper eight, even in the lower eight), while the other three (the weak indices) describe the way the lines of zero cross the BZ boundaries in the $(k_x,k_y,k_z)$-directions.

and represent $\mathcal{T} = \mathcal{K}$ (i.e. we treat electrons as spinless particles) which squares to $+1$. In this case, the matrix $\mathcal{T}(k)$ defined as in Eq. (I.91) becomes symmetric. Then the Pfaffian does not exist, but one may instead
Figure I.8: Insulators with $\mathcal{T}^2 = +1$ described by model (I.1) with $h_{0,x,z}$ even and $h_y$ an odd function of $k$. The red line indicates $\text{sign}[h_x(k)] = 0$ and the green line indicates $\text{sign}[h_z(k)] = 0$ inside BZ (the blue square). Zeros of $\mathcal{D}(k)$ occur where the two lines cross. We argue in the text, that the number of times this happens must be an integer multiple of 4, indicating the absence of the $\mathbb{Z}_2$ invariant in the absence of SOC.

consider the determinant $\mathcal{D}(k) = \det \mathcal{T}(k)$. In the absence of additional symmetries, $\mathcal{D}(k) \in \mathbb{C}$ has codimension $\delta = 2$, meaning that in 2D its zeros appear again at points. One might naively consider again the parity of the number of pairs of such zeros as a $\mathbb{Z}_2$ invariant.

But this idea does not work. The reason is that it is simply not possible to get a situation with a single pair of zeros (and we already argued that two pairs of zeros are not robust), such that the sought after “to-be-topological” phase is non-existent. We illustrate this on the simplest possible half-filled two-band model (I.1) which preserves $\mathcal{T} = \mathcal{K}$ if $h_{0,x,z}$ are even and $h_y$ is an odd function of momentum $k = (k_x, k_y)$. According to the solution (I.49), the gauge invariant absolute value $|\mathcal{D}(k)|$ becomes

$$|\mathcal{D}(k)| = \left| e^{2i\phi_h} \sin^2 \frac{\theta_h}{2} + \cos^2 \frac{\theta_h}{2} \right|. \quad (I.98)$$

This vanishes only if $\theta_h = \pi/2$ and $\phi_h = \pi/2 \pmod{\pi}$, which is equivalent to $h_x = h_z = 0$ (if furthermore $h_y = 0$, the system ceases to be insulating).

It is useful to plot $\text{sign}[h_x(k)]$ and $\text{sign}[h_z(k)]$ throughout BZ as we do in Fig. I.8. Consider moving along the contour $h_x(k) = 0$ from some starting point $k_0$ until we reach either $-k_0$ or $k_0$.

- In the case we come to $-k_0$ first, the symmetry implies that $h_z(k_0) =$
I.2. **Time-reversal symmetric insulators**

$h_z(-k_0)$ have the same sign, meaning that we had to cross $h_z(k) = 0$ an even number of times along the way. Then moving along the remainder of the contour from $-k_0$ back to $k_0$ we encounter time-reversed images of these zeros. Altogether, we encountered $4n$ zeros of $D(k)$.

- If we return back to $k_0$ without passing through $-k_0$, then there must be two disjoint contours of $h_z(k) = 0$ that are time-reversed images of each other. Since we returned to the original point, the sign of $h_z(k)$ had to change an even number of times along each of the two contours, meaning that there are $4n$ zeros of $D(k)$ again.

### I.2.6 Wilson loop description of 2D systems

We conclude this section with another perspective on the origin of the $\mathbb{Z}_2$ charge in (spinful) TRS-preserving insulators. This approach uses the notion of Wilson loops, and it is very convenient because it allows for the characterization of many further topological invariants within a unified language [56, 70, 71]. Because of the equivalence between Wilson loop spectra and the Wannier orbital centres, this approach also provides a clear physical interpretation of what the non-trivial topology microscopically corresponds to.

Consider a two-dimensional system with Hamiltonian $\mathcal{H}(k_x, k_y)$. We will fix one momentum (e.g. $k_x$) and treat the other one ($k_y$) as describing some 1D system [i.e. we write $\mathcal{H}_{k_x}(k_y)$]. Then it is natural to determine the Wilson operators along BZ of the 1D systems, obtaining $\mathcal{W}(k_x)$. For $k_x = 0$ and $k_x = \pi$, the one-dimensional Hamiltonian $\mathcal{H}_{k_x}(k_y)$ becomes time-reversal symmetric, meaning that according to Subsec. I.2.3 its eigenvalues come in doubly-degenerate pairs. These degeneracies split for the intermediate momenta. Finally, the spectrum of $\mathcal{W}(k_x)$ and $\mathcal{W}(-k_x)$ are identical, because the states along one closed loop are time-reversed images of states along the other loop, such that the arguments of Subsec. I.2.3 apply again. This indicates, that all the useful information about the insulating state is already encoded in half of the Wilson loop spectra, $\mathcal{W}(k_x)$ with $k_x \in [0, \pi]$. As we show in Fig. I.9, there are basically two possibilities: Either each pair of degenerate states at $k_x = 0$ becomes degenerate again at $k_x = \pi/a$ (trivial case), or the pairs get mixed (topological case).

A useful interpretation of these connectivities is obtained if we re-
Figure I.9: Two species of Wilson loop spectra in 2D time-reversal symmetric (spinful) insulators with six occupied bands. (a) Spectrum with no winding indicates a trivial $\mathbb{Z}_2$ invariant, while (b) a “zig-zag” spectrum indicates a non-trivial value of the $\mathbb{Z}_2$ invariant. The double degeneracies at $k_x a \in \{0, \pi\}$ are protected by TRS as explained in Subsec. I.2.3. Since there is no symmetry that could protect a band crossing at a generic $0 \neq k_x a \neq \pi$, these two options exhaust all the possibilities. Only spectra for $k_x a \in [0, \pi]$ are plotted, since the spectra for $k_x a \in [-\pi, 0]$ are mirror-symmetric versions of the plotted images.

place momentum $k_x a$ by time $t$. Periodicity in $k_x$ is replaced by $\mathcal{H}_t(k_y) = \mathcal{H}_{t+T}(k_y)$, i.e. the 1D Hamiltonian performs periodic cycles in time, and TRS is translated into $\mathcal{H}_t(k_y) = \mathcal{H}_{-t}(k_y)$. Then the lines in Fig. I.9 describe the motion of Wannier charge centres between the atomic sites during one half of the cycle. Completing these spectra with their mirror images for $k_x a \in [\pi, 2\pi]$, we observe that the situation in Fig. I.9(b) “pumps” a pair of orbitals in opposite directions, while no such motion takes place in situation in Fig. I.9(a). This means that $\mathcal{H}_t(k)$ describes a $\mathbb{Z}_2$ pump [62] which becomes a spin pump if $s_z$ is conserved.

One can similarly interpret the Hamiltonian of a Chern insulator, e.g. (I.1). In this case, the TRS condition is dropped, meaning that $\mathcal{W}(0)$ and $\mathcal{W}(\pi)$ do not contain the double degeneracies, and we need to plot $\mathcal{W}(k_x)$ for all $k_x a \in [0, 2\pi]$ to obtain the complete information about the bands. After one cycle $T$, the Wannier charge centres reach the original set of positions, but they might have been shifted one-by-one as shown in Fig. I.10(a). This is associated with pumping one electron charge across the unit cell.\[23\] However, the Wannier orbitals might as well have been shifted by any integer number of positions, e.g. by two

\[23\]Since such a shift takes place within each unit cell, one electron charge has, in fact, been pumped along the entire 1D crystal.
I.3. Tenfold way classification

In this final introductory section we review the complete topological classification of weakly interacting gapped phases (i.e. insulators and superconductors) [73] based on the spatial dimension $D$ of the system, and on its global symmetries, i.e. time-reversal symmetry (TRS, $T$), particle-hole symmetry (PHS, $P$) and chiral symmetry (CHS, $C$).

The usual crystalline symmetries (i.e. inversion, mirrors, rotations) are represented by unitary operators that commute with the Hamiltonian $\mathcal{H}$, thus allowing us to block-diagonalize $\mathcal{H}$ into sectors of different operator eigenvalues. The global symmetries act differently – they either anticommute with $\mathcal{H}$ (case of CHS), or are antiunitary (case of TRS), or both (case of PHS), such that the block-diagonalization does not apply. Upon switching to momentum space description with Hamiltonian $\mathcal{H}(k)$, the three global symmetries are defined by the presence of opera-

\[ \begin{align*}
\mathcal{H} &\rightarrow \mathcal{H} \quad \text{(case of CHS)} \\
\mathcal{H} &\rightarrow -\mathcal{H} \quad \text{(case of TRS)} \\
\mathcal{H} &\rightarrow \mathcal{P} \mathcal{H} \mathcal{P}^{-1} \quad \text{(case of PHS)}
\end{align*} \]

\[ \mathcal{P} \equiv \mathcal{P}(\mathbf{r}) \quad \text{is a periodic function of position.} \]

Figure I.10: Wilson spectra of Chern insulators with four occupied bands. (a) After one period, the Wannier charge centres return to the original set of positions, but one electron charge has been pumped across the unit cell, indicating $c = 1$. (b) Shifting the Wannier charge centres by two orbital positions indicates $c = 2$.

as in Fig. I.10(b) which corresponds to two pumped electron charges. Such a charge pump offers an alternative understanding of the $\mathbb{Z}$-valued Chern number [72], i.e. $c = 1$ in Fig. I.10(a) and $c = 2$ in Fig. I.10(b).
Table I.1: Tenfold way classification table. The column CL lists all ten AZ symmetry classes according to their Cartan label. The next three columns indicate the presence (1) or the absence (×) of time-reversal (T), particle-hole (P) and chiral (C) symmetry in a given class. The ± sign represents the square of the corresponding operator. The remaining columns list the range of values of the strong topological invariant $\nu^{(D)}_{\text{CL}}$ for the symmetry class of arbitrary spatial dimension D. All symmetry classes exhibit the Bott periodicity [74]. In complex cases (rows A and AIII) this means that the pattern repeats after two entries, while for the real cases (rows AI to CI) the period comprises eight entries.

<table>
<thead>
<tr>
<th>CL</th>
<th>symmetry</th>
<th>topological invariant $\nu^{(D)}_{\text{CL}}$ for D = …</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>× × × †</td>
<td>0 1 2 3 4 5 6 7 8</td>
</tr>
<tr>
<td>AIII</td>
<td>× × † 1</td>
<td>0 0 0 0 0 0 0 0 0</td>
</tr>
<tr>
<td>AI</td>
<td>+1 × × 1</td>
<td>Z 0 Z 0 Z 0 Z 0 Z 0 Z 0</td>
</tr>
<tr>
<td>BDI</td>
<td>+1 +1 1 ×</td>
<td>Z_2 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0</td>
</tr>
<tr>
<td>D</td>
<td>× +1 × †</td>
<td>Z_2 Z_2 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0</td>
</tr>
<tr>
<td>DIII</td>
<td>−1 +1 1</td>
<td>0 Z_2 Z_2 Z 0 Z 0 Z 0 Z 0 Z 0</td>
</tr>
<tr>
<td>AII</td>
<td>−1 × × †</td>
<td>0 Z 0 Z_2 Z_2 Z 0 Z 0 Z 0 Z 0</td>
</tr>
<tr>
<td>C</td>
<td>× −1 × 1</td>
<td>0 0 0 Z 0 Z 0 Z 2 Z 2 Z 0 Z 2 Z 2 Z 0 Z 2 Z 0 Z 0 Z 2 Z 2 Z 0 Z 0</td>
</tr>
<tr>
<td>Cl</td>
<td>+1 −1 1 †</td>
<td>0 0 0 Z 0 Z 0 Z 2 Z_2 Z 2 Z 0 Z 0 Z 0</td>
</tr>
</tbody>
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The operators fulfilling

$$\mathcal{T}\mathcal{H}(k)\mathcal{T}^{-1} = \mathcal{H}(-k) \quad \mathcal{T}^2 = \pm 1 \quad (\text{AU}) \quad (I.99a)$$
$$\mathcal{P}\mathcal{H}(k)\mathcal{P}^{-1} = -\mathcal{H}(-k) \quad \mathcal{P}^2 = \pm 1 \quad (\text{AU}) \quad (I.99b)$$
$$\mathcal{C}\mathcal{H}(k)\mathcal{C}^{-1} = -\mathcal{H}(k) \quad \mathcal{C}^2 = 1 \quad (U) \quad (I.99c)$$

where (AU) indicates antiunitarity and (U) unitarity. The fact that $\mathcal{T}^2 = \pm 1$ has been explained in Subsec. I.2.1, and we will see in chapter IV that $\mathcal{P}^2 = \pm 1$ has a natural realization in triplet/singlet superconductors [21].

We observed in Subsec. I.2.5 that the square $\mathcal{T}$ matters for the topological classification. The same dichotomy also appears for $\mathcal{P}^2$. Because of the antiunitarity of these operators, the value of their square is unchanged upon a $U(1)$ phase multiplication, i.e.

$$(e^{i\varphi}\mathcal{T})^2 = e^{i\varphi}\mathcal{T}e^{i\varphi}\mathcal{T} = e^{i\varphi}e^{-i\varphi}\mathcal{T}^2 = \mathcal{T}^2 \quad (I.100)$$

and similarly for $\mathcal{P}$. On the other hand, the square $\mathcal{C}^2$ of the unitary oper-
I.3. Tenfold way classification

Operator $C$ can be made to take any complex phase using such a phase multiplication. Furthermore, whenever the system has both $T$ and $P$, then it also has $C = TP$, although $C$ can also be present when both $T$ and $P$ are absent. Taken together, Eqs. (I.99) define 10 possible Atland-Zirnbauer (AZ) symmetry classes [41] which we list in Table I.1 alongside their Cartan label.

Using mathematical methods which are beyond the scope of this thesis, a series of Refs. [73, 75, 76] derived the range of values of the strong topological invariant $\nu_{\text{CL}}^{(D)}$ for all AZ symmetry classes of arbitrary spatial dimension $D$. We reproduce this result in Tab. I.1. An accessible overview of the meaning of most of these topological invariants appears in chapter 1 of Ref. [77].

Let us locate within this table the three systems discussed explicitly in previous sections. Chern insulators of Sec. I.1 do not have any of the global symmetries (I.99), meaning that they belong to class A which indeed has a $\mathbb{Z}$-valued topological invariant in 2D. Topological insulators of Sec. I.2 have $T^2 = -1$, meaning that they belong to class AII which has $\mathbb{Z}_2$ classification in both 2D and 3D. Finally, the insulators without SOC such that effectively $T^2 = +1$ which we briefly tackled in Subsec. I.2.5 belong to class AI which does not have a topological invariant in 2D.

Reference [75] used $K$-theory to go one step further. It showed that because of the finiteness and periodic boundary conditions of BZ, additional weak indicates can appear. In $D$ spatial dimensions, these indices describe the $d$-dimensional hyperplanes winding around BZ in all $(D_d)$ possible orientations, for all values of $1 \leq d \leq D - 1$. Consequently, the total topological classification becomes

$$\tilde{\nu}_{\text{CL}}^{(D)} = \bigoplus_{d=1}^{D} \left( \nu_{\text{CL}}^{(D)} \right)^{\oplus (D_d)} \tag{I.101}$$

This is compatible with our observation of three weak indices appearing in 3D topological insulators in Subsec. I.2.5, when the direct sum (I.101) explicitly expands as

$$\tilde{\nu}_{\text{AII}}^{(3)} = 0^{\oplus 3} \oplus \mathbb{Z}_2^{\oplus 3} \oplus \mathbb{Z}_2. \tag{I.102}$$
SYMMETRY of solids is significantly decreased relative to the Galilean and Poincaré groups. Consequently, many terms are allowed in the Hamiltonian that are not permissible in high-energy physics theories. This leads to electron spectra that disperse differently in various directions. Furthermore, the finite size of the unit cell leads to a natural momentum cut-off – the Brillouin zone (BZ) – causing the spectrum to bend down on the BZ boundary. Furthermore, the multitude of atomic orbitals and the possibly large number of atoms per unit cell lead to the presence of many such complicated electron bands. The seemingly messy band structure “spaghetti” plots that come out of first-principle calculations can be understood using the remnant symmetry of the crystal – its space group – and the theory of its irreducible representations.

In the following two chapters we discuss how space group symmetries sometimes enforce multiple bands to come together and to become degenerate at a point or along a line in momentum space. The electron spectrum in the vicinity of such band structure nodes can be very different from the dispersion of free particles. If such a node occurs very close to the Fermi level, the unusual electron dispersion leads to special signature in various physical properties like conductivity or the surface states. Importantly, since a typical band width is much larger than the room temperature, one can perform a series expansion (usually called $k \cdot p$ expansion in this context) to derive an effective low-energy theory, which often becomes very symmetric.

However, sometimes a band structure node cannot be sufficiently
explained by space group symmetry alone, and one has to start explicitly considering the topology of the underlying electron wave functions. The most prominent example of such a situation is offered by Weyl points – touching points of conduction and valence bands which act as monopoles of the Berry curvature field $\mathcal{F}(k)$ in momentum space. Weyl points, and their close cousins the Dirac points, share certain similarities with ultrarelativistic particles and have incited much research interest. They are the main actors of the present chapter.

We start the discussion in Sec. II.1 with a brief overview of the current research status of Weyl and Dirac semimetals, i.e. materials having Weyl or Dirac points in the vicinity of the Fermi level. Among the many interesting topics within this field, we pay attention only to those that are directly relevant to our work. We first clarify the topological protection and the role of symmetries in the appearance of Weyl points. We show that Weyl points are actually closely related to Chern insulators and we use this connection to explain the presence of Fermi arcs located on the surfaces of such materials. We further make a few comments on the chiral anomaly present in such systems, specifically how this leads to anomalous negative longitudinal magnetoresistance. At various places we mention known material examples and further predicted candidates for these semimetallic phases. Numerous references direct the reader to the original research articles.

In Sec. II.2 we introduce the reader to pyrochlore oxides. These are materials with a frustrated lattice, hosting $5d$ electrons with strong spin-orbit coupling and intermediate interaction strength. Because of these features, pyrochlore oxides have been predicted to host numerous exotic electronic phases. We add one more ingredient to the description of electrons on such a lattice, namely the leading coupling to an elastic degree of freedom. At the same time, we drop electron interactions to keep the discussion simple. We show that for special integer fillings of the band structure, such a model may at low temperatures exhibit a spontaneous lattice distortion. Importantly, the change in the crystalline structure is accompanied with the evolution of the electron band structure from Dirac semimetal through Weyl semimetal to an insulator.

We dedicate the next Sec. II.3 to theoretically explain the observations of the previous section. We apply the methods of group theory to explain the presence of three Dirac points in the band structure of undistorted pyrochlore oxides, and in much detail discuss why the inversion-
breaking lattice distortion splits each Dirac point into four Weyl points. This section is supplemented with Appendix A which provides a theoretical underpinning of some of the applied mathematical methods. This section is rather technical, and can be easily skipped without losing understanding of the subsequent text.

We conclude in Sec. II.4 with the analysis of the surface states of the developed model for various surface terminations, and for various amplitudes of the lattice distortion. We observe that the variation of the parameters sometimes leads to a reconnection of the surface Fermi arcs. Alternatively, such a reconnection can also be achieved with the application of a surface gate potential. We refer to such a phenomenon as a Weyl-Lifshitz transition. We indicate, how this phenomenon might be observed experimentally by detecting quantum oscillations in a magnetic field.

II.1 Research overview

II.1.1 Topological protection

Let us first state here what we mean by an ideal Weyl and Dirac point, and we will worry about their possible realizations in crystalline solids afterwards. Inspired by massless Weyl and massless Dirac particles in high-energy physics (HEP), we write

\[ H_\text{ideal}^\text{Weyl}(k) = (\pm)v_k \cdot \sigma \quad \text{and} \quad H_\text{ideal}^\text{Dirac}(k) = v_k \cdot \Gamma, \quad (II.1a) \]

where \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) are anticommuting 2 \( \times \) 2 Pauli matrices, \( \Gamma = (\Gamma_1, \Gamma_2, \Gamma_3) \) are anticommuting 4 \( \times \) 4 Dirac matrices, and \( v \) has dimension of velocity.\(^1\) In both cases, the energy spectrum is \( \varepsilon_{\pm}(k) = \pm k. \) The difference is that in the Weyl case the bands are non-degenerate, while in the Dirac case they are both doubly degenerate. At this level of discussion we do not bother about the microscopic meaning of the two-level (four-level) degree of freedom appearing in the Weyl (Dirac) point Hamiltonian.

In solids, one typically finds anisotropic Weyl and Dirac points. These

---

\(^1\)Our definition of Dirac matrices deviates slightly from the standard HEP definition. This is related to the different metric tensor. See the discussion at the beginning of chapter III for more details.
still disperse linearly in all directions; in the most general case

\[
\mathcal{H}_{\text{Weyl}}(k) = \sum_{i=1}^{3} w_i k_i \sigma_i + \sum_{i,j=1}^{3} \nu_{ij} k_i \sigma_j \quad (\text{II.1b})
\]

\[
\mathcal{H}_{\text{Dirac}}(k) = \sum_{i=1}^{3} w_i k_i \Gamma_i + \sum_{i,j=1}^{3} \nu_{ij} k_i \Gamma_j \quad (\text{II.1c})
\]

where \( \nu \) is an invertible matrix. In both cases

\[
\epsilon_{\pm}(k) = w \cdot k \pm \|\nu k\| \quad (\text{II.1d})
\]

The \( w \) terms tilts the conical spectrum, and plays a crucial role in the appearance of the tipped “type-II” points [78, 79]. Double/triple Weyl and Dirac points which have a quadratic/cubic dispersion in two perpendicular directions are also possible in the presence of certain crystalline symmetries [35, 80, 81] but we do not consider them in the present work.

Note that the ideal Weyl Hamiltonian is mathematically equivalent to the Hamiltonian of spin-\(^{-1}\)\(^2\) particle in magnetic field which we analysed in Subsec. I.1.5. As derived therein, this leads to the appearance of Berry curvature

\[
\Omega(k) = \pm \frac{k}{2k^3} \quad (\text{II.2})
\]

which yields a \( \pm 2\pi \) flow through any closed surface surrounding the point. This is in a seeming contradiction with the conservation of Berry field lines in Eq. (I.55a), but there we assumed non-degenerate bands. We observe that a Weyl point acts as \( \pm 2\pi \) monopole of the \( \Omega(k) \) field in the occupied bands [50]. The sign is tied to the sign in Eq. (II.1a) and is called the chirality \( h \) of the Weyl point. In the most general case of Eq. (II.1b), the monopole strength can still be shown be \( 2\pi \), and the chirality is defined as \( h = \text{sign} |\det \nu| \). The monopole character implies that Weyl points can be viewed as topological defects in \( k \)-space. The topological stability of a Weyl point can also be seen be adding the most general\(^2\) perturbation \( a \cdot \sigma \) to Hamiltonian (II.1b) which only shifts the band degeneracy from \( k = 0 \) to \( k = -\nu^{-1} a \), but cannot remove it.

\(^2\) By the “most general” we mean one that does not break translational invariance, such that the Fourier transformation to \( \mathcal{H}(k) \) is still meaningful, although the characteristic features of Weyl semimetals can survive quite a lot of disorder too, see e.g. [82]. The constant (\( k \)-independent) term \( a \cdot \sigma \) is dominant in the vicinity of the Weyl point. Another possibility to gap out a Weyl (semi)metal is through superconductivity, but even this may require the additional breaking of certain symmetries [83].
II.1. Research overview

Figure II.1: Symmetry transformation of Weyl points. (a) In systems with \( I \) (and no \( T \)), the Berry curvature \( \Omega(-k) = \Omega(k) \) [derived in Eq. (I.77)], which is represented by the parallel light blue arrows. Consequently, a pair of Weyl points related by \( I \) have \textit{opposite} chiralities. (b) In systems with \( T \) (and no \( I \)) the opposite relation \( \Omega(-k) = -\Omega(k) \) holds [derived in Eq. (I.75)], as exemplified by the antiparallel light blue arrows. It follows that a pair of Weyl points related by \( T \) have the \textit{same} chirality.

An important observation is that a Weyl point is not possible in a system respecting both time-reversal \( T \) and inversion symmetry \( I \). As mentioned in Subsec. I.2.5, their composition \( TI \) is an antiunitary operator squaring to \(-1\) which preserves momentum. Consequently, states \(|u(k)\rangle\) and \(TI|u(k)\rangle\) form a Kramers pair, being located at the same momentum and the same energy. In other words, because of the presence of the \( TI\)-symmetry, all bands are doubly degenerate, which contradicts the properties of a Weyl point. We say that the Dirac spectrum is \textit{spin-degenerate}, while the Weyl spectrum is \textit{spin-split}.

This means that to realize a Weyl semimetal, one has to break \( T \) or \( I \). If one breaks \( T \) while keeping \( I \), Weyl points appear in pairs of \textit{opposite} chiralities located at \( \pm k \), as shown in Fig. II.1(a). On the other hand, systems breaking \( I \) while keeping \( T \) have pairs of Weyl points of the \textit{same} chirality located at \( \pm k \), as illustrated in Fig. II.1(b). Both scenarios were investigated in the context of normal insulator vs. topological insulator (NI-TI) multilayers [84–86] early after the concept of Weyl points in solids was introduced in the context of magnetic pyrochlore iridates [29].

These two realization are also characterized with a different minimal number of Weyl points. First, note that the net flow of Berry curvature through the BZ boundary must vanish. This is because the BZ boundary consists of pairs of opposite faces, which are (due to the periodicity of \( k \)-space) the \textit{same} surfaces of \textit{opposite orientations}. This implies that the contributions to the Berry flow through the BZ boundary from these two faces trivially cancel out. On the other hand, the flow of Berry curvature through the BZ boundary can also by expressed as the sum of the chiralities of all the contained Weyl points. Hence, the number of
Weyl points of one chirality must equal the number of Weyl points of the opposite chirality [87]. Comparing this result to the discussion in the previous paragraph, we find that the minimal number of Weyl points is 2 in $\mathcal{I}$-symmetric systems, while it is 4 in $\mathcal{T}$-symmetric ones.

One may consider codimension arguments to see how much fine tuning is necessary to obtain a band touching of spin-split bands. In the absence of symmetries, the effective two band model of bands that may potentially touch is (I.1), which we previously considered in the context of 2D Chern insulators. According to the analysis therein, a band touching occurs at $k_0$ if the three conditions $\forall i \in \{x, y, z\} : h_i(k_0) = 0$ are simultaneously fulfilled. Setting three real-valued function to zero corresponds to codimension $\delta = 3$, meaning that the solutions in $D = 3$ generically occurs at (0-dimensional) points. This means that Weyl points can easily occur anywhere inside BZ, making them more difficult to notice.

If the crystal obeys a mirror symmetry $M_z$ (which we choose without the loss of generality to flip the $z$-coordinate), then points $k = (k_x, k_y, 0)$ [as well as points $k = (k_x, k_y, \pi)$] are mapped by $M_z$ back onto themselves. We say that they form a mirror-invariant plane inside BZ. The relation $M_z \mathcal{H}(k_x, k_y, 0) M_z^\dagger = \mathcal{H}(k_x, k_y, -k_z)$ implies that within the mirror-invariant plane

$$[M_z, \mathcal{H}(k_x, k_y, 0)] = 0 \quad (\text{II.3})$$

commute, meaning that every band can be labelled by a mirror eigenvalue. If the two bands forming model (I.1) have the same mirror eigenvalue, then $M_z \propto \mathbb{1}_\sigma$ and no constraints on $\mathcal{H}(k_x, k_y, 0)$ is obtained. However, if their eigenvalues are different, then $^3 M_z \propto \sigma_z$, and relation (II.3) together with anticommutation relations of Pauli matrices yield

$$\mathcal{H}(k_x, k_y, 0) = h_0(k_x, k_y) \mathbb{1}_\sigma + h_z(k_x, k_y) \sigma_z. \quad (\text{II.4})$$

The gap closes when $h_z = 0$ such that the codimension is $\delta = 1$. But we have two remaining momenta $k_x, k_y$ that can be tuned, meaning that solutions in general occur along lines. This is not a Weyl semimetal, but an example of a nodal line semimetals which are studied in chapter III.

The same symmetry-invariant plane is also obtained in the presence of combined $\mathcal{T}C_{2z}$ symmetry, where $\mathcal{T}$ is time-reversal symmetry and $C_{2z}$ is a rotation around $z$-axis by $\pi$. Obtaining the appropriate operator representation of $\mathcal{T}C_{2z}$ is a bit more tricky. We already know from

\footnote{The codimension argument works equally well for any $M_z \propto n \cdot \sigma$, the choice $M_z = \sigma_z$ is quite arbitrary.}
II.1. Research overview

Subsec. I.2.1 that within the full lattice model

\[ T = e^{-i \frac{\pi}{2} \sigma_y} \otimes 1_{\tau} \mathcal{K} = -i \sigma_y \otimes 1_{\tau} \mathcal{K} \]  

(II.5a)

where \( \sigma \) is the spin and \( \tau \) is an (unaffected) orbital degree of freedom. According to the discussion of spin rotations in Subsec. I.1.5,

\[ C_{2z} = e^{-i \frac{\pi}{2} \sigma_z} \otimes c_{\tau} = -i \sigma_z \otimes c_{\tau} \]  

(II.5b)

where \( c_{\tau} \) is a possible permutation of orbitals under the spatial rotation, i.e. a real-valued matrix squaring to \( +1 \). The composed symmetry is

\[ TC_{2z} = i \sigma_x \otimes c_{\tau} \mathcal{K} \]  

(II.5c)

which squares to \( +1 \). Hence the representation of \( TC_{2z} \) within the effective model (I.1) must also be antiunitary and has to square to \( +1 \). Without the loss of generality, we can set \( TC_{2z} = \mathcal{K} \). The condition

\[ [TC_{2z}, \mathcal{H}(k_x, k_y, 0)] = 0 \]  

(II.6)

then leads to

\[ \mathcal{H}(k_x, k_y, 0) = h_0(k_x, k_y) 1_\sigma + h_x(k_x, k_y) \sigma_x + h_z(k_x, k_y) \sigma_z. \]  

(II.7)

This has codimension \( \delta = 2 \), which within the two-dimensional symmetric plane generically leads to 0-dimensional solutions, i.e. Weyl points. Such a fixation of Weyl points to a high-symmetry plane occurs for the four Weyl points of the (type-II) Weyl semimetal MoTe\(_2\) [88].

Finally, Weyl points can occur along rotation-invariant lines in systems with rotation or screw symmetries. Such possibilities have been investigated in Refs. [80, 81]. We remark that the proper analysis of symmetry constraints in the presence of nonsymmorphic screw and glide symmetries is more complicated and we will present a suitable mathematical apparatus in Sec. II.3.

Weyl semimetals (WSMs) have originally been proposed by Ref. [29] in magnetic pyrochlore iridates, such as \( Y_2\text{Ir}_2\text{O}_7 \). Most of the subsequent investigations of Weyl semimetals focused on their realizations in interacting models with broken time-reversal symmetry [29, 89, 90] and in normal insulator vs. topological insulator (NI-TI) multilayers [84–86]. Weyl and Dirac semimetals also arise naturally as the intermediate phase in a TI to NI phase transition [91–94]. It was further been
proposed [95, 96] and subsequently confirmed in experiments [97, 98] that certain non-centrosymmetric transition metal monophosphides are nonmagnetic WSMs. Our work on Weyl semimetals from spontaneous lattice distortion presented in subsequent sections has for the most part been completed before the experimental findings in these materials.

Before moving on with the discussion of the chiral anomaly in WSMs, we make here a few comments about Dirac semimetals. First note that one possible realization of Dirac matrices is \( \Gamma = \sigma_z \otimes \sigma \), which automatically implies that a Dirac point can be understood as if composed of two Weyl points of opposite chirality.\(^4\) Furthermore, to realize a Dirac point in the absence of symmetries, many parameters need to be tuned. There are as many as 15 linearly independent zero-trace Hermitian \( 4 \times 4 \) matrices, although the relevant number is brought down to\(^5\) 5 in the presence of \( T \circ \mathcal{I} \). The model (II.1c) with only three matrices therefore cannot occur just by chance. Nevertheless, with the help of crystalline symmetry, a Dirac point can be stabilized either at a TRIM on the BZ boundary of a non-symmorphic space group [34, 101, 102] or along a rotation-invariant line in systems with a rotation/screw symmetry [35]. The first possibility is realized in the pyrochlore model of Sec. II.2 and has also been proposed for \( \beta \)-cristobalite BiO\(_2\) [34] and for distorted spinels [103], while the latter option is realized in real materials Na\(_3\)Bi and Cd\(_3\)As\(_2\) [104–109]. A Weyl semimetal can then be obtained by starting with a 3D Dirac semimetal and then breaking \( \mathcal{I} \) or \( T \) symmetry [30, 84–86]. In fact, this is our strategy in the developed model on the elastic pyrochlore lattice described in Sec. II.2.

### II.1.2 Chiral anomaly

One of the peculiar properties of Weyl semimetals is that they provide a condensed matter realization of the chiral anomaly. In this subsection we keep \( \hbar \) explicitly to show the quantum nature of this effect. To derive the chiral anomaly, we consider the ideal Weyl Hamiltonian (II.1a) in parallel magnetic and electric fields, which we orient along the \( z \)-direction, i.e.

\[
\mathbf{B} = (0, 0, B) \quad \text{and} \quad \mathbf{E} = (0, 0, E).
\]  
\(^{4}\)Two Weyl points of the same chirality sitting on top of each other are also possible. Such a node is called a double Weyl point and is suspected to exist in HgCr\(_2\)Se\(_4\) [99] and SrSi\(_2\) [100]. We will encounter another possible realization of double Weyl points in superconducting systems in chapter IV.

\(^{5}\)This number is derived in chapter IV.
II.1. Research overview

We model the presence of magnetic field by performing the Peierls substitution,

\[
(\hbar k_x, \hbar k_y, \hbar k_z) \mapsto (-i\hbar \partial_x + eA_x, -i\hbar \partial_y + eA_y, \hbar k_z)
\]

≡ \((\Pi_x, \Pi_y, \hbar k_z)\) \hspace{1cm} (II.9a)

so that the commutator

\[
[\Pi_x, \Pi_y] = i\hbar (\partial_y A_x - \partial_x A_y) = -i\hbar e B.
\]

This allows us to express the \(\Pi\)-operators using the usual ladder operators \([a, a^\dagger] = 1\) as

\[
\Pi_x = \sqrt{\frac{\hbar |B|}{2}} (a + a^\dagger) \quad \text{and} \quad \Pi_y = i \text{sign}(B) \sqrt{\frac{\hbar |B|}{2}} (a - a^\dagger). \hspace{1cm} (II.9c)
\]

Assuming further that \(B > 0\), the Peierls substitution changes the ideal Weyl Hamiltonian into

\[
\mathcal{H}(k_z) = \hbar \nu \begin{pmatrix} \hbar k_z & \sqrt{2\hbar e B a} \\ \sqrt{2\hbar e B a^\dagger} & -\hbar k_z \end{pmatrix}. \hspace{1cm} (II.10)
\]

To find eigenvalues of Hamiltonian (II.10), note that the square \(\mathcal{H}^2(k_z)\) is diagonal,

\[
\mathcal{H}(k_z) = v^2 \begin{pmatrix} \hbar^2 k_z^2 + 2\hbar e B (a^\dagger a + 1) & 0 \\ 0 & \hbar^2 k_z^2 + 2\hbar e B a^\dagger a \end{pmatrix}. \hspace{1cm} (II.11)
\]

But \(a^\dagger a\) is the number operator, such that we can simply read out the eigenenergies of \(\mathcal{H}^2(k_z)\). These are

\[
\varepsilon^2_0(k_z) = v^2 \hbar^2 k_z^2 \quad \text{(once)} \hspace{1cm} \text{(II.12a)}
\]

\[
\forall n \in \mathbb{Z}^+: \varepsilon^2_n(k_z) = v^2 \left( \hbar^2 k_z^2 + 2\hbar e B n \right) \quad \text{(each twice).} \hspace{1cm} \text{(II.12b)}
\]

Eigenvalues of (II.10) are obtained by taking square root of (II.12). It turns out that for (II.12b) both \(\pm\) roots are physical, but for (II.12a) only one is physical, namely \(-\hbar \nu k_z\) for chirality \(\hbar[110]\).\footnote{The corresponding eigenstate in both cases is} Put together, the
**Figure II.2: Chiral anomaly of a single Weyl point in the quantum limit.** The spectrum of a Weyl point in magnetic field $B$ consists of quasi-1D LLs. In the case of an ideal Weyl point (II.1a), the spectrum takes the simple symmetric form, with the exception of the chiral LL which only disperses in one direction determined by the chirality $\hbar$. The motion of electrons in such bands under the action of electric field $E$ leads to pumping of electric charge between Weyl points of opposite chirality as described by Eq. (II.17b).

The spectrum of (II.10) is

$$
\varepsilon_0(k_z) = -\hbar v k_z \quad \text{(II.15a)}
$$

$$
\forall n \in \mathbb{Z} \setminus \{0\} : \varepsilon_n(k_z) = \text{sign}(n) v \sqrt{\hbar^2 k_z^2 + 2e\hbar|n|}. \quad \text{(II.15b)}
$$

These are the dispersive Landau levels (LLs) of a Weyl point in a magnetic field. The $\varepsilon_0(k_z)$ mode is called the *chiral* LL because it does not have a counterpart dispersing in the opposite direction.

We now include the effect of the electric field semiclassically using

$$
\partial_t k_z = -\frac{e}{\hbar} E, \quad \text{(II.16)}
$$

meaning that electrons will move along the 1D bands (II.15) opposite to the direction of $E$. We illustrate the situation in Fig. II.2. Due to the

where $|0\rangle$ is the vacuum of ladder operator $a$. We also remark that for $B < 0$, the Hamiltonian takes the Hermitian conjugate form of (II.10). Its spectrum is identical to (II.15) with the exception of $\tilde{\varepsilon}_0 = +\hbar v k_z$ with eigenstate

$$
|\psi_0\rangle = \begin{pmatrix} |0\rangle \\ 0 \end{pmatrix}. \quad \text{(II.14)}
$$
II.1. Research overview

finiteness of the crystal, the spacing between the neighboring $k_z$ points is $2\pi/L_z$ where $L_z$ is the length of the crystal in the $z$-direction. Furthermore, each LL has a degeneracy $\Phi/\Phi_0$ where $\Phi = BL_xL_y$ is the magnetic flux through the crystal and $\Phi_0 = 2\pi\hbar/e$ is the magnetic flux quantum. Consequently, we deduce from Fig. II.2 that electric charge is being pumped into the Weyl point at a rate \[ 1 \frac{\partial Q_e}{\partial t} = -\hbar \frac{e^3}{(2\pi\hbar)^2} E B \] (II.17a)

where $V = L_xL_yL_z$ is the volume of the crystal. This non-conservation of electric charge in a single Weyl point is called the chiral anomaly. The charge conservation is saved by the Nielsen-Ninomiya doubling theorem [87] which states that in a crystal Weyl points of the two chiralities $\hbar = \pm 1$ come in pairs. We remark that using field-theoretical methods it is possible to derive \[ 1 \frac{\partial Q_e}{\partial t} = -\hbar \frac{e^3}{(2\pi\hbar)^2} E \cdot B \] (II.17b)

for arbitrary direction of the electric and magnetic field.

Note that the chiral anomaly leads to an anomalous behaviour of conductivity $\sigma$ in a magnetic field. Assuming a system with a single pair of Weyl points, and a relaxation time $\tau$, the charge imbalance leads to \[ \sigma(B) = \frac{e^3}{2\pi^2\hbar} B\tau \] (II.18)

This is the result in the quantum limit when only the chiral LL contributes to transport. It remains valid if the Weyl point is partially filled with electrons/holes provided that \[ |\mu| \lesssim v\sqrt{2e\hbar B}. \] (II.19)

We compare result (II.18) to the semiclassical limit when many LLs are partially occupied. Such a situation was in much detail analyzed in Ref. [32]. In such a case it is easier to forget about the LL structure and to treat the magnetic field semiclassically too. Without going too deep into the subtleties, we reproduce here an overview of the derivation.

The semiclassical equations of motion for a wave packet centred at position $r$ and at momentum $k$ in the presence of electric and magnetic
fields for a band with energy $\varepsilon_k$ with a non-vanishing Berry curvature $\Omega$ are [112]

$$\dot{r} = \frac{1}{\hbar} \nabla_k \varepsilon_k - \dot{k} \times \Omega \quad (\text{II.20a})$$
$$\hbar \dot{k} = -eE - e\dot{r} \times B. \quad (\text{II.20b})$$

These equations can be separated, leading to

$$\dot{r} = \frac{v + \frac{e}{\hbar} E \times \Omega + \frac{e}{\hbar} (\Omega \cdot v)B}{1 + \frac{e}{\hbar} B \cdot \Omega} \quad (\text{II.21a})$$
$$\dot{k} = -\frac{\frac{e}{\hbar} E + \frac{e}{\hbar} v \times B + \frac{e^2}{\hbar^2} (E \cdot B)\Omega}{1 + \frac{e}{\hbar} B \cdot \Omega} \quad (\text{II.21b})$$

where we used $v = \frac{1}{\hbar} \nabla_k \varepsilon_k$ which can be perceived as a yet another field (with vanishing curl) characterizing the bands in $k$-space. Expressions (II.21) enter the Boltzmann equation

$$\dot{r} \cdot \nabla_r n + \dot{k} \cdot \nabla_k n + \partial_t n = I_{\text{coll.}} \quad (\text{II.22})$$

where $n = n(r, k, t)$ is the occupation function in phase space and $I_{\text{coll.}}$ is the collision integral. The final ingredient for the semiclassical dynamics is the modified density of states in $k$-space[^7][113]

$$\rho_k = \rho_0 \left(1 + \frac{e}{\hbar} B \cdot \Omega \right) \quad (\text{II.24a})$$

where $\rho_0 = 1/(2\pi)^3$ is the (constant) density of states in the absence of fields. We also need expression (II.2) for the Berry curvature in the vicinity of the Weyl point, which can be used to derive the density of states.

[^7]: A rather painful derivation shows that a phase space volume element $\Delta V$ changes under the semiclassical equations of motion (II.21), namely

$$\frac{d}{dt} \log \Delta V = \frac{1}{\Delta V} \frac{d\Delta V}{dt} = \sum_i \frac{\partial \dot{x}_i}{\partial x_i} + \sum_k \frac{\partial \dot{k}_i}{\partial k_i} = \ldots = -\frac{d}{dt} \log \left(1 + \frac{e}{\hbar} B \cdot \Omega \right) \quad (\text{II.23})$$

leading to a violation of the Liouville’s theorem [113]. This influences the density of states in $k$-space in the indicated manner.
II.1. Research overview

states in energy

\[ \rho(\epsilon) = \sum_{\pm} \int \frac{d^3k}{(2\pi)^3} \left( 1 + \frac{e}{\hbar} B \cdot \Omega \right) \delta(\pm \hbar v_k - \epsilon) \]

\[ = \frac{1}{(2\pi)^2} \sum_{\pm} \int_{0}^{\infty} dk k^2 \int_{0}^{\pi} d\theta \sin \theta \left( 1 + \frac{\hbar}{2k^2} \right) \delta(\pm \hbar v_k - \epsilon) \]

\[ = \frac{\epsilon^2}{2\pi^2 \hbar^3 v^3} \]  

(II.24b)

where \( \delta \) is the Dirac delta function. Note that this quantity is not influenced by the \( B \) and \( \Omega \) fields, opposed to Eq. (II.24a).

Now we put everything together. Since a pair of Weyl points usually has a large separation in momentum space, the inter-valley relaxation time \( \tau \) is assumed much longer than the intra-valley relaxation processes. Consequently, we can assume that within a single Weyl cone the occupation function \( n \) depends only on energy \( \epsilon_k \) and not on momentum \( k \). We also assume homogeneity (\( \nabla_r n = 0 \)) and equilibrium state (\( \partial_t n = 0 \)), such that the Boltzmann equation gives

\[- \left( 1 + \frac{e}{\hbar} B \cdot \Omega \right)^{-1} \left[ \frac{e}{\hbar} E + \frac{e}{\hbar} v \times B + \frac{e^2}{\hbar^2} (E \cdot B) \Omega \right] \cdot \nabla_k n(\epsilon_k) = I_{\text{coll.}}. \]  

(II.25)

We will now use the relaxation time approximation, such that \( I_{\text{coll.}}(\epsilon) \approx -\frac{\delta n(\epsilon)}{\tau} \) where \( \delta n(\epsilon) \) is the deviation of the occupation function relative to the situation in the absence of \( E \) and \( B \) fields. Furthermore,

\[ \nabla_k n(\epsilon_k) = \hbar v \partial_{\epsilon} n(\epsilon). \]  

(II.26)

Multiplying (II.25) by \( (1 + \frac{e}{\hbar} B \cdot \Omega) \delta(\epsilon_k - \tilde{\epsilon}) \) and integrating both side with \( \int \frac{d^3k}{(2\pi)^3} \) (and flipping the overall sign) leads to

\[ \frac{\rho(\tilde{\epsilon}) \delta n(\tilde{\epsilon})}{\tau} = \frac{e}{(2\pi)^3} \int d^3k \left[ E + v \times B + \frac{e}{\hbar} (E \cdot B) \Omega \right] \cdot v \partial_{\epsilon} n(\epsilon) \delta(\epsilon - \tilde{\epsilon}) \]

\[ = \frac{e}{4\pi^2} \int_{0}^{\pi} d\theta \sin \theta \int_{0}^{\infty} k^2 dk \left[ E v \cos \theta + (\nu \times B) \cdot v + \frac{e}{\hbar} (E \cdot B) (\Omega \cdot v) \right] \frac{\partial n(\epsilon)}{\partial \epsilon} \bigg|_{\tilde{\epsilon}} \delta(\epsilon - \epsilon') \]

\[ = - \text{sign} (\tilde{\epsilon}) \hbar \frac{e^2}{4\pi^2 \hbar^2} (E \cdot B) \frac{\partial n(\epsilon)}{\partial \epsilon} \bigg|_{\tilde{\epsilon}} \]  

(II.27)

where the polar angle \( \theta \) is defined with respect to \( E \), we shortened \( \epsilon_k \equiv \epsilon \) for simplicity, and on the LHS we used the result of integration
in (II.24b). For small enough temperatures we can approximate
\[
\frac{\partial n(\varepsilon)}{\partial \varepsilon} \bigg|_{\tilde{\varepsilon}} \approx \frac{\partial f_{\text{FD}}(\varepsilon)}{\partial \varepsilon} \bigg|_{\tilde{\varepsilon}} \approx -\delta(\varepsilon' - \mu) \tag{II.28}
\]

where \( f_{\text{FD}}(\varepsilon) \) is the Fermi-Dirac distribution function. Inverting Eq. (II.27) and using Eqs (II.24b) and (II.28) gives
\[
\delta n(\varepsilon) \approx \text{sign}(\mu) \frac{e^2 \tau \hbar \nu^3}{2 \mu^2} (\mathbf{E} \cdot \mathbf{B}) \delta(\varepsilon - \mu) \tag{II.29}
\]

We calculate the current appearing due to \( \delta n \). Using Eq. (II.21a) and correcting for the density of states as in Eq. (II.24a) we obtain
\[
\begin{align*}
\mathbf{j} &= -e \int d^3k \, \mathbf{v}_k \cdot \mathbf{r} \delta n(k) \\
&= - \int \frac{d^3k}{(2\pi)^3} \left[ v + \frac{e}{\hbar} \mathbf{E} \times \mathbf{\Omega} + \frac{e}{\hbar} (\mathbf{\Omega} \cdot \mathbf{v}) \mathbf{B} \right] \text{sign}(\mu) \hbar \frac{e^3 \tau \hbar \nu^3}{2 \mu^2} (\mathbf{E} \cdot \mathbf{B}) \delta(\varepsilon - \mu) \\
&= \frac{e^4 \nu^3 \tau}{8\pi^2 \hbar \mu^2} (\mathbf{E} \cdot \mathbf{B}) \mathbf{B} \tag{II.30}
\end{align*}
\]

For a pair of Weyl cones for a longitudinal field, we obtain
\[
\sigma(B) = \frac{e^4 \nu^3 \tau}{4\pi^2 \hbar \mu^2} B^2. \tag{II.31}
\]

This result applies away from the quantum limit, i.e. for \( |\mu| \gg v \sqrt{2e\hbar B} \). One should also keep in mind that there are additional contributions to conductivity for both (II.18) and (II.31) due to redistribution of electrons by the applied \( \mathbf{E} \) and \( \mathbf{B} \) fields within the Weyl cones.

The results for conductivity in both limits indicate negative longitudinal magnetoresistance
\[
\text{MR} = \frac{\rho(B) - \rho(0)}{\rho(0)} \tag{II.32}
\]

where \( \rho \) is electrical resistance. This result is considered to be one of the main experimental signatures of WSMs, especially because under very general assumptions MR of metals can be shown to be negative [114]. Negative longitudinal MR has been confirmed in the most studied Weyl semimetal material TaAs [115].
II.1. Research overview

Figure II.3: Surface states of the minimal Weyl semimetal. A pair of Weyl points (green and red dot) are located inside a box-shaped BZ (pale blue). We divide the BZ into many 2D sheets (pale violet) by fixing the value of $k_x$. Every such a sheet corresponds to some 2D insulator (with the exception of the two sheets that pass through a Weyl point which are metallic). Since these sheets are homeomorphic to tori $\mathbb{T}^2$, the Berry flow passing through each such a sheet is quantized to an integer multiple of $2\pi$, cf. Sec. I.1. Since Weyl points act as sources/sinks of $2\pi$ Berry phase, some sheets must necessarily be non-trivial, i.e. characterized by a finite Chern number. In the illustrated example, we choose the central sheets to be topologically non-trivial. Consequently, each of these sheets is characterized with an in-gap edge mode (dark blue dots) in its edge BZ (orange lines). Gluing the individual edge BZs into the surface BZ (SBZ) reveals the appearance of an arc (dashed blue) joining the projections (dashed black lines) of the bulk Weyl points – the Fermi arcs.

II.1.3 Surface states

Consider the simplest case of only two Weyl points inside a box-shaped BZ. We may further imagine “slicing” the 3D BZ into many parallel sheets, as shown in Fig. II.3. Every such a sheet is homeomorphic to a torus $\mathbb{T}^2$, meaning that it corresponds to some two-dimensional system. More precisely, since most of these sheets are gapped, they correspond to 2D insulators. The only exceptions are the two sheets passing through one of the two Weyl points.

Recall that Weyl points acts as sources/sinks of $2\pi$ Berry phase, and that this phase has to flow somewhere with zero divergence. This flow is thus picked up by the pair of parallel 2D sheets lying on the two sides of the Weyl point. But since these sheets do not have a boundary, their Berry flow is also quantized to integer multiples of $2\pi$ (I.48). The simplest solution is that one sheet picks up all the $2\pi$ phase (and has $c = 1$),
Figure II.4: Quantum oscillations of electrons in Weyl semimetals. In an applied magnetic field, electrons move along constant energy contours. For electrons at the Fermi arcs, this indicates motion \textit{along} the arc. Once the electron reaches the endpoint of the arc, it uses the chiral LL (II.15a) to traverse the bulk. When it reaches the opposite surface, the electron moves along a surface Fermi arc again, until it eventually reaches the original position. Such unusual closed orbits lead to special signatures in the Schubnikov-de Haas and the de Haas-van Alphen effects.

while the other sheet has zero phase (and $\epsilon = 0$). In Fig. II.3 we choose the non-trivial sheets to lie between the pair of Weyl points. An alternative situation where the \textit{outer} sheets are topological is also possible.

As we discussed in Subsec. I.1.1, the boundary of a Chern insulator is characterized with a gapless edge, meaning that an edge mode crosses the chemical potential $\mu$ located within the gap of the bulk band structure. Such a state has to exist in the 1D edge BZ of every topologically non-trivial sheet between the pair of Weyl points. We can now collect all the 1D edge BZs of the individual 2D sheets and “glue” them together into a 2D surface BZ (SBZ). The collection of all the edge modes creates a Fermi arcs which connects the projections of the two Weyl points into SBZ. The same procedure can be also performed with the bottom surface, where a complementary arc appears. Such open-ended Fermi arcs are not possible in truly 2D systems, only on the surfaces of 3D systems. Such Fermi arcs have indeed been reported for Weyl semimetal TaAs [97, 98, 116].

One of the peculiar phenomena that are linked to the presence of the surface Fermi arcs in Weyl semimetals occurs when the sample is sub-
II.2 Model on a pyrochlore lattice

II.2.1 Physics of pyrochlore iridates

Pyrochlore oxides have over the past decade received much interest as potential hosts of novel electronic phases. Due to the presence of strong SOC and intermediate strength electron correlation effects, pyrochlore oxides with 5\(d\) transition-metal ions have been identified as a playground for topological phases [119] including exotic spin liquids [120, 121], topological insulators [122–124], topological crystalline insulators [125], topological semimetals [89, 90] and unusual forms of mag-
netism [126, 127]. Besides these intrinsic three dimensional phases, heterostructuring of pyrochlore oxides offers the possibility to access two-dimensional topological phases, such as quantum spin Hall, integer or fractional Chern insulators [128–132].

In this work, we add an additional ingredient to the physics of pyrochlore oxides: The leading coupling of the electronic degrees of freedom to the lattice. Our starting point is a general Hamiltonian on the pyrochlore lattice, which, as a consequence of the non-symmorphic space group symmetry, realizes a Dirac semimetal with three Dirac points at the Fermi level [34]. We find that for an intermediate stiffness of the crystal, an inversion-symmetry breaking staggered strain can spontaneously develop. The symmetry-broken phase realizes a Weyl semimetal, whose Fermi surface consists of twelve Weyl points with linearly dispersing valence and conduction bands. If the staggered strain reaches a critical value, the system turns into a fully gapped trivial insulator phase. Our model exhibits a peculiar phase diagram that includes a reentrant Weyl semimetal, which can be reached from a more symmetric phase present at both lower and higher temperatures.

### II.2.2 Tight-binding model

We study a system of non-interacting electrons on the lattice of corner-sharing tetrahedra called the pyrochlore lattice. These tetrahedra form a bipartite lattice and can therefore be labelled as even and odd [illustrated in blue and orange in Fig. II.5(d)] in such a way that every even tetrahedron touches only odd ones and vice versa. The pyrochlore lattice is a face-centred cubic (FCC) lattice belonging to a non-symmorphic space group #227 ($Fd\bar{3}m$). Its BZ has the form of a truncated octahedron illustrated in Fig. II.5(b).

We consider the following Hamiltonian in real space to describe the dynamics of the electrons on the pyrochlore lattice [90],

\[
H_0 = \sum_{\langle i,j \rangle} c_i^\dagger \left( t_1 + i t_2 d_{ij} \cdot \sigma \right) c_j + \\
+ \sum_{\langle\langle i,j \rangle\rangle} c_i^\dagger \left[ t'_1 + i (t'_2 R_{ij} + t'_3 D_{ij}) \cdot \sigma \right] c_j. \tag{II.34}
\]

The electron annihilation operator at site $i$ is given by $c_i = (c_{i\uparrow}, c_{i\downarrow})^\top$, where $\alpha = \uparrow, \downarrow$ refers to a (pseudo-)spin-$\frac{1}{2}$ degree of freedom. The first
II.2. Model on a pyrochlore lattice

Figure II.5: Pyrochlore lattice and its Brillouin zone. (a) Illustration of vectors $x_c$, $a_{ij}$, $b_{ij}$, and $d_{ij}$ used in the definition of Hamiltonians (II.34) and (II.38). (b) The BZ of both the pyrochlore and the breaching pyrochlore lattice has the form of a truncated octahedron. (c) Definition of the high-symmetry points of the FCC lattice within one eighth of BZ and the path $\Gamma XWL\Gamma KX$ in the $k$-space used for plotting energy spectra in Fig. II.8. The U point can be related to the K point using the system symmetries. (d) Pyrochlore lattice with differently colored even (blue) and odd (orange) tetrahedra. (e) The $I$-broken (breathing) pyrochlore lattice considered in the elastic model.

The sum runs over the nearest neighbor (NN) and the second sum over the next-to-nearest neighbor (NNN) bonds. The Pauli matrices captured by $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ correspond to the spin degree of freedom, and the terms containing them represent spin-orbit coupling (SOC). The real space vectors appearing in the NN part of $H_0$ are defined via

\begin{align}
  d_{ij} &= 2a_{ij} \times b_{ij} \\
  a_{ij} &= \frac{1}{2} (b_i + b_j) - x_c \\
  b_{ij} &= b_j - b_i \\
  x_c &= \frac{1}{2} (b_1 + b_2 + b_3 + b_4)
\end{align}

and those in the NNN part are defined as

\begin{align}
  \mathcal{R}_{ij} &= b_{ik} \times b_{kj} \quad \text{and} \quad \mathcal{D}_{ij} = d_{ik} \times d_{kj}
\end{align}

where $k$ is the common NN of the NNN sites $i$ and $j$. We further use
position vectors $b_i$ pointing to the site $i$ of the tetrahedron

$$b_1 = a(0,0,0), \ b_2 = a(0,1,1), \ b_3 = a(1,0,1), \ b_4 = a(1,1,0) \quad \text{(II.35g)}$$

and position vector $x_c$ pointing to the centre of the tetrahedron

$$x_c = \frac{1}{4} \sum_{i=1}^{4} b_i \quad \text{(II.35h)}$$

Example choices of $b_{ij}$, $a_{ij}$ and $d_{ij}$ are illustrated in Fig. II.5(a). We denote the length of the edge of the cube circumscribed to the tetrahedra [Fig. II.5(a)] as “a” so that $|b_{ij}| = a\sqrt{2}$. The edge length of the conventional FCC unit cell is $4a$.

Hamiltonian (II.34) is the most general single-orbital Hamiltonian with SOC up to NNN terms respecting the full symmetry of the pyrochlore lattice\(^8\) [124]. Such a situation arises for the five $5d$-electrons coming from each Ir\(^{4+}\) site of the pyrochlore oxides. The crystal field of the octahedral oxygen cage splits the $5d$ orbitals into the six $t_{2g}$ states and the four $e_g$ states, the latter being higher in energy. The on-site SOC further splits the six degenerate $t_{2g}$ states into an effective pseudospin $j_{\text{eff}} = 1/2$ doublet and an effective $j_{\text{eff}} = 3/2$ quadruplet, the latter being lower in energy. The five $5d$-electrons of Ir\(^{4+}\) sites completely fill the $j_{\text{eff}} = 3/2$ quadruplet and half-fill the $j_{\text{eff}} = 1/2$ doublet [121]. Hamiltonian (II.34) can then be viewed as an effective model for electrons residing in the $j_{\text{eff}} = 1/2$ orbitals. In this way one can relate the parameters $t_{1,2}$ and $t'_{1,2,3}$ to particular orbital overlaps as is thoroughly explained in Ref. [90]. This discussion also clarifies why index $\alpha$ in Eq. (II.34) describes a pseudospin rather than spin degree of freedom.

A generic spectrum of Hamiltonian (II.34) is plotted in Fig. II.8(a). Note that the site fillings $n = 1/4$ and $n = 3/4$ correspond to a semimetallic phase. In pyrochlore iridates, such a commensurate filling may be realized by considering alloys of the form $A_{2-x}B_x\text{Ir}_2\text{O}_7$ where $A$ and $B$ are nonmagnetic but have different oxidation states [134–136]. For example, we expect that $\text{Y}_{1.5}\text{Ca}_{0.5}\text{Ir}_2\text{O}_7$ [134] realizes the site filling $n = 1/4$ and the (hypothetical) compound $\text{Bi}_{1.5}\text{Se}_{0.5}\text{Ir}_2\text{O}_7$ site filling $n = 3/4$ of our model. To be concrete, throughout our study we consider

$$n = 3/4. \quad \text{(II.36)}$$

---

\(^8\) The $d$, $\mathcal{R}$ and $\mathcal{D}$ vectors appearing in the SOC terms are constrained by symmetries in the same way as the $\mathcal{D}$ vector of Ref. [133] in the context of anisotropic superexchange.
II.2. Model on a pyrochlore lattice

II.2.3 Elastic lattice

Electron-phonon coupling can lead to a softening of certain phonon modes (i.e. the Kohn anomaly) and to a distortion of the lattice akin to the Peierls transition. The leading instabilities can be found by investigating the Lindhard function. We argue that the leading lattice instability of model (II.34) occurs for momentum $q = 0$. To show this, we ignore the two occupied bands far from the chemical potential and consider only the conduction and the valence bands. Defining $\xi^\alpha_k = \epsilon^\alpha_k - \mu$ where $\alpha$ stands for the band index, Fig. II.8(a) indicates an approximate electron-hole symmetry\(^9\) $\xi^\text{con.}_k \approx -\xi^\text{val.}_k$. In the case of a perfect electron-hole symmetry $\xi^\text{con.}_k = -\xi^\text{val.}_k \equiv \xi_k$, the static ($\omega = 0$) Lindhard function at zero temperature satisfies

$$0 < -\chi(q) = -\frac{1}{\Omega} \sum_{k \in \text{BZ}} \sum_{\alpha, \alpha'} f(\xi^\alpha_{k+q}) - f(\xi^{\alpha'}_k) \frac{\xi^\alpha_{k+q} - \xi^{\alpha'}_k}{\xi^\alpha_{k+q} - \xi^{\alpha'}_k} = \frac{1}{\Omega} \sum_{k \in \text{BZ}} \frac{2}{\xi_k} \xi_{k+q} + \xi_k \leq \frac{1}{\Omega} \sum_{k \in \text{BZ}} \left( \frac{1}{2\xi_{k+q}} + \frac{1}{2\xi_k} \right) = -\chi(0) \quad (\text{II.37})$$

\(^9\)Note that we understand electron-hole symmetry as a symmetry of eigenenergies, while particle-hole and chiral symmetries (I.99) are defined on Hamiltonians!
Chapter II. Weyl semimetals

Figure II.7: Crystal structure of pyrochlore iridate \( \text{Y}_2\text{Ir}_2\text{O}_7 \). a Every iridium site (blue) is surrounded by an octahedral cage (blue) of oxygen atoms (red) with a small trigonal distortion. The yttrium atoms (grey) do not enter the effective tight-binding model, only the \( j_{\text{eff.}} = 1/2 \) doublets originating from the \( t_{2g} \) orbitals of iridium 5d electrons do, cf. Fig. II.6. b The \( j_{\text{eff.}} = 1/2 \) states located at the Iridium sites form a pyrochlore lattice which consists of corner-sharing tetrahedra (black). Figures were plotted using VESTA [139].

where we used the arithmetic-harmonic mean inequality. The equality sign applies only if \( q = 0 \) or if both bands are perfectly flat. The result indicates that the Lindhard function has a peak at \( q = 0 \) which corresponds to the leading instability. We expect this peak to be preserved for Hamiltonian (II.34) where the electron-hole symmetry is approximately valid and additional bands are present.

Inspired by this observation, we consider the most symmetric \( q = 0 \) phonon mode which corresponds to the simultaneous expansion of the even and shrinking of the odd tetrahedra as illustrated in Fig. II.5(e). We call it the breathing mode of the pyrochlore lattice. Similar breathing pyrochlore lattice has been observed in certain A-site ordered spinel oxides [137, 138].

We treat the breathing mode classically and refer to its amplitude as staggered strain \( \varepsilon \). We model its effect on the electron Hamiltonian by multiplying the NN terms by a factor \((1 \pm \varepsilon)\) for the short (long) bonds. We ignore the higher order influence on both the NN and the NNN terms as these are assumed to have a quantitative but not qualitative effect on the phase diagram of the model. The elastic energy of the lattice deformation is set to be proportional to the square \( \varepsilon^2 \). The
II.2. Model on a pyrochlore lattice

The complete Hamiltonian then reads

\[
H_\varepsilon = \frac{1}{2} \Upsilon \varepsilon^2 + \sum_{\langle i,j \rangle} (1 \pm \varepsilon) \epsilon_i \left( t_1 + i t_2 d_{ij} \cdot \sigma \right) \epsilon_j + p \sum_{\langle\langle i,j \rangle\rangle} \epsilon_i \left[ 1 + i R (\mathcal{R}_{ij} + \mathcal{D}_{ij}) \cdot \sigma \right] \epsilon_j \tag{II.38}
\]

where \( \Upsilon \) is elasticity of the lattice analogous to the Young modulus, and \( V \) is the volume of the sample. The equilibrium value of \( \varepsilon \) is determined by minimizing the energy of the electron-lattice system which, by the Hellmann–Feynman theorem, corresponds to solving the self-consistency equation

\[
\varepsilon = \frac{1}{\Upsilon V} \sum_{\langle i,j \rangle} \langle \Psi_\varepsilon | \epsilon_i \left( t_1 + i t_2 d_{ij} \cdot \sigma \right) \epsilon_j | \Psi_\varepsilon \rangle \tag{II.39}
\]

where \( | \Psi_\varepsilon \rangle \) is the ground state of the electron Hamiltonian for a staggered strain amplitude \( \varepsilon \).

Hamiltonians (II.34) and (II.38) have many free parameters. To simplify the situation, we reduce the parameter space by setting

\[
R := \frac{t_2}{t_1} = \frac{t'_2}{t'_1} = \frac{t'_3}{t'_1} = \frac{t'_2}{t'_3} \tag{II.40a}
\]

for the relative strength of the spin orbit coupling and

\[
p := \frac{t'_1}{t_1} = \frac{t'_2}{t_2} \tag{II.40b}
\]

for the relative strength of the NNN terms. We further define a variable

\[
s = \text{sign}(t_1) = \pm 1. \tag{II.40c}
\]

These substitutions modify Hamiltonian (II.38) to

\[
H_\varepsilon = \frac{1}{2} \Upsilon \varepsilon^2 + s \left\{ \sum_{\langle i,j \rangle} (1 \pm \varepsilon) \epsilon_i \left( 1 + i R d_{ij} \cdot \sigma \right) \epsilon_j + p \sum_{\langle\langle i,j \rangle\rangle} \epsilon_i \left[ 1 + i R (\mathcal{R}_{ij} + \mathcal{D}_{ij}) \cdot \sigma \right] \epsilon_j \right\} \tag{II.41}
\]

where all energies are now counted in units of \( |t_1| \). We will work with

\[
R = -0.4, \quad p = -0.1 \quad \text{and} \quad s = +1 \tag{II.42}
\]
unless stated otherwise. This choice approximately corresponds to the parameters used in Ref. [90].

It may happen that the energy of the Hamiltonian (II.41) is minimized for a non-zero value of $\mathcal{E}$. This indicates that the cost of the deformation is compensated for by the electron energies, thus making the lattice deformation energetically favourable. Such a transition decreases the symmetry of the lattice. In particular, it breaks the inversion symmetry $I$. The $I$-broken lattice still has the FCC Bravais lattice and an unchanged BZ, but it belongs to a symmorphic space group $\#216 (F\bar{4}3m)$.

**II.2.4 Evolution of the band structure**

In this subsection, we describe the evolution of the spectrum of Hamiltonian (II.41) as we tune the staggered strain amplitude $\mathcal{E}$. These observations are based on a direct numerical diagonalization of the Hamiltonian and are summarized in Fig. II.8. The next Sec. II.3 contains a detailed group theoretical explanation of the observed behaviour.

In the absence of a staggered strain, i.e. when $\mathcal{E} = 0$ [Fig. II.8(a)], we find that all bands are doubly degenerate as a consequence of the simultaneous presence of time-reversal $T$ and inversion symmetry $I$, cf. Subsec II.1.1. At each X point on the BZ surface, we find two energetically separated Dirac points where four bands reach the same energy and disperse linearly in all directions. This is similar to the spectrum of graphene but in 3D rather than just 2D. Since the inequivalent X points are related by crystal symmetries, all the higher lying (as well as all the lower lying) Dirac points are realized at the same energy. It is therefore possible to tune the chemical potential to this value, which corresponds to a site filling of $n = 3/4$ (six electrons per unit cell) for the upper and $n = 1/4$ (two electrons per unit cell) for the lower Dirac points. Such a system has a Fermi surface consisting of a discrete set of $k$-points and is usually referred to as a *Dirac semimetal* (DSM) [34].

A non-vanishing staggered strain, i.e. $\mathcal{E} \neq 0$ [Fig. II.8(b)], leads to a splitting of each Dirac point into four *Weyl points*. These are points where only two (rather than four) bands touch each other, and they still disperse linearly in all directions around the touching. As we increase the value of $\mathcal{E}$, these Weyl points move along the XW lines. The upper (or lower) 12 Weyl points of the model are mutually related by crystal symmetries. As a consequence, they are all realized at the same energy and the chemical potential resumes to be tuned to them if either $n = 1/4$
II.2. Model on a pyrochlore lattice

Figure II.8: Typical band structure of the developed model (II.41). For parameters (II.42) and (a) $\varepsilon = 0$, there are Dirac points located at the high-symmetry points $X$. For the $n = 1/4$ and $n = 3/4$ fillings of the model, they appear the Fermi level and enable a Dirac semimetal (DSM) phase. We explain the origin of these Dirac points in Sec. II.3. (b) Value $\varepsilon = 0.08$ corresponds to the Weyl semimetal (WSM) phase with 12 distinct Weyl points. They are all related by symmetries of the system and therefore occur at the same energy. (c) Value $\varepsilon = 0.13 > \varepsilon_c$ of Eq. (II.43) at the same filling corresponds to a trivial band insulator (INS). Upper row shows the spectra in the three cases along the path indicated in Fig. II.5(c), while the bottom row shows the spectra over the square face of the BZ. The arrows indicate the position of one of the Weyl points for the WSM phase, and the place where the Weyl points have annihilated for the INS phase.

or $n = 3/4$. Such a phase is called the Weyl semimetal (WSM) [140, 141]. The spectrum in the vicinity of each Weyl point can be approximated by Eq. (II.1b). As indicated in footnote (2) in Subsec. II.1.1, gapping out the spectrum requires enlarging of the effective low-energy Hilbert space and can be achieved either by scattering between different Weyl points (which breaks translational symmetry) or by forming a superconducting state (which requires breaking the global $U(1)$ symmetry) [31].

Consistent with the Nielsen-Ninomiya doubling theorem [87], we find that there are 6 Weyl points of both chiralities. Weyl points related by TRS or a rotation symmetry are characterized by the same chirality, while those related by mirror symmetry (which is a rotation composed with $\mathcal{I}$) carry opposite chirality, cf. Fig. II.1. At a critical value of the staggered strain $\varepsilon = \varepsilon_c$, pairs of Weyl points with opposite chirality meet at the W points where they are about to annihilate. At this stage,
the spectrum disperses quadratically along the XW lines, which correspond to the direction of motion of the Weyl points [92]. Such a quadratic band touching point does not carry a topological charge [94]. Finally, for \( \mathcal{E} > \mathcal{E}_c \), we find a gapped phase, which is a topologically trivial band insulator (INS). For the chosen parameters (II.42) and filling factor (II.36), the critical staggered strain is

\[
\mathcal{E}_c \approx 0.1112. \tag{II.43}
\]

## II.2.5 Phase diagrams for elastic lattices

To find the phase diagrams for the filling factor \( n = 3/4 \) at zero temperature, we numerically solve the self-consistency equation (II.39) for varying hopping parameters and elasticities of the lattice. For finite temperatures, we determine \( \mathcal{E} \) by minimizing the free energy

\[
F(\mathcal{E}) = \frac{1}{2} YV \mathcal{E}^2 + \sum_{\alpha, k} \varepsilon_\mathcal{E}^\alpha f_{\text{FD}}(\varepsilon_\mathcal{E}^\alpha - \mu) \tag{II.44}
\]

where \( f_{\text{FD}}(x) = 1/(1 + e^x/T) \) is the Fermi-Dirac distribution function, \( \varepsilon_\mathcal{E}^\alpha \) are the (\( \mathcal{E} \)-dependent) band energies of Hamiltonian (II.38), and the chemical potential \( \mu \) is such that the number of electrons

\[
N = \sum_{\alpha, k} f_{\text{FD}}(\varepsilon_\mathcal{E}^\alpha - \mu) \tag{II.45}
\]

is kept constant. In general, we expect that the deformation of a stiff lattice (i.e. with a large value of \( Y \)) is energetically too costly, so that the system will remain in the \( \mathcal{I} \)-preserving DSM phase. Decreasing the elasticity should allow for a transition to an \( \mathcal{I} \)-broken state that can be either a WSM or an INS.

We first study the role of the relative SOC strength \( R \) for temperatures \( T = 0 \) and \( T = 0.5 \) (expressed in units of \( |t_1| \)), see Figs. II.9(a) and (b). Throughout this subsection, we fix \( p = -0.1 \) and \( s = +1 \) and we vary \( R \) inside the interval \((-0.774, +0.364)\) for which the undistorted system realizes a DSM phase. For values of \( R \) outside this interval, the valence bands at \( \Gamma \) rise above the Dirac points at \( X \), leading to a metallic state with a hole-like Fermi pocket at the \( \Gamma \) point and three electron-like Fermi pockets at the inequivalent \( X \) points. The value \( R = 0 \) corresponds to the absence of SOC. In this case, the spectrum of the symmetric phase does
II.2. Model on a pyrochlore lattice

![Figure II.9: Phase diagrams of Hamiltonian (II.41) in the \( R, \Upsilon \)-plane for values of \( p \) and \( s \) listed in Eq. (II.42), and for temperatures (a) \( T = 0 \), and (b) \( T = 0.5 \). The vertical blue arrow in diagram (b) corresponds to the same set of parameters as the horizontal blue arrow in Fig. II.10(a). At \( T = 0 \) (\( T = 0.5 \)), the transition from the DSM phase to the WSM phase is of the first (second) order for the chosen parameters.](image)

not exhibit Dirac nodes, but instead *line* nodes running along the XW lines [34]. These line degeneracies are gapped out by any \( \mathcal{E} \neq 0 \), indicating the instability of such an \( \mathcal{I} \)-symmetric phase at \( T = 0 \) in Fig. II.9(a). The transition from \( R < 0 \) to \( R > 0 \) also changes the degeneracies at the \( \Gamma \) point (bottom-to-top) from \( 2 - 4 - 2 \) to \( 4 - 2 - 2 \), but this is irrelevant for the physics at the \( n = 3/4 \) filling.

At zero temperature, see Fig. II.9(a), the transition from \( \mathcal{E} = 0 \) to \( \mathcal{E} \neq 0 \) is always first order. Furthermore, for \( R \in (-0.35, 0.28) \setminus \{0\} \) a narrow WSM phase is found by varying the elasticity.\(^{10}\) For values of \( R \) outside of the mentioned interval, the first-order transition goes directly from DSM into the INS phase, i.e. the staggered strain directly jumps to a value \( \mathcal{E} > \mathcal{E}_c \). In an equivalent calculation at \( T = 0.5 \), the transition is found to be second order for all values of \( R \). By reducing \( \Upsilon \), staggered strain \( \mathcal{E} \) smoothly increases from 0 in the DSM phase to a value \( \mathcal{E} > \mathcal{E}_c \) in the INS, leading to a larger WSM region than at zero temperature.

We further study the phase diagram in the \( \Upsilon, T \)-plane for fixed SOC strength \( R = -0.4 \), see Fig. II.10(a). The diagram reveals that the WSM phase is most robust at intermediate temperatures. We further observe a reentrant phase behaviour: Starting in the symmetric DSM phase at high temperatures, the system spontaneously breaks the inversion sym-

\(^{10}\)Our numerical accuracy does not allow a definite conclusion on the presence of the WSM phase for \(|R| \lesssim 0.02\).
Figure II.10: **Phase diagrams of Hamiltonian (II.41) in the $\Upsilon, T$-plane** for parameters in Eq. (II.42).  
(a) The WSM phase is most robust at intermediate temperatures. The green line indicates the first-order transition between the $\mathcal{I}$-symmetric DSM phase and the $\mathcal{I}$-broken WSM/INS phases and ends at a tricritical point TP (green dot). At higher temperatures, the transition is always second order. The horizontal blue arrow corresponds to the same set of parameters as the vertical blue arrow in Fig. II.9(b). The red rectangle corresponds to the range of temperatures and elasticities that are used in the three-dimensional diagram on the right.  
(b) Phase diagram for the same parameters with included coupling to a symmetry-breaking staggered stress $\Upsilon \varepsilon_0$. In the presence of such a field, the distinction between the DSM and the WSM phases ceases to have a meaning. Only the structural first-order transition (the dark green sheet in the back) and the transition between the WSM and INS phases (the pale blue sheet in the front) are therefore present. Where the two transitions occur simultaneously, the dark red sheet is plotted. Various 2D slices through this 3D plot are provided by Fig II.11.

But upon further cooling, it returns to the symmetric DSM phase again. For the chosen parameters, we observe this behaviour in the range $\Upsilon \alpha^3 \in (0.513, 0.594)$. The reentrance can be traced back to the peculiar form of the density of states (DOS) in the symmetric DSM, which vanishes at the Fermi energy. Thermal broadening at finite $T$ then *enhances* the effective DOS at the chemical potential, rendering the system more susceptible to a symmetry-breaking transition at elevated temperatures than at low temperatures. A similar reentrant phase behaviour has also been observed in models of metallic metamagnetic systems [142]. At low temperatures, the transition between the $\mathcal{I}$-symmetric and the $\mathcal{I}$-broken phase is first order. The first-order transition line obeys the Clausius-Clapeyron relation, and has to approach zero temperature vertically. The first-order transition might also lead to
II.2. Model on a pyrochlore lattice

Figure II.11: Phase diagram in a symmetry-breaking field $\Upsilon E_0$. (a,b) Horizontal cuts of the three-dimensional phase diagram in Fig. II.10(b) corresponding to fixed temperature $T$, and (c,d) vertical cuts through the same diagram corresponding to a fixed staggered strain $\Upsilon E_0$. In these four diagrams, the dotted green lines correspond to the first-order structural transition, the dashed blue lines to the WSM-to-INS transition, and the solid red lines is drawn where the two transitions coincide.

A hysteretic behaviour with temperature [142]. Slightly below the tip of the belly-shaped WSM region, there is a tricritical point (TP). For temperatures above the tricritical point, the transition between the $I$-symmetric and the $I$-broken phase is of the second order.

To further explore the interesting structure of the phase diagram, we study the effect of a symmetry-breaking field, which is conjugate to the staggered strain (i.e. a staggered stress). We incorporate such an $I$-breaking field in the elastic lattice model (II.41) by modifying the elastic energy term as

$$\frac{1}{2} \Upsilon V \varepsilon^2 \mapsto \frac{1}{2} \Upsilon V (\varepsilon - \varepsilon_0)^2,$$

where $\Upsilon E_0$ parametrizes the staggered stress. The resulting 3D phase diagram in the $(\Upsilon, \varepsilon_0, T)$-space is shown in Fig. II.10(b). Due to the complexity of this 3D plot, we show in Figs. II.11 several 2D slices at either a fixed temperature $T$ or at a fixed staggered stress $\Upsilon E_0$.

A non-vanishing $\varepsilon_0$ explicitly breaks the inversion symmetry. Therefore, the DSM phase automatically transforms into a WSM phase with a small separation of the Weyl points proportional to $\varepsilon_0$. This means that the second-order transition line separating DSM from WSM at $\varepsilon_0 = 0$ ceases to exist in the presence of $\varepsilon_0$. However, the first-order line below the tricritical point survives also for $\varepsilon_0 > 0$, forming a sheet of first-order transitions (a so-called Griffiths wing [143]), which extends up to a finite value of $\varepsilon_0$. The Griffiths wing either signals a structural transition within the WSM phase [dark green sheet in Fig. II.10(b)] or between
the WSM and the INS phases [dark red sheet in Fig. II.10(b)]. Note that
the Griffiths wing takes an unusual form with a “belly” at finite temper-
atures: the end point at $T = 0.1$ occurs at $\delta_0 \approx 0.0030$ while at $T = 0$
it occurs at $\delta_0 \approx 0.0016$, see Figs. II.11(a) and (b). Finally, we note that
the boundary between the WSM phase and the INS phase remains well-
defined for all values of $\delta_0$ and $T$ [light blue sheet in Fig. II.10(b)].

### II.3 Analysing the space group symmetry

#### II.3.1 The general strategy

In this section, we demonstrate how the symmetry of the pyrochlore lat-
tice inevitably leads to the Dirac spectrum at the X point of the Brillouin
zone, and why this Dirac point has to split into four Weyl points upon
breaking the inversion symmetry $I$. The pyrochlore lattice belongs to
the same space group as the diamond lattice (#227, $Fd\bar{3}m$) so the same
reasoning as that of Ref. [34] applies. Further crystal structures belong-
ing to this space group are $\beta$-cristobalite and spinel oxides.

Our main tool to determine the spectrum degeneracies at a given $k$-
point is the relation between representations\footnote{For the precise definition of $\mathcal{D}_k(R_i)$, see Appendix A.} $\mathcal{D}_k(R_i)$ of point group
operations in the vector space spanned by the Bloch wave functions at $k$,

$$
\mathcal{D}_k(R_i) \mathcal{D}_k(R_j) = \exp (-i g_i \cdot t_j) \mathcal{D}_k(R_i \circ R_j). \tag{II.47}
$$

Here, $R_i$ is a point-symmetry operation that maps the considered $k$-
point onto itself modulo a reciprocal lattice vector $g_i = (R_i^{-1} k) - k$, and $t_i$ is
the non-symmorphic shift associated with the point operation $R_i$. The
set of all such $k$-preserving operations $R_i$ forms a group $\mathcal{G}^k$ called the
little co-group of $k$. The function

$$
\Theta(R_i, R_j) = \exp (-i g_i \cdot t_j) \tag{II.48}
$$

is called the factor system of the representation and it is completely fixed
by the lattice symmetries. A derivation of equation (II.47) can be found
e.g in Ref. [144], and we reproduce it in Appendix A.

In many situations, the factor system in Eq. (II.48) becomes trivial. This is the case especially for

(i) symmorphic lattices, because then all $t_j = 0$,
II.3. Analysing the space group symmetry

(ii) for momenta $k$ inside BZ, because then all $g_i = 0$.

In these cases, the definition (II.47) reduces to that of an “ordinary” representation. On the other hand, if the factor system is non-trivial, Eq. (II.47) defines a projective representation. This situation arises for $k$-points on the surface of BZ of non-symmetric lattices. Interestingly, irreducible projective representations (IPRs) of a group can be higher-dimensional than their ordinary counterparts.

This section is structured in the following way. In Subsec. II.3.2 we explain how the symmetries of SG #227 of the $I$-symmetric pyrochlore lattice protect a fourfold degeneracy at the X-point of BZ and why the spectrum disperses linearly around it, thus leading to a Dirac point. In Subsec. II.3.3 we show how the breaking of the inversion symmetry splits the fourfold degeneracy at X into two linearly dispersing twofold degeneracies at a higher and a lower energy. The down-dispersing band of the upper representation crosses the up-dispersing band of the lower representation along a closed loop in momentum space. In Subsec. II.3.4 we explain why this nodal loop gaps out everywhere except of four points where it is protected by lattice symmetries. These four points are the Weyl points of the WSM phase of our model.

II.3.2 The X point in the symmetric pyrochlore lattice

In this juicy subsection\textsuperscript{12} we use Eq. (II.47) to explain how the symmetries of the non-symmetric pyrochlore lattice protect the Dirac points located at the X points on the BZ boundary. Taking SOC into account, such that the $2\pi$-rotation $E$ differs from the identity operation $E$, the little co-group $\mathcal{F}^X$ contains 32 unique elements and is isomorphic to the double-valued $D_{4h}$. According to the tables in Ref. [144], the only projective IR compatible with the factor system is four-dimensional. This already explains the four-fold degeneracy observed in Fig. II.8(a). It also implies that at a commensurate filling with $4n + 2$ ($n \in \mathbb{Z}_0$) electrons per unit cell, a band insulator is not possible. This result complements a similar result found in Ref. [145] for the case of vanishing SOC but with arbitrary electron-electron interactions.

By considering the generators of $\mathcal{F}^X$, it is possible to find the factor system and a symmetry-adapted basis functions that spans the 4D IR.

\textsuperscript{12}Recommended to be read on a hot summer day!
Chapter II. Weyl semimetals

**Table II.1: Factor system of the generators of the little co-group \( \mathcal{G}^X \).** The vector indicated next to each point operation in the column headers is the non-Bravais lattice shift associated with it. The vector indicated next to the point operations in the left column indicates the reciprocal lattice shift of the X point under that point operation. The column and row with TRS operator \( T \) (displayed in gray) are included as they will come into play when analyzing the spectrum dispersion around the 4D IR.

<table>
<thead>
<tr>
<th>( \mathcal{I} ) ((t_0))</th>
<th>( \mathcal{I} ) ((g))</th>
<th>( C_{2z}^+ ) ((0))</th>
<th>( C_{4x}^+ ) ((t_0))</th>
<th>( T ) ((g))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathcal{I} ) ((t_0))</td>
<td>(-1)</td>
<td>(+1)</td>
<td>(-1)</td>
<td>(+1)</td>
</tr>
<tr>
<td>( C_{2z}^+ ) ((g))</td>
<td>(-1)</td>
<td>(+1)</td>
<td>(-1)</td>
<td>(+1)</td>
</tr>
<tr>
<td>( C_{4x}^+ ) ((0))</td>
<td>(+1)</td>
<td>(+1)</td>
<td>(+1)</td>
<td>(+1)</td>
</tr>
<tr>
<td>( T ) ((g))</td>
<td>(-1)</td>
<td>(+1)</td>
<td>(-1)</td>
<td>(+1)</td>
</tr>
</tbody>
</table>

This is achieved in Eq. (II.53). We further construct the effective low-energy Hamiltonian, given by Eq. (II.73), which demonstrates that the spectrum indeed disperses linearly around the 4D IR.

Let us first discuss the factor system constraining the projective IR at the X point. To be specific, we consider specifically the point with coordinates \( X = \frac{\pi}{2a}(1,0,0) \). The little co-group \( \mathcal{G}^X \) is generated by point operations \( \mathcal{I}, C_{2z}^+ \) and \( C_{4x}^+ \) where \( C_{n_i}^+ \) is an \( n \)-fold rotation around axis \( i \) in the positive (counter-clockwise) direction. We set the point of symmetry to be the centre of any (but fixed) tetrahedron. Of these generators,

- \( \mathcal{I} \) and \( C_{4x}^+ \) are associated with a non-Bravais shift \( t_0 = -a(1,1,1) \),
- \( \mathcal{I} \) and \( C_{2z}^+ \) transform the X point to an equivalent point displaced by \( g = -\frac{\pi}{a}(1,0,0) \).

With this information and knowing that \( e^{-ig \cdot t_0} = -1 \), we obtain the factor system between the group generators listed in Tab. II.1.

An important consequence of the non-trivial factor system in Tab. II.1 is that certain commuting point operations are represented by anticommuting operators and vice versa. We illustrate this fact with the relation between space inversion \( \mathcal{I} \) and the two-fold rotation \( C_{2z}^+ \). These point operations (i.e. ignoring the non-symmorphic translation) commute,

\[
\mathcal{I} \circ C_{2z}^+ = C_{2z}^+ \circ \mathcal{I}.
\]

(II.49a)

However, from Table II.1 it follows that their projective representations
II.3. Analysing the space group symmetry

Figure II.12: Action of inversion symmetry $\{I \mid t_0\}$. The point of symmetries is indicated by the star in middle of the blue tetrahedron, and $t_0$ is the non-Bravais translation vector indicated by the dark blue arrow in the upper left tetrahedron. Symmetry operation $\{I \mid t_0\}$ maps the non-primed sites $(1, 2, 3, 4)$ to the primed ones $(1', 2', 3', 4')$ and is equivalent to the space inversion around site 1. Note that sites 1 and 2 do not change their $x$-coordinate under the transformation while sites 3 and 4 are shifted by $-2a$. This means that $\{I \mid t_0\}$ preserves the amplitudes of Bloch wave functions with $k = X = \frac{\pi}{2a} (1, 0, 0)$ on sites 1 and 2, but it changes the amplitudes on sites 3 and 4 by a factor $\exp (i \frac{\pi}{2a} \cdot 2a) = -1$. The non-uniformity of these factors is a consequence of the non-symmorphic character of the lattice.

(which take into account the non-symmorphic translations) anticommutate:

$$\overline{\mathcal{G}}_X(I) \overline{\mathcal{G}}_X(C_{22}^+) = -\overline{\mathcal{G}}_X(C_{22}^+) \overline{\mathcal{G}}_X(I). \quad (II.49b)$$

The origin of the sign change can be understood from the geometry of the pyrochlore lattice. Recall from Fig. II.5 that the primitive unit cell of the pyrochlore lattice consists of four sites located at the corners of tetrahedra of one orientation\(^{13}\) (blue in Fig. II.12). As shown in Fig. II.12,\(^{13}\)

\(^{13}\)The tetrahedra of the other orientation (shown red in Fig. II.12) are then located in-
Table II.2: Eigenvalues of the states (II.53) under $\mathcal{D}_X(I)$ and $\mathcal{D}_X(C^{+}_{2x})$. Here, $P$ and $Q$ can both assume values $\pm i$.

|                | $|\psi_1\rangle$ | $|\psi_2\rangle$ | $|\psi_3\rangle$ | $|\psi_4\rangle$ |
|----------------|-------------------|-------------------|-------------------|-------------------|
| $\mathcal{D}_X(I)$ | $+P$              | $-P$              | $-P$              | $+P$              |
| $\mathcal{D}_X(C^{+}_{2x})$ | $+Q$              | $-Q$              | $+Q$              | $-Q$              |

inversion $\{I, t_0\}$ maps three out of four sites in one unit cell to neighbouring unit cells. As a result, when inversion acts on Bloch wave functions at $X$, non-uniform exponential factors $\exp(iX \cdot r)$ have to be taken into account. Indeed, in the convention of Fig. II.12, the amplitudes at sites 1 and 2 are unchanged, while the amplitudes at sites 3 and 4 acquire a factor

$$\exp(-iX \cdot 2b_{13}) = -1 = \exp(-iX \cdot 2b_{14}).$$  (II.50)

However, the operation $C^{+}_{2x}$ exchanges sites 1, 2 with sites 3, 4 i.e. those that change sign under $\mathcal{D}_X(I)$ with those that do not. Consequently, the amplitudes at the four sites transform under the two symmetry operations as

$$ (\psi_1, \psi_2, \psi_3, \psi_4) \xrightarrow{I} (\psi_1, \psi_2, -\psi_3, -\psi_4) \xrightarrow{C^{+}_{2x}} (-\psi_4, -\psi_3, \psi_2, \psi_1) $$  (II.51)

$$ (\psi_1, \psi_2, \psi_3, \psi_4) \xrightarrow{C^{+}_{2x}} (\psi_4, \psi_3, \psi_2, \psi_1) \xrightarrow{I} (\psi_4, \psi_3, -\psi_2, -\psi_1) $$  (II.52)

thus manifesting the anticommutation in Eq. (II.49b).

We now move on with the explanation of the four-fold degeneracy appearing at the $X$ point. To do so, we explicitly construct the four states that span the representation space of the corresponding 4D IR. Note that the representation $\mathcal{D}_X(C^{+}_{2x}) = \mathcal{D}_X(C^{+}_{4x})^2$ commutes with the representation $\mathcal{D}_X(I)$. They also both naturally commute with $\mathcal{H}(X)$ since $C^{+}_{4x}$ and $I$ are elements of the little co-group $\mathcal{G}X$. Hence, a basis can be found that diagonalizes these three operators simultaneously.

Because $\mathcal{D}_X(I)^2 = -1$ (see Table II.1) and $\mathcal{D}_X(C^{+}_{2x})^2 = \mathcal{D}_X(\overline{X}) = -1$, both $\mathcal{D}_X(I)$ and $\mathcal{D}_X(C^{+}_{2x})$ have imaginary eigenvalues $\pm i$. Let

$$ |\psi_1\rangle $$  (II.53a)

be an eigenvector of $\mathcal{H}(X)$ with eigenvalue $P = \pm i$ under $\mathcal{D}_X(I)$ and $\mathcal{D}_X(C^{+}_{2x})$. Thus, between the unit cells, and do not contain new sites entering the model.
II.3. Analysing the space group symmetry

The eigenvalue $Q = \pm i$ under $\mathcal{D}_X(C_{2\pi}^+)$. Then, the states

$$|\psi_2\rangle = \mathcal{D}_X(C_{2\pi}^+) |\psi_1\rangle \quad \text{(II.53b)}$$

$$|\psi_3\rangle = \mathcal{D}_X(C_{2\pi}^+) |\psi_1\rangle \quad \text{(II.53c)}$$

$$|\psi_4\rangle = \mathcal{D}_X(C_{2\pi}^+) \mathcal{D}_X(C_{4\pi}^+) |\psi_1\rangle \quad \text{(II.53d)}$$

are eigenvectors at the same energy. A careful application of the factor system in Tab. II.1 reveals that these four states have distinct pairs of eigenvalues under $\mathcal{D}_X(I)$ and $\mathcal{D}_X(C_{2\pi}^+)$, which we list in Tab. II.2. Hence, the four states (II.53) are mutually orthogonal and span the (projective) 4D IR at the X point. We also see that the 4D IR splits, if any of the symmetry elements $\{I \mid t_0\}, \{C_{4\pi}^+ \mid t_0\}$ and $\{C_{2\pi}^+ \mid 0\}$ is removed from the space group symmetry. Note that the presence of time-reversal symmetry $\mathcal{T}$ is not relevant for the existence of the 4D IR. However, we will see in the following pages, that $\mathcal{T}$ is essential to get a Dirac dispersion around this four-fold degeneracy.

We continue with the analysis of the spectrum dispersion around the identified Dirac point. We present a reasoning that explicitly reveals the role of symmetries. Using the symmetry-adapted basis (II.53), the spectrum to the linear order in momentum displacement $p$ is given by

$$\left[ \mathcal{H}^X_{\text{pert.}}(p) \right]_{ij} = \langle \psi_i \left| \left( \frac{\partial \mathcal{H}(k)}{\partial k} \right)_X \cdot p \right| \psi_j \rangle \approx \langle \psi_i \left| \left( \mathcal{H}(X + p) - \mathcal{H}(X) \right) \right| \psi_j \rangle. \quad \text{(II.54)}$$

If for a given direction of $p$ some of the matrix elements (II.54) are non-vanishing, then the spectrum may disperse linearly in that direction. Otherwise, the spectrum disperses at least quadratically along $p$.

Symmetries pose constraints on the matrix elements (II.54). To identify them, we use the transformation laws of the Bloch functions (II.53) deduced from Tabs. II.1 and II.2 together with the fact that the $k \cdot p$ Hamiltonian (II.54) transforms according to a (co-)vector representation

$$R : \left( \frac{\partial \mathcal{H}(k)}{\partial k} \right)_X \cdot p \mapsto \left( \frac{\partial \mathcal{H}(k)}{\partial k} \right)_X \cdot \left( R^{-1} p \right). \quad \text{(II.55a)}$$
under a point operation \( R \in \mathcal{G} \). Equation (II.55a) follows from

\[
R \left( \frac{\partial \mathcal{H}(k)}{\partial \mathbf{k}} \right)_X \cdot \mathbf{p} \right) R^{-1} = R \left[ \mathcal{H}(X + \mathbf{p}) - \mathcal{H}(X) \right] R^{-1} = \mathcal{H}(R^{-1}X + R^{-1}p) - \mathcal{H}(R^{-1}X) = \mathcal{H}(X + R^{-1}p) - \mathcal{H}(X) = \frac{\partial \mathcal{H}(k)}{\partial \mathbf{k}} \bigg|_X \cdot \left( R^{-1} \mathbf{p} \right) .
\] (II.55b)

We start by considering \( I \), which flips the sign of all components of the vector \( \mathbf{p} \). If the Bloch functions \( \langle \psi_i | \) and \( | \psi_j \rangle \) have \( \mathcal{D}_X(I) \) eigenvalues \( P_i^* \) and \( P_j \), then

\[
\left[ \mathcal{H}_{\text{pert.}}^X(\mathbf{p}) \right]_{ij} = \langle \psi_i | \mathcal{D}_X(I)^\dagger \mathcal{D}_X(I) \left( \frac{\partial \mathcal{H}(k)}{\partial \mathbf{k}} \right)_X \cdot \left( - \mathbf{p} \right) | \psi_j \rangle = (-P_i^* P_j) \left[ \mathcal{H}_{\text{pert.}}^X(\mathbf{p}) \right]_{ij} .
\] (II.56)

If \( P_i^* = -P_j \), then \( -P_i^* P_j = -1 \) and the corresponding matrix element (II.54) must be zero. This reasoning forces the matrix elements indicated in Tab. II.3 by the crossed font “\( p_i \)” to vanish.

We further consider the operation \( C_{2x}^+ \), which flips the sign of \( p_y \) and \( p_z \), and preserves the sign of \( p_x \). According to a calculation analogous to Eq. (II.56), if the Bloch functions \( \langle \psi_i | \) and \( | \psi_j \rangle \) have \textit{the same} eigenvalue \( Q_i^* = Q_j \) under \( \mathcal{D}_X(C_{2x}^+) \), they produce a factor \((\pm Q)^2 = -1\) under that transformation. This means that the corresponding \( p_x \) matrix element maps to minus itself and has to vanish. On the other hand, if the two Bloch functions have \textit{opposite} eigenvalues, they produce a factor +1, and the corresponding \( p_y \) and \( p_z \) matrix elements are forced to be zero. Both of these constraints are indicated in Tab. II.3 by the back-crossed terms “\( p_i \)” . It turns out that the remaining symmetry generators \( C_{4x}^+, C_{2z}^+ \) and \( \mathcal{T} \) do not force any of the remaining matrix elements to be zero. Since there are \( p_x \), \( p_y \) and \( p_z \) terms left uncrossed for some pair of wave functions in Tab. II.3, the spectrum disperses linearly in all directions.

The remaining 12 terms in Tab. II.3 are not all independent, but some of them are related by symmetries. In fact, a careful analysis shows that
the $k \cdot p$ Hamiltonian (II.54) has only two free parameters. To identify these constraints, we first analyse rotation $C_{2z}^+$. This leads to\textsuperscript{14}

\[
\begin{align*}
[H_{\text{pert.}}(p_x)]_{13} &= - [H_{\text{pert.}}(p_x)]_{24} \tag{II.58a} \\
[H_{\text{pert.}}(p_y)]_{12} &= + [H_{\text{pert.}}(p_y)]_{21} \tag{II.58b} \\
[H_{\text{pert.}}(p_z)]_{12} &= - [H_{\text{pert.}}(p_z)]_{21}. \tag{II.58c}
\end{align*}
\]

Additional three constraints are obtained if we permute $(1, 2, 3, 4) \mapsto (3, 4, 1, 2)$. Similarly, the little co-group generator $C_{4x}^+$ leads to

\[
\begin{align*}
[H_{\text{pert.}}(p_y)]_{12} &= (-Q) [H_{\text{pert.}}(p_z)]_{34} \tag{II.59a} \\
[H_{\text{pert.}}(p_z)]_{12} &= (+Q) [H_{\text{pert.}}(p_y)]_{34} \tag{II.59b} \\
[H_{\text{pert.}}(p_x)]_{13} &= (+Q) [H_{\text{pert.}}(p_x)]_{31}. \tag{II.59c}
\end{align*}
\]

\textsuperscript{14} Here is an example derivation of one of these constraints,

\[
\begin{align*}
[H_{\text{pert.}}(p_x)]_{13} &= \langle \psi_1 | \left( \frac{\partial H(k)}{\partial k_x} \right)_x p_x | \psi_3 \rangle \\
&= \langle \psi_1 | \mathcal{D}_x(C_{2z}^+)^\dagger \mathcal{D}_x(C_{2z}^+) \left( \frac{\partial H(k)}{\partial k_x} \right)_x p_x \mathcal{D}_x(C_{2z}^+)^\dagger \mathcal{D}_x(C_{2z}^+) | \psi_3 \rangle \\
&= \langle \psi_2 | \left( \frac{\partial H(k)}{\partial k_x} \right)_x (-p_x) | \psi_4 \rangle = - [H_{\text{pert.}}(p_x)]_{24}. \tag{II.57}
\end{align*}
\]
and opposite sign relations\textsuperscript{15} with \((1, 2, 3, 4) \mapsto (4, 3, 2, 1)\). However, only nine of the twelve derived constraints are linearly independent, meaning that the most general admissible Hamiltonian at this stage of the derivation has three free parameters. Taking hermiticity into account, the most general admissible Hamiltonian without time-reversal is

\[
\hat{H}^X_{\text{pert.}}(\mathbf{p}) = \begin{pmatrix}
0 & b p_y + ic p_z & \frac{a}{\sqrt{2}} (1 + Q) p_x & 0 \\
bp_y - ic p_z & 0 & 0 & -\frac{a}{\sqrt{2}} (1 + Q) p_x \\
\frac{a}{\sqrt{2}} (1 - Q) p_x & 0 & 0 & Q(b p_z + ic p_y) \\
0 & -\frac{a}{\sqrt{2}} (1 - Q) p_x & -Q(b p_z + ic p_y) & 0
\end{pmatrix} \quad (\text{II.66})
\]

where \(a, b, c \in \mathbb{R}\). This is not yet a Dirac Hamiltonian. The 4D IR splits into four separate bands away from the X point.

\textsuperscript{15} As an example, we show here a derivation of Eq. (II.59a). First, note that

\[
C_{4x}^+ \circ C_{2z}^+ = C_{2z}^+ \circ C_{4x}^+.
\]

This is best seen by looking at the transformation of spin degree of freedom, for which the representation of \(C_{n_i}^+\) is

\[
e^{-\frac{2n\pi}{m} \varepsilon_i} = \cos \left( \frac{\pi}{n} \right) \mathbb{1} - i \sigma_i \sin \left( \frac{\pi}{n} \right) \quad (\text{II.61})
\]

and the proof of Eq. (II.60) follows from checking that

\[
\frac{1}{\sqrt{2}} (\mathbb{1} - i \sigma_x) (-i \sigma_z) = (-i \sigma_x) (-i \sigma_z) \frac{1}{\sqrt{2}} (\mathbb{1} - i \sigma_x).
\]

We use this to show that

\[
\bar{\mathbb{X}}(C_{4x}^+) |\psi_2\rangle = \begin{pmatrix} (\text{II.53b}) \\
(\text{II.60})
\end{pmatrix} \bar{\mathbb{X}}(C_{2x}^+ \circ C_{4x}^+) |\psi_1\rangle = \begin{pmatrix} (\text{II.47}) \\
(\text{II.64})
\end{pmatrix} \bar{\mathbb{X}}(C_{4x}^+ \circ C_{2z}^+) |\psi_1\rangle = \begin{pmatrix} (\text{II.53d}) \\
(\text{II.62})
\end{pmatrix} - \bar{\mathbb{X}}(C_{2z}^+) |\psi_4\rangle = Q |\psi_4\rangle.
\]

On the other end, \( (\psi_1 | \bar{\mathbb{X}}(C_{4x}^+) \rangle \dagger = |\psi_3\rangle \), therefore

\[
[H^X_{\text{pert.}}(p_y)]_{12} = \langle \psi_1 | \left( \frac{\partial H(k)}{\partial k_y} \right)_x | p_y \rangle |\psi_2\rangle = \langle \psi_1 | \bar{\mathbb{X}}(C_{4x}^+) \left( \frac{\partial H(k)}{\partial k_y} \right)_x | p_y \rangle \bar{\mathbb{X}}(C_{4x}^+) \dagger \bar{\mathbb{X}}(C_{4x}^+) |\psi_2\rangle = \langle \psi_3 | \left( \frac{\partial H(k)}{\partial k_z} \right)_x |(p_z)\rangle = +Q [H^X_{\text{pert.}}(p_z)]_{34} \quad (\text{II.64})
\]

where in the last step we used [cf. Eq. (II.55b)] that

\[
(C_{4x}^+)^{-1} : (0, p_y, 0) \mapsto (0, 0, -p_y).
\]

(II.65)
We finally incorporate time-reversal symmetry $\mathcal{T}$. This is an antiunitary operator, which commutes with all point group symmetries. We find that

\begin{equation}
\mathcal{D}_X(I) (\mathcal{D}_X(\mathcal{T}) | \psi_i \rangle)^{2 \times \text{Tab. II.1}} = - \mathcal{D}_X(\mathcal{T}) \mathcal{D}_X(I) | \psi_i \rangle \\
= - \mathcal{D}_X(\mathcal{T}) | \psi_i \rangle = P_i \mathcal{D}_X(\mathcal{T}) | \psi_i \rangle \quad \text{(II.67)}
\end{equation}

\begin{equation}
\mathcal{D}_X(C_{2x}^+)(\mathcal{D}_X(\mathcal{T}) | \psi_i \rangle)^{4 \times \text{Tab. II.1}} = \mathcal{D}_X(\mathcal{T}) \mathcal{D}_X(C_{2x}^+) | \psi_i \rangle \\
= \mathcal{D}_X(\mathcal{T}) Q_i | \psi_i \rangle = - Q_i \mathcal{D}_X(\mathcal{T}) | \psi_i \rangle \quad \text{(II.68)}
\end{equation}

where we used the fact that the eigenvalues $P_i$ and $Q_i$ are imaginary and therefore switch sign when commuted with $\mathcal{D}_X(\mathcal{T})$. The way that time-reversal symmetry changes the eigenvalues indicates that $\mathcal{D}_X(\mathcal{T}) | \psi_1 \rangle \propto | \psi_4 \rangle$, $\mathcal{D}_X(\mathcal{T}) | \psi_2 \rangle \propto | \psi_3 \rangle$ and vice versa. More specifically, if $\mathcal{D}_X(\mathcal{T}) | \psi_1 \rangle = e^{i \phi_1} | \psi_4 \rangle$, then $^\dagger \mathcal{D}_X(\mathcal{T}) | \psi_2 \rangle = - e^{i \phi_1} | \psi_3 \rangle$.

\begin{footnote}{A careful reader may get confused at this point: How come that TRS does not conjugate both of the eigenvalues, but instead keeps that imaginary eigenvalue of $\mathcal{D}_X(I)$ intact? The superficial answer is that the factor system $\theta$ does it, but that does not provide a physical understanding. In reality, the physical inversion operation $\{I| t_0 \}$ squares to $+1$, meaning that it has eigenvalues $\pm 1$ and these are left invariant under the action of TRS. However, as explained in Appendix A, when switching from the language of little group representations $\tilde{\rho}_X$ to projective representations $\mathcal{D}_X$ in Eq. (A.9), we multiply these two eigenvalues by $e^{i X \cdot t_0} = i$ which means that eigenvalues of $\mathcal{D}_X(I)$ become $\pm i$. But this multiplication with a constant does not change the objective fact, that the eigenvalue is invariant under commutation with TRS. The factor system captures this well. This is in contrast with $\{C_{2x}^+| 0 \}$ which has imaginary eigenvalues $\pm i$ to start with, which therefore anticommute with TRS. When switching to the language of $\mathcal{D}_X(C_{2x}^+)$, we multiply by $e^{i X \cdot 0} = 1$, meaning that the eigenvalues are unaffected, still imaginary.}

\end{footnote}

\begin{footnote}{To derive this,}

\begin{equation}
\mathcal{D}_X(\mathcal{T}) | \psi_2 \rangle = \mathcal{D}_X(\mathcal{T}) \mathcal{D}_X(C_{2x}^+) | \psi_1 \rangle^{2 \times \text{Tab. II.1}} = \mathcal{D}_X(C_{2x}^+) \mathcal{D}_X(\mathcal{T}) | \psi_1 \rangle \\
= \mathcal{D}_X(C_{2x}^+) e^{i \phi_1} | \psi_4 \rangle \quad ^\dagger \mathcal{D}_X(C_{2x}^+) \mathcal{D}_X(\mathcal{T}) | \psi_3 \rangle \\
= e^{i \phi_1} \mathcal{D}_X(\mathcal{T}) | \psi_3 \rangle = - e^{i \phi_1} | \psi_3 \rangle. \quad \text{(II.69)}
\end{equation}

\end{footnote}
It follows\(^{18}\) that

\[
\begin{bmatrix}
H_{\text{pert.}}^X (p_y) \\
\end{bmatrix}_{12} = \begin{bmatrix}
H_{\text{pert.}}^X (p_y) \\
\end{bmatrix}_{34} \tag{II.71}
\]

such that we are down to only two free parameters. Combining these results with hermiticity, which determines the *phase* of the two free parameters, we obtain

\[
H_{\text{pert.}}^X (p) = \begin{pmatrix}
0 & b(p_y + Qp_z) & \frac{a}{\sqrt{2}}(1 + Q)p_x & 0 \\
b(p_y - Qp_z) & 0 & 0 & -\frac{a}{\sqrt{2}}(1 + Q)p_x \\
\frac{a}{\sqrt{2}}(1 - Q)p_x & 0 & 0 & b(p_y + Qp_z) \\
0 & -\frac{a}{\sqrt{2}}(1 - Q)p_x & b(p_y - Qp_z) & 0
\end{pmatrix} \tag{II.72}
\]

where \(a, b \in \mathbb{R}\). This is just the Hamiltonian (II.66) with \(c = ibQ\). The \(k \cdot p\) Hamiltonian (II.72) can be written compactly as

\[
H_{\text{Dirac}}^X (p) = \varepsilon(X)1 + ap_x \Gamma_1 + b (p_y \Gamma_2 + p_z \Gamma_3) \tag{II.73}
\]

where \(\varepsilon(X)\) is the energy of the 4D IR at point \(X\), and the Dirac matrices \(\Gamma_i\) are given by

\[
\begin{align*}
\Gamma_1 &= \frac{1}{\sqrt{2}} (\rho_x + iQ\rho_y) \otimes \tau_z, \\
\Gamma_5 &= \frac{1}{\sqrt{2}} (iQ\rho_x - \rho_y) \otimes \tau_z, \\
\Gamma_2 &= 1 \rho \otimes \tau_x, \\
\Gamma_3 &= iQ 1 \rho \otimes \tau_y, \\
\Gamma_4 &= \rho_z \otimes \tau_z
\end{align*} \tag{II.74}
\]

where the \(\rho_i\) Pauli matrices act on the \(2 \times 2\) blocks of the matrix Hamiltonian (II.73), and the \(\tau_i\) Pauli matrices act within these blocks\(^{19}\) and fulfill

\[^{18}\text{To see this,}\]

\[
\begin{align*}
\begin{bmatrix}
H_{\text{pert.}}^X (p_y) \\
\end{bmatrix}_{12} &= \langle \psi_1 | \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} p_y | \psi_2 \rangle \\
&= \langle \psi_1 | \mathcal{F}_X (\mathcal{T})^{-1} \left[ \mathcal{F}_X (\mathcal{T}) \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} p_y \right] \mathcal{F}_X (\mathcal{T})^{-1} | \psi_2 \rangle \\
&= \langle \psi_1 | \mathcal{F}_X (\mathcal{T})^{-1} \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} (-p_y) \rangle \left( -| \psi_3 \rangle e^{i\varphi_1} \right) \\
&= e^{-i\varphi_1} \langle \psi_3 | \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} p_y \rangle \mathcal{F}_X (\mathcal{T}) | \psi_1 \rangle \\
&\overset{(I.72)}{=} e^{-i\varphi_1} \langle \psi_3 | \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} p_y \rangle \\
&= \langle \psi_3 | \left( \frac{\partial H(k)}{\partial k_y} \right)_{X} p_y \rangle | \psi_4 \rangle = \left[ H_{\text{pert.}}^X (p_y) \right]_{34}.
\end{align*} \tag{II.70}
\]

\[^{19}\text{Note also that according to Tab. II.2, \(\mathcal{F}_X (\mathcal{I}) = p \rho_z \otimes \tau_z\) and \(\mathcal{F}_X (C_{2x}^+) = Q 1 \rho \otimes \tau_z\).}\]
the anticommutation relation $\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}$. Diagonalizing the Dirac Hamiltonian (II.73) leads to a spectrum with two doubly degenerate linearly dispersing bands

$$\varepsilon(X + p) = \varepsilon(X) \pm \sqrt{(ap_x)^2 + b^2(p_y^2 + p_z^2)}.$$  (II.75)

### II.3.3 The X point in the breathing pyrochlore lattice

In this subsection we show that breaking of the inversion symmetry decreases the allowed degeneracy at the X point from 4 to 2, i.e. the 4D IR splits into two 2D IRs with the chemical potential located in-between. The dispersion around each of these nodes is linear within the square face of the BZ, and quadratic\(^{20}\) in the perpendicular $p_x$ direction.

We do not have to start from scratch – we can adopt the rather painfully derived $k \cdot p$ Hamiltonian (II.73). As explained in Ref. [30], an $\mathcal{I}$-breaking perturbation\(^{21}\) of a Dirac Hamiltonian compatible with $\mathcal{T}$ can only be a combination of $\Gamma_4, \Gamma_{14}, \Gamma_{24}, \Gamma_{34}$ and $\Gamma_{45}$ where the double-indexed Dirac matrices are defined by

$$\Gamma_{ij} = -\frac{i}{2} [\Gamma_i, \Gamma_j].$$  (II.76)

We only have to check which of the five matrices are compatible with the point-group generators.

The little co-group at the X point of the $\mathcal{I}$-broken pyrochlore lattice is isomorphic to the double-valued $D_{2d}$ crystallographic point group. It is generated by the rotation $C_{2z}^+$ and the improper rotation

$$S_{4x}^- = \mathcal{I} \circ C_{4x}^+ : (x, y, z) \mapsto (-x, z, -y),$$  (II.77)

that satisfies $(S_{4x}^-)^2 = C_{2x}^\pm$. With the information already obtained about the states (II.53), it is relatively easy to check that

$$\mathcal{D}_X(C_{2z}^+) = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = 1_0 \otimes (-i \tau_y)$$  (II.78a)

\(^{20}\)This indicates that these two degeneracies are not Weyl points!

\(^{21}\)More precisely, this is true for zeroth order (i.e. $k$-independent) perturbation. Analysis of higher-order perturbations is more complicated.
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Table II.4: Determining the symmetry-compatible $\mathcal{I}$-breaking perturbations.
As explained in Ref. [30], only perturbations proportional to the five listed Dirac matrices are compatible with TRS. This is because they commute ($\mathcal{C}$ with $\mathcal{D}_X(\mathcal{T})$. Of the five matrices, only $\Gamma_{14}$ also commutes with the representation of the little co-group generators $\mathcal{D}_X(C_{2x}^+)$ and $\mathcal{D}_X(S_{4x}^-)$. The other other four matrices either anticommute with one of the generators (A), or do not have a simple commutation relation ($\times$)

<table>
<thead>
<tr>
<th>$\mathcal{D}_X(\mathcal{T})$</th>
<th>$\Gamma_4$</th>
<th>$\Gamma_{14}$</th>
<th>$\Gamma_{24}$</th>
<th>$\Gamma_{34}$</th>
<th>$\Gamma_{45}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{D}<em>X(C</em>{2x}^+)$</td>
<td>A</td>
<td>C</td>
<td>C</td>
<td>A</td>
<td>C</td>
</tr>
<tr>
<td>$\mathcal{D}<em>X(S</em>{4x}^-)$</td>
<td>A</td>
<td>C $\times$</td>
<td>$\times$</td>
<td>A</td>
<td></td>
</tr>
</tbody>
</table>

and

\[
\mathcal{D}_X(S_{4x}^-) = \begin{pmatrix} 0 & 0 & -PQ & 0 \\
0 & 0 & 0 & -P \\
P & 0 & 0 & 0 \\
0 & -PQ & 0 & 0 \end{pmatrix} = \frac{P}{2} (\rho_x - i Q \rho_y) \otimes (\tau_z - Q \mathbb{1}_\tau). \tag{II.78b}
\]

With Eqs. (II.74) and (II.78) it is straightforward to check the necessary commutation relations. We list them in Tab. II.4. We see that the only symmetry-compatible $\mathcal{I}$-breaking perturbation is $w \Gamma_{14}$. The spectrum of the resulting Hamiltonian can be shown to be

\[
\varepsilon(X + p) = \pm \left[ (ap_x)^2 + (w \pm b \sqrt{p_y^2 + p_z^2})^2 \right]^{1/2} \tag{II.79}
\]

which disperses linearly in the $p_y, p_z$-plane and quadratically in the $p_x$-direction.

If we do not include higher-order corrections to the perturbation Hamiltonian, energies (II.79) cross along a circular nodal loop with radius $|w/b|$. We argue in the following subsection that the crystalline symmetries gap out this nodal loop everywhere except for four discrete points.

II.3.4 Appearance of the Weyl points

A generic point lying on the nodal line described by Eq. (II.79) has only a single symmetry in its little co-group, namely the antiunitary $C_{2x}^+ \circ \mathcal{T}$. This symmetry squares to $+\mathbb{1}$ (hence it does not enforce Kramers degeneracy) and has only a single IR. We therefore expect the band crossing
II.3. Analysing the space group symmetry

to be gapped out at such a low-symmetry \( k \)-point. Potential exceptions are the XU and the XW lines which have more symmetries. In this subsection we show that the spectrum along the XU opens a gap, but the band crossings along the XW lines are protected and therefore imply the presence of Weyl points.

We first discuss the XU \( \equiv \Sigma \) high-symmetry line. Its little co-group is generated by a diagonal mirror symmetry \( M_d = \mathcal{I} \circ C_{2d} \) and the antiunitary \( C_{2x}^+ \circ T \) symmetry. We first show that such a symmetry group has only 1D IRs. To see this, note that states can be labelled by their \( \pm i \) eigenvalue \( \Sigma^2 \) of \( \Sigma (M_d) \). But this operator anticommutes \( \Sigma (C_{2x}^+ \circ T) \) which implies that if \( | \psi_0 \rangle \) is an eigenstate of \( \Sigma (M_d) \) with eigenvalue \( \varphi \), then \( \Sigma (C_{2x}^+ \circ T) | \psi_0 \rangle \) has the same eigenvalue. Since \( \Sigma (C_{2x}^+) = +1 \), this is the same state that we started with. After checking all the symmetries, we see that there are two 1D IRs which differ by their \( \Sigma (M_d) \) eigenvalue.

We want to see whether the two crossing bands of spectrum (II.79) along the \( \Sigma \) line belong to the same or to different 1D IRs. This can be deduced with a pair of considerations. First, if we restore the inversion symmetry, then \( T \circ \mathcal{I} \) enters the little co-group, and the bands 1 and 2 in Fig. II.13(a) become degenerate. This symmetry commutes with \( M_d \).

Furthermore, both \( T \circ \mathcal{I} \) and \( M_d \) are associated with zero shift \( g = 0 \) in momentum space, leading to a trivial factor system, therefore

\[
[\Sigma (T \circ \mathcal{I}), \Sigma (M_d)] = 0.
\]  (II.83)

\[22\] Since \( \mathcal{I} \) commutes will all point operation and the factor system of the symmorphic \( \mathcal{I} \)-broken phase is trivial, we find that

\[
\Sigma (M_d)^2 = \Sigma (\mathcal{I}) \Sigma (C_{2d}) \Sigma (\mathcal{I}) \Sigma (C_{2d}) = \Sigma (\mathcal{I})^2 \Sigma (C_{2d})^2 = \Sigma (\mathcal{I}) \Sigma (\mathcal{I}) = -1
\]  (II.80)

meaning that the eigenvalues of \( \Sigma (M_d) \) are \( \pm i \).

\[23\] To see this, we use the decomposition \( M_d = \mathcal{I} \circ C_{2d} \). Recall that two-fold rotations \( C_{2i}, C_{2j} \) with respect to perpendicular axes fulfil \( C_{2i} \circ C_{2j} = C_{2j} \circ C_{2i} \mathcal{E} \) as a consequence of the half-integer spin rotation matrices. Furthermore, \( T \) and \( \mathcal{I} \) commute with all point symmetry operations. Because of the trivial factor system, we find that

\[
\Sigma (M_d) \Sigma (C_{2x}^+ \circ T) = \Sigma (\mathcal{I}) \Sigma (C_{2d}) \Sigma (C_{2x}^+) \Sigma (T) = \Sigma (\mathcal{I}) \Sigma (C_{2x}^+) \Sigma (\mathcal{I}) \Sigma (T) = -\Sigma (C_{2x}^+ \circ T) \Sigma (M_d).
\]  (II.82)

The sign of \( \Sigma (M_d) \) eigenvalues is switched twice. Once upon anticommutation, and once because of antiunitary of \( C_{2x}^+ \circ T \) and their imaginary character.
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Figure II.13: Searching for Weyl point vestiges of the nodal loop. (a) A schematic sketch of the four bands (II.79) along the $XU \equiv \Sigma$ lines. The little co-group $\mathcal{F}^\Sigma$ admits two 1D IRs, indicated in the plot with the dashed red and solid blue lines. We argue in the text that the crossing bands belong to the same 1D IR and therefore gap out. (b) Analogous analysis along the $XW \equiv Z$ line reveals that in this case the crossing bands belong to different representations. Such a crossing is protected by the symmetry and acts as a Weyl point. Four such Weyl points emanate from every Dirac point upon breaking the inversion symmetry.

But $D_\Sigma(\mathcal{T} \circ \mathcal{I})$ is antiunitary, meaning that it changes the sign of the $D_\Sigma(M_d)$ eigenvalue. Consequently, bands 1 and 2 belong to different 1D IRs, and are plotted with a different colour in Fig. II.13(a). The same reasoning also applies to bands 3 and 4.

As a second step, consider the $\mathcal{I}$-broken system and move along the $\Sigma$ line to the $X$ point. When we reach the $X$ point, a perpendicular mirror symmetry $M_{d'}$ enters the little co-group, which fulfils\(^{24}\)

$$M_d \circ M_{d'} = \mathcal{E} \circ M_{d'} \circ M_d.$$  (II.84)

But because of the trivial factor system of the $\mathcal{I}$-broken phase,

$$D_X(M_d)D_X(M_{d'}) = -D_X(M_{d'})D_X(M_d),$$  (II.85)

meaning that $D_X(M_{d'})|\psi_0\rangle$ has a different $D_X(M_d)$ eigenvalue than $|\psi_0\rangle$. This implies that bands 1 and 3 of Fig. II.13(a) belong to different 1D IRs. The same conclusion can be found for bands 2 and 4. Combining the arguments of the last two paragraphs, we find that the crossing bands belong to the same IR along the $\Sigma$ line. Such a crossing is not protected by symmetry, and hybridization opens an energy gap.

\(^{24}\)See footnote (23) again.
II.3. Analysing the space group symmetry

Table II.5: Factor system of little co-group $\mathcal{G}_{\text{Z}}$ in the inversion symmetric phase.

We use these to understand the spectrum along the $XW \equiv Z$ line.

<table>
<thead>
<tr>
<th></th>
<th>$C^+_{2z}$</th>
<th>$M_x$</th>
<th>$M_y$</th>
<th>$\mathcal{T}\mathcal{I}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C^+_{2z}$ (g)</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$M_x$ (g)</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$M_y$ (0)</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>$\mathcal{T}\mathcal{I}$ (0)</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
</tr>
</tbody>
</table>

We finally investigate the crossing along the $XW \equiv Z$ lines. For concreteness, we consider the $Z$-line parallel to the $z$-axis passing through $X = \frac{\pi}{2a} (1, 0, 0)$. The little co-group is generated by a two-fold rotation $C^+_{2z}$ and an antiunitary symmetry $C^+_{2z} \circ \mathcal{T}$ as before. The same argumentation as in the case of the $\Sigma$-lines reveals that this symmetry supports two 1D IRs which are characterized by the $\pm i$ eigenvalues of $\mathcal{D}_Z(C^+_{2z})$.

Now we perform again an analogous pair of considerations to assign the four bands in Fig. II.13(b) to the two IRs. First, if we restore the inversion symmetry, then $\mathcal{T} \circ \mathcal{I}$ as well as mirror symmetries $M_x$ and $M_y$ appear in the little co-group, and bands 1 and 2 become degenerate. Furthermore, the system restores non-symmorphicity and the factor system is non-trivial, see Tab. II.5. A careful calculation reveals\(^25\) that representations $\mathcal{D}_Z(C^+_{2z}), \mathcal{D}_Z(M_x)$ and $\mathcal{D}_Z(M_y)$ mutually commute, hence a basis can be found that diagonalizes all of them simultaneously. Let $|\psi_1\rangle$ be an element of such a basis with eigenvalues\(^26\) $Q = \pm i, \mathcal{P}_x = \pm 1, \mathcal{P}_y = \pm i$.

\(^25\) Recall from footnote (23) that two rotations with respect to perpendicular axes anticommute (i.e. they have to composed with the $2\pi$ rotation $\mathcal{E}$). The same is true if one or both of the rotations is replaced by a mirror symmetry, which is just a composition of the rotation with spatial inversion. The reason for this is that spatial inversion commutes with all point operations. Combining this knowledge with the factor system in Tab. II.5 gives

\[ \mathcal{D}_Z(M_x)\mathcal{D}_Z(M_y) = -\mathcal{D}_Z(M_x \circ M_y) = \mathcal{D}_Z(M_y \circ M_x) = \mathcal{D}_Z(M_y)\mathcal{D}_Z(M_x) \] \hspace{1cm} (II.86a)

\[ \mathcal{D}_Z(M_x)\mathcal{D}_Z(C^+_{2z}) = \mathcal{D}_Z(M_x \circ C^+_{2z}) = -\mathcal{D}_Z(C^+_{2z} \circ M_x) = \mathcal{D}_Z(C^+_{2z})\mathcal{D}_Z(M_x) \] \hspace{1cm} (II.86b)

\[ \mathcal{D}_Z(M_y)\mathcal{D}_Z(C^+_{2z}) = \mathcal{D}_Z(M_y \circ C^+_{2z}) = -\mathcal{D}_Z(C^+_{2z} \circ M_y) = \mathcal{D}_Z(C^+_{2z})\mathcal{D}_Z(M_y) \] \hspace{1cm} (II.86c)

\(^26\) To understand why these eigenvalues are real or imaginary, we use Tab. II.5 to show

\[ \mathcal{D}_Z(C^+_{2z})^2 = +\mathcal{D}_Z(\mathcal{E}) = -1 \] \hspace{1cm} (II.87a)

\[ \mathcal{D}_Z(M_x)^2 = -\mathcal{D}_Z(\mathcal{E}) = +1 \] \hspace{1cm} (II.87b)

\[ \mathcal{D}_Z(M_y)^2 = +\mathcal{D}_Z(\mathcal{E}) = -1 \] \hspace{1cm} (II.87c)
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respectively, which corresponds to band 1. Since

\[ D_{XW}(\sigma_x)D_{XW}(-\sigma_y) = -D_{XW}(C_{2z}^+) \] (II.88)

the eigenvalues are constrained by \( p_x p_y = -Q \). It turns out that the state \( \mathcal{T}_Z(T \circ I)|\psi_1\rangle \) from band 2 has the same energy and eigenvalues \( (Q, -p_x, -p_y) \), respectively. The unchanged sign of the eigenvalue of \( \mathcal{T}_Z(C_{2z}^+) \) implies that bands 1 and 2 in Fig. II.13(b) belong to the same 1D IR of the \( I \)-broken phase. Analogous statement can be made about bands 3 and 4.

Second, if we move towards the X point, then \( C_{2y}^+ \) enters the little co-group and bands 1 and 3 become degenerate. Since \( C_{2x}^+ \circ C_{2y}^+ = E \circ C_{2y}^+ \circ C_{2x}^+ \), we find that

\[ D_{X}(C_{2x}^+)D_{X}(C_{2y}^+) = -D_{X}(C_{2y}^+)D_{X}(C_{2x}^+). \] (II.89)

This means that the state \( D_{X}(C_{2y}^+)|\psi_1\rangle \) from band 3 is an eigenstate at \( X \) degenerate with \( |\psi_1\rangle \) and with eigenvalue \(-Q\) under \( D_{X}(C_{2z}^+) \). This implies that bands 1 and 3 in Fig. II.13(b) belong to different representations. Analogous conclusion can be derived for the pair of bands 2 and 4. Note that the bands crossing along the Z line belong to different representations. This means that the crossing is protected and corresponds to a Weyl point. There are four such Weyl points emanating from each Dirac point upon breaking the inversion symmetry. This completes the explanation of our observations in Fig. II.8.

II.4 Surface states and Weyl-Lifshitz transitions

II.4.1 Terminations of a (111) slab

The topological nature of the WSM phase is manifested in the exotic surface states that have the form of open-ended Fermi arcs and that are robust against all local perturbations [29, 31]. As discussed in Subsec. II.1.3, the endpoints of the Fermi arcs are given by the projections of the bulk Weyl points into the surface BZ (SBZ).

Throughout this section, we focus on the \{111\} and \{11\bar{1}\} surfaces as these are the natural cleavage planes of the pyrochlore oxides. Besides
II.4. Surface states and Weyl-Lifshitz transitions

The crystal can terminate either at the triangular (T) or the kagome (K) lattice, and for $\mathcal{E} \neq 0$ we further have to specify whether the bonds connecting the outermost layer of sites to the next one are strong (S) or weak (W). In the considered slab geometry, only TW and KS terminations are possible on the top, and only TS and KW are possible on the bottom.

The topological surface states exhibited by the WSM of model (II.41), we also identify non-topological surface states in the DSM and the INS phase for certain terminations of the pyrochlore lattice.

Along the $\{111\}$ directions, the pyrochlore lattice can be viewed as a stack of alternating layers of triangular and kagome lattices. Hence, the two simplest open boundary conditions correspond to terminating the crystal at sites making up either the kagome lattice (K) or the triangular lattice (T). Note that the kagome termination splits the outermost tetrahedra. This observation will help us interpret some of the observed surface states in Subsec. (II.4.2).

Because of the inequivalent bonds in the $I$-broken state, we further have to specify whether the bonds connecting the outermost layer of sites to the next layer are strong (S) or weak (W). This gives four possible terminations illustrated in Fig. II.14. For the DSM phase, the labels S and W are redundant and can be dropped. A suitable geometry for experimental studies is a thin slab with large lateral dimensions [117]. If we set the $(111)$ surface on the top and we limit our attention to $\mathcal{E} > 0$, then only KS and TW can be realized on the top, and only KW and TS can be realized on the bottom surface, as illustrated in Fig. II.14.

The SBZ has the shape of a regular hexagon and its construction is in-
Figure II.15: The surface Brillouin zone of a (111) slab. (a) The TRIMs of the surface Brillouin zone (SBZ) are obtained by projecting (brown dashed lines) pairs of bulk TRIMs on top of each other. The chirality of the twelve Weyl points located on the BZ boundary is indicated by the red vs. green dots. (b) Definition of the high-symmetry points \( \Gamma, M \) and \( K \) of SBZ. The three inequivalent M points and the \( \Gamma \) point are TRIMs. The solid red and dashed green lines indicate the trajectories of the projections of Weyl points of the two chiralities upon increasing the value of \( \varepsilon \). The crosses indicate where the Weyl points annihilate for the critical value \( \varepsilon_c \). (c) and (d) The DSM phase develops a tiny gap for finite thickness of the slab. The \( \mathbb{Z}_2 \) invariant of the insulating phase depends on the number of TRIMs encircled by the surface Fermi lines. Situation (c) corresponds to a NI and situation (d) to a TI.

In this subsection we provide a detailed discussion of the surface states plotted in Fig. II.16. The organization is such that we sequentially increase the value of \( \varepsilon \geq 0 \), and for each value we discuss all the relevant surface terminations.

We begin with the case \( \varepsilon = 0 \) which corresponds to the DSM phase. We find no surface states for the triangular termination. For the kagome termination, we find a single non-degenerate Fermi line connecting the
II.4. Surface states and Weyl-Lifshitz transitions

Figure II.16: Surface states for various surface terminations as a function of $\varepsilon$. The surface spectral function is plotted within the hexagonal SBZ constructed in Fig. II.15(a). The blue circles in the DSM row indicate the projections of the bulk Dirac points into SBZ. In the same way, the red square and the green triangle markers in the WSM rows indicate the projection of Weyl points of the two chiralities, and the pale crosses in the $E_c$ row represent the $k$-points where pairs of Weyl points annihilate. In the INS phase, the chemical potential is set to the middle of the bulk gap. The detailed discussion of the surface states for the individual terminations as a function of $\varepsilon$ is provided in Subsec. II.4.2.
M points of the hexagonal SBZ, which are the projections of the bulk Dirac points. However, since the surface explicitly violates some of the symmetries that protect the bulk Dirac points, a small gap (which shrinks with an increasing slab width) opens in the (111) film. As a consequence, the surface states for the kagome termination of the DSM phase do not pass exactly through the M points but slightly circumvent them.

In general for band insulators, the surface Fermi line has to avoid the time-reversal invariant momenta (TRIMs) of SBZ. The parity of the number of enclosed TRIMs depends on the strong $\mathbb{Z}_2$ invariant of the band structure [16, 17]. Because of the threefold rotation symmetry of the slab, we expect that either the situation shown in Fig. II.15(c) (normal insulator, NI) or in Fig. II.15(d) (topological insulator, TI) occurs. We numerically find that the NI possibility is realized. This is consistent with the fact that there are no surface states for the triangular termination.

We proceed with the discussion of the WSM phase. In this case, the surface states form Fermi arcs connecting the projections of Weyl points (WPs) of opposite chirality. Interestingly, the connectivity of the Fermi arcs, i.e. the way the WPs are paired into the arcs, depends on the termination of the sample. In Ref. [146], a similar dependence appears naturally in a toy model consisting of a stack of alternating electron and hole Fermi surfaces. Here, we directly observe this phenomena in a microscopic model. Let us be more specific:

- For the TW termination, we observe six Fermi arcs developing between the projections of WPs in neighbouring SBZs as $\varepsilon$ increases from zero. At the critical $\varepsilon_c$, three Fermi arcs surrounding a K point form a closed Fermi line. For even larger values of $\varepsilon_c$, all surface bands are shifted away from the bulk chemical potential.

- For the KS termination, the very opposite happens. The closed Fermi line present in the DSM phase splits into six Fermi arcs upon breaking the inversion symmetry. Increasing the staggered strain $\varepsilon$ leads to a shrinkage of the Fermi arcs and to a complete disappearance of the surface states at $\varepsilon_c$.

- For the TS termination when $\varepsilon \gtrsim 0.04$, the same pairs of WPs as for the KS termination are connected but with opposite curvature. They also disappear at $\varepsilon_c$. In Subsec. II.4.3, we separately discuss the interesting parameter range $0 < \varepsilon \lesssim 0.04$. 
For the KW termination, additional Fermi arcs appear very close to the Fermi lines present in the DSM phase. This fact makes their observation obscured in Fig. II.16. For the INS phase we find a pair of closed Fermi lines encircling the $\Gamma$ point.

We further investigate the surface states of the INS phase. In this case we observe no surface states for the TS, TW and KS terminations. However, for the KW termination, there are two surface bands crossing the bulk chemical potential that encircle the $\Gamma$ point. These observations are in accordance with the trivial $\mathbb{Z}_2$ invariant of the INS phase.

One possibility to understand the non-topological surface states of the KW termination is to consider the (unphysical) limit $\mathcal{E} \to 1$ and $p \to 0$ which corresponds to a lattice of isolated tetrahedra. Such a lattice is reminiscent of the atomic limit and exhibits only flat bands. The boundary of such a lattice consists of

(i) isolated tetrahedra for the TS and KS terminations,

(ii) isolated triangles for the KW termination,

(iii) isolated points for the TW termination.

In situation (i), the bulk and the surface have identical spectra so the chemical potential lies in the gap of both. For sufficiently weak coupling between the tetrahedra, this observation has to remain valid and we do not expect surface states for the TS and KS terminations.

For the other two situations, we need to know the eigenenergies of the corresponding boundary objects. Focusing on $s = +1$, the states of an isolated tetrahedron with SOC parametrized by $R$ lie at energies

$$
\varepsilon^{(4)}_1 = 6, \quad \varepsilon^{(4)}_2 = -2(1 - 4R), \quad \varepsilon^{(4)}_{3,4} = -2(1 + 2R).
$$

Due to TRS, all levels are doubly degenerate. It follows that for $R = -0.4$ (as in the calculation of Fig. II.16), the chemical potential satisfies

$$
\varepsilon^{(4)}_2 < \varepsilon^{(4)}_{3,4} < \mu < \varepsilon^{(4)}_1.
$$

On the other hand, the energy levels of an isolated triangle appearing at the KW termination are

$$
\varepsilon^{(3)}_{\pm} = 1 + 2R \pm \sqrt{3 \left[ 3 + 4(1 - R)R \right]},
$$

$$
\varepsilon^{(3)}_3 = -2(1 + 2R).
$$
Chapter II. Weyl semimetals

The highest energy level $\varepsilon^{(3)}_+$ also satisfies

$$\varepsilon^{(4)}_{3,4} < \varepsilon^{(3)}_+ < \varepsilon^{(4)}_1 \quad (II.93)$$

which pins $\mu$ at $\varepsilon^{(3)}_+$ for $T = 0$ in a charge neutral system. The eigenenergy of an isolated point appearing at the TW termination is simply

$$\varepsilon^{(1)}_1 = 0, \quad (II.94)$$

which too lies between $\varepsilon^{(4)}_{3,4}$ and $\varepsilon^{(4)}_1$ for $R = -0.4$. We therefore expect that there are surface states in the bulk gap both for the KW and the TW termination, even if we reintroduce the coupling between the tetrahedra. We indeed do observe this. In Fig. II.16, we fixed the chemical potential in the INS phase at the bulk value. For the KW termination, the surface states cross the bulk chemical potential, for the TW termination they lie below it.

II.4.3 Weyl-Lifshitz transitions

We observed in Fig. II.16 that the connectivity and the shape of Fermi arcs in the WSM phase depend on the termination of the sample. For the studied surfaces of our model, there are three possible connectivities that respect the symmetries of the system, see Fig. II.17(a-c). Interestingly, it is possible to continuously move from one connectivity to another, giving rise to a Lifshitz transition of the Fermi arcs that we dub Weyl-Lifshitz transition. More precisely, the Weyl-Lifshitz transition is characterized by a topological change of the closed Fermi lines formed by joining the Fermi arcs on the top and bottom surface. A similar transition was also observed and discussed in Ref. [147].

We have observed such a transition for the TS termination when varying the amplitude of staggered strain $\varepsilon$. For small $\varepsilon$, the connectivity of the Fermi arcs is identical to that of the TW termination, see Fig. II.16. At $\varepsilon \approx 0.015$, a part of the topological surface band crosses the chemical potential from below at the two K points. The corresponding Fermi lines grow and at $\varepsilon \approx 0.04$ they touch the original Fermi arcs. A reconnection of the Fermi arcs from situation in Fig. II.17(b) to that of Fig. II.17(a) occurs.

Another possibility is to tune the shape and connectivity of the Fermi arcs by applying a surface gate potential. We model such an experiment
II.4. Surface states and Weyl-Lifshitz transitions

Figure II.17: Symmetry compatible connectivities of the surface Fermi arcs. (a,b,c) The three Fermi arc connectivities that preserve the symmetry of the system. The dark red and pale green points indicate the projections of the bulk WPs of opposite chiralities. The bending bright blue arrows connecting the WPs indicate the direction of motion of the electrons in the quantum oscillations experiment proposed in Ref. [117] when a magnetic field is applied perpendicular to the surface. (d) The oriented vertical lines correspond to the chiral Landau levels emanating from the WPs, cf. Subsec II.1.2, and act as “conveyor belts” transporting the electrons between the top and bottom surfaces of the slab. If the indicated connectivity of the Fermi arcs is realized on the bottom surface (pale red), the electron orbits traverse the bulk 2, 6 and 12 times, respectively, if connectivities (a),(b) and (c) are realized on the top surface (pale blue). Realizing the situations (b) and (c) on the opposite surfaces leads to electron orbits traversing the bulk 4 times.

in a simplified manner by adding an on-site potential \( V \) to the outermost layer of atoms. This effectively shifts the energy of the surface states, and those that were originally away from the Fermi level can be tuned to cross it. The surface states are then allowed to hybridize with the Fermi arcs, leading to a reconnection of the Weyl points. Fig. II.18(a) shows the transition between the connectivities shown in Fig. II.17(a) and (b) by applying a positive surface potential to the KS termination. Similarly, we observe a transition between the situations shown in Fig. II.17(a) and (c) if we apply a negative surface potential.

An interesting aspect of the Weyl-Lifshitz transition is that it changes the number of times an electron crosses the bulk in order to complete
For fixed $\mathcal{E} = 0.08$ we observe a Weyl-Lifshitz transition by changing the on-site potential on the outermost layer of atoms by applying a surface gate. Assuming the TS termination on the opposite surface as in Fig. II.17(d), we find that (a) the transition at positive $V = 0.93$ changes the number of times the electron orbits cross the bulk from 2 to 6, and (b) the transition at negative $V = -0.82$ changes the same number from 2 to 12.

Figure II.18: Example Weyl-Lifshitz transitions for the KS termination. For fixed $\mathcal{E} = 0.08$ we observe a Weyl-Lifshitz transition by changing the on-site potential on the outermost layer of atoms by applying a surface gate. Assuming the TS termination on the opposite surface as in Fig. II.17(d), we find that (a) the transition at positive $V = 0.93$ changes the number of times the electron orbits cross the bulk from 2 to 6, and (b) the transition at negative $V = -0.82$ changes the same number from 2 to 12.

Such a dramatic change might be observable in quantum oscillation experiments in very clean samples for which the mean-free path $\lambda$ exceeds the system width $L_z$. As mentioned in Subsec. II.1.3, according to Ref. [117] the surface-state response shows periodic-in-$1/B$ oscillations for both the resistivity and the magnetization. An energy level periodically crosses the chemical potential $\mu$ when condition (II.33) is fulfilled for some $n \in \mathbb{Z}^+$. Hence, by measuring the dependence on the field-direction, one can extract the second term $ecL_z/\hbar k_0$ of Eq. (II.33). In an experiment with a surface gate potential similar to Fig. II.18, the change in $ecL_z/\hbar k_0$ originates both from the change of the length of the Fermi arcs $k_0$, and from the change in the number of bulk crossings $2c$. 

its semiclassical orbit in an external magnetic field. For example, if we assume the TS termination on the bottom and the KS termination on the top surfaces, the transitions shown in Fig. II.18 change the number of bulk crossings from 2 to 6 in example (a) and from 2 to 12 in case (b).
We already encountered in Eq. (II.4) of Sec. II.1 the possibility of creating a nodal line – i.e. a one-dimensional touching of the conduction and valence bands inside the Brillouin zone. At that stage, we treated such a node only as a curiosity, and did not pay much attention to it. In this chapter, we return to these objects and examine them in much detail.

We begin in Sec. III.1 with a discussion of the symmetry requirements to realize a nodal line (semi-)metal. While the only conditions on the possible occurrence of Weyl semimetals were the absence of $T \circ I$ symmetry and the presence of SOC, we find that nodal lines can appear in systems with a very differing level of symmetry. We follow (and slightly supplement) here Ref. [148] in an attempt to organize all these various realizations into several categories. We observe that the unifying feature of all known nodal lines is a topological $\mathbb{Z}_2$ charge corresponding to a quantized Berry phase on a loop enclosing the nodal line, although an additional protection is sometimes also present. We further use this introductory section to explain the origin of the nearly-flat “drumhead” surface bands appearing in systems exhibiting a nodal line.

The rest of the chapter contains our original results. While in Sec. II.3 we discussed how non-symmorphic symmetry may enforce high-order degeneracies on the BZ boundary via the non-trivial factor system, in Sec. III.2 we show that non-symmorphicity may also impose band degeneracies along high-symmetry lines or planes inside BZ via the non-trivial compatibility relations between the IRs at high-symmetry points.
We apply these arguments to spin-orbit coupled systems with a glide plane and no inversion centre to show that such materials are automatically furnished with nodal lines. We refer to such symmetry-imposed nodal lines as non-symmorphic nodal lines and contrast them to accidental nodal lines which need certain degree of luck on the band structure side to be realized. In spite of the differences, both species of nodal lines are characterized with the same $\mathbb{Z}_2$ invariant. We further show that if a system respects a pair of glide planes, space group symmetry enforces the presence of a pair of touching nodal loops (i.e. circular nodal lines) which stretch all the way across BZ. Consequently, the node looks like a chain in the extended $k$-space. We thereby dub materials exhibiting such a feature near the Fermi level nodal-chain metals. By systematically going through all non-magnetic space groups, we develop a complete catalog of possible nodal chains.

It turns out, that the addition of the spatial inversion to the space group of a non-symmorphic nodal line (NSNL) leads to the contraction of the NSNL into a Dirac point located at a TRIM on the BZ boundary. We use Sec. III.3 to comment on the relation between Dirac points and NSNLs. This connection helps us to understand the peculiar structure of Landau levels (LLs) of a NSNL which is very sensitive to the direction of the applied magnetic field. Based on the character of the LLs, we hypothesize that NSNLs exhibit a direction-selective chiral anomaly manifested by a very anisotropic magnetoresistance. However, we fail to reproduce such a result in the semiclassical limit. We make a few remarks on this disagreement, but we ultimately conclude that a more careful analysis which takes into account non-adiabatic corrections is necessary to determine the nature of magnetoresistance in materials with a NSNL in the vicinity of the Fermi level.

In Sec. III.4 we present the results of numerical calculations performed by our colleague Dr. Quan-Sheng Wu, which indicate that the existing material IrF$_4$ might be a nodal-chain metal. We present the calculated surface spectral function, develop an effective tight-binding model, and use group theory and Wilson loop operators to explain the presence of all the surface bands of this material. A situation with detached NSNLs can be obtained by applying the appropriate strain to a nodal-chain metal.

To completely comprehend the surface states predicted for IrF$_4$, we make use of the sublattice structure of this material. It turns out that
in the presence of a *perfect* sublattice symmetry (i.e. in a model with only NN hopings included), the symmetries impose the presence of a *third* nodal loop. This additional loop touches both of the glide-imposed nodal loops, thus forming a peculiar three-dimensional *nodal net* structure. We present the symmetry arguments explaining the appearance of this complex nodal structure in Sec. III.5. The sublattice symmetry is only mildly broken in realistic IrF$_4$, such that we observe a small vestigial gap in its band structure where the third nodal loop would have appeared in an idealized scenario.

### III.1 Research Overview

#### III.1.1 Weyl lines in spin-orbit coupled systems

We begin with a reformulation of the nodal lines encountered in Sec. II.1. We consider a mirror-symmetric system breaking the $\mathcal{T} \circ \mathcal{I}$ symmetry, such that the bands are spin-split. Then a pair of non-degenerate bands with different mirror eigenvalues may cross within a mirror-invariant plane, thus forming a nodal line. To see this, consider a mirror symmetry that flips the orientation of the $z$-axis, represented by $^1 M_z = -i\sigma_z$, acting on the effective two-band Hamiltonian

$$
\mathcal{H}(k) = h_0(k)\mathbb{1}_\sigma + h(k) \cdot \sigma
$$

(III.1a)

where $h_{0,x,y,z}$ are real-valued functions of momentum. The invariance under the mirror symmetry

$$
\mathcal{H}(k_x, k_y, -k_z) = M_z \mathcal{H}(k_x, k_y, k_z) M_z^{-1}
$$

(III.1b)

implies that $h_{x,y}$ are *odd* in $k_z$ while $h_{0,z}$ are *even* in $k_z$. The first pair of conditions imply that on the mirror-invariant plane $k_z = 0$ the Hamiltonian reduces to that of Eq. (II.4) which closes the band gap with codimension $\delta = 1$ and therefore enables the appearance of nodal lines.

We wish to formulate a topological invariant that protects such a nodal line. To do so, note that the spinor character of Hamiltonian (III.1a)

---

1This form of the operator is motivated by the action of $M_z = C_2^+ \circ \mathcal{I}$ on the spin degree of freedom. Inversion symmetry leaves spin unaffected, $\mathcal{I} = \mathbb{1}_\sigma$, and the rotation part is represented by $C_2^+ = e^{-i\pi \sigma_z} = -i\sigma_z$. Nevertheless, the microscopic meaning of the two-level degree of freedom described by Pauli matrices $\sigma_i$ is irrelevant for the argument. In fact, the argument proceeds equally well for any $M_z = e^{i\alpha} (\mathbf{n} \cdot \sigma)$ where $\mathbf{n}$ is an arbitrary unit vector in $\mathbb{R}^3$. 

---
allows us to harbour the discussion of spin rotations in Subsec. I.1.5. More specifically, consider a closed path $\gamma \subset BZ$ with a gapped spectrum, and interpret $h(k)$ as a magnetic field $B$ acting on a spin-$\frac{1}{2}$ particle. The magnetic field evolves in time, which corresponds to the dependence of vector $h(k)$ on the momentum along the path. We have discussed in the introductory chapter that the geometric phase picked up by such a system equals half the area of the (oriented) solid angle spanned by the unit vectors

$$n(k) = \frac{h(k)}{||h(k)||}. \quad \text{(III.2)}$$

Not much can be deduced about the phase $\varphi_B(\gamma)$ for a generic closed path. However, for a mirror-symmetric closed path, i.e. $M_z \gamma = -\gamma$ (where the minus sign takes care of the orientation), the spanned solid angle becomes quantized.

To see the quantization, notice that for momenta within the mirror-invariant plane, there are only two possible unit vectors $n = (0, 0, \pm 1)$ which we call the north (N) and the south (S) pole. This corresponds to a positive vs. negative value of $h_z(k_x, k_y, 0)$, meaning that the two regions are separated by the nodal line. We illustrate these regions with a different colour in Fig. III.1(a). Note that a path $\gamma_1$ which encloses the nodal line has to pass through both the north and the south pole. Because of the symmetry of functions $h_i$, the pair of points $(k_x, k_y, \pm k_z) \in \gamma_1$ are represented by unit vectors $(\pm n_x, \pm n_y, n_z)$ which are related by a $\pi$-rotation around the vertical axis. This implies that the differential area spanned by momentum increments $dk$ and $-M_z dk$ is proportional to half the circumference of the local parallel of the unit sphere “globe”, see Fig. III.1(b). Since $\gamma_1$ passes through both of the poles, the net area it spans corresponds to the integral of the half-circumferences, which is simply half the area of the unit sphere. This corresponds to Berry phase $\varphi_B = \frac{1}{2}2\pi = \pi$. On the other hand, a mirror-symmetric path $\gamma_2$ that does not contain the nodal line passes twice through one of the poles. As illustrated in Fig. III.1(c), in such case the trajectory of $n(k)$ encloses two regions of the same area but of opposite orientation, meaning that the spanned oriented angle is $\omega = 0$, corresponding to $\varphi_B = 0$.

The geometric arguments of the previous paragraph can be formalized using the results of Subsec. I.2.3. We derived in Eq. (I.87) that the Berry phase of a 1D system with a unitary symmetry relating $\mathcal{H}(k)$ to $\mathcal{H}(-k)$ quantizes the Zak phase to $\varphi_{\text{Zak}} \in \{0, \pi\}$. This applies regardless
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of the number of bands. Obviously, if we define a one-component momentum running along a mirror-symmetric closed path $\gamma$, such a symmetry is present, hence the quantization is guaranteed. A non-trivial value of such a $\mathbb{Z}_2$ invariant indicates that the corresponding path is not contractible without encountering a band degeneracy, i.e. that it encloses

Figure III.1: Quantization of Berry phase acquired on a mirror-symmetric path. (a) Within the mirror-invariant plane (parallelogram), the unit vector $n(k)$ points either to the north (N, blue) or to the south (S, red) pole. The two regions are separated by the nodal line (NL, black). (b) The trajectory of $n(k)$ corresponding to a path $\gamma_1$ which encloses the nodal line has to pass through both N and S. As explained in the text, because of the mirror symmetry (III.1b) the images of the parts of $\gamma_1$ in the upper and in the lower half-space are related by a $\pi$-rotation around the vertical axis. Consequently, the trajectory of $n(k)$ spans half the unit sphere surface, which leads to Berry phase $\varphi_B = \pi$. (c) The same analysis for a path $\gamma_2$ that does not enclose the nodal line. In this case, $n(k)$ spans two regions of the same area but opposite orientation, hence the net oriented solid angle vanishes. The solid angle orientation is best seen by assigning explicit orientation to $\gamma_2$, which we indicate be the arrows, and then applying the right-hand rule. The thumb points inward vs. outward for the two regions.
Figure III.2: The incompleteness of the Berry phase invariant. Example band structures that exhibit a pair of nodal lines protected by a mirror symmetry. The red and blue lines indicate bands with even vs. odd mirror eigenvalue, meaning that all the drawn band crossings are protected by the mirror symmetry. In both cases, we consider a (mirror-symmetric) path $\gamma$ that encloses both nodal lines. The locations where $\gamma$ intersects the mirror-invariant plane are indicated with the black crosses. In case (a), the Berry phase $\varphi_B = 0$ is trivial and the two nodal lines can indeed be annihilated by shifting the two bands in energy in opposite directions. On the other hand, the Berry phase in case (b) is again trivial, but the bands cannot be separated. This is because the $\mathbb{Z}$-valued invariant (III.4b) remains non-trivial. The background colours in both plots indicate the value of quantity (III.4a) which is used to determine the $\mathbb{Z}$-valued invariant (III.4b).

a nodal line. We formally write for this invariant

$$z_2(\gamma) = \frac{\varphi_B(\gamma)}{\pi} \mod 2.$$

(III.3)

However, as pointed out in Sec. 2 of Ref. [148], the Berry phase invariant is incomplete. Since it is a $\mathbb{Z}_2$-valued quantity, it suggests that a pair of nodal lines is always able to annihilate. But this is not true. Consider the pair of situations in Fig. III.2 where we plot two simple band structures along a mirror-invariant momentum. The red and blue colour indicate the two possible mirror eigenvalues, and the black crosses indicate where the mirror-symmetric path $\gamma$ crosses the high-symmetry plane. In both situations, $\gamma$ encloses a pair of nodal lines, meaning that $\varphi_B(\gamma) = 0$ is trivial. However, while the pair of nodal lines contained by $\gamma$ in Fig. III.2(a) can be trivially removed, the pair of nodal lines in Fig. III.2(b) cannot. The reason is that the number of occupied bands of a prescribed eigenvalue is different at the two crosses. More precisely we
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define a quantity

\[ n_M(k) = \sum_{\alpha \in \text{occ.}} \langle u^\alpha(k) | M_2 | u^\alpha(k) \rangle \]  

(III.4a)

which counts the sum of mirror eigenvalues of all the occupied bands at a mirror-invariant momentum \( k \). We further denote the two points where \( \gamma \) intersects the mirror-invariant plane as \( k_{1,2} \). Then

\[ c(\{k_1, k_2\}) = \frac{n_M(k_2) - n_M(k_1)}{2} \in \mathbb{Z} \]  

(III.4b)

defines an integer topological invariant. The invariant is indeed trivial for the situation in Fig. III.2(a) and equals +2 for the situation in Fig. III.2(b). We observe that

\[ c(\{k_1, k_2\}) = \frac{\phi_B(\gamma)}{\pi} \mod 2. \]  

(III.4c)

Note that the expression on the left of Eq. (III.4c) correctly expresses that the precise choice of path \( \gamma \) is irrelevant. In chapter IV we will encounter a few more invariants defined on a pair of \( k \) points, and we will refer to such a pair as a zero-dimensional sphere \( S^0 \).

On the other hand, the surface states are only sensitive to the parity of invariant (III.4b), i.e. only to the \( \mathbb{Z}_2 \) Berry phase again. To understand this, note that topologically protected surface states of semimetals can be understood through a dimensional reduction to gapped systems. Similar to the explanation of Fermi arcs in Weyl semimetals by cutting the 3D BZ into 2D slices characterized by a \( \mathbb{Z} \)-valued Chern number, we can now divide the BZ into vertical 1D “fibers” characterized by a \( \mathbb{Z}_2 \)-valued Zak phase. This quantization appears due to the mirror symmetry of the 1D fibers [49]. As discussed in Subsec. I.2.3, \( \varphi_{\text{Zak}} = \pi \) is associated with the presence of an edge state [57]. The nodal line separates fibers with a trivial vs. non-trivial Zak phase, as is explained in the caption to Fig. III.3. Collecting all the edge modes of the fibers which pass through the interior of the nodal line, we find a “drumhead” surface band living inside the projection of the NL inside the surface BZ (SBZ). Since the \( \mathbb{Z} \)-valued invariant (III.4b) does not have a direct equivalent in 1D insulators, we cannot use it to construct edge states.

\[ ^2 \text{In the presence of an electron-hole symmetry, this edge state occurs at zero energy and leads to a } \pm e/2 \text{ excess charge located at the edge of the system. This is especially relevant for the chiral symmetry models discussed in Subsec. III.1.4.} \]
Chapter III. Nodal line semimetals

III.1.2 Dirac lines in spin-orbit coupled systems

In spinful systems with $T \circ I$ symmetry, the Kramers theorem implies a double degeneracy of all bands. We have already mentioned in Subsec. II.1.1 that the codimension to create a gap closing in such a system without additional symmetries is too high, but that such a touching point can be stabilized with the help of certain crystalline symmetries. We call such a touching a Dirac point. Stabilizing a Dirac line sounds even
more daunting, but Ref. [38] showed that it is possible with the help of non-symmorphic symmetries. Here, we briefly review their proof reformulated into the mathematical language of Subsec. II.3.

We consider a primitive orthogonal space group, meaning that the unit cell consists of a simple block with sides a, b and c and BZ is a box with dimensions $\frac{2\pi}{a}$, $\frac{2\pi}{b}$ and $\frac{2\pi}{c}$. We assume the presence of a symmorphic\(^3\) inversion symmetry $I$ and time-reversal symmetry $T$, and a non-symmorphic two-fold rotation around the $z$-axis. We require the square of the rotation to yield a shift by one unit cell along the $z$-axis.

Such a non-symmorphic rotation symmetry is commonly referred to as a screw axis. This forces the non-symmorphic shift associated with $C^+_{2z}$ to be\(^4\) $(x_0, y_0, \frac{c}{2})$. Then the composition $I \circ C^+_{2z}$ is a non-symmorphic mirror, leading to a pair of mirror-invariant planes at $k_z c = 0$ and $k_z c = \pi$.

Furthermore, the composition $I \circ T$ also belongs to the little co-group of points lying in these planes. One can therefore construct a factor system in a way similar to Tab. II.1, which we do in Tab. III.1.

Operator $\overline{\mathcal{G}}_{k_z c}(I \circ C^+_{2z})$ which properly represents the non-symorphic mirror $I \circ C^+_{2z}$ in the high-symmetry plane $k_z c$ has to be unitary. To find its eigenvalues, we calculate the square

$$
\overline{\mathcal{G}}_{k_z c}(I \circ C^+_{2z})^2 = e^{-i k_z c} \overline{\mathcal{G}}_{k_z c}(I \circ C^+_{2z} \circ I \circ C^+_{2z}) = e^{-i k_z c} \overline{\mathcal{G}}_{k_z c} (E) = -e^{-i k_z c} \quad (\text{III.6})
$$

where we used the information in Tab. III.1 and the fact that $I$ commutes with all other point operations. We see that the mirror eigenvalues are imaginary in the $k_z c = 0$ plane, and real in the $k_z c = \pi$ plane.

Let $|\psi_1\rangle$ be an eigenstate of $\overline{\mathcal{G}}_{k_z c}(I \circ C^+_{2z})$ with eigenvalue $\mathcal{P}$. Since $\overline{\mathcal{G}}_{k_z c}(T \circ I)$ is an antunitary operator squaring to $-\mathbb{1}$, $\overline{\mathcal{G}}_{k_z c}(T \circ I)|\psi_1\rangle$

\(^3\)It is always possible to find such a point of symmetry that $I$ is symmorphic. If $I : \vec{r} \mapsto (-\vec{r} + \vec{t})$, then $I : (\frac{t}{2} + \vec{r}) \mapsto (\frac{t}{2} - \vec{r})$, meaning that the spatial inversion acts symmorphically with respect to point $t/2$.

\(^4\)Let the screw axis transform the real space as

$$
C^+_{2z} : (x, y, z) \mapsto (-x + x_0, -y + y_0, z + z_0). \quad (\text{III.5a})
$$

Applying $C^+_{2z}$ twice leads to

$$
(C^+_{2z})^2 : (x, y, z) \mapsto (x, y, z + 2z_0). \quad (\text{III.5b})
$$

Since we demand this to be a translation by one unit cell in the $z$-direction, we conclude that $z_0 = c/2$. Crystalline symmetry further implies that $x_0 = n_x \frac{a}{2}$ and $y_0 = n_y \frac{b}{2}$ where $n_i \in \mathbb{Z}$, but these finer constraints do not enter the argument.
Chapter III. Nodal line semimetals

Table III.1: Factor system for momenta in mirror-invariant planes. The little co-group is generated by only two point operations $R$, namely $T \circ I$ and $I \circ C_{2z}^+$. The vectors in the column headers indicate the associated shift $t_j$ in real space, and the vectors in rows indicate a reciprocal lattice vector $g_i = (R^{-1}k) - k$. The four values in the table are the structure factors $e^{-ig_i \cdot t_j}$ which depend on the choice of the high-symmetry plane. Only the plane on the BZ boundary ($k_{zc} = \pi$) has a non-trivial factor system because of the non-symmorphic symmetry.

<table>
<thead>
<tr>
<th>$T \circ I$</th>
<th>$I \circ C_{2z}^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(0,0,0)$</td>
<td>$(-x_0, -y_0, -\frac{c}{2})$</td>
</tr>
<tr>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>+1</td>
<td>$e^{-ik_{zc}}$</td>
</tr>
</tbody>
</table>

is a different state degenerate with $|\psi_1\rangle$. It is also an eigenstate of the non-symmorphic mirror with eigenvalue $P^*$.\(^5\) Since a generic $k$ point in the mirror-invariant planes does not have additional symmetries, we collected all the information necessary to describe all the irreducible representations:

- For $k_{zc} = 0$, there is only one 2D IR with mirror eigenvalues $(i, -i)$.
- For $k_{zc} = \pi$ plane, there are two 2D IRs with mirror eigenvalues $(1, 1)$ and $(-1, -1)$.

The latter result indicates, that a crossing of the two 2D IRs may occur within the mirror-invariant plane on the BZ boundary, which facilitates four-fold degenerate Dirac lines. Such a nodal line has been predicted for a perovskite material SrIrO$_3$ [151, 152].

Dirac lines are associated with a $Z_2$ topological invariant which corresponds to the Berry phase in one\(^6\) spin sector $\varphi_B^\sigma$. This invariant pro-

\(^5\)To see this,

\[ \mathcal{D}_{k_{zc}}(I \circ C_{2z}^+) \mathcal{D}_{k_{zc}}(T \circ I) |\psi_1\rangle = \mathcal{D}_{k_{zc}}(I \circ C_{2z}^+ \circ T \circ I) |\psi_1\rangle = \mathcal{D}_{k_{zc}}(T \circ I \circ I \circ C_{2z}^+) |\psi_1\rangle = \mathcal{D}_{k_{zc}}(T \circ I) \mathcal{D}_{k_{zc}}(I \circ C_{2z}^+) |\psi_1\rangle = \mathcal{D}_{k_{zc}}(T \circ I) \varphi |\psi_1\rangle = \varphi^* \mathcal{D}_{k_{zc}}(T \circ I) |\psi_1\rangle \quad \text{(III.7)} \]

where we used Tab. III.1, the fact that both $I$ and $T$ commute with all other point symmetries, and the antiunitary of $T \circ I$. The non-trivial elements of the factor system did not enter this calculation.

\(^6\)Taking both spins into account leads to $\varphi_B^\sigma(\gamma) = 0$ on all mirror-invariant paths.
tects spin-degenerate drumhead surface band inside the projection of the nodal line. One can also define a $\mathbb{Z}$-valued topological invariant analogous to (III.4b), but it does not enable additional states on the surface.

**III.1.3 Nodal lines without spin-orbit coupling**

A further kind of nodal lines exists in materials without spin-orbit coupling (SOC) which respect composed $\mathcal{T} \circ \mathcal{I}$ symmetry. The absence of SOC implies that $\mathcal{H}(k) \propto 1_\sigma$ in the spin degree of freedom, meaning that it is natural to drop spin out from the problem description altogether. At the level of time-reversal symmetry, this is achieved by considering its composition with a $\pi$ rotation in spin space around arbitrary axis. If we choose this to be the negative $y$-axis, then such a composition is

$$\tilde{T} = e^{i \frac{\pi}{2} \sigma_y} (-i \sigma_y K) = K. \quad (III.8)$$

This operator squares to $+1$ and preserves spin, as expected for “spinless electrons”. Furthermore, $\mathcal{I}$ commutes with both $\mathcal{T}$ and spin rotations, and also squares to $+1$. This implies that the composition $\mathcal{I} \circ \tilde{T}$ is an antiunitary operator squaring to $+1$ and mapping any $k$-point back to itself. With a suitable rotation of the basis, such an operator can be always represented simply as the complex conjugation $K$, meaning that $\mathcal{H}(k)$ can be brought into a real form.

We now check that such symmetry constraints indeed allow for nodal lines. To see this, we can again consider the effective two-band model Eq. (III.1a) expanded using a set of Pauli matrices. The reality condition implies that we cannot use the imaginary Pauli matrix, therefore $\delta = 2$, which allows for nodal lines in a 3D BZ [38]. Note that this species of nodal lines is *not* constrained to a high-symmetry plane.

We wish to derive the topological invariant characterizing these nodal lines. Since $\mathcal{H}(k)$ is now a real symmetric matrix, its eigenstates $|u^a(k)\rangle$ can be chosen real, meaning that the Wilson loop operator on any closed path $\mathcal{W}(\gamma)$ is an *orthogonal* matrix. According to Eq. (I.18), this leads to the quantization of Berry phase into 0 vs $\pi$. This is similar to Subsec. III.1.1 with the important difference that in the presence case we admit paths of *arbitrary* shape. The Berry phase reaches the non-trivial value whenever the path contains a nodal line. In chapter IV we will look at this topological invariant again from a different perspective.

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7The fact that $\tilde{T}^2 = +1$ does *not* depend on the specific choice of the rotation axis.
To find these species of nodal lines in real systems, one has to consider light elements, such that the condition on the absence of SOC is well satisfied. For example, multiple nodal lines of this kind were predicted to exist in certain 3D graphene networks [153]. Four nodal lines also exist in common graphite (also called alpha, hexagonal, or Bernal graphite) [154]. These four nodal lines are connected along a high-symmetry line, forming a complex nexus structure [155]. The less frequent allotrope of graphite (called beta or rhombohedral graphite) exhibits a pair of nodal lines with a peculiar spiral structure [160]. A plethora of other, more recently discovered nodal line materials belonging to this class is listed in “Type B” row of Tab. 1 in Ref. [148].

The surface states of these nodal line semimetals can be understood in the same way as those in Subsec. III.1.1. We remark here, that if the effective model describing a nodal line exhibits an approximate electron-hole symmetry, then the topological surface band has a tendency to flatten, leading to a huge density of states at zero energy. Ref. [160] considered the effect of such surface flat bands on the enhancement of superconductivity. More recent Ref. [161] studied the competition between superconducting, magnetic, and charge density instabilities in such surface flat band systems, and found the superconducting order becomes more stable if the chemical potential is moved slightly away from the flat band energy through doping.

### III.1.4 Nodal lines from chiral symmetry

The final category of nodal line materials corresponds to systems with the chiral symmetry defined in Eq. (I.99c). Although such a situation more naturally arises in superconductors, it may in principle also appear in non-superconducting systems with a bipartite lattice and nearest-neighbour hoppings only. In realistic crystals, such a symmetry is usually only approximately valid, hence we are not able to mention here any material examples. We nevertheless include this possibility in our list, because it will help us to understand the surface states of IrF$_4$ in Sec. III.5. These nodal lines will also appear in the more general classification of nodal objects developed in chapter IV.

If we represent chiral symmetry as $\sigma_z$, then $\mathcal{H}(k)$ can according to Eq. (I.99c) only contain terms proportional to $\sigma_x$ and $\sigma_y$, meaning that it

---

8This is also reminiscent of the triple point metals [156–159].
III.2. Nodes imposed by non-symmorphicity

has a block-off-diagonal form

\[ \mathcal{H}(k) = \begin{pmatrix} 0 & \hat{h}(k) \\ \hat{h}^\dagger(k) & 0 \end{pmatrix}. \quad (III.9) \]

where \( \hat{h}(k) \in \text{GL}(n, \mathbb{C}) \). Hamiltonian (III.9) has a zero energy state (indicating the presence of a node) whenever the complex-valued determinant of \( \hat{h}(k) \) vanishes, meaning that the codimension is \( \delta = 2 \). Consequently, nodes of this symmetry classes in 3D take the form of lines that are not constrained to a high-symmetry plane, similar to the case of Subsec. III.1.3.

The invariant defined on a closed path \( \gamma \) is a \( \mathbb{Z} \)-valued winding number of \( \det \hat{h}(k) \), that means

\[ \omega(\gamma) = \frac{1}{2\pi i} \oint_\gamma dk \cdot \nabla_k \log \det \hat{h}(k). \quad (III.10a) \]

It was proved in Ref. [73] that

\[ \omega(\gamma) = z_2(\gamma) \mod 2 \quad (III.10b) \]

meaning that the \( \mathbb{Z}_2 \) Berry phase corresponds to the parity of the winding number. Since their derivation is rather technical, we provide in this thesis a somewhat simplified version of it. However, we postpone that until footnote (5) in chapter IV, after we get to know certain properties of chiral-symmetric systems.

The surface states in this class can be understood in the same way as presented in Fig III.3 with the important difference that the 1D fibers are characterized by a \( \mathbb{Z} \)-valued winding number. As a consequence, this class of nodal line metals is able to protect an integer number of coinciding surface bands. We will see an example in Sec. III.5.

III.2 Nodes imposed by non-symmorphicity

All the nodal-line semimetals encountered in Sec. III.1 needed some degree of “luck” for the occurrence of the band crossing. In this section, we show that non-symmorphic symmetries can impose nodal lines to appear in the band structure automatically, regardless of any further material details. We begin with demonstrating the existence of the so-called non-symmorphic nodal lines (NSNLs) in non-centrosymmetric spin-orbit
coupled systems with a glide-plane symmetry. The presence of time-reversal (TRS) is also assumed. We then show that a pair of glides can similarly enforce two circular nodal lines (i.e. nodal loops) that have to touch, and that together look like an infinite chain in the extended $k$-space.

**III.2.1 Non-symmorphic nodal lines**

We first recall a few definitions, which we need for the presented arguments. Reciprocal lattice vectors $g$ fulfil

$$g \cdot R = 0 \mod 2\pi$$  \hspace{1cm} (III.11a)

for every Bravais vector $R$. Two momenta are called equivalent if they differ by a reciprocal lattice vector $g$. Especially, time-reversal invariant momenta (TRIMs) $\Gamma$ are equivalent to their time-reversed images, $\Gamma = -\Gamma + g$. Combining this relation with equation (III.11a), we obtain

$$\Gamma \cdot R = 0 \mod \pi.$$  \hspace{1cm} (III.11b)

Similarly, in a mirror-symmetric crystal, a mirror-invariant momentum $k$ is equivalent to its mirror image $M_n k$ if

$$2n (k \cdot n) = 0 \mod g,$$  \hspace{1cm} (III.11c)

where $n$ is the normal vector of the mirror plane.

A mirror invariant plane contains four inequivalent TRIMs. To see this, pick two arbitrary reciprocal lattice vectors $g_{1,2}$ such that they both have non-zero in-plane components ($g_{i,\parallel} \neq 0$) which are mutually non-collinear ($g_{1,\parallel} \nmid g_{2,\parallel}$). By symmetry, the mirror images $M_n g_i$ are also reciprocal lattice vectors, and hence $2g_{i,\parallel} = g_i + M_n g_i$ are in-plane reciprocal lattice vectors. Let $\tilde{g}_i$ be the shortest reciprocal lattice vector in the direction of $g_{i,\parallel}$. Then, by taking all linear combinations $n_1 \tilde{g}_1 + n_2 \tilde{g}_2$, $n_{1,2} \in \mathbb{Z}$, we construct all in-plane reciprocal lattice vectors. These vectors form a grid of equivalent $k$-points. The midpoints of these vectors form a four-times denser mesh of all the in-plane TRIMs. Thus, there are four inequivalent in-plane TRIMs.

We further become more specific. We consider a spin-orbit coupled (SOC) system with only two symmetries: Time-reversal $T$ and a glide plane $G_n = \{ M_n | t \}$, i.e. a mirror symmetry $M_n$ followed by a uniform translation by vector $t$. Such a system supports only 1D IRs everywhere
III.2. Nodes imposed by non-symmorphicity

except for TRIMs, where the Kramers theorem implies double degeneracies. The square of the glide plane is

\[ G_n^2 = \{ \overline{E} | 2t_\parallel \} \]  

(III.12)

where \( t_\parallel = \frac{1}{2} (t + M_n t) \) is the in-plane component of the translation vector, and \( \overline{E} \) is a 2\( \pi \)-rotation, represented by \(-1\) in SOC systems. Result (III.12) corresponds to a pure translation, which implies that \( 2t_\parallel \) is a Bravais vector. Consequently, \( G_n^2 \) is represented at any \( k \in \text{BZ} \) by \(-e^{-ik \cdot 2t_\parallel}\), from which we conclude that the possible glide eigenvalues are [101]

\[ \eta_{k,\pm} = \pm ie^{-ik \cdot t_\parallel}. \]  

(III.13)

Since \( 2t_\parallel \) is a Bravais vector, we find from (III.11b) that

\[ \mathbf{\Gamma} \cdot t_\parallel = 0 \mod \frac{\pi}{2}. \]  

(III.14a)

Relation (III.14a) enables two possibilities. Either \( \mathbf{\Gamma} \cdot t_\parallel = 0 \mod \pi \) at all four mirror-invariant TRIMs, in which case the glide eigenvalues (III.13) are imaginary at all TRIMs and no band crossings are enforced. The second possibility is that

\[ \mathbf{\Gamma}_1 \cdot t_\parallel = 0 \mod \pi \quad \text{and} \quad \mathbf{\Gamma}_2 \cdot t_\parallel = \frac{\pi}{2} \mod \pi \]  

(III.14b)

for two TRIMs \( \mathbf{\Gamma}_{1,2} \) inside the mirror-invariant plane. We argue that in such a case \( \mathbf{\Gamma}_1 \) and \( \mathbf{\Gamma}_2 \) have to be separated by a nodal line (NL) lying within the mirror-invariant plane.

To see how conditions (III.14b) impose a NL, consider any in-plane path \( \gamma \) that connects \( \mathbf{\Gamma}_1 \) to \( \mathbf{\Gamma}_2 \). The Kramers theorem forces the bands to be doubly degenerate at \( \mathbf{\Gamma}_{1,2} \), and the trivial commutator \([G_n, T] = 0\) makes the glide eigenvalues of a Kramers doublet complex conjugate. According to equations (III.13) and (III.14b), the glide eigenvalues of a Kramers doublet at \( k = \mathbf{\Gamma}_1 \) are \((+i, -i)\). As one moves along \( \gamma \), the phase of the eigenvalues has to change by

\[ (\mathbf{\Gamma}_1 - \mathbf{\Gamma}_2) \cdot t_\parallel = \frac{\pi}{2} \mod \pi, \]  

(III.15)

so they evolve into \((+1, -1)\) at \( \mathbf{\Gamma}_2 \). However, these are not complex conjugate anymore and hence belong to different Kramers doublets. We
Figure III.4: Non-symmorphic nodal line.  (a) Any path $\gamma$ connecting a pair of TRIMs $\Gamma_{1,2}$ in a glide-invariant plane (blue) fulfilling conditions (III.14b) must exhibit a gap closing point, which lies on a non-symmorphic nodal line (red).  (b) A generic spectrum along an in-plane path $\gamma$ that connects $\Gamma_{1,2}$.  The evolution of the glide eigenvalues along the path is shown in colour for all bands.  

therefore infer that Kramers doublets have to switch partners along $\gamma$, and a band crossing has to appear in the glide-invariant plane.  Since the argument holds for any in-plane path $\gamma$, there is a line of band crossings separating $\Gamma_{1,2}$ within the plane: the non-symmorphic nodal line (NSNL). We illustrate the argument in Fig. III.4.  

In the absence of additional symmetries, the band structure consists of the quadruplets illustrated in Fig. III.4(b).  Simple electron counting suggests that the NSNL is formed between a conduction and a valence band whenever there are

$$n = 4v + 2, \quad v \in \mathbb{Z}_0^+,$$

(III.16)

filled bands. Additional symmetries may lead to additional spectrum degeneracies and change the above filling criterion. For example, in the presence of inversion symmetry $I$ the whole argument ceases to be applicable, since $T \circ I$ enforces the spin degeneracy of all bands throughout BZ. We will pursue considerations along these lines in Subsec. III.3. In Tab. III.2 we list all the 47 non-centrosymmetric space groups (SGs) that contain a glide plane fulfilling criterion of Eq. (III.14b).

### III.2.2 Nodal chains

We further narrow down to non-centrosymmetric spin-orbit coupled systems with (1) two mutually orthogonal glide planes $G_{1,2} = \{M_{1,2}|t_{1,2}\}$. According to the discussion above, each of them may create a NSNL in a mirror-invariant plane. These NSNLs necessarily touch if (2) the choice of TRIMs $\Gamma_{1,2}$ fulfilling Eq. (III.14b) for both $t_{1,2}$ coincides with the TRIMs
Table III.2: Non-centrosymmetric SGs with a suitable glide-plane symmetry. For every Bravais lattice we identified all non-centrosymmetric SGs furnished with a glide plane fulfilling criterion (III.14b). Column \( P \) indicates the corresponding point group. The color scheme indicates the number of such glide planes: One = green, two = blue, three = violet, four = red, six = orange.

<table>
<thead>
<tr>
<th>Bravais lattice</th>
<th>( P )</th>
<th>non-centrosymmetric + glide plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monoclinic P</td>
<td>( C_s )</td>
<td>#7</td>
</tr>
<tr>
<td>Monoclinic C</td>
<td>( C_s )</td>
<td>#9</td>
</tr>
<tr>
<td>Orthorhombic P</td>
<td>( C_{2v} )</td>
<td>#26, #27, #28, #29, #30, #31 #32, #33, #34</td>
</tr>
<tr>
<td>Orthorhombic A,C</td>
<td>( C_{2v} )</td>
<td>#36, #37, #39, #40, #41</td>
</tr>
<tr>
<td>Orthorhombic F</td>
<td></td>
<td>#43</td>
</tr>
<tr>
<td>Orthorhombic I</td>
<td></td>
<td>#45, #46</td>
</tr>
<tr>
<td>Tetragonal P</td>
<td>( C_{4v} )</td>
<td>#100, #101, #102, #103, #104 #105, #106</td>
</tr>
<tr>
<td></td>
<td>( D_{2d} )</td>
<td>#112, #114, #116, #117, #118</td>
</tr>
<tr>
<td>Tetragonal I</td>
<td>( C_{4v} )</td>
<td>#108, #109, #110</td>
</tr>
<tr>
<td>Trigonal R</td>
<td>( C_{3v} )</td>
<td>#161</td>
</tr>
<tr>
<td>Trigonal P</td>
<td>( C_{3v} )</td>
<td>#158, #159</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>( C_{6v} )</td>
<td>#184, #185, #186</td>
</tr>
<tr>
<td></td>
<td>( D_{3h} )</td>
<td>#188, #190</td>
</tr>
<tr>
<td>Cubic P</td>
<td>( T_d )</td>
<td>#218</td>
</tr>
<tr>
<td>Cubic F</td>
<td></td>
<td>#219</td>
</tr>
<tr>
<td>Cubic I</td>
<td></td>
<td>#220</td>
</tr>
</tbody>
</table>

along an intersection of the two mirror-invariant planes. Moreover, (3) the high-symmetry line connecting \( \Gamma_1 \) and \( \Gamma_2 \) should support only 1D IRs in the \( T \)-symmetric case for the eigenvalue argument to remain valid.

Of the SGs listed in Table III.2, only nine satisfy criteria (1-3). Eight of them also lead to the filling condition of Eq. (III.16) and are listed in Fig. III.5. The additional space group \#110 (\( I4_1cd \)) is more complicated since the minimal number of detached bands is eight rather than four [162, 163], and because it supports only 2D IRs at high-symmetry point \( P = (\Gamma_1 + \Gamma_2)/2 \) [144]. This leads to a rather complicated nodal line structure clarified in the caption to Fig. III.6(b).
Chapter III. Nodal line semimetals

Figure III.5: Catalog of nodal chain metals. A nodal chain appears in metals with these space groups whenever there are $4\nu + 2$ electrons per primitive unit cell. The blue and red lines show the nodal loops (NLs) located in mutually orthogonal planes. The additional 4D IRs are marked with green circles. The high-symmetry lines supporting a two-fold degeneracy of valence (conduction) bands are highlighted in orange. In space groups 109 and 122 the NLs touching point is at the point $\bar{P}$.

The presence of a pair of glide planes has an additional effect on the band structure. It can be shown using the mathematical tools of Subsec. II.3 that if condition (III.14b) is valid for both glide planes, then their representations $\overline{D}_\Gamma(M_1)$ and $\overline{D}_\Gamma(M_2)$ anticommute at some other TRIM $\bar{\Gamma}$. This leads to the appearance of a four-fold degeneracy at point $\bar{\Gamma}$. Because of the absence of $I$, the spectrum dispersion around these 4D IRs does not have the Dirac form. We indicate the location of such degeneracies for the space groups supporting nodal chains with green circles in Fig. III.5.

While the appearance of NSNLs and nodal chains formed by conduction and valence bands requires the filling of Eq. (III.16), the experimen-
III.2. Nodes imposed by non-symmorphicity

Figure III.6: Nodal chain spectra along the high-symmetry line from $\Gamma_1$ to $\Gamma_2$. (a) The generic spectrum along the high-symmetry line for space groups listed in Fig. III.5. The labels 1 to 4 (also distinguished by colours) correspond to four different irreducible representations (IRs) characterized by pairs of glide eigenvalues. Bands appear in quadruplets, and Kramers doublets at $\Gamma_{1,2}$ have switched partners. The imposed band crossing corresponds to the touching point of the two NSNLs. In groups #109 and #122, the crossing is pinned to $P = (\Gamma_1 + \Gamma_2)/2$. (b) Space group #110 also supports only 1D IRs along the high-symmetry line, but forces pairs of IRs $1 + 1$, $2 + 3$ and $4 + 4$ to become degenerate at $P$, leading to band octuplets. As a consequence, there are multiple imposed nodal lines: The squares indicate single NLs, the circles correspond to crossing of straight NLs along high-symmetry lines, and triangles correspond to a pair of NSNLs crossed by a pair of straight NLs along high-symmetry lines, i.e. a nexus of four NLs.

tal observation of the transport properties of NSNLs and nodal chains requires their proximity to the Fermi level. Notice that in general in metals the condition of Eq. (III.16) does not guarantee this proximity. Especially, any additional carrier pockets has to be charge-compensated, meaning that chemical potential may be away from the node even at integer fillings (III.16). For example, in nodal chain metals such pocket automatically arises around the unavoidable 4D IRs. Thus, candidate materials for experimental probes of nodal chains and NSNLs should be chosen such that the nodal loops are realized reasonably close to the Fermi level.

On the other hand, in materials with additional Fermi pockets a nodal chain or a NSNL can be probed experimentally even when the condition of Eq. (III.16) is not fulfilled. For $n = 4\nu$ a NSNL or a nodal chain formed within the conduction (or within the valence) bands can still have significant effects on transport provided that it appears sufficiently close to the Fermi level. Examples of such materials are provided by the CuTlSe$_2$ material class of space group #122 ($I4_1md$). These materials were recently predicted to host Weyl points occurring between
the valence and conduction bands [164], but the presence of the NSNLs formed by conduction or valence bands was missed. Since in many of these compounds the NSNLs are located close to the Fermi level, we expect both the Weyl points and the NSNLs to be relevant for transport properties of these materials.

**III.3 Relation to Dirac semimetals**

Introducing inversion symmetry $I$ into a time-reversal symmetric spin-orbit coupled system results in spin degeneracy of all bands. Thus, if the inversion-breaking terms in the Hamiltonian of a NSNL are taken to zero, the NSNL shrinks into a four-fold degeneracy at either $\Gamma_1$ or $\Gamma_2$. In a system with time-reversal and glide-plane symmetries this four-fold degeneracy corresponds to a Dirac points on the BZ boundary, or to a Dirac line running along a high-symmetry axis. We thus observe a direct connection between NSNLs and Dirac Hamiltonians. This section investigates the similarities between these two species of semimetals.

Possible antiferromagnetic ordering with $T_N \lesssim 100$ K was reported for IrF$_4$ in magnetic susceptibility measurements [165]. A paramagnetic phase is expected to occur at temperatures above $T_N$, still accessible for an angle resolved photoemission spectroscopy (ARPES). We first discuss the paramagnetic phase, in which the crystal symmetries and band filling guarantee the presence of a nodal chain corresponding to Fig. III.5c.

**III.3.1 $k \cdot p$ models**

We start by considering the inverse of the last statement: Is it always possible to obtain a NSNL by a suitable distortion of a system exhibiting a Dirac points on the BZ boundary? We show in this subsection that there are situations when it is not possible to distort a NSDP into a NSNL. Along the way we manage to derive a $k \cdot p$ Hamiltonian of NSNL which will be used to study its Landau levels in the next subsection.

As shown in Ref. [129], a Dirac point at a TRIM on the BZ boundary requires a simultaneous presence of time-reversal $T$, inversion $I$, and an even n-fold non-symmorphic rotational symmetry $C_{nz}^+$ (set along the z-axis by convention). In general, non-symmorphic symmetries have to be represented by $k$-dependent operators, but this $k$-dependence can be dropped in local $k \cdot p$ expansions, as we observed in Subsec. II.3.
III.3. Relation to Dirac semimetals

The point group corresponding to the specified system contains a twofold rotational symmetry

$$C_{2z}^+ = (C_{nz}^+)^{n/2}$$  \hspace{1cm} (III.17a)

and a mirror symmetry

$$M_z = I \circ C_{2z}^+. \hspace{1cm} (III.17b)$$

The Dirac point appears in the mirror-invariant plane. Breaking $C_{2z}$ and $I$ while keeping their non-symmorphic composition $M_z$ allows for the appearance of a NSNL. To find how such a crystal distortion modifies the spectrum, we look for terms compatible with the remaining $M_z$ and $T$ symmetries.

According to Ref. [129], the Dirac Hamiltonian is

$$H^{(s)}_{\text{Dirac}} = \hbar \left[ v_x \frac{(k_x^+ + k_y^+)}{2} \Gamma_1 + v_y \frac{i(k_x^- - k_y^-)}{2} \Gamma_2 + v_z k_z \Gamma_3 \right] \hspace{1cm} (III.18)$$

where $k_{\pm}^s = (k_x \pm i k_y)^s$, and $\Gamma_1$ to $\Gamma_5$ are mutually anticommuting Hermitian matrices squaring to $1$. Together with the commutators

$$\Gamma_{ij} = -\frac{i}{2} \left[ \Gamma_i, \Gamma_j \right], \hspace{1cm} (III.19)$$

these matrices form a basis of traceless $4 \times 4$ Hermitian matrices. The value of the parameter $s = 1 \ (s = 3)$ corresponds to linear (cubic) Dirac Hamiltonians.

Terms in the Hamiltonian that are independent of $k$ and consistent with $T$ and $M_z$ can only be proportional to those of the 15 Dirac matrices that commute with both of the symmetries. For $T$, Ref. [30] shows

$$[T, \Gamma_a] = 0 \quad \text{for} \quad a \in \{4, 14, 24, 34, 45\} \hspace{1cm} (III.20)$$

and $\{T, \Gamma_a\} = 0$ for the remaining Dirac matrices. The classification developed in Ref. [129] allows us to check the anti-/commutation relations of the operator $M_z$ for all possible non-symmorphic Dirac points, which we present in Tab. III.3.

We find that for a Dirac point located along a 2-fold or 6-fold rotation axes, the only symmetry-compatible zeroth order perturbation is

$$H^{(n=2,6)}_{\text{pert.}} = w \gamma_{34}, \hspace{1cm} (III.21)$$

leading to a NSNL in the mirror-invariant plane [30]. The bands forming the NSNL have different eigenvalues of $M_z$, hence the nodal loop
Table III.3: Relation of non-symmorphic nodal loops to Dirac points. The first three columns reproduce the classification of non-symmorphic Dirac points developed in Ref. [129], where \( u_{A\uparrow} \) encodes \( C_{nz} \) eigenvalues of the four states degenerate at the nodal point and the third column indicates the type of dispersion around the nodal point. We used the \( \mathbf{k} \cdot \mathbf{p} \) models developed in Ref. [129] to check which of the \( T \)-symmetric matrices (III.20), displayed in orange, are also \( M_z \)-symmetric. Those labelled C (A) (anti)commute with the mirror and are therefore (not) present in the non-centrosymmetric \( \mathbf{k} \cdot \mathbf{p} \) expansions (III.21) and (III.22).

<table>
<thead>
<tr>
<th>( C_{nz} )</th>
<th>( u_{A\uparrow} )</th>
<th>type</th>
<th>( \gamma_1 )</th>
<th>( \gamma_2 )</th>
<th>( \gamma_3 )</th>
<th>( \gamma_4 )</th>
<th>( \gamma_5 )</th>
<th>( \gamma_{14} )</th>
<th>( \gamma_{24} )</th>
<th>( \gamma_{34} )</th>
<th>( \gamma_{45} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{2z} )</td>
<td>( \pm \exp \left[ i \frac{\pi}{2} \right] )</td>
<td>linear</td>
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<td>A</td>
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</tr>
<tr>
<td>( C_{4z} )</td>
<td>( \pm \exp \left[ \pm i \frac{\pi}{4} \right] )</td>
<td>linear</td>
<td>C</td>
<td>C</td>
<td>A</td>
<td>A</td>
<td>C</td>
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<td>A</td>
</tr>
<tr>
<td>( C_{6z} )</td>
<td>( \pm \exp \left[ \pm i \frac{\pi}{3} \right] )</td>
<td>linear</td>
<td>C</td>
<td>C</td>
<td>A</td>
<td>A</td>
<td>C</td>
<td>A</td>
<td>A</td>
<td>C</td>
<td>A</td>
</tr>
<tr>
<td>( C_{6z} )</td>
<td>( \pm \exp \left[ i \frac{\pi}{2} \right] )</td>
<td>cubic</td>
<td>C</td>
<td>C</td>
<td>A</td>
<td>A</td>
<td>C</td>
<td>A</td>
<td>A</td>
<td>C</td>
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is stable against including higher-order symmetry-preserving perturbations to the Hamiltonian. Such a situation corresponds for example to the Dirac points of \( \beta \)-cristobalite \( \text{BiO}_2 \) [34] and of distorted spinels \( \text{Ba}_X \text{SiO}_4 \) [103].

On the other hand, for Dirac points occurring along a 4-fold rotation axis, the symmetry compatible perturbation is

\[
\mathcal{H}_{\text{pert.}}^{(n=4)} = m\gamma_4 + u_x\gamma_{14} + u_y\gamma_{24}
\]

and the spectrum is gapped whenever \( m \neq 0 \), therefore not leading to a NSNL in general [30]. In the presence of an additional mirror plane parallel to the rotation axis, like in the case of \( \beta \)-cristobalite \( \text{BiO}_2 \) [34], a NSNL can still appear in this plane. However, the existence of such a mirror is not guaranteed, examples being the A and Z points of the simple tetragonal SG #84.

From now on, we will focus on linear Dirac points \((s=1)\) in situations leading to a NSNL. Combining Eqs. (III.18) and (III.21) we find a \( \mathbf{k} \cdot \mathbf{p} \) description of a NSNL,

\[
\mathcal{H}_{\text{NSNL}}(k) = \hbar \left[ v_x k_x \Gamma_1 + v_y k_y \Gamma_2 + v_z k_z \Gamma_3 \right] + w \Gamma_{34}.
\]

Using this Hamiltonian we can explicitly calculate the topological \( \mathbb{Z}_2 \) Berry phase carried by the NSNL, i.e.

\[
\frac{\varphi_B(\gamma)}{\pi} = \frac{1}{\pi} \oint_c \mathbf{dk} \cdot \text{tr} \mathbf{A}(k) \mod 2.
\]
Here, \( \gamma \) is a mirror-symmetric path enclosing the NSNL and \( \mathcal{A}(\mathbf{k}) \) is the Berry connection of the occupied bands, c.f. Subsec. I.1.2. For this purpose, we choose a specific set of Dirac matrices
\[
\begin{align*}
\Gamma_1 &= -\sigma_y \otimes \tau_z \quad \Gamma_2 = \sigma_x \otimes \tau_z \quad \Gamma_3 = \mathbf{1}_\sigma \otimes \tau_y \\
\Gamma_4 &= \mathbf{1}_\sigma \otimes \tau_x \quad \Gamma_5 = \sigma_z \otimes \tau_z.
\end{align*}
\] (III.25)
consistent with \( \mathcal{T} = i\sigma_y \otimes \mathbf{1}_\tau \mathcal{K} \) and \( M_z = \mathbf{1}_\sigma \otimes \tau_z \), and a path enclosing the NSNL
\[
\gamma = \left\{ \left( \frac{w + u \cos \alpha}{\hbar v_x}, 0, \frac{u \sin \alpha}{\hbar v_z} \right) \bigg| \alpha \in [0, 2\pi) \right\}.
\] (III.26)
where \( u \) is the radius of path \( \gamma \).

The spectrum along path \( \gamma \) is non-degenerate. The lower of the two occupied bands is contractible to a point without encountering a band degeneracy, it therefore carries zero Berry phase. On the other hand, the band that participates in the formation of the NSNL in smooth gauge is
\[
|\psi(\alpha)\rangle = \frac{e^{-i\alpha/2}}{\sqrt{2}} \left( -\sin \frac{\alpha}{2}, i \cos \frac{\alpha}{2}, i \sin \frac{\alpha}{2}, \cos \frac{\alpha}{2} \right) \dagger.
\] (III.27)
The corresponding Berry connection is
\[
\mathcal{A}_\alpha = \langle \psi(\alpha) | \partial_\alpha | \psi(\alpha) \rangle = -\frac{i}{2}
\] (III.28)
which, upon integration over \( \alpha \), yields the topologically non-trivial value \( \varphi_B(\gamma) = \pi \), as expected for a NSNL.

**III.3.2 Landau levels in a perpendicular field**

The rest of this section is analogous to the treatment of Weyl points in Subsec. II.1.2. We use the derived \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian of a NSNL in Eq. (III.23) to study the Landau levels in a magnetic field. We first consider a *perpendicular* magnetic field \( \mathbf{B} = (0, 0, B) \) with \( B > 0 \). We perform the Peierls substitution (II.9a) again, but this time we fulfil the commutation relation (II.9b) using
\[
\Pi_x = \sqrt{\frac{e\hbar \nu_y B}{2\nu_x}} \left( a + a^\dagger \right) \quad \text{and} \quad \Pi_y = i \sqrt{\frac{e\hbar \nu_x B}{2\nu_y}} \left( a - a^\dagger \right).
\] (III.29)
Adopting Dirac matrices of Eq. (III.25) and representing Pauli matrices $\tau_i$ by $2 \times 2$ blocks and matrices $\sigma_i$ as elements within the blocks, we obtain the matrix Hamiltonian

$$H(k_z) = \begin{pmatrix} -w & i\sqrt{b}a & -i\hbar v_z k_z & 0 \\ -i\sqrt{b}a^\dagger & -w & 0 & -i\hbar v_z k_z \\ i\hbar v_z k_z & 0 & w & -i\sqrt{b}a \\ 0 & i\hbar v_z k_z & i\sqrt{b}a^\dagger & w \end{pmatrix}$$  (III.30)

where we introduced a rescaled magnetic field $b = \frac{2v_y v_z e\hbar}{v^2}$. When squared, this Hamiltonian has a block-diagonal form

$$\tilde{H}^2 = \begin{pmatrix} b (a^\dagger a + 1) & -2i\omega \sqrt{b} a & 0 & 0 \\ -2i\omega \sqrt{b} a & b a^\dagger a & 0 & 0 \\ 0 & 0 & b (a^\dagger a + 1) & -2i\omega \sqrt{b} a \\ 0 & 0 & 2i\omega \sqrt{b} a^\dagger & b a^\dagger a \end{pmatrix}$$

where $\tilde{H}^2 = H^2(k_z) - \left(\omega^2 + \hbar^2 v_z^2 k_z^2\right) \mathbb{1}_\tau \otimes \mathbb{1}_\sigma$. Clearly, the eigenvalues of $H(k_z)$ and of $\tilde{H}^2$ are related through $\varepsilon^2(k_z) = \tilde{\varepsilon}^2 + \omega^2 + \hbar^2 v_z^2 k_z^2$.

We look for the eigenstates of $\tilde{H}^2$ in the form

$$|\tilde{\psi}\rangle = \left(\sum_{n=0}^{+\infty} \tilde{\psi}^{s,+}_n |n\rangle \right) \begin{pmatrix} \sum_{n=0}^{+\infty} \tilde{\psi}^{s,+}_n |n\rangle \\ \sum_{n=0}^{+\infty} \tilde{\psi}^{s,-}_n |n\rangle \\ \sum_{n=0}^{+\infty} \tilde{\psi}^{s,+}_n |n\rangle \\ \sum_{n=0}^{+\infty} \tilde{\psi}^{s,-}_n |n\rangle \end{pmatrix}$$  (III.31)

where $|n\rangle$ is the eigenstate of the number operator $a^\dagger a |n\rangle = n |n\rangle$. Using the standard algebra of ladder operators

$$a |n\rangle = \sqrt{n} |n-1\rangle, \quad a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$  (III.32)

we find the eigenstates of $\tilde{H}^2$ corresponding to the eigenvalue $\tilde{\varepsilon}^2$ to satisfy conditions

$$b (n+1) \tilde{\psi}^{s,+}_n + 2i\omega \sqrt{b} \sqrt{n+1} \tilde{\psi}^{s,-}_{n+1} = \tilde{\varepsilon}^2 \tilde{\psi}^{s,+}_n$$  (III.33)

$$2i\omega \sqrt{b} \sqrt{n} \tilde{\psi}^{s,+}_{n-1} + b n \tilde{\psi}^{s,-}_n = \tilde{\varepsilon}^2 \tilde{\psi}^{s,-}_n$$  (III.34)

where $n \geq 0$ and $s = +, -$. This leads to solutions of the form

$$\begin{pmatrix} 0 & |0\rangle & 0 & 0 \end{pmatrix}^\dagger \quad \text{and} \quad \begin{pmatrix} 0 & 0 & 0 & |0\rangle \end{pmatrix}^\dagger$$  (III.35)
Figure III.7: Landau levels of a non-symmorphic nodal loop. (a-c) Landau levels of Hamiltonian (III.23) for a perpendicular magnetic field are always gapped except when condition (III.40) is fulfilled, which is the case for diagram (b). (d-f) Gapless Landau levels for an in-plane magnetic field. The zero energy crossing is symmetry protected and present for all values of $b/w^2$.

for the lowest eigenvalue $\tilde{\varepsilon}^2 = 0$, and to solutions

$$\frac{1}{\sqrt{2}} \begin{pmatrix} |n\rangle \\ \pm i |n + 1\rangle \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ |n\rangle \\ \pm i |n + 1\rangle \end{pmatrix}$$

(III.36)

with eigenvalues $\tilde{\varepsilon}^2 = b(n + 1) \pm 2w \sqrt{b} \sqrt{n + 1}$, where $n \in \mathbb{Z}_0^+$. It is now easy to check that suitable linear combinations of states in Eq. (III.35) form eigenstates of $\mathcal{H}$ with the corresponding Landau level energies

$$\varepsilon_{0,\pm} = \pm \sqrt{(\hbar v_z k_z)^2 + w^2}$$

(III.37)

while the appropriate linear combinations of states in Eq. (III.36) give the
eigenstates of $\mathcal{H}$ with the Landau level energies

$$\varepsilon_{\pm n, \pm} = \pm \sqrt{\left(\hbar v_z k_z\right)^2 + \left(w \pm \sqrt{n} b\right)^2} \quad (\text{III.38})$$

where $n \in \mathbb{Z}^+$. Results of Eqs. (III.37)-(III.38) can be written compactly in a single equation

$$\varepsilon_{n, \pm}(k_z) = \pm \left[\left(\hbar v_z k_z\right)^2 + \left(w \pm \text{sign } n \sqrt{|n|} b\right)^2\right]^{1/2} \quad (\text{III.39})$$

where $n \in \mathbb{Z}$. Sample spectra are plotted in Fig. III.7(a-c).

The spectrum (III.39) is gapped unless $w^2 / b \in \mathbb{Z}$, i.e. the gap closes for magnetic fields

$$B_c = \frac{w^2}{2e\hbar v_x v_y n}, \quad n \in \mathbb{Z}\setminus\{0\}. \quad (\text{III.40})$$

These gap closings correspond to topological phase transitions, in which a charge $e/2$ is topologically pumped to the surface of the sample, orthogonal to the direction of the field. To see this, notice that the perturbation of Eq. (III.21) is proportional to the mirror operator $M_z \propto \gamma_{34}$. As a consequence, tuning the magnitude of the perturbation $w$ shifts the energy of the eigenstates with different mirror eigenvalues in opposite directions, and thus a gap closure in the LL spectrum interchanges “valence” and “conduction” LLs with different mirror eigenvalues. This gap closing corresponds to a 1D topological phase transition, in which the Zak phase (I.45) changes by $\pi$. This change corresponds to pumping a charge of $e/2$ to the surface of the sample parallel to the plane of NSNL [55]. For this reason, a change in the Hall response of the metallic surface states is expected to occur at the critical values of the magnetic field (III.40).

**III.3.3 Landau levels in an in-plane field**

We proceed with the discussion of an in-plane magnetic field $\mathbf{B} = (B, 0, 0)$ with $B > 0$. In this case, the appropriate Peierls substitution is

$$\begin{align*}
(\hbar k_x, \hbar k_y, \hbar k_z) &\quad \mapsto \quad (\hbar k_x, -i\hbar \partial_y + eA_y, -i\hbar \partial_z + eA_z) \\
&\equiv (\hbar k_x, \Pi_y, \Pi_z) \quad (\text{III.41})
\end{align*}$$
with the commutation relationship

$$\left[ \Pi_y, \Pi_z \right] = i\hbar e \left( \partial_z A_y - \partial_y A_z \right) = -i\hbar e B.$$  \hspace{1cm} \text{(III.42)}

We express the \( \Pi \) operators as

$$\Pi_y = \sqrt{\frac{\hbar v_x B}{2v_y}} \left( a + a^\dagger \right), \quad \Pi_z = i\sqrt{\frac{\hbar v_y B}{2v_z}} \left( a - a^\dagger \right).$$  \hspace{1cm} \text{(III.43)}

Substituting this into the Hamiltonian of Eq. (III.23) and using a different set of Dirac matrices

$$\Gamma_1 = 1_\sigma \otimes \tau_y, \quad \Gamma_2 = \sigma_x \otimes \tau_z, \quad \Gamma_3 = \sigma_y \otimes \tau_z, \quad \Gamma_4 = 1_\sigma \otimes \tau_x, \quad \Gamma_5 = \sigma_z \otimes \tau_z$$  \hspace{1cm} \text{(III.44)}

we arrive at the Hamiltonian matrix

$$\mathcal{H}(k_x) = \begin{pmatrix} 0 & \sqrt{b}a & -i\hbar v_x k_x & -w \\ \sqrt{b}a^\dagger & 0 & w & -i\hbar v_x k_x \\ i\hbar v_x k_x & w & 0 & -\sqrt{b}a \\ -w & i\hbar v_x k_x & -\sqrt{b}a^\dagger & 0 \end{pmatrix}. \hspace{1cm} \text{(III.45)}$$

We were not able to diagonalize Hamiltonian (III.3.3) analytically, we therefore proceed with some interesting special cases. Applying the parametrization of Eq. (III.31) and setting \( k_x = 0 \), we find recurrence equations for the eigenstates of \( \mathcal{H}(k_x = 0) \) with zero energy

$$\psi_{s,+}^{r,+} = -\psi_{n,s,+}^{r,-} \frac{\sqrt{n+1}}{w} \hspace{1cm} \text{(III.46a)}$$

$$\psi_{n+1,s,-}^{r,-} = \psi_{n,s,-}^{r,-} \frac{1}{\sqrt{n+1}} \frac{w}{\sqrt{b}}. \hspace{1cm} \text{(III.46b)}$$

We can construct four linearly independent solutions for the system of Eqs. (III.46). Starting with a single non-trivial component, \( \psi_0^{s,r} = 1 \). The solutions generated for \( r = + \) are not normalizable because of a cumulative divergent factor \( \sqrt{n!} \), and are therefore non-physical. The two normalized physical solutions for \( r = - \) are

$$|\psi^{+,r}\rangle = e^{-\frac{w^2}{2b}} \begin{pmatrix} 0 & \cosh \left( \frac{w a^\dagger}{\sqrt{b}} \right) |0\rangle & 0 & \sinh \left( \frac{w a^\dagger}{\sqrt{b}} \right) |0\rangle \end{pmatrix} \hspace{1cm} \text{(III.47)}$$

$$|\psi^{-,r}\rangle = e^{-\frac{w^2}{2b}} \begin{pmatrix} 0 & \sinh \left( \frac{w a^\dagger}{\sqrt{b}} \right) |0\rangle & 0 & \cosh \left( \frac{w a^\dagger}{\sqrt{b}} \right) |0\rangle \end{pmatrix} \hspace{1cm} \text{(III.48)}$$
where we used
\[ \sum_{n=0}^{+\infty} \frac{\omega^{2n}}{n! b^n} = e^{\omega^2/b} \] (III.49)
to obtain the normalization factor.

For \( k_x \neq 0 \), the first order (linear) correction to zero energy can be obtained by diagonalizing the matrix
\[ M_{rs} = \hbar \nu x k_x \langle \psi_r^r, - | \Gamma_1 | \psi_s^s, - \rangle. \] (III.50)
Evaluating the matrix leads to
\[ M = \hbar \nu x k_x e^{-2\omega^2/b} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \] (III.51)
and the linear correction to the LL energy is
\[ \Delta \varepsilon(k_x) = \pm \hbar \nu x k_x e^{-2\omega^2/b}. \] (III.52)

We see that the dispersion of zeroth LLs is exponentially suppressed for weak magnetic fields \( b \lesssim \omega^2 \), and it saturates at \( \pm \hbar \nu x k_x \) for \( b \gg \omega^2 \). This behaviour is confirmed by the numerical results in Fig. III.7(d-f).

We argue that the crossing of the lowest LLs is protected by system symmetries. Notice that the composition of the time-reversal and the glide plane
\[ S = G_z \circ T = \left\{ M_z T \right\} \] (III.53)
remains a symmetry of the system even in the presence of an in-plane magnetic field,\(^9\) even though both \( T \) and \( G_z \) are violated. The square of this operation
\[ S^2 = \left\{ E^2 | 2t \parallel \right\} \sim e^{-2ik \cdot t \parallel} \] (III.54)
which is according to Eq. (III.14b) represented at the centre of our \( k \cdot p \) expansion by \( -\mathbb{1} \). Additionally, \( S \) is an antiunitary operator, meaning that enforces Kramers eigenstate doublets. One can then understand the zero-energy LLs of a NSNL in an in-plane field as a remnant of the chiral LLs of a Dirac Hamiltonian. These exist in the Dirac Hamiltonian with

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\(^9\)Since magnetic field \( \mathbf{B} \) is an axial vector, its in-plane components flip sign under the mirror symmetry. Time-reversal also flips direction of \( \mathbf{B} \), hence the composition (III.53) brings an in-plane magnetic field back onto itself.
III.3. Relation to Dirac semimetals

$w = 0$, and including an $S$-compatible $w \Gamma_{34}$ perturbation preserves this property. This result should be contrasted with accidental nodal loops (ANLs) such as those of Subsec III.1.1. ANLs do not have a symmetry that can protect a zero-energy Landau level crossing, hence they do not produce chiral LLs and therefore should have transport properties qualitatively different from those of NSNLs.

### III.3.4 Semiclassical description

The results of the two previous subsections suggest the presence of a direction-selective chiral anomaly, which only exists if the applied magnetic field does not have a perpendicular component. Of course, the physical magnetoresistance response should not have such a singular behaviour! To consider this problem a bit more, we present here the semiclassical description of the magnetoresistance of $k \cdot p$ model (III.23). Unfortunately, we will arrive at another singularity.

To simplify the discussion, we define coordinates\(^10\) $k, \phi$ and $\theta$ as

\[
\begin{align*}
    k_x &= \frac{1}{\hbar v_x} (w + k \sin \theta) \cos \phi \\
    k_y &= \frac{1}{\hbar v_y} (w + k \sin \theta) \sin \phi \\
    k_z &= \frac{1}{\hbar v_z} k \cos \theta,
\end{align*}
\]

where $\theta \in [0, 2\pi), \phi \in [0, 2\pi)$ and $k \in [0, \infty)$, together with an additional constraint on $k$, namely

\[
w + k \sin \theta > 0,
\]

for $w = 0$ they correspond to spherical coordinates.

To prevent non-uniqueness. Assuming that the chemical potential $\mu$ is close to the NSNL, we only need to determine the Berry curvature of the two bands forming the NSNL. We further rotate to a yet another Dirac basis

\[
\begin{align*}
    \Gamma_1 &= -\sigma_y \otimes \tau_y, & \Gamma_2 &= \sigma_x \otimes \tau_y, & \Gamma_3 &= \sigma_z \otimes \tau_y, \\
    \Gamma_4 &= 1 \sigma \otimes \tau_z, & \Gamma_5 &= 1 \sigma \otimes \tau_x.
\end{align*}
\]

such that $\Gamma_{34} = \sigma_z \otimes \tau_x$. Then Hamiltonian (III.23) becomes

\[
\mathcal{H}_{k,\theta,\phi} =
\begin{pmatrix}
    0 & 0 & w - ikC & (w + kS) e^{-i\phi} \\
    0 & 0 & - (w + kS) e^{i\phi} & -w + ikC \\
    w + ikC & - (w + kS) e^{-i\phi} & 0 & 0 \\
    (w + kS) e^{i\phi} & -w - ikC & 0 & 0
\end{pmatrix},
\]

\(^{10}\)For $w = 0$ they correspond to spherical coordinates.
where $C, S$ are shorthand notations for $\cos \theta$ and $\sin \theta$. Then the two states forming the NSNL are

$$|\psi^c(k, \theta, \phi)\rangle = \frac{1}{2} \left( e^{-i\phi} e^{i\theta} e^{i(\theta+\phi)} \right)^\top \quad \text{with} \quad \varepsilon^c = k,$$

$$|\psi^v(k, \theta, \phi)\rangle = \frac{1}{2} \left( e^{i\phi} e^{i\theta} e^{-i(\theta+\phi)} \right)^\top \quad \text{with} \quad \varepsilon^v = -k,$$

which do not depend on coordinate $k$. The non-vanishing components of the single-band Berry connection are $A^c_\phi = A^v_\phi = A^c_\theta = A^v_\theta = i/2$, which lead to vanishing $\Omega^c = \Omega^v = 0$. In fact, the same result can also be found for the two bands further away from the Fermi level.

In other words, Berry curvature is flat. On the other hand, there is a singular $\pi$ Berry curvature flow along the NSNL, which corresponds to a diverging $\Omega(k)$ at the line. The first of these results indicate a zero magnetoresistance at $\mu \neq 0$ because of the vanishing $(E \cdot B) \Omega$, cf. Eq. (II.27), while the semiclassical description suddenly breaks down for $\mu = 0$ because of the infinitely strong field $\Omega$. We see, that the problem of magnetoresistance of NSNLs cannot be treated well semiclassically.

As a possible solution to this problem, we suggest to study the magnetoresistance using the Landau level formalism, but with explicit corrections to the adiabatic dynamics. Such corrections should be able to remove the singular behaviour predicted previously: Since the gap between the lowest energy LLs is very small for a very small $B_\perp$, there is a chance that the electrons would be able to tunnel across the gap. Amplitude of such a process should decrease with increasing $B_\perp$, until at some point the signatures of the chiral anomaly disappears altogether. However, the finite length of the doctoral studies did not allow us to pursue this direction further, and we leave it for future studies.

### III.4 Iridium tetrafluoride

Our colleague Dr. Quan-Sheng Wu performed an exhaustive search using the Inorganic Crystal Structure Database [166] and discovered the presence of a nodal chain in an existing compound IrF$_4$. We spend this section discussing the predicted properties of this material. These results were published in Ref. [37], together with predictions of other nodal chain materials belonging to the same material class, which we do not discuss in this thesis.
III.4. Iridium tetrafluoride

III.4.1 Crystal structure and symmetry

The face-centred orthorhombic crystal structure of this compound belongs to space group #43 (Fdd2). The conventional unit cell parameters are [165]

$$a = 9.64(1) \, \text{Å}, \quad b = 9.25(1) \, \text{Å}, \quad c = 5.67(1) \, \text{Å}. \quad (\text{III.59})$$

and the primitive unit cell contains two formula units, so that the number of electrons satisfies Eq. (III.16). Each Ir site is surrounded by an octahedron of six F atoms, four of which are shared with the neighbouring octahedra. The IrF$_6$ octahedra form a bipartite lattice as shown in Fig. III.8. The space group contains two mutually orthogonal glide planes: $G_x$ and $G_y$ formed by the reflection with respect to the (100) and (010) planes, followed by a translation of $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ in the reduced coordinates. Possible antiferromagnetic ordering with $T_N \lesssim 100$ K was reported for IrF$_4$ in magnetic susceptibility measurements [165]. A paramagnetic phase is expected to occur at temperatures above $T_N$, still accessible for an angle resolved photoemission spectroscopy (ARPES). Throughout the thesis, we discuss only the paramagnetic phase, in which the crystal symmetries and band filling guarantee the presence of a nodal chain corresponding to Fig. III.5(c). Some comments on the possible antiferromagnetic phase are included in Ref. [37].

Figure III.8: Crystal structure of IrF$_4$. (a) The iridium atoms are surrounded by an octahedron of six fluorine atoms. Four of the six fluorines on each octahedron are shared with neighbouring octahedra. The IrF$_6$ octahedra form two symmetry-related sublattices, coloured in green and orange. (b) The same structure viewed along the z-direction. The crystal structures were plotted using VESTA 3 [139].
**III.4.2 Band structure**

In this subsection we present two complementary approaches to describe the band structure of IrF$_4$: First-principles calculations and tight-binding (TB) modelling. The first was performed by Dr. Quan-Sheng Wu, and the latter was performed by the author of the thesis.

The first-principles calculations have been performed within the framework of density functional theory (DFT) [167], using the generalized gradient approximation [168] with the projector augmented-wave [169] implemented in the VASP simulation program [170, 171]. Spin-orbit coupling was included into considerations via pseudopotentials. Further numerical specifications appear in the Supplementary Information File to Ref. [37]. The calculated band structure around the Fermi level

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**Figure III.9: Band structure of IrF$_4$.** (a) The band structure along the high-symmetry lines. The solid red line corresponds to the first-principle calculations as described in the text. The dashed blue line represents the TB model (III.60) with five free parameters (III.61) fitted to the first-principle results. The dotted green line corresponds to the chiral TB model with two free parameters (III.62) which we use to explain the surface states of IrF$_4$, which are presented in Fig. III.11. The orange arrows indicate cross-sections with the two loops of the nodal chain. The pink arrow indicates the 4D IR at the Z point where the entire band quadruplet collapses onto a single energy. (b) Fermi surface of IrF$_4$ consists of touching electron pockets (cyan) and hole pockets (red & dark blue). They touch where the energy of the nodal chain equals the chemical potential, indicated by green arrows. The approximately torical electron pocket in the centre does not correspond to a nodal line, and appears because of the approximate sublattice symmetry, as discussed in the following subsections.
is plotted along high-symmetry lines in Fig. III.9(a). The corresponding Fermi surface is shown in Fig. III.9(b).

We now complement the first-principle calculations with a short-ranged symmetry-based TB model of IrF$_4$. The DFT calculations predict the set of bands originating from the 5$d$ Ir orbitals to be separated from the 5$s$ Ir orbitals above and the 2$p$ F orbitals below. Analogous to Fig. II.6 in the context of pyrochlore iridates, the local octahedral crystal field splits the 5$d$ Ir orbitals into a partially filled lower-lying $t_{2g}$ manifold and an empty higher-energy $e_g$ states. SOC further splits the $t_{2g}$ orbitals into a filled $J_{\text{eff}} = \frac{3}{2}$ quadruplet$^{11}$, and a half-filled $J_{\text{eff}} = \frac{1}{2}$ doublet, which are well separated in energy – see the additional red lines in Fig. III.9(a).

Since there are two Ir sites per primitive unit cell, each carrying a 2-level degree of freedom well-separated in energy from the other orbitals, it is possible to formulate an effective four-band TB model. To simplify the analysis, we assume a perfect $C_4z$ screw rotational symmetry, which is very weakly broken in IrF$_4$ – see the orientation of green and orange octahedra in Fig. III.8(b). Such simplification changes the relevant SG from the face-centred orthorhombic #43 ($F\bar{d}d2$) to the body-centred tetragonal #109 ($I4_1md$). According to Fig. III.5(c), these two SGs are characterized with nodal chains of the same geometry.

We construct such a symmetry-based TB model, which reproduces the central four bands of IrF$_4$ to better than 4% fraction of the overall bandwidth.$^{12}$ It contains five independent real parameters, $t_1, T_1, t_2, T_3, t_4$, where the small letters indicate spin-independent hopping amplitudes, and the capital ones the SOC processes. The subscript of the amplitudes indicates the relative position of pairs of sites connected by the corresponding hopping process according to the legend in Fig III.10.

The resultant TB Hamiltonian can be written compactly, using a set of Pauli matrices $\sigma_i$ for the pseudospin degree of freedom. The electron annihilation operator at site $i$ with position vector $r_i$ is given by $c_i = (c_{i\uparrow}, c_{i\downarrow})^\top$. The constructed real space Hamiltonian in the second

$^{11}$In fact, the NNN crystal field further splits $J_{\text{eff}} = \frac{3}{2}$ into two doublets, but that is not relevant for the construction of the TB model.

$^{12}$This number is determined as root-mean-square average of the difference between the original bands and the fit.
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Figure III.10: Construction of the tight-binding model. The lattice of iridium atoms (green spheres) inside IrF$_4$ looks like a vertically compressed diamond lattice. The numbers along the bonds and arrows coincide with the subscripts of the corresponding hopping amplitudes in Hamiltonian (III.60). We warn the reader that this illustration is misleading when it comes to symmetry analysis, because the omitted fluorine octahedra break some of the symmetries exhibited by the displayed lattice of iridium atoms.

The quantized form is\(^\text{13}\)

\[
H = \sum_{\{i,j\} \in 1} c_i^\dagger (t_1 + iT_1 [r_{ij} \times e_z] \cdot \sigma) c_j + t_2 \sum_{\{i,j\} \in 2} c_i c_j + t_4 \sum_{\{i,j\} \in 4} c_i^\dagger c_j + iT_3 \sum_{\{i,j\} \in 3} c_i^\dagger [(e_z \cdot r_{ij})(e_z \times d_{ij})] \cdot \sigma c_j, \quad \text{(III.60)}
\]

where \(d_{ij} = r_{ik} + r_{jk}\) with \(k\) being the shared NN of sites \(\{i,j\} \in 3\), \(r_{ik} = r_k - r_i\), and \([v] = v / |v|\) is the unit vector in a prescribed direction.

The values of the TB parameters fitted to the first-principle results together with the chemical potential corresponding to the half-filling are

\[
t_1 = 0.0548, \quad T_1 = -0.0577, \quad t_2 = -0.0153, \quad T_3 = 0.0071, \quad t_4 = -0.0068, \quad \mu = 0.0179. \quad \text{(III.61)}
\]

where all the value are listed in eV. The fitted TB band structure is plotted with dashed blue line in Fig. III.9(a).

\(^{13}\)Additional hopping processes and SOC terms up to the considered distance are possible, but we found their fitted amplitudes to be small compared to the terms already present in Eq. (III.60). We therefore decided to drop them out from the Hamiltonian altogether.
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The hopping amplitudes between the two sublattices \((t_1, T_1)\) strongly dominate over intra-sublattice ones \((t_2, T_3, t_4)\). This indicates that the sublattice realization of the chiral symmetry, defined in Eq. (I.99c), is only weakly broken. Indeed, turning off the intra-sublattice hoppings altogether leads to an ideal chiral symmetry in the model, while still producing a reasonable fit to the band structure, see the dotted green line in Fig. III.9(a). The parameters of such a chiral-symmetric TB model are

\[
\begin{align*}
t_1 &= 0.0548, & T_1 &= -0.0577, & t_2 &= 0 \\
T_3 &= 0, & t_4 &= 0, & \mu &= 0.
\end{align*}
\]  

The chiral symmetry (CHS) operator is

\[
C = \tau_z,
\]  

where Pauli matrices \(\tau_i\) correspond to the sublattice degree of freedom.

### III.4.3 Surface states

We only focus on the \((100)\) surface throughout this and the following subsections. The nodal chain produces topological surface states on such a surface of IrF\(_4\), which are plotted in Fig. III.11(a,b). On this surface, the projection of \((010)\) and of the \((100)\) NSNL is a line and an oval, respectively, which are indicated with black dashed lines in Fig. III.11b.

Fermi arcs arise from the touching points of the electron and hole Fermi pockets. For the projection of the \((100)\) NSNL\(^{14}\) a single such arc, produced by the drumhead states clarified in Fig. III.3, emerges from the touching point. However, the touching points that appear on a linear projection of the \((010)\) NSNL produce two Fermi arcs, consistent with the fact that there are two such Fermi pocket touchings that project onto the same point in the surface BZ (SBZ).

The arcs originating on different NSNLs are connected either directly, or through a carrier pocket. Moreover, the \(\mathbb{Z}_2\) invariant computed on the gapped \(\mathcal{T}\)-symmetric plane\(^{15}\) projected onto the magenta path in Fig. III.11(b) is non-trivial. Therefore, the path corresponds to an edge of a 2D TI, and has to host an odd number of Kramers pairs of edge

---

\(^{14}\)Also shown as region 1 in Fig. III.11d.

\(^{15}\)Points M and T correspond to a projection of a pair of bulk TRIMs into SBZ, see also Fig. III.12(b).
Figure III.11: Surface density of states of IrF$_4$. (a) The (100) surface density of states along the high-symmetry lines of the surface BZ (SBZ). Various number of surface bands is clearly visible along the individual segments of the path. (b) The cut of the surface density of states in (a) at the Fermi energy, plotted in the (100) SBZ. End points of the surface Fermi arcs coincide with the projections of the bulk touching points of the electron and hole Fermi pockets. The dashed black lines indicate the projection of the nodal chain into the SBZ. The magenta line is the projection of the curved plane in Fig. III.12(b), which is used to determine the bulk $Z_2$ invariant. The meaning of (c,d) is analogous to (a,b) but for the chiral TB model. The white numbers in (d) indicate the number of topological surface bands in the corresponding region, and the thick black lines correspond to the projection of the additional nodal loop imposed by CHS, as we discuss in Subsec. III.5. Calculations were performed and results plotted by Dr. Quan-Sheng Wu.

states [11]. In agreement with the observed connectivity of the Fermi arcs, there is a single Kramers pair of such edge states, see Fig. III.12(a). In fact, we reason in Subsec. III.4.4 that the glide symmetry enforces the
III.4. Iridium tetrafluoride

\(Z_2\) invariant to be non-trivial, regardless of the model details.

To understand why both Fermi arcs of the (010) NSNL appear on the same side of its projection onto the (100) surface, we take use of the approximate chiral symmetry (CHS) present in the material, which we explained above Eq. (III.62). It turns out that the avoided crossing along the \(Z\Gamma\) line in Fig. III.9(a) originates from intra-sublattice hoppings. If we restore perfect CHS by setting the intra-sublattice hopping amplitudes to zero, i.e. by the choice of parameters (III.62), we obtain the band structure plotted with dotted green lines in Fig. III.9(a). One can see that now the gap along the \(Z\Gamma\) line vanishes, and an additional NL appears. It connects to the nodal chain, thus creating a nodal net, which we plot in Fig. III.13. The projection of the additional NL onto the (100) surface is indicated with the thick black lines in Fig. III.11(d).

Endowed with the CHS, the Hamiltonian allows for a richer topological classification, as discussed in Subsec. III.5, which predicts two/one/-zero surface modes to exist in regions marked as 2/1/0 in Fig. III.11(d). In the presence of the CHS, all these regions are topologically distinct and separated by NLs. When the CHS is weakly broken, only the parity of the number of surface states remains topologically protected, cf. Eq. (III.10b). This gaps out the additional NL in Fig. III.11(d), which separates regions “two” and “zero”. However, since the breaking of the CHS in realistic IrF\(_4\) is weak, the location of surface modes in the SBZ of IrF\(_4\) is inherited from the chiral symmetric structure. This explains the position of the Fermi arcs originating from the (010) NSNL.

**III.4.4 \(Z_2\) invariant on a curved plane**

In the previous subsection, we alluded to a \(Z_2\) invariant on a \(T\)-symmetric curved plane, the projection of which onto the (100) surface is given by the magenta line in Fig. III.11(b). We claimed that the invariant is non-trivial, suggesting an odd number of Kramers pairs of edge states to cross the bulk gap along the magenta line. The corresponding surface spectral function shown in Fig. III.12(a) confirms this prediction.

Let us be more precise now. We claim that the value of the topological \(Z_2\) invariant is, in fact, constrained to be non-trivial by the crystalline symmetries. To motivate this assertion, we apply the established technique of Refs. [172, 173] to compute the value of the topological invariant by tracking the changes in the Wannier charge centre (WCC) positions – or, equivalently, in the Wilson loop operator spectrum. In particular, we
Figure III.12: **Finding the $\mathbb{Z}_2$ invariant on the curved plane.** (a) The surface spectral function along the magenta line in Fig. III.11(b) reveals a non-trivial $\mathbb{Z}_2$ invariant. Points T and M are projections of pairs of bulk TRIMs, and P corresponds to the point where the magenta line crosses the SBZ boundary. (b) The curved magenta cut $\mathcal{H}$ through bulk BZ is $T$-symmetric. The projection of $\mathcal{H}$ to the right (with points T,P,M) corresponds to the magenta line in III.11(b), while the projection to the top (with points A,B,C) does not correspond to any physical surface. The dashed yellow lines indicate two paths in $k$-space related by glide reflection $G_x$. The dark points on the sheet correspond to bulk TRIMs. The green plane is mirror-invariant with respect to $G_x$. (c) Wannier charge centres (WCCs) along vertical threads of the magenta sheet $\bar{l}(k_x)$ computed from ab initio for IrF$_4$. The vertical shift associated with $G_x$ leads to glide symmetry of the WCC plot with respect to the central dashed line. This enforces the $\mathbb{Z}_2$ invariant of a system with $4\nu+2$ occupied bands to be non-trivial [70].

consider a cut $\mathcal{H} = (k_x,k_\ell)$, shown as a magenta plane in Fig. III.12(b). The cut is formed by momentum $k_x$ and a curved line parametrized by $k_\ell$. The plane contains four inequivalent bulk TRIMs, and exhibits a gapped spectrum. The projection of this cut onto the (100) surface is the magenta line in Fig. III.11(b).

We determine the WCCs $\bar{l}^a(k_x)$ by carrying out the non-Abelian parallel transport (I.13) along $k_\ell$ at different values of $k_x$. The $k_\ell$ lines that connect TRIMs at $k_x = A$ or $k_x = C$ of Fig. III.12(b) are mapped onto themselves by TRS, and hence the WCCs at these values of $k_x$ should appear in Kramers degenerate pairs [62, 172], as we explained in Subsec. I.2.6. At values of $k_x$ other than A and C the degeneracies have to split, as is indeed observed in Fig. III.12(c).

However, since the lines located at $B \pm \delta k_x$ [like the pair of dashed yellow lines in Fig. III.12(b)] are related by $G_x$ which contains a vertical shift by half-unit cell, the WCCs $\bar{l}^a$ at $B \pm \delta k_x$ must also be displaced by half-unit cell along $\ell$, as is confirmed by Fig. III.12(c). Because of
this shift, the connectivity of the WCCs between \( k_x = A \) and \( k_x = C \) is constrained in such a way that the \( \mathbb{Z}_2 \) invariant is trivial (non-trivial) if there are 4\( \nu \) (4\( \nu + 2 \)) occupied bands [70], meaning that the WCCs do not exchange (do exchange) partners when \( k_x \) increases from A to C.

### III.5 Nodal nets

In this section, we explain the appearance of the third nodal loop in the chiral TB model of IrF\(_4\). As explained in Subsec. III.1.4, the presence of CHS enables the block-off-diagonal form (III.9) of the Hamiltonian, which facilitates a \( \mathbb{Z} \)-valued winding number (III.10a). We claimed therein [and we prove it in footnote (5) of chapter IV], that the winding number \( w(\gamma) \) and the (rescaled) Berry phase \( z_2(\gamma) \) on a mirror-invariant path \( \gamma \) are related by [73]

\[
w(\gamma) = z_2(\gamma) \mod 2. \tag{III.64}
\]

Two paths \( \gamma_{a,b} \) with \( w(\gamma_{a,b}) = \pm 1 \) are topologically distinct in the chiral-symmetric case, but the distinction is lost once the CHS is broken. In the spirit of Fig. (III.3), if a pair of vertical 1D fibers have distinct chiral charges, they need to be separated by a gapless nodal line in the bulk BZ. However, if the chiral charge of the two fibers differs by a multiple of 2, the gapless nodal line separating the two fibers becomes unstable upon breaking the chiral symmetry. This is precisely what happens when going from Fig. III.11(d) to Fig. III.11(b).

To explain the appearance of the third nodal loop, we use that in a crystal with a symmetry \( S \), the winding numbers \( w(\gamma) \) and \( w(S\gamma) \) are not independent. Specifically, we derive that

\[
w(S\gamma) = \zeta w(\gamma) + \frac{n}{2\pi} \oint_{\gamma} dk \cdot \nabla_k [\text{arg}(v_k)], \tag{III.65}
\]

where \( n \) is the dimension of the off-diagonal block \( h(k) \) (i.e. the number of occupied bands of the TB model), and the appropriate form of \( v_k \in U(1) \) and \( \zeta \) for various operators \( S \) are listed in Table III.4. The integral in (III.65) vanishes if \( \gamma \) does not wind around the BZ torus.\(^{16}\)

To outline the derivation of (III.65), we explicitly discuss the case of a unitary symmetry \( S \) that exchanges the two sublattices, corresponding

\(^{16}\)The quantity \( v_k \in U(1) \) is well-defined also at NLs, meaning that a NL does not pose a topological obstacle for the integral in Eq. (III.65).
Figure III.13: Nodal chain and nodal net of IrF$_4$. (a) Nodal chain structure of IrF$_4$. (b) Nodal net in the chiral-symmetric TB model of IrF$_4$ plotted in the same region. (c) The form of the nodal net in the extended $k$-space. Different colours correspond to different orientations of the nodal loops.

Table III.4: Transformation of chiral winding number under crystal symmetries. The four rows characterize the possible crystal symmetries $\mathcal{S}$ as commuting (C) vs. anticommuting (AC) with the chiral symmetry $\mathcal{C}$, and as being unitary (U) vs. antiunitary (AU). The third column indicates the most general form of such an operator $\mathcal{S}(k)$, where $\mathcal{K}$ is the complex conjugation. The columns $\zeta$ and $\nu_k$ indicate the appropriate choice of variables in relation (III.65). The last column categorizes all symmetry operations of IrF$_4$ into the four defined classes.

<table>
<thead>
<tr>
<th>SLS type</th>
<th>$\mathcal{S}(k)$</th>
<th>$\zeta$</th>
<th>$\nu_k$</th>
<th>in IrF$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC</td>
<td>$U_k \otimes (a_k \tau^x + b_k \tau^y)$</td>
<td>$-$</td>
<td>$(a^<em>_k - ib^</em>_k)(a_k - ib_k)$</td>
<td>$G_x, G_y$</td>
</tr>
<tr>
<td>C</td>
<td>$U_k \otimes (a_k \mathbb{1} + b_k \tau^z)$</td>
<td>$+$</td>
<td>$(a^<em>_k - b^</em>_k)(a_k + b_k)$</td>
<td>$C_{2z}^+$</td>
</tr>
<tr>
<td>AC</td>
<td>$U_k \otimes (a_k \mathbb{1} + b_k \tau^z)$ $\mathcal{K}$</td>
<td>$+$</td>
<td>$(a^<em>_k - ib^</em>_k)(a_k - ib_k)$</td>
<td>$\mathcal{T} \circ G_x, \mathcal{T} \circ G_y$</td>
</tr>
<tr>
<td>C</td>
<td>$U_k \otimes (a_k \mathbb{1} + b_k \tau^z)$ $\mathcal{K}$</td>
<td>$-$</td>
<td>$(a^<em>_k - b^</em>_k)(a_k + b_k)$</td>
<td>$\mathcal{T}, \mathcal{T} \circ C_{2z}^+$</td>
</tr>
</tbody>
</table>

to the first row of Table III.4. Such a symmetry is off-diagonal in the sublattice basis, hence

$$S^{\text{AC}}_U(k) = U_k \otimes (a_k \tau^x + b_k \tau^y)$$ (III.66)

where $U_k$ captures any other degree of freedom besides sublattice, i.e. pseudospin in the case of IrF$_4$. The $k$-dependence of $U_k \in U(n)$ and $a_k, b_k \in \mathbb{C}$ is continuous, and non-trivial for non-symmorphic space groups. The unitarity of (III.66) implies $|a_k|^2 + |b_k|^2 = 1$ and $a_k b^*_k - b_k a^*_k = 0$. 
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Since for symmetries in general
\[
\mathcal{H}(Sk) = S(k)\mathcal{H}(k)S^{-1}(k),
\] (III.67)
we find that operator (III.66) alters the upper right block of (III.9) as
\[
h(Sk) = v_k U(k) h^\dagger(k) U^\dagger(k)
\] (III.68)
where \( v_k = (a^*_k - ib^*_k)(a_k - ib_k) \in U(1) \). Consequently
\[
det h(Sk) = (v_k)^n [det h(k)]^*,
\] (III.69)
from which we conclude the relation (III.65) with \( \zeta \) and \( v_k \) given in the first row of Table III.4. In the same fashion, we find \( \zeta \) and \( v_k \) for symmetries that do not exchange the two sublattices and for antiunitary symmetries that commute or anticommute with \( C \).

Before explaining the origin of the nodal chain, we do a quick sanity check of relation (III.65). We consider two loops \( \gamma_1,2 \) in Fig. III.14 related by \( \gamma_2 = -C_{2z}^+ \gamma_1 = G_x \gamma_1 \) where we are careful to capture the orientation properly. The relation (III.65) implies \( w(\gamma_2) = -w(\gamma_1) \). Loops \( \gamma_1,2 \) enclose a NL so that \( z_2(\gamma_2) = z_2(\gamma_1) = 1 \). The last two relations imply\(^{17}\)
\[
|w(\gamma_2) - w(\gamma_1)| = 2.
\] (III.70)
This means that within the chiral-symmetric TB model, deforming \( \gamma_1 \) onto \( \gamma_2 \) must be associated with encountering at least two NLs. This is indeed true: The red NL in Fig. III.14 needs to be intersected twice. We can analogously consider loops \( \gamma_3,4 \) in Fig. III.14 related by \( \gamma_4 = -C_{2z}^+ \gamma_3 = G_y \gamma_3 \), and infer
\[
|w(\gamma_4) - w(\gamma_3)| = 2.
\] (III.71)
Therefore, deforming \( \gamma_3 \) onto \( \gamma_4 \) is associated with encountering at least two NLs in the CHS case. This time it is the blue NL in Fig. III.14 that needs to be intersected twice to relate the two loops.

After the warm-up exercise, let us explain the appearance of the additional NL imposed by CHS. Consider a pair of horizontal loops \( \gamma_5,6 \) in Fig. III.14 related by \( \gamma_6 = -(G_x \circ T) \gamma_5 \). The relation (III.65) implies that \( w(\gamma_6) = -w(\gamma_5) \). But since both \( \gamma_5,6 \) encircle the red NL, we obtain
\[
|w(\gamma_6) - w(\gamma_5)| = 2.
\] (III.72)
\(^{17}\)More precisely, they imply \( |w(\gamma_2) - w(\gamma_1)| = 4n + 2 \) with \( n \in \mathbb{Z}^+_0 \), but we expect small values.
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Figure III.14: Paths considered in the analysis of the chiral symmetric model I.
The difference (III.70) between $\omega(\gamma_1)$ and $\omega(\gamma_2)$ can be explained by the red NL separating them. Similarly, the blue NL explains the difference (III.71) between $\omega(\gamma_3)$ and $\omega(\gamma_4)$. However, the nodal chain alone does not explain the difference (III.72) between $\omega(\gamma_5)$ and $\omega(\gamma_6)$. This implies the presence of an additional NL in the $k_z = 0$ plane of the chiral symmetric TB model, which has to touch the red NL.

Consequently, a deformation of $\gamma_5$ into $\gamma_6$ must be accompanied by crossing two nodal lines. In this case, the the nodal chain alone is not able to explain the obstacle. Therefore, we must conclude that CHS imposes an additional NL located in the $k_z = 0$ plane, such that $\gamma_{5,6}$ become separated. We indicate such possible NLs by dashed green lines in Fig. III.14.

We can go one step further: A suitable choice of considered paths can explain the actual topology of the nodal net. First, note that Eq. (III.72) implies that the additional NL cannot terminate at the red NL, because that would correspond to just a single gap closing between $\gamma_5$ and $\gamma_6$, such that it would not be possible to change the topological invariant by 2. This implies that the additional NL really has to pass through the red NL. Because of the periodicity of $k$-space, this leaves us with only two possibilities indicated by the dashed green and magenta lines in Fig III.15. We argue below that the first option is realized.

Consider a path $\gamma_7 = C_2^+ \gamma_5$, such that $\omega(\gamma_7) = \omega(\gamma_5)$. The paths $\gamma_{5,7}$ can be merged into $\gamma_8$ with $|\omega(\gamma_8)| = 2$. If we finally consider a path $\gamma_9 = -(G_x \circ T) \gamma_8$, we conclude using Eq. (III.65) that

$$|\omega(\gamma_9) - \omega(\gamma_8)| = 4.$$  \hspace{1cm} (III.73)

Therefore, deforming $\gamma_8$ onto $\gamma_9$ is accompanied by crossing of four NLs. This implies that the topology of the nodal net cannot take the form (2) of
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Figure III.15: Paths considered in the analysis of the chiral symmetric model II.

The invariants for paths $\gamma_{8,9}$ are related by Eq. (III.73), which is consistent with the green NL (1), but not with the magenta NL (2). This uniquely determines the topology of the nodal net in the extended $k$-space as plotted in Fig. III.13(c).

Fig. III.15. Consequently, the topology of the nodal net in the extended $k$-space is fixed to take the form plotted in Fig. III.13(c). We expect analogous findings for all the eight space groups listed in the catalog of Fig. III.5, although we did not check this explicitly.

Let us finally tackle the distinction of the regions labelled by “0” and “2” in Fig. III.11(d). The labels correspond to the winding numbers of straight paths (“fibers”) traversing the Brillouin zone in the [100] direction. The two regions are related by $C_2^+ z$ (which also reverses the orientation of the fibers). Since these loops are non-contractible, we have to take into account the integral term in Eq. (III.65). We adopt the tight-binding convention with phase factors $e^{i k \cdot R}$ where $R$ are the Bravais vectors. With such a choice, $\mathcal{H}(k) = \mathcal{H}(k + G)$. The representation of $C_2^+ z$ in this convention is

\[ C_2^+(k) = -i \sigma_z \otimes \begin{pmatrix} e^{-i(k_z-k_y)/2} & 0 \\ 0 & e^{-i(k_z+k_x)/2} \end{pmatrix} \] (III.74)

and the phase $v_k$ in Eq. (III.65) becomes

\[ v_k = (a_k^* - b_k^*) (a_k + b_k) = e^{i(k_x+k_y)/2}, \] (III.75)

which winds once for any one-dimensional path threading the Brillouin zone in the [100] direction. Since in our case $n = 2$, we obtain from Eq. (III.65) that

\[ c(k_y, k_z) = -c(-k_y, k_z) + 2, \] (III.76)
where we also took into account the reversed orientation of the two fibers related by $C_{2z}^+$. This condition is compatible with the region labels in Fig. III.11(d).
In the previous two chapters, we studied how space group symmetry facilitates the appearance of nodes in band structures. Such nodes are typically constrained to lie at high-symmetry lines or planes in momentum space. Specifically, the Dirac points of pyrochlore iridates in chapter II lie at TRIMs on the BZ boundary, and the Weyl points they produce upon breaking move along rotation invariant axes. In chapter III, we observed the formation of nodal lines in mirror-invariant planes. Similar confinement to a lower-dimensional subspace of momentum space is also present for other nodes recently discussed in the literature, e.g. hyper-Dirac points [174], emergent spin-1 fermions [175], and nexus of nodal lines [155–159], which are not explicitly discussed in this thesis.

However, we also went across a few examples where such a confinement is absent. First, we discussed in Subsec. II.1.1 that Weyl points are robust against essentially all perturbation, especially all those that break point group symmetries [29, 31]. This means that breaking all the remnant rotation and mirror symmetries of the breathing pyrochlore lattice does not gap out the observed Weyl points, but only moves them away from the rotation-symmetric axes. Second, we mentioned in Subsec. III.1.3 that in systems preserving both \( T \) and \( I \) in the absence of SOC, nodal lines may appear which can take arbitrary shape [38]. Electrons in such systems are described as effectively spinless. As a non-trivial example of such nodal lines, we mentioned the nodal spiral in rhombohedral graphite [160]. Finally, the three nodal loops observed
in the chiral-symmetric TB model of Subsec. III.5 would start traversing the momentum space if point group symmetries were removed, because they are protected by the winding number invariant of Eq. (III.10a).

While Weyl points do not require the presence of any symmetry for their appearance, the common property of the latter two examples is that they exhibit a symmetry \textit{local in }k\textit{ space}, i.e. one posing a constraint on \( \mathcal{H}(k) \) for all \( k \in \text{BZ} \). Such local constraints influence the codimension \( \delta \) of the node formation at such a generic \( k \)-point. In the case of the spinless nodal line semimetals, such a symmetry is \( e^{i\pi \sigma_y/2} \circ \mathcal{T} \circ \mathcal{I} \), i.e. a composition of space inversion, time-reversal and a spin-rotation symmetry [38]. In the case of the nodal net, the local symmetry corresponds to the sublattice realization of the chiral symmetry \( \mathcal{C} \) of Eq. (III.63). In both cases, the codimension is decreased from \( \delta = 3 \) in the absence of symmetries (leading in 3D to Weyl points), to a lower \( \delta = 2 \) (leading in 3D to the mentioned nodal lines).

The confinement of the other mentioned nodes to a lower-dimensional part of \( k \)-space stems from the fact, that a typical point group symmetry \( R \) relates \( \mathcal{H}(k) \) to \( \mathcal{H}(Rk) \), which is \textit{not} a local condition for a generic \( k \). However, the example of the spinless nodal line semimetals suggest a viable generalization: A composition of spatial inversion \( \mathcal{I} \) (which flips \( k \) to \( -k \)) with a time reversal \( \mathcal{T} \) or particle-hole symmetry \( \mathcal{P} \) (which also flip \( k \) to \( -k \)) \textit{becomes} local in \( k \)-space. This motivates us to develop a modified version of the Atland-Zirnbauer (AZ) classification based on the presence of such global symmetries (i.e. \( \mathcal{T}, \mathcal{P} \) and \( \mathcal{C} \)) which would be better tailored for centrosymmetric systems.

We develop such a modified classification scheme, which we call the \( AZ+I \) classification, in Sec. IV.1. We refer to the ten symmetry possibilities of this scheme as the \textit{centrosymmetrically extended AZ classes}, or just \( AZ+I \) classes, for short. The generalization is done in such a way, that non-centrosymmetric systems can also be assigned into one of the ten extensions. We then apply codimension arguments to determine the dimension of the nodes exhibited by the individual \( AZ+I \) classes in an arbitrary spatial dimension, and we apply homotopy theory to determine their topological characteristics, which we call \textit{topological charges}.

One of the interesting findings of Sec. IV.1 is the observation of nodes characterized by \textit{multiple topological charges}. More specifically, we show that in three spatial dimension, four of the ten centrosymmetrically extended AZ classes support nodes characterized with a \textit{pair} of charges [40].
Two of these have been previously known, namely the spinless nodal lines\footnote{Up until now, we only exposed one of the two charges, namely the $Z_2$ Berry phase in Eq. (III.3). The other charge is also $Z_2$-valued and has been identified by Ref. [38]. We will explain this additional charge in Sec. IV.6. This $Z_2$ invariant has been more recently investigated also by Refs. [176, 177].} of $AZ+I$ class AI [38], and the Bogolyubov Fermi surfaces appearing in certain time-reversal breaking multi-orbital superconductors [39], which correspond to $AZ+I$ class D. The second example forms a *nodal surface* in the sense that a pair of Bogolyubov-de Gennes (BdG) bands touches along a 2D manifold inside 3D $k$-space. The further two examples include doubly charge nodal lines of $AZ+I$ class CI, and doubly charged nodal surfaces of $AZ+I$ class BDI.

Such multiply-charged nodes may reach the very high degree of stability usually associated with Weyl points: Continuous deformation of the underlying Hamiltonian can move these nodes across the $k$-space, but the only way to remove them is through a pairwise annihilation. Since $I$ is preserved in the usual straining experiments and since no further point group symmetries are necessary for the appearance of these nodes, they are robust against a very wide range of perturbation. We describe this property as *robustness*. Of all the nodes alluded to in the previous chapters, only Weyl points are robust in this sense.

In Sec. IV.2, we follow the logic of Ref. [21] in order to relate the abstractly defined $AZ+I$ classes to various physical systems. For systems characterized by a particle-hole symmetry, we divide the discussion into systems with a sublattice symmetry (treated in Subsec. IV.2.1) and into superconducting systems (treated in Subsec. IV.2.2). The developed classification applies beyond semimetals. For example, it captures nodes of the gap function of various superconductors [178–180], of excitation spectra of superfluids [15] and even of magnon bands [181].

In the remaining sections, we discuss individually the four $AZ+I$ classes supporting doubly charged nodes in three spatial dimensions. We develop a simple TB model on a hexagonal SrPtAs-like lattice [182] for each class, and provide a geometric interpretation of both of the two topological charges of the nodes exhibited by the TB models. We sequentially go through: The $AZ+I$ class D exhibiting $Z_2 \oplus 2Z$ nodal surfaces in Sec. IV.3, class BDI with $Z_2 \oplus Z_2$ nodal surfaces in Sec. IV.4, class CI with $Z \oplus Z_2$ nodal lines in Sec. IV.5, and finally class AI with $Z_2 \oplus Z_2$ nodal lines in Sec. IV.6. While most of the formulated charges are in some way already present in the ten-fold way classification [73], on three occasions...
we encounter a somewhat unusual $\mathbb{Z}_2$ charge corresponding to a closed path winding inside Lie group $SO(n)$ [38], which we formalize using Wilson loop spectra [70, 183].

IV.1 Mathematical considerations

In this section we derive most of the main results of the present chapter. The later sections mostly serve to strengthen our claims by providing explicit tight-binding (TB) models that exhibit the doubly charged nodes. They also explain in more detail the geometric meaning of the pair of topological charges.

To derive the results, which are summarized in Tab. IV.1, we begin in Subsec. IV.1.1 by developing the centrosymmetrically extended Atland-Zirnbauer ($AZ+I$) classification. We use codimension arguments to determine the dimension of the nodes of the individual $AZ+I$ classes in Subsec. IV.1.2. Finally, in Subsec. IV.1.3 we apply the homotopy theory to derive the topological charges of the nodes. The last subsection is supplemented by Appendix B which presents the derivation of the classifying spaces relevant for the individual $AZ+I$ classes.

IV.1.1 Symmetry classification

A classification of Hamiltonians according to their global symmetries was developed in Ref. [41]. By these we mean time-reversal ($T$), particle-hole ($P$) and chiral ($C$) symmetry. They are defined by Eqs. (I.99) as presented in the introductory Sec. I.3. There are ten possibilities which are listed alongside their Cartan label (CL) in the first four columns of Tab. I.1 in the same section. This classification is reproduced again in the left part of Tab. IV.1.

Apart from the discrete set of $2^D$ time-reversal invariant momenta (TRIMs), where $D$ is the number of spatial dimensions, $T$ and $P$ relate Hamiltonians at two different $k$-points. These non-local constraints have to be incorporated when developing the ten-fold way classification of gapped topological insulators and superconductors [73, 75, 76, 184]. However, when characterizing nodes of a gapless system, one only needs to know the Hamiltonian in the vicinity of the node, which is typically not constrained by conditions (I.99a) and (I.99b). Consequently, a $D = 3$ system exhibits nodal points (lines) in the absence (presence) of $C$, as is
Table IV.1: Summary of the main results of chapter IV. The first four columns list the ten possible symmetry classes together with their Cartan label (CL). The headers $T, P, C$ (in gray) correspond to the AZ classification [41], while the headers $\mathcal{Z}, \mathcal{W}, \mathcal{C}$ correspond to the AZ+$\mathcal{I}$ classification developed in Subsec. IV.1.1 and considered throughout the following sections. The rest of the table applies to the AZ+$\mathcal{I}$ case only. The fifth column lists the classifying spaces $\mathbb{M}_{CL}$ [75] relevant for each symmetry class as explained in Subsec. IV.1.2. Here, $n, \ell$ indicate the number of occupied and unoccupied bands ($n = \ell$ whenever $\mathcal{W}$ or $\mathcal{C}$ is present), except cases labelled by ($\dagger$) when we denote these as $2n, 2\ell$ instead. The next block of the table lists the large $n, \ell$ limit homotopy groups of $\mathbb{M}_{CL}$ with the exception of $\pi_0(\mathbb{M}_{CL})$ which counts the number of connected components of $\mathbb{M}_{CL}$. As discussed in Subsec. IV.1.3, the homotopy groups $\pi_p(\mathbb{M}_{CL})$ that determine the charges of a node are those with $d_{CL} - 1 \leq p \leq D - 1$ where $d_{CL}$ is the node codimension listed for all AZ+$\mathcal{I}$ classes in Tab. IV.2, and $D$ is the spatial dimension. The homotopy groups relevant for $D = 3$ are typesetted in bold. We observe that AZ+$\mathcal{I}$ classes $\text{AI}, \text{BDI}, \text{D}$ and $\text{CI}$ support doubly charged nodes in this spatial dimension. The last three columns indicate the corresponding topological charges, namely $\int \mathcal{F}$ is the (first) Chern number, $\int q^{-1}dq$ is the winding of the off-diagonal block of $Q(k)$, $\int A$ is the Berry phase, $\text{sign Pf}$ is the sign of the Pfaffian of the Hamiltonian, and $\pi_1[\text{SO}(n)]$ is the homotopy class of a closed path inside the orthogonal group.

<table>
<thead>
<tr>
<th>CL</th>
<th>$\mathcal{Z}, \mathcal{W}, \mathcal{C}$</th>
<th>$\mathbb{M}_{CL}$</th>
<th>homotopy group $\pi_p(\mathbb{M}_{CL})$ for $p = 0, 1, 2, 3, 4, 5, 6, 7, 8$</th>
<th>topological charge $\epsilon_{CL}(S^p)$ for $p = 0, 1, 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$\times \times \times$</td>
<td>$U(n + \ell)/U(n) \times U(\ell)$</td>
<td>$0 \ 0 \ \mathbb{Z}$</td>
<td>$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0$</td>
</tr>
<tr>
<td>AIII</td>
<td>$\times \times 1$</td>
<td>$U(n)$</td>
<td>$0 \ \mathbb{Z}$</td>
<td>$0 \ 0 \ 0 \ 0 \ 0 \ 0$</td>
</tr>
<tr>
<td>AI</td>
<td>$+1 \times \times$</td>
<td>$O(n + \ell)/O(n) \times O(\ell)$</td>
<td>$0 \ \mathbb{Z}_2 \ \mathbb{Z}_2$</td>
<td>$0 \ 2\mathbb{Z} \ 0 \ 0 \ 0 \ 0 \ \mathbb{Z}$</td>
</tr>
<tr>
<td>BDI</td>
<td>$+1 +1 1$</td>
<td>$O(n)$</td>
<td>$\mathbb{Z}_2 \ \mathbb{Z}_2 \ 0$</td>
<td>$2\mathbb{Z} \ 0 \ 0 \ 0 \ \mathbb{Z} \ \mathbb{Z}_2$</td>
</tr>
<tr>
<td>D</td>
<td>$\times +1 \times$</td>
<td>$O(2n)/U(n)$</td>
<td>$\mathbb{Z}_2 \ 0 \ 2\mathbb{Z}$</td>
<td>$0 \ 0 \ 0 \ \mathbb{Z} \ \mathbb{Z}_2 \ \mathbb{Z}_2$</td>
</tr>
<tr>
<td>DIII</td>
<td>$\times +1 1$</td>
<td>$U(2n)/\text{Sp}(n)(\dagger)$</td>
<td>$0 \ 2\mathbb{Z} \ 0$</td>
<td>$0 \ 0 \ \mathbb{Z} \ \mathbb{Z}_2 \ \mathbb{Z}_2 \ 0$</td>
</tr>
<tr>
<td>AII</td>
<td>$-1 \times \times$</td>
<td>$\text{Sp}(n + \ell)/\text{Sp}(n) \times \text{Sp}(\ell)(\dagger)$</td>
<td>$0 \ 0 \ 0$</td>
<td>$0 \ \mathbb{Z} \ \mathbb{Z}_2 \ \mathbb{Z}_2 \ 0 \ 2\mathbb{Z}$</td>
</tr>
<tr>
<td>CII</td>
<td>$-1 -1 \times$</td>
<td>$\text{Sp}(n)(\dagger)$</td>
<td>$0 \ 0 \ \mathbb{Z}$</td>
<td>$\mathbb{Z} \ \mathbb{Z}_2 \ \mathbb{Z}_2 \ 0 \ 2\mathbb{Z} \ 0$</td>
</tr>
<tr>
<td>C</td>
<td>$\times -1 \times$</td>
<td>$\text{Sp}(n)/U(n)$</td>
<td>$0 \ 0 \ \mathbb{Z}$</td>
<td>$\mathbb{Z}_2 \ \mathbb{Z}_2 \ 0 \ 2\mathbb{Z} \ 0 \ 0$</td>
</tr>
<tr>
<td>CI</td>
<td>$+1 -1 \times$</td>
<td>$U(n)/O(n)$</td>
<td>$0 \ \mathbb{Z} \ \mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2 \ 0 \ 2\mathbb{Z} \ 0 \ 0 \ 0$</td>
</tr>
</tbody>
</table>
shown using homotopy theory in the subsequent sections. These two scenarios correspond precisely to the Weyl points and to nodal lines characterized by the winding number, which were mentioned in the introduction to this chapter. Further nodal points imposed by conditions (I.99a) and (I.99b) may be imposed at TRIMs, but these are unremovable and immobile, and thus not of relevance to us.

The conclusion that $T$ and $P$ do not affect the classification of nodes is changed in the presence of crystalline symmetries [185]. In this chapter, we consider the presence of inversion symmetry ($I$) which is typically robust against simple straining. It fulfills

$$I\mathcal{H}(k)I^{-1} = \mathcal{H}(-k) \quad I^2 = 1 \quad (U) \quad (IV.1)$$

such that compositions

$$TI = \mathcal{I} \quad \text{and} \quad PI = \mathcal{P} \quad (IV.2)$$

impose local antiunitary constraints in $k$-space [38, 176] and become relevant for the characterization of nodes. Apart from the (non-)locality in $k$-space, the set of operators $\mathcal{I}, \mathcal{P}, C$ is mathematically equivalent to the set $T, P, C$. It is therefore natural to define ten symmetry classes based on the presence of operators fulfilling

$$\mathcal{I}\mathcal{H}(k)\mathcal{I}^{-1} = \mathcal{H}(k) \quad \mathcal{I}^2 = \pm 1 \quad (AU) \quad (IV.3a)$$

$$\mathcal{P}\mathcal{H}(k)\mathcal{P}^{-1} = -\mathcal{H}(k) \quad \mathcal{P}^2 = \pm 1 \quad (AU) \quad (IV.3b)$$

$$\mathcal{C}\mathcal{H}(k)\mathcal{C}^{-1} = -\mathcal{H}(k) \quad C^2 = 1 \quad (U). \quad (IV.3c)$$

We call them the centrosymmetrically extended AZ classes, or just AZ+$I$ classes for brevity. We list them together with their CL in the first four columns of Tab. IV.1.

We remark that CLs of the AZ class and of the AZ+$I$ class corresponding to a given system may be different – a subtlety that is more carefully explained in Sec. IV.2. Furthermore, classification (IV.3) also applies to systems without spatial inversion. Especially, symmetries (IV.2) can be present even when $T, P, I$ themselves are absent.

**IV.1.2 Node dimensionality**

In this subsection we systematically determine the dimension of nodes supported by the individual AZ+$I$ classes in arbitrary spatial dimension
Table IV.2: Determining the node codimension $\delta_{\text{CL}}$. The first four columns indicate for every $AZ+I$ class our representation of $\mathcal{Z}$, $\mathcal{P}$ and $\mathcal{C}$, if present. The fifth column lists the basis matrices $\sigma_i$ of a two-band Hamiltonian $\mathcal{H}_{2\times2}$ that are compatible with the listed operators, and the sixth column achieves the same for basis matrices $\sigma_i \otimes \tau_j$ of a four-band Hamiltonian $\mathcal{H}_{4\times4}$. For classes DIII and CII, Kramers degeneracy associated with $\mathcal{Z}^2 = -1$ together with the presence of $\mathcal{P}$ necessitates a minimum of four bands, such that $\mathcal{H}_{2\times2}$ is non-existent ($\emptyset$). Similarly, $\mathcal{Z}^2 = -1$ of class AII implies a double degeneracy of bands for all $k$, meaning that a minimum of four bands is necessary to obtain a node formed by touching valence and conduction bands. The column $\delta_{\text{CL}}$ indicates the node codimension for each $AZ+I$ class. It is obtained by counting the number of traceless basis elements of the minimal model (typesetted in black). As explained in Subsec. IV.1.2, stable nodes exist when $D \geq \delta_{\text{CL}}$ and their dimension is given by the difference $D - \delta_{\text{CL}}$. We list the node type appearing in $D = 3$ explicitly in the last column.

<table>
<thead>
<tr>
<th>CL</th>
<th>$\mathcal{Z}$</th>
<th>$\mathcal{P}$</th>
<th>$\mathcal{C}$</th>
<th>basis of $\mathcal{H}_{2\times2}$</th>
<th>basis of $\mathcal{H}_{4\times4}$</th>
<th>$\delta_{\text{CL}}$</th>
<th>nodes in $D = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
<td>${1, \sigma_x, \sigma_y, \sigma_z}$</td>
<td>${1, \sigma_x, \sigma_y, \sigma_z} \otimes {1, \tau_x, \tau_y, \tau_z}$</td>
<td>3</td>
<td>point</td>
</tr>
<tr>
<td>AIII</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\sigma_z$</td>
<td>${\sigma_x, \sigma_y}$</td>
<td>${\sigma_x, \sigma_y} \otimes {1, \tau_x, \tau_y, \tau_z}$</td>
<td>2</td>
<td>line</td>
</tr>
<tr>
<td>AI</td>
<td>$\mathcal{K}$</td>
<td>$\times$</td>
<td>$\times$</td>
<td>${1, \sigma_x, \sigma_z}$</td>
<td>${1, \sigma_x, \sigma_y} \otimes {1, \tau_x, \tau_y}$</td>
<td>2</td>
<td>line [38]</td>
</tr>
<tr>
<td>BDI</td>
<td>$\mathcal{K}$</td>
<td>$\sigma_z \mathcal{K}$</td>
<td>$\sigma_z$</td>
<td>${\sigma_x}$</td>
<td>$\sigma_x \otimes {1, \tau_x, \tau_y} \cup {\sigma_y \otimes \tau_y}$</td>
<td>1</td>
<td>surface</td>
</tr>
<tr>
<td>D</td>
<td>$\times$</td>
<td>$\mathcal{K}$</td>
<td>$\times$</td>
<td>${\sigma_y}$</td>
<td>$\sigma_y \otimes {1, \tau_x, \tau_y} \cup {1, \sigma_x, \sigma_z} \otimes \tau_y$</td>
<td>1</td>
<td>surface [39]</td>
</tr>
<tr>
<td>DIII</td>
<td>$i\sigma_y \mathcal{K}$</td>
<td>$\sigma_y \mathcal{K}$</td>
<td>$\sigma_z$</td>
<td>$\emptyset$</td>
<td>${\sigma_x, \sigma_y} \otimes \tau_y$</td>
<td>5</td>
<td>line</td>
</tr>
<tr>
<td>AII</td>
<td>$i\sigma_y \mathcal{K}$</td>
<td>$\times$</td>
<td>$\times$</td>
<td>${1}$</td>
<td>$1 \otimes {1, \tau_x, \tau_y} \cup {\sigma_x, \sigma_y, \sigma_z} \otimes \tau_y$</td>
<td>2</td>
<td>(none)</td>
</tr>
<tr>
<td>CII</td>
<td>$i\tau_y \mathcal{K}$</td>
<td>$-i\sigma_z \otimes \tau_y \mathcal{K}$</td>
<td>$\sigma_z$</td>
<td>$\emptyset$</td>
<td>${\sigma_x \otimes 1} \cup \sigma_y \otimes {\tau_x, \tau_y, \tau_z}$</td>
<td>4</td>
<td>(none)</td>
</tr>
<tr>
<td>C</td>
<td>$\times$</td>
<td>$i\sigma_y \mathcal{K}$</td>
<td>$\times$</td>
<td>${\sigma_x, \sigma_y, \sigma_z}$</td>
<td>${\sigma_x, \sigma_y, \sigma_z} \otimes {1, \tau_x, \tau_y} \cup {1 \otimes \tau_y}$</td>
<td>3</td>
<td>point</td>
</tr>
<tr>
<td>CI</td>
<td>$\mathcal{K}$</td>
<td>$i\sigma_y \mathcal{K}$</td>
<td>$i\sigma_y$</td>
<td>${\sigma_x, \sigma_z}$</td>
<td>${\sigma_x, \sigma_z} \otimes {1, \tau_x, \tau_z}$</td>
<td>2</td>
<td>line</td>
</tr>
</tbody>
</table>
D. To achieve this, we fix canonical representations of operators (IV.3) and use them to determine the codimension $\delta_{\text{CL}}$ of the node formation, i.e. the number of conditions to be fulfilled to make two bands touch. Provided that $D \geq \delta_{\text{CL}}$, nodes of dimension $D - \delta_{\text{CL}}$ occur.

Our choice of representing operators $\mathcal{T}, \mathcal{P}, \mathcal{C}$ is shown in Tab. IV.2 where $\mathcal{K}$ indicates complex conjugation, and $\sigma_i$ and $\tau_i$ are Pauli matrices corresponding to two different degrees of freedom. The choice is rather arbitrary, but this freedom does not influence the analysis of the node codimension and of the node charges in the subsequent text. Specifically, we apply the following rules:

(i) Set $\mathcal{C} = \sigma_z$ to enforce a block-off-diagonal form (IV.6) of the Hamiltonian.

(ii) Represent antiunitary operators squaring to $+1$ by $\mathcal{K}$, and those squaring to $-1$ by $i\sigma_y\mathcal{K}$.

These requirements are incompatible if all $\mathcal{T}, \mathcal{P}$ and $\mathcal{C}$ are present, hence classes BDI, DIII, CII and CI contain some exceptions. Finally, we always apply the rule:

(iii) Set $\mathcal{T}\mathcal{P} = \mathcal{C}$ if all three symmetries are present.

Having fixed the representations of $\mathcal{T}, \mathcal{P}$ and $\mathcal{C}$, the node codimension $\delta_{\text{CL}}$ is determined by considering the minimal model capturing degeneracies between the valence and the conduction bands. This is either a two-band Hamiltonian

$$\mathcal{H}_{2\times2}(k) = \sum_{i=0}^{3} f_i(k) \sigma_i$$  \hspace{1cm} (IV.4a)

where $\sigma_i$ are Pauli matrices, or a four-band model

$$\mathcal{H}_{4\times4}(k) = \sum_{i,j=0}^{3} g_{ij}(k) \sigma_i \otimes \tau_j$$  \hspace{1cm} (IV.4b)

expanded using product of pairs of Pauli matrices (i.e. Dirac matrices) $\sigma_i \otimes \tau_j$, and $f_i$ and $g_{ij}$ are real-valued functions. Model (IV.4) can be always locally obtained by projecting out bands that do not participate in the node formation. By Kramers theorem, the minimal model is (IV.4b) whenever the symmetry class contains $\mathcal{T}^2 = -1$, and (IV.4a) otherwise.
Local constraints (IV.3) forbid the presence of some of the basis matrices in expansions (IV.4). For the representation of operators given in Tab. IV.2 we systematically analyse these constraints, and we list the symmetry-compatible basis matrices and their number $\delta_{\text{CL}}$ further in Tab. IV.2. The unit matrix is not relevant for the node dimension (although it may be relevant for its experimental signatures [78]) and is therefore not counted in $\delta_{\text{CL}}$. We observe that the remaining basis matrices of the minimal model are always anticommuting, which implies that a node occurs at $k_0$ whenever the $\delta_{\text{CL}}$ function values $f_i(k_0)$ [or $g_{ij}(k_0)$] vanish. Solutions to $\delta_{\text{CL}}$ equations in $D$ dimensions generically occur on a $(D - \delta_{\text{LC}})$-dimensional manifold – the node dimension of the corresponding $\text{AZ}+\mathcal{I}$ class. We provide the explicit outcome of the analysis for $D = 3$ in the last column of Tab. IV.2.

We remark that for classes with $\mathfrak{P}$ or $\mathcal{C}$ the presented arguments only work for zero energy (i.e. Fermi level) nodes. For nodes located at a non-zero energy (i.e. ones formed entirely within the valence or within the conduction bands), symmetries $\mathfrak{P}$ and $\mathcal{C}$ do not restrict the effective model (IV.4) and can be dropped from the $\text{AZ}+\mathcal{I}$ description. This a rather trivial observation and we do not return to it again.

### IV.1.3 Topological charges

Knowing the dimensionality of the nodes for all the $\text{AZ}+\mathcal{I}$ classes, we now determine the corresponding topological charges by considering $p$-spheres $S^p$ wrapping around them. The largest sphere fitting into the Brillouin zone (BZ) is $S^{D-1}$, and by $S^0$ we mean a pair of points (rather than just a single one). However, not all of these come into play. For example, all circles $S^1 \subset \text{BZ}$ in a class supporting nodal points are continuously contractible to a single point without encountering a gap closing, and therefore cannot host any topological obstruction. The same is true for $S^0$ in such a system, and a few more similar examples are illustrated in Fig. IV.1. Simple counting reveals that only $p$-spheres with $\delta_{\text{CL}} - 1 \leq p \leq D - 1$ can be non-contractible and may therefore accommodate a topological charge.

To find the topological charge supported by $S^p$, we first perform spectral flattening [73]. For a system with $n$ occupied and $\ell$ unoccupied bands, we decompose the Hamiltonian $\mathcal{H}(k)$ on $S^p$ using the eigensys-
Chapter IV. Nodes from spatial inversion

\[ \{ \varepsilon^a(k), |u^a(k)\rangle \}_{a=1}^{n+\ell} \]

which can be continuously deformed without closing the gap on \( S^p \) into a flat-band Hamiltonian

\[ Q(k) = \sum_{a=1}^{n+\ell} |u^a(k)\rangle \text{sign} [\varepsilon^a(k)] \langle u^a(k)|. \] (IV.5b)

Note that the description using \( \{|u^a(k)\rangle\}_{a=1}^{n+\ell} \in \mathbb{U}(n+\ell) \) is redundant because rotating the occupied (unoccupied) states by a \( \mathbb{U}(n+\ell) \) matrix leaves \( Q(k) \) invariant, meaning that \( Q(k) \) is an element of \( \mathbb{U}(n+\ell)/\mathbb{U}(n) \times \mathbb{U}(\ell) \equiv \mathbb{M}_A \) [or, alternatively, \( Q(k) \) corresponds to a fiber in \( \mathbb{U}(n+\ell) \)] which is the classifying space in the absence of \( AZ+I \) symmetries. The decompositions (IV.5) may not be achieved with a smooth gauge in the case of Chern bands, nevertheless, the flat-band Hamiltonian \( Q(k) \in \mathbb{M}_A \) is still smooth within the fiber bundle \( \mathbb{M}_A \).

Conditions (IV.3) of a given symmetry class \( CL \) constrain \( Q(k) \) to be an element of a smaller classifying space \( \mathbb{M}_{CL} \subseteq \mathbb{M}_A \). For example, \( C = \sigma_z \) leads to

\[ Q(k) = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix} \] (IV.6)

with \( q(k) \in \mathbb{U}(n) \equiv \mathbb{M}_{AIII} \). All relevant classifying spaces appeared in Ref. [75] and we reproduce them in Tab. IV.1. A curious reader can find the derivation of all the classifying spaces in Appendix B.

Every \( S^p \subset \text{BZ} \) with a gapped spectrum is associated with a continuous map \( \mathcal{F} : S^p \to \mathbb{M}_{CL} \). Continuous deformations of \( S^p \) as well as of \( \mathcal{H}(k) \) (such that the spectrum on \( S^p \) is kept gapped) lead to continuous changes of \( \mathcal{F} \). One may thus consider the class \( [\mathcal{F}] \) of maps continuously reachable from \( \mathcal{F} \). Especially, if a constant map \( \mathcal{F}_m : S^p \to m \) with a fixed element \( m \in \mathbb{M}_{CL} \) cannot be reached from \( \mathcal{F} \), then \( S^p \) cannot be shrunk to a single point \( k_0 \in \text{BZ} \). This implies that \( S^p \) contains an unremovable node. We therefore deduce a connection between the class \( [\mathcal{F}] \) and the charge \( c_{CL}(S^p) \) accommodated by the \( p \)-sphere. The order of the charge for \( p \geq 1 \) corresponds to the number of inequivalent classes \( [\mathcal{F}] \), which is captured by the homotopy group \( \pi_p(\mathbb{M}_{CL}) \) [42]. The charge on \( S^p \) is then some element

\[ c_{CL}(S^p) \in \pi_p(\mathbb{M}_{CL}). \] (IV.7a)
**Table IV.3: Relevant few-band homotopy groups I.** We list here the homotopy groups $\pi_p(M_{CL})$ for $AZ+I$ symmetry classes supporting doubly charged nodes in $D = 3$ for systems not reaching the large $n$ limit. Class $AI$ contains more special cases and is treated separately in Tab. IV.4. The exceptional values are typesetted in a bold font, while the values following the large $n$ result of Tab. IV.1 are displayed in gray. Note that in all cases a minimum of four bands ($n = 2$) is necessary to realize a node with a pair of non-trivial topological charges.

<table>
<thead>
<tr>
<th>$n$</th>
<th>BDI</th>
<th>D</th>
<th>CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (2 bands)</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>2 (4 bands)</td>
<td>$\mathbb{Z}_2 \times \mathbb{Z}$</td>
<td>$\mathbb{Z}_2 \times \mathbb{Z}$</td>
<td>$\mathbb{Z} \times \mathbb{Z}$</td>
</tr>
<tr>
<td>$\geq 3$</td>
<td>$\mathbb{Z}_2 \times \mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2 \times \mathbb{Z}_2$</td>
<td>$\mathbb{Z} \times \mathbb{Z}_2$</td>
</tr>
</tbody>
</table>

Homotopy groups of $M_{CL}$ for large $n, \ell$ can be found in Ref. [74], and we reproduce them in Tab. IV.1. The special $p = 0$ case $\pi_0(M_{CL})$ counts the number of connected components of $M_{CL}$ and also happens to have a group structure (although this is not true about $\pi_0(M)$ for a general manifold $M$).

Collecting the charges supported by all $p$-spheres enclosing a node of a given $AZ+I$ class, the complete topological charge of the node is

$$c^{(D)}_{CL} \in \bigoplus_{p=0}^{D-1} \pi_p(M_{CL}). \quad (IV.7b)$$

A node is termed *multiply charged* whenever more than one of the groups in the direct sum (IV.7b) are non-trivial. We read from Tabs. IV.1 and IV.2 that for $D = 3$ in the large $n, \ell$ limit, doubly charged nodal lines appear in $AZ+I$ classes $AI$ and $CI$, and doubly charged nodal *surfaces* exist in classes BDI and D.

More care is required if one studies *few-band* models not reaching the large $n, \ell$ limit of Ref. [74]. In that case, the homotopy groups may differ from those listed in Tab. IV.1. If $M_{CL}$ is a Lie group (classes AIII, BDI and CII), the homotopy groups can be readily found in various sources (e.g. [186]), while if $M_{CL}$ is a fiber bundle, $M_{CL} = E/F$ (all other classes), one can determine $\pi_p(M_{CL})$ from the long exact sequence of homomorphisms [187]

$$\ldots \rightarrow \pi_p(E) \rightarrow \pi_p(M_{CL}) \rightarrow \pi_{p-1}(F) \rightarrow \pi_{p-1}(E) \rightarrow \ldots \quad (IV.8)$$
Chapter IV. Nodes from spatial inversion

Table IV.4: Relevant few-band homotopy groups II. We list here the relevant homotopy groups $\pi_p(M_{AI})$ for systems not reaching the large $n, \ell$ limit. They contain multiple exceptions (displayed in bold) differing from the large $n, \ell$ limit (displayed in gray) of Tab. IV.1. We briefly tackle these exceptions in Sec. IV.6.

<table>
<thead>
<tr>
<th>$\pi_1(M_{AI})$</th>
<th>$n = 1$</th>
<th>$n \geq 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell = 1$</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>$\ell \geq 2$</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\pi_2(M_{AI})$</th>
<th>$n = 1$</th>
<th>$n = 2$</th>
<th>$n \geq 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell = 1$</td>
<td>0</td>
<td>$2\mathbb{Z}$</td>
<td>0</td>
</tr>
<tr>
<td>$\ell = 2$</td>
<td>$2\mathbb{Z}$</td>
<td>$\mathbb{Z} \oplus \mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>$\ell \geq 3$</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
</tbody>
</table>

We carried out the analysis for the classes supporting doubly charged nodes in $D = 3$, and we list the results in Tabs. IV.3 and IV.4. We find that in all four instances, the minimal half-filled model with doubly charged nodes contains four bands.

Let us briefly discuss the concept of node robustness, which is characterized by the presence of such a charge that a set of nodes can mutually annihilate only if their net charge vanishes. Clearly, the nodal loop in Fig. IV.1(e) with a non-trivial $c(S^1)$ and trivial $c(S^2)$ is not robust: It can be shrunk to a single point, and since at that stage $c(S^1)$ ceases to be defined (there is no “loop interior”), nothing prevents us from gapping out the spectrum entirely. The result would be different if $c(S^2)$ were non-trivial too, because then the nodal point is enclosed with a non-contractible sphere carrying a topological obstruction [38]. On the other hand, the winding nodal line in Fig. IV.1(e) cannot be shrunk to a point and thus $c(S^1)$ never ceases to be meaningful. Such winding nodal lines are robust regardless of $c(S^2)$.

An analogous dichotomy exists for the nodal torus and the nodal cylinder with non-trivial $c(S^1)$ and trivial $c(S^2)$ that are illustrated in Fig. IV.1(d): The cylinder is robust while the torus is not. In the same spirit, a nodal surface with a non-trivial $c(S^0)$ also becomes robust if both of its dimensions wind around BZ. Generally, if the highest non-trivial homotopy group in expansion (IV.7b) corresponds to $\tilde{p}$-sphere, the nodal object has to possess $D - \tilde{p} - 1$ winding coordinates to become robust.

IV.2 Realizations of $AZ^{+I}$ classes

We have already warned the reader that the Cartan labels of the AZ and of the $AZ^{+I}$ class corresponding to a given centrosymmetric system
IV.2. Realizations of AZ+I classes

Figure IV.1: Enclosing nodes (red) by $p$-spheres $S^p$ (blue) for $D = 3$. (a) The only non-contractible $S^p$ wrapping around a nodal point is $S^2$. Any $S^1$ would be trivially shrinkable to a point, as indicated, and similarly for a pair of points $S^0$. (b) A nodal line can be wrapped by both $S^1$ and $S^2$, but not by $S^0$. It follows that nodal lines may be doubly charged. (c) A spherical nodal surface can be clearly encased by $S^2$ (shown), as well as by a pair of points $S^0$ located on the opposite sides of the surface. (d) If the nodal surface takes the form of a cylinder winding around BZ (black frame) or of a torus, it can be wrapped by $S^1$, too. If the nodal cylinder is characterized by a non-trivial charge on $S^1$, it becomes robust and a Nielsen-Ninomiya type of argument [110] implies the presence of another such a cylinder. The same is not true for torical nodal surface which can be gapped out by itself. The pair of points indicated by arrows is an example of $S^0$ “enclosing” the cylinder. (e) Two kinds of nodal lines. The dashed ones wind around BZ, while the solid one does not and is hence called a nodal loop. Similar to the previous case, a non-trivial charge on $S^1$ makes only the winding loops robust.

may be different. In this section we explain that this disagreement occurs when $I P \neq P I$, and we further discuss how the individual AZ+I classes are realized as various semimetallic and superconducting phases. Throughout the section we focus on centrosymmetric systems only. The generalization to non-centrosymmetric cases is straightforward.

Before delving into the scrutiny of operators $P$ and $Q$, let us show that time-reversal behaves “nicely” in the sense that always $T^2 = \bar{I}^2$, thus not leading to a Cartan label difference. The reason is that $T$ and
Chapter IV. Nodes from spatial inversion

$\mathcal{I}$ act on different degrees of freedom (flipping the sign of time vs. position), therefore the commutator $[\mathcal{T}, \mathcal{I}] = 0$ and

$$\mathcal{I}^2 = \mathcal{T}\mathcal{I}\mathcal{T}\mathcal{I} = \mathcal{T}\mathcal{I}\mathcal{T}\mathcal{I} = \mathcal{T}^2$$  \hspace{1cm} (IV.9)

where $\mathcal{I}^2 = 1$ is true for any system.

In the following two subsections we show that always $\mathcal{Q}^2 = \pm \mathcal{P}^2$, where the sign depends on the specific system realization. The discussion is split into Subsec. IV.2.1 dealing with non-superconducting systems with sublattice symmetry (SLS), and Subsec. IV.2.2 dealing with superconducting (SC) systems. A visual summary of the entire Sec. IV.2 is provided by Fig. IV.3.

**IV.2.1 $\mathcal{P}$ from sublattice symmetry**

The sublattice realization of $\mathcal{C}$ corresponds to acting on the two sets of sites with opposite sign, therefore $\mathcal{C}^2 = 1$. Furthermore, this operation is insensitive to spin, such that $\mathcal{C}$ and $\mathcal{T}$ commute. The composition $\mathcal{P} = \mathcal{T}\mathcal{C}$ fulfills

$$\mathcal{P}^2 = \mathcal{T}\mathcal{C}\mathcal{T}\mathcal{C} = \mathcal{T}\mathcal{C}\mathcal{T}\mathcal{C} = \mathcal{T}^2\mathcal{C}^2 = \mathcal{T}^2.$$  \hspace{1cm} (IV.10)

This subsection is thus relevant only to AZ classes BDI and CII, which are themselves distinguished by the presence or absence of spin-orbit coupling (SOC). We want to find the associated AZ+$\mathcal{I}$ classes.

Let us begin with the example of the graphene lattice which contains two sublattices [red and blue in Fig IV.2(a)]. Within the nearest-neighbour (NN) TB description, electrons only hop between the two sublattices, meaning that the Hamiltonian is block-off-diagonal in the sublattice (orbital) basis captured by Pauli matrices $\tau_i$. The Hamiltonian therefore anticommutes with $\mathcal{C} = \tau_z$. On the other hand, inversion symmetry switches the two sublattices, such that $\mathcal{I}(a) = \tau_x$ and $\mathcal{I}(a)\mathcal{C} = -\mathcal{C}\mathcal{I}(a)$. It follows that $\mathcal{Q} = \mathcal{P}\mathcal{I}(a)$ obeys

$$\mathcal{Q}^2(a) = \mathcal{T}\mathcal{C}\mathcal{I}(a)\mathcal{T}\mathcal{C}\mathcal{I}(a) = -(\mathcal{T}\mathcal{C})^2\mathcal{I}^2(a) = -\mathcal{P}^2$$  \hspace{1cm} (IV.11a)

meaning that the AZ + $\mathcal{I}$ class relevant for graphene differs from the underlying AZ class. We refer to this situation as having $\mathcal{I}$-odd SLS. The Cartan labels are changed as

$$\text{BDI} \xrightarrow{+\mathcal{I}} \text{CI} \quad \text{and} \quad \text{CII} \xrightarrow{+\mathcal{I}} \text{DIII}.$$  \hspace{1cm} (IV.11b)
Figure IV.2: Two species of sublattice symmetry. The two displayed bipartite lattices are characterized with a different representation of the inversion operator $I$. The red and blue discs represent atoms on the two sublattices – each unit cell contains one atom of each colour. The black dots in lattice (b) indicate atoms that do not enter the effective TB model, but that still influence the hopping amplitudes by distorting the crystal field. The atoms of both colours are identical in all respects, such that the Hamiltonian is block-off-diagonal in the sublattice basis, leading to $\mathcal{C} = \tau_z$.

While in (a) the inversion symmetry $I_{(a)} = \tau_x$ anticommutes with $\mathcal{C}$ ($I$-odd SLS), in (b) the inversion operator $I_{(b)} = 1\tau$ commutes with it ($I$-even SLS). In case (a), the Cartan labels of the relevant AZ and AZ+$I$ classes are different.

On the other hand, the lattice in Fig. IV.2(b) has $\mathcal{C} = \tau_z$ and $I_{(b)} = 1\tau$ which commute ($I$-even SLS). In this case

$$\mathcal{P}^2_{(b)} = TCI_{(b)} TC I_{(b)} = (TC)^2 I^2_{(b)} = \mathcal{P}^2,$$

meaning that the AZ and AZ+$I$ Cartan labels coincide. Such a situation arises in various non-symmorphic lattices including various distorted perovskites with doubled unit cells [188, 189].

IV.2.2 $\mathcal{P}$ from superconductivity

The commutation relation of $\mathcal{P}$ and $I$ in SC systems depends on the parity of the gap function $\Delta_k$. Furthermore, the relevant AZ and AZ+$I$ classes finely depend on the presence of time-reversal symmetry (TRS) and on the degree of spin-rotation symmetry (SRS). To systematically treat all the possibilities, we largely follow Sec. II.C of Ref. [21] which similarly treats the case of AZ classification. For simplicity, we only consider SC with zero momentum and even frequency pairing.
The most general SC Hamiltonian takes form \[41\]

\[
H(k) = \frac{1}{2} \begin{pmatrix} c_{a}^{\dagger} & c_{b}^{\dagger} \end{pmatrix} \mathcal{H}_{\text{BdG}}^{ab}(k) \begin{pmatrix} c_{a} & c_{b} \end{pmatrix}
\] (IV.12a)

where indices \(a\) and \(b\) encode both the spin and the orbital degree of freedom, and

\[
\mathcal{H}_{\text{BdG}}^{ab}(k) = \begin{pmatrix} \Xi_{ab}^{k} & \Delta_{ab}^{k} \\ -\Delta_{ab}^{*} & -\Xi_{ba}^{k} \end{pmatrix}
\] (IV.12b)

is the Bololyubov-de Gennes (BdG) Hamiltonian, in which \(\Xi_{k} = \Xi_{k}^{\dagger}\) describes the underlying normal metal band structure, and \(\Delta_{k} = -\Delta_{-k}^{\dagger}\) due to the fermionic statistics. Hamiltonian (IV.12b) is automatically furnished with particle-hole operator

\[
\mathcal{P}_{t} = s_{x} \mathcal{K}
\] (IV.13)

where Pauli matrices \(s_{i}\) act on the particle-hole degree of freedom. Operator (IV.13) squares to \(\mathcal{P}_{t}^{2} = +1\).

The system described by (IV.12) is assumed to be centrosymmetric. We can decompose the inversion operator of the normal metal state as \(I_{0} = I_{\tau} \otimes 1_{\sigma}\) where \(I_{\tau}\) is the orbital component, Pauli matrices \(\sigma_{i}\) represent the spin degree of freedom, and the \(1_{\sigma}\) part follows because spin is an axial vector, i.e. it is unaffected by \(I\). The symmetry relates \(I_{0} \Xi_{k} I_{0}^{-1} = \Xi_{-k}\). Operator \(I_{0}\) is real because it only permutes the orbitals. Furthermore, inversion symmetry does not mix electrons and holes, hence the inversion operator of (IV.12b) is diagonal in \(s\), leaving only two options

\[
I_{\text{BdG}} = I_{0} \oplus (\pm I_{0}) \in \{I_{0} \otimes 1_{s}, I_{0} \otimes s_{z}\}.
\] (IV.14)

These translate to a constraint on the gap function

\[
\pm I_{0} \Delta_{k} I_{0}^{-1} = \Delta_{-k} = -\Delta_{k}^{\dagger}
\] (IV.15a)

where in the second step we used the fermionic statistics.

In single-orbital SCs, Eq. (IV.15a) contains \(2 \times 2\) matrices in the spin-degree of freedom with \(I_{0} = 1_{\sigma}\). Eq. (IV.15a) therefore simplifies to

\[
\pm \Delta_{k} = -\Delta_{k}^{\dagger}
\] (IV.15b)
IV.2. Realizations of AZ+I classes

The fields highlighted in green indicate the example models discussed explicitly in Secs. IV.3 to IV.6. Only the classification of centrosymmetric systems is given.

where the $\pm$ sign is inherited from Eq. (IV.15a). We see that single-orbital SCs have to follow one of two scenarios. Either “$+$” is realized in Eq. (IV.15b) (singlet, $I$-even $\Delta_k$), such that $\Delta_k = \psi_k(i\sigma_y)$ with a complex-valued scalar function $\psi_k$ even in $k$. In this case $I_{BdG} = I_0 \otimes 1_s$ commutes with $P_t$, such that $P_t^2 = +\mathbb{I}$. Alternatively, the “$-$” sign in Eq. (IV.15b) is realized (triplet, $I$-odd $\Delta_k$), and the gap function takes the form $\Delta_k = (d_k \cdot \sigma)(i\sigma_y)$ with a complex-valued vector function $d_k$ odd in $k$. In this case $I_{BdG} = I_0 \otimes s_z$ anticommutes with $P_t$, such that $P_t^2 = -\mathbb{I}$. However, as explained in Ref. [21], the presence of SRS renders description (IV.12) redundant and a finer examination is necessary. We do so below after first commenting on the case of multi-orbital superconductivity.

In multi-orbital SCs, the presence of inversion symmetry may be insuf-
ficient to enforce the singlet/triplet separation. The gap function can be a mixture of both, provided that the parity in the spin degree of freedom is compensated by the parity in the orbital one. Let us illustrate this on the graphene lattice of Fig. IV.2(a) with $\mathcal{I}_0 = \tau_x \otimes 1_\sigma$. The symmetry group permits two mixed representations. First, the even one ($\mathcal{I}$-even $\Delta_k$) with

$$\Delta_k^+ = \sum_{j=0,x,y} \psi_j^0(i\sigma_y) \otimes \tau_j + \sum_{i=x,y,z} d_k^{ijz} \sigma_i(i\sigma_y) \otimes \tau_z$$

where $\psi_k^0, \psi_k^x$ are even and $d_k^{iyz}, d_k^{ijz}$ are odd functions of $k$. In this case $\mathcal{I}_{\text{BdG}} = \mathcal{I}_0 \otimes 1_s$ commutes with $\mathcal{P}_t$ such that $\mathcal{P}^2 = \mathcal{P}_t^2 = +1$. The second options is the odd representation ($\mathcal{I}$-odd $\Delta_k$)

$$\Delta_k^- = \psi_k^z(i\sigma_y) \otimes \tau_z + \sum_{i=x,y,z} d_k^{ij0} \sigma_i(i\sigma_y) \otimes \tau_j$$

where $\psi_k^z, d_k^{iy}$ are even and $d_k^{ij0}, d_k^{ijx}$ are odd in $k$. In this case $\mathcal{I}_{\text{BdG}} = \mathcal{I}_0 \otimes s_z$ anticommutes with $\mathcal{P}_t$ such that $\mathcal{P}^2 = -\mathcal{P}_t^2 = -1$. Contrastingly, the lattice of Fig. IV.2(b) has a trivial $\mathcal{I}_0 = 1_\tau \otimes 1_\sigma$, such that the simplification to Eq. (IV.15b) becomes valid, and the singlet/triplet separation of the previous paragraphs applies again.

We now combine the obtained information with the arguments of Ref. [21]. We begin with systems without SRS. If the system breaks TRS, the only AZ symmetry is $\mathcal{P}_t^2 = +1$ which corresponds to AZ class D. Depending on the inversion-parity of $\Delta_k$ in Eq. (IV.15a) we obtain $\mathcal{P}^2 = \pm \mathcal{P}_t^2 = \pm 1$. The positive sign ($\mathcal{I}$-even $\Delta_k$) leads to AZ+I class D while the negative sign ($\mathcal{I}$-odd $\Delta_k$) moves us to AZ+I class C. On the other hand, a system respecting TRS has additional

$$\mathcal{T} = i\sigma_y K$$

squaring to $-1$, and belongs to AZ class DIII. The corresponding AZ+I class for $\mathcal{I}$-even $\Delta_k$ remains DIII, while $\mathcal{I}$-odd $\Delta_k$ leads to AZ+I class CII. Note that such realizations of AZ+I classes D and DIII are only possible in multi-orbital SCs, because $\mathcal{I}$-even $\Delta_k$ in single-orbital case indicates a pure singlet state having the full SU(2) SRS, which contradicts the original assumption.

We further consider SCs with a U(1) SRS. As shown in Ref. [21], the Hamiltonian (IV.12b) now canonically decouples into two blocks, rendering the original description redundant. If we rotate the coordinates
Table IV.5: Overview of the sets of Pauli matrices used in this chapter. The last two entries are only relevant for Secs. IV.4 to IV.6 when developing TB models on a SrPtAs-like lattice. We use the words “orbital” and “sublattice” interchangeably if the orbitals reside at different lattice sites.

<table>
<thead>
<tr>
<th>symbol</th>
<th>corresponding two-level degree of freedom</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma$</td>
<td>spin ($\uparrow \leftrightarrow \downarrow$)</td>
</tr>
<tr>
<td>$s$</td>
<td>particle-hole ($p^{\uparrow} \leftrightarrow h^{\uparrow}$)</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>reduced particle-hole ($p^{\uparrow} \leftrightarrow h^{\downarrow}$)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>orbital [same colour interlayer (A $\leftrightarrow$ B) in Fig. IV.5]</td>
</tr>
<tr>
<td>$r$</td>
<td>orbital (intralayer red $\leftrightarrow$ blue in Fig. IV.5)</td>
</tr>
<tr>
<td>$\varrho$</td>
<td>orbital (interlayer red $\leftrightarrow$ blue in Fig. IV.5)</td>
</tr>
</tbody>
</table>

such that the conserved spin component is $\sigma_z$, then one of the blocks becomes

$$H_{1/2}(k) = \frac{1}{2} \begin{pmatrix} c_{k\uparrow}^\alpha & c_{-k\downarrow}^\alpha \end{pmatrix} H_{1/2}^{\alpha\beta}(k) \begin{pmatrix} c_{k\uparrow}^\beta \\ c_{-k\downarrow}^\beta \end{pmatrix}$$  \hspace{1cm} (IV.18a)

where $\alpha, \beta$ stand for the orbital degree of freedom, and

$$H_{1/2}^{\alpha\beta}(k) = \begin{pmatrix} \Xi_{k\uparrow\uparrow}^{\alpha\beta} & \Delta_{k\uparrow\downarrow}^{\alpha\beta} \\ -\Delta_{-k\uparrow\uparrow}^{\alpha\beta} & -\Xi_{-k\downarrow\downarrow}^{\beta\alpha} \end{pmatrix}$$ \hspace{1cm} (IV.18b)

is the reduced BdG Hamiltonian. Operator $\mathcal{P}_t$ of Eq. (IV.13) relates the two blocks, and in the absence of TRS the single block (IV.18b) contains none of the AZ symmetries (I.99). We thus end up in AZ class A which corresponds to the same AZ$+\mathcal{I}$ class. The additional presence of TRS manifests within a single block as chiral symmetry $C = \zeta_y$ where Pauli matrices $\zeta_i$ correspond to the particle-hole degree of freedom of Eqs. (IV.18). Consequently, such SCs correspond to AZ and AZ$+\mathcal{I}$ class AIII.

Finally, we tackle SCs with the complete SU(2) SRS. These are automatically of pure singlet character. In this case, the block (IV.18b) develops particle-hole symmetry

$$\mathcal{P}_s = i\zeta_y \mathcal{K}$$  \hspace{1cm} (IV.19)
squaring to $-\mathbb{1}$. In the absence of TRS, this corresponds to AZ class C. Depending on the inversion-parity of $\Delta_k$ in Eq. (IV.15a), the inversion operator induced into the block (IV.18b) from $I_{BdG}$ is

$$I_{1/2} = I_\tau \oplus (\pm I_\tau) \in \{ I_\tau \otimes 1, I_\tau \otimes \zeta, I_\tau \otimes \zeta_z \}.$$  \hspace{1cm} (IV.20)

The “+” sign of Eq. (IV.20) corresponds to $I$-even $\Delta_k$, when $P_s$ and $I_{1/2}$ commute and the AZ+$I$ class remains C. This is the case of single-orbital singlet SCs, and of multi-orbital SC in which the three $d_{ij}^{\ell z}$ terms in Eq. (IV.16a) vanish. On the other hand, the “−” sign relates to the $I$-odd case $\Delta_k$ with $\Psi^2 = -P_s^2 = +1$ such that the AZ+$I$ class switches to D. This situation corresponds to a very fine-tuned multi-orbital case when the nine $d_{ij}^k$ of Eq. (IV.16b) vanish, and as such may be relevant only to certain artificially engineered systems. Ultimately, if the singlet SC preserves TRS, the block (IV.18b) develops $T_s = K$ squaring to $+\mathbb{1}$ leading to AZ class CI. Then the $I$-even $\Delta_k$ case keeps AZ+$I$ class CI, while the $I$-odd $\Delta_k$ case moves us to AZ+$I$ class BDI.

**IV.3 \( \mathbb{Z}_2 \oplus 2\mathbb{Z} \) nodal surfaces in class D**

In the remainder of the manuscript we individually discuss each of the four AZ+$I$ symmetry classes supporting doubly charged nodes in $D = 3$. As shown in Tabs. IV.3 and IV.4, the minimal half-filled model capable of supporting doubly charged nodes always contains four bands, hence we begin each section by introducing the most general four-band Hamiltonian compatible with the AZ+$I$ symmetries (IV.3). We continue with an explanation of the two topological charges, and conclude by constructing a concrete TB model on a SrPtAs-like lattice.

The present section focuses on AZ+$I$ class D. According to Tabs. IV.1 and IV.2, its zero-energy nodes take the form of surfaces characterized by a pair of topological charges

$$\varepsilon_D^{(3)} \in \pi_0(\mathbb{I}_D) \oplus \pi_2(\mathbb{I}_D) = \mathbb{Z}_2 \oplus 2\mathbb{Z}. \hspace{1cm} (IV.21)$$

We show that the $\pi_0$-charge can be understood as the sign of the Pfaffian of the Hamiltonian and the $\pi_2$-charge as the (first) Chern number, as is indicated in the rightmost block of Tab. IV.1. In the last subsection we discuss how such nodal surfaces naturally appear in TRS breaking multi-orbital superconductors [39].
IV.3.1 General 4-band Hamiltonian

The six $4 \times 4$ matrices compatible with $\mathcal{P} = \mathcal{K}$ which appear in Tab. IV.2 can be arranged into a pair of vectors

\begin{align*}
v &= (\sigma_x \otimes \tau_y, \sigma_y \otimes 1, \sigma_z \otimes \tau_y) \\
w &= (\sigma_y \otimes \tau_x, 1 \otimes \tau_y, \sigma_z \otimes \tau_y)
\end{align*}

such that $\{v_i, v_j\} = \{w_i, w_j\} = 2\delta_{ij}$ and $[v_i, w_j] = 0$. The most general four-band Hamiltonian of this class is

$$H(k) = a(k) \cdot v + b(k) \cdot w$$

where $a(k)$ and $b(k)$ are real-valued vector functions. The spectrum of (IV.23a) is easily found to be

$$\epsilon(k) = \pm \|a(k)\| \pm \|b(k)\|.$$  

The gap closes whenever $\|a(k)\| = \|b(k)\|$. This is a single condition, manifesting the codimension $\delta_D = 1$ listed in Tab. IV.2.

Although the $4 \times 4$ matrices $v_i$ (as well as $w_i$) are anticommuting, they do not form a Dirac basis because their algebra is closed under commutator, $[v_i, v_j] = 2i\epsilon_{ijk}v_k$. Following Ref. [176], we refer to such a it as a double Weyl basis. An important characteristic is that a double Weyl Hamiltonian $H_{d,W.} \propto k \cdot v$ describes two superimposed Weyl points of the same chirality (which can be separated in energy using terms $\propto w_i$). This is to be contrasted with a Dirac Hamiltonian $H_D. \propto k \cdot \Gamma$ which creates two superimposed Weyl points of opposite chirality (which can be separated in energy using a term $\propto \Gamma_{45}$). Consequently, a double Weyl point is a source of two Berry phase quanta, while the Chern number of a Dirac point vanishes.

IV.3.2 Interpretation of $\pi_0(\Gamma M_D) = \mathbb{Z}_2$

The six matrices (IV.22) are antisymmetric and imaginary. The hermiticity of $H(k)$ along with $\mathcal{P} = \mathcal{K}$ entail

$$H^\top(k) = H^*(k) = \mathcal{P}H(k)\mathcal{P}^{-1} = -H(k).$$

As a consequence, $iH(k)$ is a skew-symmetric and even-dimensional matrix with real entries. One can therefore construct a non-vanishing
Chapter IV. Nodes from spatial inversion

Pfaffian \( \text{Pf}[i\mathcal{H}(k)] \) which is a real-valued function of \( k \). Specifically, for (IV.23a) one finds

\[
\text{Pf}[i\mathcal{H}(k)] = b^2(k) - a^2(k) \tag{IV.25}
\]

which changes sign at the nodal surface. This observation generalizes to an arbitrary class D model: The presence of a node at \( k_0 \) is revealed by a pair of zero energy states. This enforces \( \text{det}[\mathcal{H}(k)] = \prod a \varepsilon^a(k) \) to vanish at \( k_0 \) and to depend quadratically on \( (k - k_0) \). By the identity

\[
\text{det}[\mathcal{H}(k)] = \text{Pf}[\mathcal{H}(k)]^2 = (-1)^n \text{Pf}[i\mathcal{H}(k)]^2, \tag{IV.26}
\]

the Pfaffian also vanishes at \( k_0 \), but it varies linearly with \( (k - k_0) \). This implies that \( \text{Pf}[i\mathcal{H}(k)] \) has a different sign at two points \( \{k_1, k_2\} \cong S^0 \) located on the opposite sides of the nodal surface. We can therefore formulate the zeroth homotopy charge as

\[
\mathcal{c}_D(S^0) = \text{sign} \left\{ \prod_{k \in S^0} \text{Pf}[i\mathcal{H}(k)] \right\} \in \{+1, -1\}. \tag{IV.27}
\]

This charge has very recently also been identified in Ref. [39].

**IV.3.3 Interpretation of \( \pi_2(\mathbb{M}_D) = 2\mathbb{Z} \)**

A natural candidate for an integer topological charge on a 2-sphere is the (first) Chern number. We show below that this is indeed the case here, and we explain why the particle-hole symmetry enforces it to be even.

We explained in Subsec. I.1.4 that in \( D = 3 \) there is a canonical isomorphism which allows us to formulate Berry curvature as an (axial) vector \( \Omega \), defined using Eqs. (I.54) and (I.22). The Chern number is then defined as [73]

\[
\mathcal{c}_D(S^2) = \frac{i}{2\pi} \oint_{S^2} d^2k \cdot \text{tr} \Omega(k) \in \mathbb{Z} \tag{IV.28}
\]

We also discussed in that section, that in the case of locally non-degenerate bands, \( \Omega \) separates into the contributions of individual bands,

\[
\text{tr} \Omega(k) = \sum_{a=1}^{n} \langle \nabla_k u^a(k) | \times | \nabla_k u^a(k) \rangle = \sum_{a=1}^{n} \Omega^a(k) \tag{IV.29}
\]

where \( a \) labels the occupied bands. One can similarly determine the Berry curvature and the Chern number of the unoccupied bands.
**Figure IV.4: Double Weyl vs. Dirac Hamiltonian.** (a) Spectrum of Hamiltonian (IV.33) consists of two Weyl points (black dots) of the same chirality with energy offset $\pm m$, crossing on a nodal sphere with radius $|m|$. The two species of lines indicate Berry curvatures of opposite signs, which integrate to opposite Chern numbers $\pm 1$ on a closed surface surrounding $k = 0$. The total Chern number over the occupied states is 0 inside, while it equals $\pm 2$ outside the nodal sphere, meaning that the nodal sphere is a source of a pair of Berry phase quanta. (b) Spectrum of Dirac Hamiltonian with $m \Gamma_{45}$ perturbation creates identical spectrum, but with different Berry curvature. The total Chern number vanishes both inside and outside of the spherical crossing, and the nodal sphere is not topologically protected.

The Berry curvature of an occupied band $|u^a(k)\rangle$ and the Berry curvature of a particle-hole related unoccupied band $|\tilde{u}^a(k)\rangle = \mathcal{K}|u^a(k)\rangle$ differ only by the overall sign. To see this, recall from Eq. (I.40) that the Berry connection $\mathcal{A}(k)$ is skew-Hermitian,

$$0 = \nabla_k \delta^{ab} = \nabla_k \langle u^a(k)|u^b(k)\rangle = \mathcal{A}^{ab} + (\mathcal{A}^{ba})^*, \quad \text{(IV.30)}$$

such that its diagonal terms are imaginary. Taking the curl in Eq. (I.54) preserves this property, hence the single-band Berry curvatures that appear in Eq. (IV.29) are imaginary, too. It follows that

$$\tilde{\Omega}^a(k) = \langle \nabla_k \tilde{u}^a(k) | \times | \nabla_k \tilde{u}^a(k) \rangle = \left[ \langle \nabla_k u^a(k) | \times | \nabla_k u^a(k) \rangle \right]^* = -\Omega^a(k) \quad \text{(IV.31)}$$

as we wanted to show.

Relation (IV.31) readily explains why the Chern number (IV.28) takes only even values: Consider a nodal surface $S^2_{\text{node}}$, together with a surface $S^2_{\text{in}}$ inside of it and a surface $S^2_{\text{out}}$ enclosing it. Since $S^2_{\text{in}}$ can be trivially shrunk to a point without encountering a node, $\varepsilon_D(S^2_{\text{in}}) = 0$. The node $S^2_{\text{node}}$ is created by switching one occupied and one empty band, which by Eq. (IV.31) carry opposite Berry curvatures, which integrate to opposite Chern numbers $c$ and $-c$. Consequently, the charge
\[ c_D(S^2_{out}) = c_D(S^2_{in}) + c - (-c) = 2c \]
is indeed even. These considerations give the nodal surface a peculiar interpretation as an inflated double Weyl point \cite{39}. The reason is that \( S^2_{node} \) is a source of an even number of Berry phase quanta, reminiscent of double Weyl points. This is consistent with our discussion of the double Weyl basis in Subsec. IV.3.1. Work \cite{39} also dubbed these objects as Bogolyubov Fermi surfaces, which is in line with our findings in Sec. IV.2 that AZ+I class D is relevant for certain superconducting phases.

We demonstrate these observations by setting \( a(k) = (0, m, 0) \) and \( b(k) = k \) in the general 4-band model (IV.23a). This produces a nodal sphere with radius \( |m| \). We further rotate the basis as \( \sigma_x \mapsto \sigma_y \mapsto \sigma_z \mapsto \sigma_x \) using \( U_\sigma \), where

\[ U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}. \]  

This is accompanied by a transformation \( \mathcal{P} = \mathcal{K} \mapsto \sigma_z \mathcal{K}. \) Then, the Hamiltonian decouples into two blocks, \( \mathcal{H}(k) = \mathcal{H}_1(k) \oplus \mathcal{H}_2(k) \), with

\[ \mathcal{H}_1(k) = +m \tau_x + k_x \tau_x + k_y \tau_y + k_z \tau_z \]  
\[ \mathcal{H}_2(k) = -m \tau_x - k_x \tau_x + k_y \tau_y - k_z \tau_z. \]

Clearly, this is a pair of Weyl points of the same chirality with energy offset \( \pm m \), as illustrated in Fig. IV.4(a). We observe that indeed \( c_D(S^2_{in}) = 0 \) and \( |c_D(S^2_{out})| = 2 \). We remark for completeness, that Ref. \cite{39} also presents torical nodal surfaces that are characterized with a non-trivial \( c_D(S^0) \) but trivial \( c_D(S^2) \), which are interpreted as inflated nodal lines.

### IV.3.4 Example class \( D \) model

We provide the reader with a simple way of testing the presented ideas by introducing a tight-binding (TB) model on a SrPtAs-like lattice adapted from Ref. \cite{182}. This work observed the appearance of nodal surfaces in a multi-orbital \( d \pm id \) SC phase \cite{180} with an admixed \( p \)-wave component. These nodal surfaces correspond precisely to the doubly charged nodes of AZ+I class D.

As illustrated in Fig. IV.5(a), the centrosymmetric structure of SrPtAs consists of graphene-like layers with platinum (Pt) and arsenic (As) atoms on the two sublattices, and of intercalated strontium (Sr) atoms. Our goal here is not to provide a realistic description of SrPtAs, but to demonstrate the possible appearance of the doubly charged nodal
surfaces in a superconducting phase on this lattice for the properly set values of the TB parameters.

We assume that $s$-like orbitals located at the Pt sites enter the TB model. The primitive Bravais vectors are

$$
R_{1,2} = \frac{3a}{2} \left( 1, \pm \frac{1}{\sqrt{3}}, 0 \right) \quad \text{and} \quad R_3 = (0,0,2c)
$$

and the positions of the two orbitals corresponding to a given Bravais vectors are

$$
r_A = (0,0,0) \quad \text{and} \quad r_B = \left( \frac{a}{2}, -\frac{a\sqrt{3}}{2}, c \right).
$$

To write the Hamiltonian compactly, we use vectors

$$
t_{1,2} = a \left( -\frac{1}{2}, \mp \frac{\sqrt{3}}{2}, 0 \right) \quad \text{and} \quad t_3 = a (1,0,0)
$$

that are indicated in Fig. IV.5(b), and their differences $T_i = \frac{1}{2} \sum_{jk} \epsilon_{ijk} (t_k - t_j)$.

We further define complex numbers $\omega_n = e^{i2\pi n/3}$, and functionals

$$
S_f^{p,v}(k) = \sum_{n=1}^{3} (\omega_n)^p f(k \cdot v_n)
$$
where the subscript $f$ is a function on $\mathbb{R}$, the first superscript $p \in \mathbb{Z}$, and the second superscript indicates a set of three vectors, $v = \{v_n\}_{n=1}^{3}$. We will specifically use the sets
\[ t = \{t_n\}_{n=1}^{3} \quad \text{and} \quad T = \{T_n\}_{n=1}^{3}. \] (IV.35)

The NN intra-layer hopping with amplitude $t_0/2$ and the intra-orbital hopping across two layers with amplitude $t'_z/2$ produce
\[ \mathcal{H}_1(k) = \left[ t_0 S_{\cos}(k) + t'_z \cos(2k_z c) \right] \mathbb{1}_\sigma \otimes \mathbb{1}_\tau, \] (IV.36a)
while the inter-layer hopping with amplitude $t_z/2$ gives
\[ \mathcal{H}_2(k) = t_z \cos(k_z c) \mathbb{1}_\sigma \otimes \left[ S_{\cos}^{0,t}(k) \tau_x + S_{\sin}^{0,t}(k) \tau_y \right]. \] (IV.36b)

We further include the intra-layer SOC term
\[ \mathcal{H}_3(k) = \alpha_{so} S_{\sin}^{0,T}(k) \sigma_z \otimes \tau_z. \] (IV.36c)
which reduces the SRS of $\mathcal{H}(k)$ down to $U(1)$. The meaning of Pauli matrices $\sigma_i$ and $\tau_i$ follows Tab. IV.5.

We set the parameters of TB model (IV.36) to
\[ t = 1, \quad t_z = -1, \quad t'_z = 1, \quad \alpha_{so} = -1 \quad \text{and} \quad \mu = -3.5 \] (IV.37)
where $\mu$ is the chemical potential. Then the Fermi surface consists of a pair of pockets centred on the corners of BZ as shown in Fig. IV.6(a). We further let the system develop a SC $d + id$ order parameter
\[ \Delta^d_k = \psi^0 S_{\cos}^{1,T}(k) (i\sigma_y) \otimes \mathbb{1}_\tau \] (IV.38a)
which is $I$-even.\(^2\) Order parameter (IV.38a) vanishes along the vertical edges of the BZ, meaning that nodal points are formed where these edges cross the Fermi pockets. This is compatible with the scheme in Fig. IV.3: The complexity of the order parameter breaks TRS, and the combined Eqs. (IV.36) and (IV.38a) preserve $U(1)$ SRS. This locates the system in AZ+$I$ class A, which according to Tab IV.2 in $D = 3$ indeed exhibits nodal points. In fact, because of the underlying spin degeneracy of the bands,\(^3\) these are precisely the previously discussed double Weyl points – not yet inflated!

\(^2\)More exactly, it belongs to the $E_{2g}$ representation of the $D_{6h}$ point group [182].
\(^3\)This is due to the block reduction (IV.18) of the BdG Hamiltonian.
IV.3. $Z_2 \oplus 2Z$ nodal surfaces in class D

Figure IV.6: Doubly charged nodal surfaces of $AZ+I$ class D. (a) Fermi surface of TB model (IV.36) with parameters (IV.37) consists of a pair of pockets centred on the corners of BZ. (b) The $d + id$ order parameter (IV.38a) creates double Weyl points where the vertical BZ edges cross the Fermi pockets. Admixing a $p$-wave order parameter (IV.38b) inflates them into tiny nodal surfaces. (c) Plot of sign $\text{Pf} [iH(k)]$ for a horizontal slice through the nodal surface at the indicated value of $k_z c$. (d) Flow of the Berry curvature across an ellipsoid described in the text, which encloses the nodal surface. Integration reveals that the nodal surface is a source of two Berry phase quanta.

However, the multi-orbital character of the SrPtAs lattice allows us to admix a $p$-wave order parameter [182]

$$\Delta_k^p = d^{-z} \sin(2k_z c) \left( \sigma_x - i \sigma_y \right) (i \sigma_y) \otimes \tau_z,$$  

which preserves the even parity\(^4\) of $\Delta_k$ and that does not vanish along the vertical BZ edges. Importantly, (IV.38b) breaks SRS altogether, such that the system is moved to $AZ+I$ class D, which can exhibit doubly charged nodal surfaces according to Tab. IV.1. To check this, we set

$$\psi^z = 0.2 \quad \text{and} \quad d^{-z} = 0.2$$  

and find tiny nodal surfaces at the expected positions, plotted in Fig. IV.6(b). Rotating the basis by $U_s^\dagger \otimes 1 \otimes U_t^\dagger$ with matrix $U$ from (IV.32) leads to $\Psi = K$, such that we can check the sign of $\text{Pf} [iH(k)]$ on a plane crossing

\(^4\)It also preserves the $E_{2g}$ representation of $D_{6h}$, meaning that it admixes naturally.
the nodal surface, plotted in Fig. IV.6(c). Finally, we calculate the Berry curvature over the occupied states on an ellipsoid with radii \(\frac{1}{10}, \frac{1}{a}, \frac{1}{c}\) centred on the nodal surface, which is plotted in Fig. IV.6(d). Numerical integration of (IV.28) reveals that indeed \(|c_D(S_{\text{out}})| = 2\).

**IV.4 \(\mathbb{Z}_2 \oplus \mathbb{Z}_2\) nodal surfaces in class BDI**

The AZ+\(\mathbb{I}\) class BDI is the only one that supports doubly charged nodes already in \(D = 2\), namely

\[
c^{(2,3)}_{\text{BDI}} \in \pi_0(\mathbb{M}_{\text{BDI}}) \oplus \pi_1(\mathbb{M}_{\text{BDI}}) = \mathbb{Z}_2 \oplus \mathbb{Z}_2. \tag{IV.40}
\]

Most of our discussion applies equally well to both cases, although all the explicit examples are provided for \(D = 3\). In the following subsections we first construct the most general 4-band Hamiltonian of this symmetry class and determine its spectrum. We show that the \(\pi_0\)-charge is again the Pfaffian invariant (IV.27), although an alternative determinant formulation becomes applicable too. On the other hand, the \(\pi_1\)-charge is new and corresponds to the winding of a closed path inside \(SO(n) \ni q(\mathbf{k})\). We develop a way to determine this charge by plotting the spectrum of \(\pi\) along the path. In the last subsection we develop a non-SC model on a lattice consisting of dimerized AAA-stacked graphene layers, which belongs to symmetry class BDI and that exhibits robust nodal surfaces.

**IV.4.1 General 4-band Hamiltonian**

We order the four basis matrices of Tab. IV.2 into a pair of two-component vectors

\[
\begin{align*}
\mathbf{v} &= (\sigma_x \otimes 1, -\sigma_y \otimes \tau_y) \tag{IV.41a} \\
\mathbf{w} &= (\sigma_x \otimes \tau_z, -\sigma_x \otimes \tau_x) \tag{IV.41b}
\end{align*}
\]

fulfilling \(\{v_i, v_j\} = \{w_i, w_j\} = 2\delta_{ij}\) and \([v_i, w_j] = 0\). We encode the general 4-band Hamiltonian using a pair of real-valued vector functions \(\mathbf{a} = (a_1, a_2), \mathbf{b} = (b_1, b_2)\) as

\[
\mathcal{H}(\mathbf{k}) = \mathbf{a}(\mathbf{k}) \cdot \mathbf{v} + \mathbf{b}(\mathbf{k}) \cdot \mathbf{w}. \tag{IV.42a}
\]
Diagonalizing the Hamiltonian reveals the spectrum,

\[ \varepsilon(k) = \pm \|a(k)\| \pm \|b(k)\|. \]  

(IV.42b)

The gap closes whenever \( \|a(k)\| = \|b(k)\| \). Since this is a single scalar constraint, we deduce the codimension \( c_{\text{BDI}} = 1 \), thus confirming again that AZ+I class BDI in \( D = 3 \) supports nodal surfaces.

**IV.4.2 Interpretation of** \( \pi_0(M_{\text{BDI}}) = \mathbb{Z}_2 \)

The presence of \( C = \sigma_z \) guarantees a block-off-diagonal form of \( H(k) \), while \( \mathcal{T} = \mathcal{K} \) makes it real. Consequently,

\[ H(k) = \begin{pmatrix} 0 & \hat{h}(k) \\ \hat{h}^\top(k) & 0 \end{pmatrix} \quad \text{with } \hat{h}(k) \in \text{GL}(n, \mathbb{R}). \]  

(IV.43)

For the \( n = 2 \) model (IV.42a) explicitly

\[ \hat{h}(k) = a_1(k)1_\tau - b_2(k)\tau_x + a_2(k)i\tau_y + b_1(k)\tau_z. \]  

(IV.44)

Since \( \mathcal{P} \) fixes nodes to zero energy, their presence is exposed by

\[ 0 = \det H(k) = i^{2n} \left| \det \hat{h}(k) \right|^2. \]  

(IV.45)

Nodal surfaces separate regions with opposite sign of \( \det \hat{h}(k) \). This implies that for \( S^0 = \{k_1, k_2\} \) there is

\[ c_{\text{BDI}}(S^0) = \text{sign} \left[ \prod_{k \in S^0} \det \hat{h}(k) \right] \in \{+1, -1\}. \]  

(IV.46)

In fact, this is just the Pfaffian invariant (IV.27) in disguise. Rotating the basis by \( U_\sigma \) leads to \( \mathcal{T} = \sigma_x \mathcal{K}, \mathcal{P} = \mathcal{K}\) and \( C = \sigma_x \), such that the transformed Hamiltonian \( U_\sigma H(k) U_\sigma^\dagger \equiv \tilde{H}(k) \) is antisymmetric and has a well-defined Pfaffian. It follows that

\[ \left| \det \hat{h}(k) \right|^2 = \text{Pf}[i\tilde{H}(k)]^2 \]  

(IV.47)

such that formula (IV.27) is also applicable for calculating \( c_{\text{BDI}}(S^0) \).
### IV.4.3 Interpretation of $\pi_1(\mathbb{M}_{BDI}) = \mathbb{Z}_2$

We first explain why $\mathbb{M}_{BDI} = \mathbb{O}(n)$. Note that $\mathcal{C} = \sigma_z$ relates pairs of states with energies $\pm \varepsilon^a$,

$$
|u^{a,+}(k)\rangle = \left(\begin{array}{c} |u_k^{a,1}\rangle \\ |u_k^{a,2}\rangle \end{array}\right) \quad \text{with} \quad \varepsilon^a(k) > 0 \quad (IV.48a)
$$

$$
|u^{a,-}(k)\rangle = \sigma_z |u^{a,+}(k)\rangle \quad \text{with} \quad -\varepsilon^a(k) < 0 \quad (IV.48b)
$$

where $(a,+)$ and $(a,-)$ label a pair of bands. It follows from the orthogonality of states (IV.48) that\(^5\)

$$
\langle u_k^{a,1} | u_k^{b,1}\rangle = \langle u_k^{a,2} | u_k^{b,2}\rangle = \frac{1}{2} \delta^{ab} \quad (IV.50a)
$$

$$
\sum_a |u_k^{a,1}\rangle \langle u_k^{a,1}| = \sum_a |u_k^{a,2}\rangle \langle u_k^{a,2}| = \frac{1}{2} \mathbb{1}. \quad (IV.50b)
$$

Furthermore, all the eigenstates are real because of $\mathcal{F} = \mathcal{K}$. It follows that the flat-band Hamiltonian $\mathcal{Q}(k)$ acquires the block-off-diagonal form (IV.6) with

$$
q(k) = 2 \sum_a |u_k^{a,1}(k)\rangle \langle u_k^{a,2}(k)| \in \mathbb{O}(n). \quad (IV.51)
$$

Every $S^1 \subset \text{BZ}$ with a gapped spectrum therefore traces a closed path image in $\mathbb{O}(n)$. The charge $c_{BDI}(S^1)$ corresponds to the homotopy equivalence class of this image.

---

\(^5\)We use this occasion to fill in a gap left from Subsec. III.1.4. We want to prove relation (III.10b) between the Berry phase and the winding number in systems with CHS. First, we comment on the nature of gauge transformations (I.15) in chiral-symmetric systems. Obviously, such a gauge transformation multiplies the matrix $U^1(k)$ of the upper components and the matrix $U^2(k)$ of the lower components of states (IV.48b) with the same unitary matrix $\mathcal{X}(k) \in \mathbb{U}(n)$. Further, note that we can write $q(k + dk) = q(k) [\mathbb{1} + dk \cdot \mathbf{s}(k)]$. Since (in general) $q(k) \in \mathbb{U}(n)$, the small correction can be expressed as

$$
1 + dk \cdot \mathbf{s}(k) = q^\dagger(k) q(k + dk) = 4 \sum_{a,b} |u_k^{a,2}(k)\rangle \langle u_k^{a,1}(k)| u_k^{b,1}(k+dk)\rangle \langle u_k^{b,2}(k+dk)|
$$

\((IV.50a)\)

$$
= 4 \sum_{a,b} |u_k^{a,2}(k)\rangle \left( \frac{1}{2} \delta^{ab} + dk \cdot \langle u_k^{a,1}(k)| \nabla_k u_k^{b,1}(k)\rangle \right) \left( \langle u_k^{b,2}(k)| + dk \cdot \langle \nabla_k u_k^{b,2}(k)| \right)
$$

$$
= 2 \sum_a |u_k^{a,2}(k)\rangle \langle u_k^{a,2}(k)| + dk \cdot \left( 2 \sum_a |u_k^{a,2}(k)\rangle \langle \nabla_k u_k^{a,2}(k)| \right) \quad (IV.49a)
$$

\(\mathbb{1}\) by Eq. (IV.50b)

$$
+ 4 \sum_{a,b} |u_k^{a,2}(k)\rangle \langle u_k^{a,1}(k)| \nabla_k u_k^{b,1}(k)\rangle \langle u_k^{b,2}(k)|
$$
The space $O(n)$ consists of two separate components characterized by $\det q(k) = \pm 1$. This is just the $\pi_0$-charge (IV.46), i.e. the sign of $\det h(k) = \det q(k)$ is fixed unless one crosses a nodal surface. This implies that the image of a gapped $S^1 \subset BZ$ lies entirely within one of the two components. If $\det|q(k)| = -1$, we replace $q(k)$ by its composition with a mirror symmetry with respect to the $n^{th}$ coordinate, while we keep it unchanged otherwise. Then the analysed $q(k) \in SO(n)$, and we formally write down the $\pi_1$-charge as the homotopy equivalence class

$$c_{\text{BDI}}(S^1) = \left[q : S^1 \to SO(n)\right].$$

within the special orthogonal group. In the subsequent sections we will encounter a similar charge appearing also in the case of nodal lines of $AZ+\mathcal{L}$ classes CI and AI.

Determining the homotopy class (IV.52) can be achieved by tracking the eigenvalues of $q(k)$. For $n$ even, the eigenvalues come in complex conjugate pairs $e^{\pm i\alpha}$, while for $n$ odd there is an additional eigenstate

Using identity (I.29), we obtain

$$\det \left[1 + dk \cdot s(k)\right] = 1 + dk \cdot \left(2 \sum_a \langle \nabla_k u^{a,2}(k) | u^{a,2}(k) \rangle + 4 \sum_{a,b} \langle u^{b,2}(k) | u^{a,2}(k) \rangle \langle u^{a,1}(k) | \nabla_k u^{b,1}(k) \rangle \right)$$

$$= 1 + 2dk \cdot \sum_a \left(\langle u^{a,1}(k) | \nabla_k u^{a,1}(k) \rangle - \langle u^{a,2}(k) | \nabla_k u^{a,2}(k) \rangle \right).$$

(IV.49b)

It follows that

$$\frac{1}{2} \nabla_k \log \det q(k) = \sum_a \left(\langle u^{a,1}(k) | \nabla_k u^{a,1}(k) \rangle - \langle u^{a,2}(k) | \nabla_k u^{a,2}(k) \rangle \right).$$

(IV.49c)

This is a gauge-invariant quantity, because the two non-covariant terms $\lambda^\dagger \nabla_k \lambda$ and $-\lambda^\dagger \nabla_k \lambda$ [cf. Eq. (I.26)] cancel each other. On the other hand, the trace of the Berry connection over the occupied states is

$$\text{tr} \mathcal{A}(k) = \sum_a \langle u^{a,-}(k) | \nabla_k u^{a,-}(k) \rangle$$

$$= \sum_a \left(\langle u^{a,1}(k) | \nabla_k u^{a,1}(k) \rangle + \langle u^{a,2}(k) | \nabla_k u^{a,2}(k) \rangle \right).$$

(IV.49d)

This is obviously different from expression (IV.49c), but it is not gauge invariant. Finally, we show that there is a gauge in which expressions (IV.49c) and (IV.49d) coincide. This is easy, we can simply rotate with $\lambda(k) = [\tilde{U}^2(k)]^\dagger$, such that the rotated $\tilde{U}^2(k) = 1$ has zero derivatives in both of the equations (IV.49c) and (IV.49d). Since there is a gauge in which the two expressions coincide, their integrals (I.19) and (III.10b) have to coincide, too.
(axis of rotation) with eigenvalue 1. The charge $c_{\text{BDI}}(S^1)$ may be non-trivial if the eigenvalue phases $\alpha_i$ contain a non-trivial winding along $S^1$. More specifically, one has to count the number of eigenvalue crossings at $\alpha = \pm \pi$. This number is a robust $\pi_1[SO(2)] = \mathbb{Z}$ quantity for $n = 2$, while for $n \geq 3$ only the parity $\pi_1[SO(n)] = \mathbb{Z}_2$ is conserved since then a pair of $\pm \pi$ crossings is allowed to annihilate. For $n = 1$ there is just the static unit eigenvalue and the topological charge $\pi_1[SO(1)] = 0$ is absent. These observations are in agreement with the exceptional entries in Tab. IV.3.

We demonstrate this procedure on model (IV.42a). The off-diagonal block $q \in SO(2)$ can be shown to be

$$q = \frac{1}{||a||} \begin{pmatrix} a_1 & a_2 \\ -a_2 & a_1 \end{pmatrix} \quad \text{or} \quad \frac{1}{||b||} \begin{pmatrix} b_1 & -b_2 \\ b_2 & b_1 \end{pmatrix}$$

(IV.53)

where the first expression applies if $||a|| > ||b||$, and the second one otherwise. Let us be more specific by setting $a(k) = (k_x, k_y)$ and $b(k) = (m, 0)$. Then the spectrum $\epsilon(k) = \pm m \pm \sqrt{k_x^2 + k_y^2}$ exhibits a zero-energy nodal cylinder at $k_x^2 + k_y^2 = m^2$, as well as a pair of nodal lines with energies $\pm m$ coexisting at $k_x = 0 = k_y$. These nodal lines tie the pair of occupied (and the pair of unoccupied) bands in a way that makes the nodal cylinder robust: One can at best shrink the cylinder to a line by setting $m = 0$, but it reappears for both $m > 0$ and $m < 0$.

To check the topological charge of the nodal cylinder exhibited by this simple model, we consider a circular path

$$S^1: k(\phi) = (k \cos \phi, k \sin \phi, 0) \quad \text{with} \quad \phi \in [0, 2\pi].$$

(IV.54)

We find

$$q(\phi) = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(IV.55)

where the first expression applies for $k > m$ (i.e. when $S^1$ encloses the nodal cylinder), and the second one otherwise. We observe that the invariant (IV.52) is trivial inside and non-trivial outside the nodal surface.

We remark that invariant (IV.52) does not correspond to the Berry phase (I.19). Although the nodal lines at energies $\pm m$ of the considered model both carry Berry $\pi$-phase, their pairwise appearance (imposed by $\mathcal{P}$) leads to net Berry $2\pi$-phase both outside and inside of the nodal cylinder. This doubling is similar to the presence of an even Chern number in AZ+I class D. The difference here is that Berry phases $2\pi$ and 0 on
non-contractible loops are indistinguishable [cf. Eq. (I.30)] and therefore both trivial.

### IV.4.4 Example class BDI model

As an example realization of the doubly charged nodal surfaces of AZ+I class BDI, we consider AAA-stacked\(^6\) graphene layers, obtained by identifying the Pt and As sites in Fig. IV.5. The layers are further assumed dimerized into nearby pairs at distance \(c\), the pairs being separated by larger gaps \(rc\) with \(r > 1\). Importantly, we require the presence of a sub-lattice realization of \(C\) which is usually only approximately present in realistic systems.

Adhering to the Pauli matrix notation of Tab. IV.5, we consider intralayer NN hoppings

\[
\mathcal{H}_1(k) = t_1 1_{q} \otimes \left[ S_{\cos}(k) r_x - S_{\sin}(k) r_y \right] \quad \text{(IV.56a)}
\]

and vertical hoppings of different amplitude within and between the dimerized layers

\[
\mathcal{H}_2(k) = \left( t_2 e^{ik_z c} + t_3 e^{-ik_z rc} \right) q_{\pm} \otimes 1_r + \text{h.c.} \quad \text{(IV.56b)}
\]

where \(q_{\pm} = \frac{1}{2}(q_x \pm i q_y)\), and h.c. denotes the Hermitian conjugation. The spatial inversion of the system \(I = q_x \otimes r_x\) commutes with the sub-lattice symmetry \(C = q_z \otimes r_z\), making this an \(I\)-even SLS model. Since the Hamiltonian respects TRS and does not contain SOC, the scheme of Fig. IV.3 locates us in AZ+I class BDI.

To be specific, we consider parameter values

\[
t_1 = 1, \quad t_2 = 0.5, \quad t_3 = 0.1 \quad \text{and} \quad r = 2 \quad \text{(IV.57)}
\]

which create a pair of nodal cylinders centred on the vertical BZ edges, see Fig. IV.7(a). Rotating the basis by

\[
V = \frac{1}{\sqrt{2}} \left[ 1_q \otimes \left( \begin{array}{cc} 1 & 0 \\ i & 0 \end{array} \right) \otimes 1_r + q_x \otimes \left( \begin{array}{cc} 0 & 1 \\ 0 & -i \end{array} \right) \otimes 1_r \right] \quad \text{(IV.58)}
\]

\(^6\)Such an allotrope of graphite does not exist. The most abundant graphite allotrope has stacking ABA (hexagonal), and the ABC (rhombohedral) form is also stable, although less common. We mentioned both allotropes in Subsec. III.1.3 as examples of spinless nodal line semimetals.
Figure IV.7: Doubly charged nodal surfaces of AZ+ class BDI. (a) Fermi surface of model (IV.56) with parameters (IV.57) consists of a pair of nodal cylinders centred on the vertical BZ edges. (b,c) Evolution of the $q(k) \in \text{SO}(2)$ eigenvalues along a path encircling the nodal surface (green) and a path inside of it (red) indicate a non-trivial $\pi_1$-charge (IV.52). (d,e) Plot of $\text{sign det}[q(k)]$ for horizontal planes at the indicated values of $k_z$ demonstrate the non-trivial value of $\pi_0$-charge (IV.46).

leads to $\mathcal{C} = e_z \otimes 1_r$ and $\mathcal{Z} = \mathcal{K}$, as has been required for the calculation of the topological charges. In Figs. IV.7(b,c) we check the $q(k)$ eigenvalue winding (IV.52) along a path that encloses (green) and a path that is enclosed by (red) the nodal cylinder. In Fig. IV.7(d) we plot the sign of $\text{det}[q(k)]$ within the horizontal high-symmetry planes of the BZ. These two calculations confirm that both charges (IV.46) and (IV.52) of the nodal cylinders are non-trivial.

IV.5 $\mathbb{Z} \oplus \mathbb{Z}_2$ nodal lines in class CI

The AZ+ class CI in $D = 3$ exhibits nodal lines characterized by a pair of topological charges

$$\mathfrak{c}^{(3)}_{\text{CI}} \in \pi_1(M_{\text{CI}}) \oplus \pi_2(M_{\text{CI}}) = \mathbb{Z} \oplus \mathbb{Z}_2.$$ (IV.59)

According to Tab. IV.3, the minimal model supporting a non-trivial value of the higher charge contains four bands. In the following subsections, we first introduce the general 4-band Hamiltonian belonging to this symmetry class and determine its spectrum. We show that the $\pi_1$-charge cor-
responds to the winding of the determinant of \( q(k) \) – the off-diagonal block of the flat-band Hamiltonian \( Q(k) \). We further show that the \( \pi_2 \)-charge corresponds to the homotopy equivalence class inside SO\((n)\) just like for the \( \pi_1 \)-charge of the AZ+I class BDI. The difference is that the role of the Hamiltonian block \( q(k) \) is replaced by Wilson loop operators \( \mathcal{W}(S^1) \). In the last subsection we show how such doubly charged nodal lines may appear in TRS preserving singlet SC phase of nodal line metals, provided that the gap function changes sign along the Fermi surface. A viable route to realize such a phase experimentally might be through the proximity effect.

### IV.5.1 General 4-band Hamiltonian

We order the six symmetry-compatible basis matrices of Tab. IV.2 into a pair of three-component vectors

\[
\begin{align*}
\mathbf{v} &= (\sigma_z \otimes \tau_z, -\sigma_z \otimes \tau_x, \sigma_x \otimes 1) \\
\mathbf{w} &= (-\sigma_x \otimes \tau_z, \sigma_x \otimes \tau_x, \sigma_z \otimes 1)
\end{align*}
\]

such that \( \{v_i, v_j\} = \{w_i, w_j\} = 2\delta_{ij} \) and \( [v_i, w_j] = -i\delta_{ij} \sigma_y \otimes 1_\tau \). A general 4-band Hamiltonian is expressed using two real-valued vector functions \( a(k) \) and \( b(k) \) as

\[
\mathcal{H}(k) = a(k) \cdot v + b(k) \cdot w.
\]

and has spectrum

\[
\varepsilon(k) = \pm \sqrt{a^2 + b^2} \pm 2\|a \times b\|.
\]

The gap closes whenever simultaneously \( \|a(k)\| = \|b(k)\| \) and \( a(k) \cdot b(k) = 0 \). This is a pair of scalar constraints, compatible with \( \delta_{\text{CI}} = 2 \) that has been determined independently in Tab. IV.2. This means that the nodal objects in \( D = 3 \) are one-dimensional lines.

### IV.5.2 Interpretation of \( \pi_1(M_{\text{CI}}) = \mathbb{Z} \)

The presence of \( C \) implies a natural interpretation of the \( \mathbb{Z} \)-valued \( \pi_1 \)-charge as the usual winding number of Eq. (III.10a), with \( I \) not playing a role. Rotating the basis of Tab. IV.2 by \( U_{\sigma} \) of Eq. (IV.32) leads to the canonical form \( C \propto \sigma_z \), when the off-diagonal block \( q(k) \) of the flat-band
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Hamiltonian (IV.5b) acquires an integer winding

$$c_{CI}(S^1) = \omega(S^1) = \frac{i}{2\pi} \oint_{S^1} dk \cdot \text{tr} \left[q^\dagger(k) \nabla_k q(k)\right] \in \mathbb{Z}. \quad (IV.62)$$

Formula (IV.62) remains valid if we replace $q(k)$ by the off-diagonal block of the rotated $H(k)$, as we do in Eq. (III.10a).

### IV.5.3 Interpretation of $\pi_2(\mathbb{M}_{CI}) = \mathbb{Z}_2$

The $\pi_2$-charge of AZ+$I$ class CI can be understood in the way presented in the supplemental material to Ref. [38]. Here we apply a slight modification to that procedure which replaces the gauge-dependent Wilson operators on open-ended paths by gauge-invariant ones on closed loops. The invariant is also related to the $\pi_1$-charge of AZ+$I$ class BDI.

To determine the charge on a gapped $S^2$, we proceed as follows: We pick two arbitrary (but different) points $N,S \in S^2$ and consider a set of continuously varying closed paths $S^1(\theta) \subset S^2$ with $\theta \in [0, \pi]$ such that:

1. $S^1(0) = N$ and $S^1(\pi) = S$ are single points,
2. for $0 < \theta < \pi : S^1(\theta)$ are homeomorphic to a circle (not to a point),
3. for $\theta_1 \neq \theta_2 : S^1(\theta_1) \cap S^1(\theta_2) = \emptyset$.

One can visualize loops $S^1(\theta)$ as the parallels on a globe with $N,S$ the geographic poles, although any other choice is equally good. The union $\cup_\theta S^1(\theta) = S^2$ reproduces the original sphere.

We further consider the Wilson operators [48, 70, 183] as we defined them in Eqs. (I.12) and (I.14). Wilson operator $\mathcal{W}(\gamma)$ describes the adiabatic evolution of the occupied states along $\gamma$, and as such has to be unitary, $\mathcal{W}^\dagger \mathcal{W} = 1$. However, the AZ+$I$ class CI respects $\mathcal{T} = \mathcal{K}$ which allows us to find a real set of eigenvectors. It follows from the definition (I.12) that $\mathcal{W}(S^1)$ in this symmetry classes is real unitary, i.e. an element of $O(n)$.

To obtain the $\pi_2$-charge, we determine $\mathcal{W}[S^1(\theta)] \equiv \mathcal{W}(\theta)$ which depends continuously on $\theta$. Since $\mathcal{W}(0) = \mathcal{W}(\pi) = 1$, the Wilson loop $\mathcal{W}(\theta)$ traces a closed path in $SO(n)$, and $c_{CI}(S^2)$ is expressed as the homotopy equivalence class of loops in the special orthogonal group,

$$c_{CI}(S^2) = [\mathcal{W} : \theta \rightarrow SO(n)] \quad (IV.63)$$
IV.5. $\mathbb{Z} \oplus \mathbb{Z}_2$ nodal lines in class CI

The topological classification for various $n$ follows

$$\pi_1[SO(n)] = \begin{cases} \emptyset & \text{for } n = 1 \\ \mathbb{Z} & \text{for } n = 2 \\ \mathbb{Z}_2 & \text{for } n \geq 3. \end{cases} \tag{IV.64}$$

This agrees with $\pi_2[U(n)/O(n)]$, which we used to determine the entries in Tab. IV.3

A more illustrative geometric interpretation of charge (IV.63) exists for the $n = 2$ case (IV.61). To keep the discussion simple, we consider a specific choice

$$a(k) = k \quad \text{and} \quad b = (0, 0, m). \tag{IV.65}$$

This creates a nodal loop at

$$k_x^2 + k_y^2 - m^2 = 0 = k_z \tag{IV.66}$$

which has a non-trivial $\pi_2$-charge (IV.63) as is checked by calculating the Wilson operator eigenvalues in Fig. IV.8(a).

The nodal loop (IV.66) of model (IV.65) lies on a surface

$$S_{a,b}^2 = \left\{ k \bigg| k_x^2 + k_y^2 + k_z^2 = m^2 \right\} \tag{IV.67}$$

defined by $\|a(k)\| = \|b(k)\|$. Note that while vector field $b(k)$ has a fixed direction, field $a(k)$ has a hedgehog structure on $S_{a,b}^2$. The map

$$S_{a,b}^2 \ni k \longmapsto n_a(k) = \frac{a(k)}{\|a(k)\|} \in S^2 \tag{IV.68}$$

is characterized by the second homotopy group $\pi_2(S^2) = \mathbb{Z}$, and the hedgehog structure of the considered $a(k)$ corresponds to a non-trivial element of $\pi_2(S^2)$. By virtue of Eq. (IV.61b), the nodal loop separates the “northern hemisphere” of $S_{a,b}^2$ (with $a(k) \cdot b(k) > 0$) from the “southern hemisphere” (with $a(k) \cdot b(k) < 0$). Because of the non-trivial winding of map (IV.68), the two “geographic poles” with parallel vectors $a(k) \times b(k) = 0$ must appear somewhere on $S_{a,b}^2$. Since $a(k)$ varies continuously on $S_{a,b}^2$, the presence of the two “poles” makes the equator separating the two hemispheres – i.e. the nodal loop – robust.

We compare these observations to a model with

$$\tilde{a}(k) = (\sqrt{k_x^2 + k_y^2}, \tilde{m}, k_z) \quad \text{and} \quad b = (0, 0, m) \tag{IV.69}$$
Figure IV.8: Nodal lines of AZ+I class CI. (a) Non-trivial eigenvalue winding of Wilson loop operators (IV.63) for the nodal loop exhibited by model (IV.65), and (b) the trivial winding for the nodal loop of model (IV.69). Both spectra were calculated on a sphere with radius $2m$ centred at $k = 0$. (c) Torical Fermi surface of a nodal loop metal. If the system develops a singlet SC order parameter with a gap function $\Delta_k$ that changes sign (red and blue regions) along the torus, a pair of SC nodal loops appear (cyan). By locally adjusting the energy of the metallic nodal loop to the chemical potential, it is possible to shrink the SC node to a single point. However, further energy variation of the metallic node leads to a regrowth of the SC nodal loop, thus manifesting its non-trivial $\pi_2$-charge. (d) The same consideration for a torical Fermi surface without an underlying nodal loop lead to removable nodal loops of the singlet gap function, i.e. their $\pi_2$-charge is trivial. (e) Both torical Fermi surfaces admit a more complicated geometry of the SC nodal loops. Interpenetrating loops were argued to exhibit anomalous gravitomagnetoelectric response in Ref. [190].

which for $\tilde{m} = 0$ produces a nodal line at the same location as the previous model (IV.65) but with a trivial $\pi_2$-charge (IV.63) as checked in Fig. IV.8(b). In this case, the surface $S^2_{a,b} = S^2_{a,b}$ remains unchanged, but the winding (IV.68) of $n_{\tilde{a}}(k)$ is trivial because it lies on a circle with $n_y = 0$. Indeed, increasing $\tilde{m}$ from zero to $\pm m$ shrinks the nodal line to a point, and a gap opens for $|\tilde{m}| > |m|$, thus manifesting the trivial nature of its $\pi_2$-charge.

IV.5.4 Example class CI model

In Sec. IV.2 we identified two qualitatively different realizations of AZ+I class CI. Here we focus on the case of a TRS-preserving singlet SC in
**IV.5. $\mathbb{Z} \oplus \mathbb{Z}_2$ nodal lines in class CI**

the absence of SOC. First, we show how such a class of systems relates to $k \cdot p$ models (IV.65) and (IV.69). Afterwards, we develop a concrete TB model of a nodal line metal on a SrPtAs-like lattice of Fig. IV.5, and we show that its singlet SC phase exhibits doubly charged nodal loops whenever the gap function changes sign along the Fermi surface. The SC order parameter may either appear spontaneously at low enough temperatures, or it is induced at an interface through the proximity effect.

Consider a two-orbital system with $\mathcal{I} = \mathbb{1}_\tau$. According to the discussion in Subsec. IV.2.2, its singlet SC phase acquires $AZ+\mathcal{I}$ symmetries $\mathcal{P} = i\varsigma_y \otimes \mathbb{1}_\tau \mathcal{K}$ and $\mathcal{T} = \mathcal{K}$. These are precisely the forms listed in Tab. IV.2, meaning that the symmetry-compatible basis matrices of the reduced BdG Hamiltonian (IV.18) are those organized in Eqs. (IV.60) (with replaced $\sigma_i \mapsto \varsigma_i$). More specifically, model (IV.65) corresponds to the (non-reduced) BdG Hamiltonian (IV.12b) with

$$
\Xi_k = \mathbb{1}_\sigma \otimes (k_x \tau_z - k_y \tau_x + m \mathbb{1}_\tau)
$$

$$(IV.70a)$$

$$
\Delta_k = k_z (i\varsigma_y) \otimes \mathbb{1}_\tau.
$$

$$(IV.70b)$$

The metallic state described by $\Xi_k$ exhibits a cylindrical Fermi surface

$$
\text{FS} = \left\{ k | k_x^2 + k_y^2 = m^2 \right\}
$$

$$(IV.70c)$$

connected to a nodal line at energy $m$, hence we call this system a nodal line metal. Additionally, the gap function $\Delta_k$ changes sign from negative at $k_z < 0$ to positive at $k_z > 0$, leading to a zero-energy nodal loop located at $k_z = 0$ of the SC phase. If one imagines warping the cylindrical Fermi surface into a torus, then such SC nodal loops have to come in pairs as shown in Fig. IV.8(c).

The underlying nodal line of the metallic band structure (IV.70a) makes nodal loops of the SC phase (IV.70b) robust: One can at best shrink the loop to a point by setting $m = 0$, but a 1D loop reappears for $m \neq 0$ of both signs. The reason is that the underlying electron-like FS (for $m < 0$) evolves directly into a hole-like FS (for $m > 0$) through the nodal line that glues the two bands together. This touching is protected by the Berry $\pi$-phase invariant. We illustrate such a band evolution and the robustness of such SC nodal loops in Fig. IV.8(c).

We compare this to model (IV.69) which arises from

$$
\Xi_k = \mathbb{1}_\sigma \otimes \left( \sqrt{k_x^2 + k_y^2} \tau_z - m \tau_x + m \mathbb{1}_\tau \right).
$$

$$(IV.71a)$$
Figure IV.9: **Doubly charged nodal lines of $\text{AZ}+\mathcal{I}$ class CI.** (a) Fermi surface of the developed TB model with parameters (IV.72) consists of touching electron (blue) and hole (red) pockets. The pockets are topologically non-trivial because of nodal lines running along the vertical BZ edges. The SC order parameter (IV.73) creates two pairs of SC nodal loops when $|\Delta| < 1$. (b) Winding of $\mathcal{W}(\theta)$ eigenvalues on an ellipsoid described in the text which contains a pair of SC nodal loops, and (c) the same calculation on an ellipsoid containing a single SC nodal loop. These calculations indicate that both SC nodal loops carry a non-trivial value of the $\pi_2$-charge (IV.63).

This leads to a cylindrical

$$\tilde{\mathcal{F}}S = \left\{ k |k_x^2 + k_y^2 = m^2 - \tilde{m}^2 \right\} \quad \text{(IV.71b)}$$

without an underlying nodal line (apart from the fine-tuned case $\tilde{m} = 0$ which is accidental and does not carry a topological charge). This makes it possible to remove $\tilde{\mathcal{F}}S$ by setting $|\tilde{m}| > |m|$, which also eliminates the nodal loop of the SC phase (IV.70b) as illustrated in Fig. IV.8(d). We infer that doubly charged nodes of the gap function are bound to SC phase of *nodal line metals*. This observation supplements the previously known unusual SC phases enabled in topologically non-trivial Fermi surfaces [83, 191].

We now develop a concrete TB model belonging to this symmetry class to make our ideas more tangible. We consider again the lattice of Subsec. IV.4.4 but *without dimerization*. There are two orbitals per unit
cell that lead to $I = r_x$ and $C = r_z$. We consider parameters

$$t_1 = 1 \quad \text{and} \quad t_2 = 0.4, \quad (IV.72)$$

and further $t_3 = t_2$, $r = 1$ and $\mu = 0$. The hexagonal crystalline symmetry imposes nodal lines running along the vertical BZ edges. This are the “spinless” nodal lines discussed in Subsec. III.1.3. The chosen TB parameters (IV.72) lead to touching electron and hole Fermi pockets as shown in Fig. IV.9(a). We further assume that the system acquires a singlet SC order parameter

$$\Delta_k = \varphi^0 [\Delta + \cos(k_zc)] (i\sigma^y) \otimes 1_r. \quad (IV.73)$$

The AZ$+I$ symmetries of this model are $\Sigma = r_xK$, $\Psi = ir_x \otimes \zeta_yK$ and $C = i\zeta_y$. These can be modified to the choice of Tab. IV.2 if one rotates the basis by $U_r^\dagger$ with the matrix given in Eq. (IV.32).

The developed model exhibits four SC nodal loops for $|\Delta| < 1$ [one pair at heights $k_zc = \pm \arccos(-\Delta)$ at both BZ edges] which move along the touching Fermi pockets when varying $\Delta$. These nodes annihilate in pairs at $k_z = 0$ ($k_z = \pi$) for $\Delta = -1$ ($\Delta = +1$). They shrink to points for $\Delta = 0$ when they coincide with the touching points of the Fermi pockets. To check the $\pi_2$-charge of these nodal loops, we set $\varphi^0 = 0.2$ and $\Delta = -\sqrt{3}/2$ which locates them at $k_zc = \pm \pi/4$.

We plot in Fig. IV.9(b) the trivial eigenvalue winding on an ellipsoid with radii $(\pi/3a, \pi/3a, \pi/3a)$ centred at $k_c = (0, 4\pi/3\sqrt{3}a, 0)$ which contains a pair of the SC nodal loops. On the other hand, in Fig. IV.9(c) we plot the non-trivial eigenvalue winding for an ellipsoid of the same dimensions centred at $k_c = (0, 4\pi/3\sqrt{3}a, \pi/4c)$ which contains a single SC nodal loop. These observations imply a non-trivial value of the $\pi_2$-charge (IV.63). The $\pi_1$-charge (IV.62) is non-trivial for every (non-accidental) SC nodal line of this symmetry class, e.g. for the well-known $d$-wave superconductors.

### IV.6 $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ nodal lines in class AI

We finally discuss the AZ$+I$ class AI in $D = 3$, which has been to varying degree considered in Refs [38, 176, 177]. This symmetry class supports nodal lines with charge

$$c_{AI}^{(3)} \in \pi_1(M_{AI}) \oplus \pi_2(M_{AI}) = \mathbb{Z}_2 \oplus \mathbb{Z}_2. \quad (IV.74)$$
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According to Tab. IV.4, the minimal half-filled model supporting a non-trivial $\pi_2$-charge contains four bands. The nine basis matrices of Tab. IV.2 can be organized into three vectors (called \textit{real Dirac basis} by Ref. [177])

\[
\begin{align*}
\mathbf{v}^{(1)} &= (\sigma_z \otimes \tau_z, -\sigma_z \otimes \tau_x, \sigma_x \otimes 1) \quad \text{(IV.75a)} \\
\mathbf{v}^{(2)} &= (1 \otimes \tau_x, 1 \otimes \tau_z, \sigma_y \otimes \tau_y) \quad \text{(IV.75b)} \\
\mathbf{v}^{(3)} &= (-\sigma_x \otimes \tau_z, \sigma_x \otimes \tau_x, \sigma_z \otimes 1) \quad \text{(IV.75c)}
\end{align*}
\]

which fulfil an elegant anticommutation relation

\[
\{\mathbf{v}^{(a)}_i, \mathbf{v}^{(b)}_j\} = 2 \left[ \delta_{ij} \delta^{ab} 1 + \epsilon_{ijk} \epsilon^{abc} \mathbf{v}^{(c)}_k \right]. \quad \text{(IV.76)}
\]

We failed to derive analytic conditions for the occurrence of a gap closing in the most general four-band model, so we proceed directly with the discussion of the topological charges. The $\pi_1$-charge is just the Berry phase, which is for closed paths quantized to $\{0, \pi\}$ by $\mathcal{K}$, as explained in the partial coverage of this symmetry class in Subsec. III.1.3. The $\pi_2$-charge is again the $\pi_1[\text{SO}(n)]$ homotopy equivalence class of Wilson loop operators that has been explained for AZ+I class CI in Subsec. IV.5.3. In the last subsection we develop a TB model on a SrPtAs-like lattice that exhibits either singly or doubly charged nodal loops, depending on the chosen parameter values.

\section*{IV.6.1 Interpretation of $\pi_1(\mathbb{M}_{AI}) = \mathbb{Z}_2$}

The $\pi_1$-charge $\mathcal{C}_{AI}(S^1)$ of AZ+I class AI corresponds to the Berry phase acquired along $S^1$, which is defined as the phase of $\det(\mathcal{W}(S^1))$, as has been discussed in Subsec. I.1.2. We can equivalently write

\[
\hat{\mathcal{C}}_{AI}(S^1) = \frac{i}{\pi} \oint_{S^1} d\mathbf{k} \cdot \text{tr} \mathcal{A}(\mathbf{k}) \quad \text{mod} 2 \quad \text{(IV.77)}
\]

The Berry phase is quantized because $\mathcal{K} = \mathcal{K}$ makes it possible to find a \textit{real} set of eigenvectors $|u^a(\mathbf{k})\rangle$, such that $\mathcal{W}(S^1) \in \mathcal{O}(n)$ has a real-valued determinant $\pm 1$.

Note that according to Tab. IV.4 there is an exception to the order of the $\pi_1$-charge in half-filled 2-band models. In this case, the basis of symmetry-compatible Hamiltonians is two-dimensional (spanned by $\sigma_x$ and $\sigma_z$) and thus allows for a richer $\mathbb{Z}$-valued winding number.
IV.6.2 Interpretation of $\pi_2(M_{\text{AI}}) = \mathbb{Z}_2$

The $\pi_2$-charge of this symmetry class is

\[ c_{\text{AI}}(S^2) = [\mathcal{W} : \theta \to SO(n)], \tag{IV.78} \]

i.e. it corresponds to the homotopy equivalence class of Wilson loop operators $\mathcal{W}(\theta) \in SO(n)$ for a set of closed paths $S^1(\theta)$ covering $S^2$, just like for the AZ+I class CI. However, we see from Tab. IV.4 that the order of charge (IV.78) is modified whenever $\min\{n, \ell\} \leq 2$. Such exceptions were absent in symmetry class CI. We use the rest of this subsection to clarify this complication.

The key observation is that the homotopy class (IV.78) can be determined for two Wilson loop operators, $\mathcal{W}^{\text{occ.}} \in SO(n)$ over the occupied and $\mathcal{W}^{\text{un.}} \in SO(\ell)$ over the unoccupied bands. The presence of $\mathfrak{B}$ in class CI enforces the two Wilson operators to have identical spectra, so nothing is gained by considering both. On the other hand, particle-hole symmetry is absent in class AI which allows the Wilson spectra to be different. As with the other topological charges, we expect the sum of the two charges to be trivial, but the sum has to be perceived in the sense of $\pi_1[SO(n+\ell)]$, which may differ from groups $\pi_1[SO(n)]$ and $\pi_1[SO(\ell)]$, cf. (IV.64). In fact, the latter two may themselves be different.

For example, for $n = 2$ and $\ell = 1$ the two occupied bands admit $c_{\text{AI}}^{\text{occ.}}(S^2) \in SO(2) = \mathbb{Z}$, while the unoccupied band has a trivial $c_{\text{AI}}^{\text{un.}}(S^2) \in SO(1) = \mathbb{Z}_2$. The sum of the two has to be trivial within $\pi_1[SO(3)] = \mathbb{Z}_2$ which only percieves the parity, hence $c_{\text{AI}}^{\text{occ.}}(S^2)$ must be an even integer as indicated in Tab. IV.4. An example Hamiltonian with a prescribed charge $2\nu \in 2\mathbb{Z}$ is

\[ H^{(2,1)}_{2\nu}(k) = k \left[ 2n_{(\theta,\nu\phi)} \cdot n_{(\theta,\nu\phi)}^\top - 1 \right] \tag{IV.79} \]

where $k = kn_{(\theta,\phi)}$ is expressed using spherical coordinates $(k, \theta, \phi)$ and

\[ n_{(\alpha,\beta)}^\top = (\sin \alpha \cos \beta, \sin \alpha \sin \beta, \cos \alpha) \tag{IV.80} \]

with $\alpha \in [0, \pi]$ and $\beta \in [0, 2\pi)$ is the unit vector in a specified direction, expanded in Cartesian coordinates. The Wilson loop spectra $\mathcal{W}^{\text{occ.}}$ and $\mathcal{W}^{\text{un.}}$ of model (IV.79) with $2\nu = 2$ are plotted in Figs. IV.10(a,b). This enrichment to $2\mathbb{Z}$ is in a stark contrast to models with $n \geq 3$ and $\ell = 1$ when the only consistent choice of charges summing to 0 (mod 2) is
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Figure IV.10: Wilson loop spectra of exceptional class AI few-band models. (a) Wilson loop spectrum over the occupied and (b) the unoccupied states of the (2+1)-band Hamiltonian (IV.79) with $\nu = 1$. The pair of plots looks identical for the (2+2)-band Hamiltonian (IV.81) with the same $\nu$. (c,d) The corresponding Wilson loop spectra for the (2+2)-band Hamiltonian (IV.82), also with $\nu = 1$.

$c_{\text{AI}}^{\text{occ.}}(S^2) = 0 \ (\in \mathbb{Z}_2)$ and $c_{\text{AI}}^{\text{un.}}(S^2) = 0 \ (\in 0)$, such that no topological classification remains. The same conclusion is also found for $n = \ell = 1$. Clearly, the order of the charge is unchanged if we exchange $n \leftrightarrow \ell$, which is manifested by the diagonal symmetry of Tab. IV.4.

For $n = 2$ and $\ell \geq 3$ we find $\mathbb{Z}$ topologically inequivalent classes: Charges $c_{\text{AI}}^{\text{occ.}}(S^2) \in \mathbb{Z}$ and $c_{\text{AI}}^{\text{un.}}(S^2) \in \mathbb{Z}_2$ have to sum up to 0 (mod 2). Clearly, there is a unique solution to $c_{\text{AI}}^{\text{un.}}(S^2)$ for any $c_{\text{AI}}^{\text{occ.}}(S^2)$. Finally, in the case $n = \ell = 2$ we have to pick two integers that sum up to 0 (mod 2), meaning they are either both even or both odd. This corresponds to the $\mathbb{Z} \oplus \mathbb{Z}$ entry in the middle of Tab. IV.4. As a non-trivial example, consider

$$\mathcal{H}_{(2,2)}^{(2,2)}(k) = \mathcal{H}_{(2,1)}^{(2,1)}(k) \oplus (k)$$  \hspace{1cm} (IV.81)

i.e. where we just increase the dimension of Hamiltonian (IV.79) by adding “$k$” in its bottom-right corner, which produces an additional trivial unoccupied state. As indicated by the subscripts, Hamiltonian (IV.81) has charges $c_{\text{AI}}^{\text{occ.}}(S^2) = 2\nu$ and $c_{\text{AI}}^{\text{un.}}(S^2) = 0$ on any surface $S$ enclosing
$k = 0$, manifested again by the Wilson loop spectra in Fig. IV.10(a,b). On the other hand, the two charges of [177]

\[
\mathcal{H}^{(2,2)}_{(\nu,-\nu)} = \begin{align*}
\text{Re} \left[ (k_x + \text{sign}(\nu) i k_y) |\nu| \right] v_1^{(a)} + \text{Im} \left[ (k_x + \text{sign}(\nu) i k_y) |\nu| \right] v_2^{(a)} + k_z v_3^{(a)}
\end{align*}
\] (IV.82)

with a real Dirac basis (IV.75) are $\nu$ and $-\nu$. We plot the corresponding spectra of $\mathcal{W}^{\text{occ.}}$ and $\mathcal{W}^{\text{un.}}$ for $\nu = 1$ in Fig. IV.10(c,d). The somewhat unusual charge for $n = \ell = 2$ stems from the fact that $O(4)/O(2) \times O(2)$ is double covered by $S^2 \times S^2$ [192, 193].

We remark that Hamiltonians (IV.79), (IV.81) and (IV.82) are fine-tuned such that the node is contracted to a single point at $k = 0$. We did not investigate how the exceptional charges $c_{\text{occ.}}^{\text{AI}}(S^2)$ and $c_{\text{un.}}^{\text{AI}}(S^2)$ manifest themselves in the few-band spectra when the Hamiltonian becomes detuned from this simple setting.

### IV.6.3 Example class AI model

We consider a SrPtAs-like lattice with $s$-like orbitals at both the Pt and the As sites (in this case assumed inequivalent), both contributing to a TB model. In the absence of SOC, the hexagonal lattice symmetry enforces nodal lines running along the vertical BZ edges. A single unit cell extends over two layers and contains a pair of orbitals in each.

We stick to the Pauli matrix notation of Tab. IV.5, such that the two orbitals of the same species [same colour in Fig. IV.5(a)] are exchanged by $\mathcal{I} = \varrho_x \otimes r_x$. We consider intralayer hoppings with amplitude $t_1$

\[
\mathcal{H}_1(k) = t_1 \varrho_x \otimes \left[ S_{\cos(k)}^0 r_x - S_{\sin(k)}^0 r_y \right],
\] (IV.84a)

and vertical interlayer hoppings with amplitude $t_2$

\[
\mathcal{H}_2(k) = 2t_2 \cos(kz) \varrho_x \otimes \mathbb{1}_r.
\] (IV.84b)

More appropriately,

\[
\tilde{\mathcal{Gr}}(2,2) \equiv \frac{\text{SO}(4)}{\text{SO}(2) \times \text{SO}(2)} \simeq S^2 \times S^2.
\] (IV.83)

where $\tilde{\mathcal{G}}r(2, 2)$ is the space of oriented 2D planes passing though $r = 0$ in 4D real Euclidean space. This is a very peculiar statement. Unfortunately, the author remains unaware of a simple visualization of this homeomorphism.
Figure IV.11: Doubly charged nodal loops of AZ+ class AI. (a) The transparent green sheets indicate the trajectory traced out by nodal loops of TB model (IV.84) for parameters (IV.86a) and \( m \in [-2, 2] \). Snapshots of these nodal loops for \( m \in \{-2, -1.6, -0.8, 0, 0.8, 1.6, 2\} \) are shown in various shades of blue to red. The large circular grey loops inside the BZ correspond to nodes of the same model with \( t_2 = 1.5 \). (b) The Wilson Loop spectrum for one of the nodal lines for parameters (IV.86) exposes the non-trivial value of their \( \pi_2 \)-charge defined in Eq. (IV.78). This observation is related to the underlying nodal lines formed within the (un)occupied bands along the vertical BZ edges, running through the interior of the plotted nodal loops. (c) The \( \pi_2 \)-charge is trivial for nodal loops with \( t_2 = 1.5 \) on the other side of the topological phase transition (IV.87).

We further consider vertical hoppings to the second nearest layer with amplitudes \( t_0 \pm t_3 \), and a staggered on-site potential \( \pm m \) on the two elemental sublattices,

\[
\mathcal{H}_3(k) = [m + 2t_3 \cos(2k_zc)] \varrho_z \otimes r_z + 2t_0 \cos(2k_zc) \mathbb{1}_q \otimes \mathbb{1}_r. \tag{IV.84c}
\]

The representation \( \mathcal{K} = \varrho_x \otimes r_x \mathcal{K} \) in the employed basis differs from that of Tab. IV.2, but there is no need for a basis transformation as the Wilson loop formulation of charges (IV.77) and (IV.78) applies to any basis.

Model (IV.84) exhibits a gap closing at momentum \( k \) with energy
IV.6. $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ nodal lines in class AI

$-mt_0 / t_3$ whenever the pair of conditions

$$2t_3 \cos(2k_zc) + m = 0 \quad \text{(IV.85a)}$$

$$\left[ S^{0,t}_\cos(k) \right]^2 + \left[ S^{0,t}_\sin(k) \right]^2 = \frac{2t_2^2}{t_1^2} \left(1 - \frac{m}{2t_3}\right) \quad \text{(IV.85b)}$$

are fulfilled. Nodal loops appear in the model for $|m| < 2$ and a small enough ratio $|t_2/t_1|$. These loops annihilate in pairs at the $k_zc = 0$ plane for $m = -2$, and at the $k_zc = \pi/2$ plane for $m = 2$. We plot their trace for the intermediate values of $m$ and for parameters

$$t_1 = 1, \quad t_2 = 0.4, \quad \text{and} \quad t_3 = 1 \quad \text{(IV.86a)}$$

in Fig. IV.11(a).

We determine the $\pi_2$-charge (IV.78) of these nodal loops for

$$m = 0 \quad \text{(IV.86b)}$$

which sets their vertical location to $k_zc = \pi/4$. In Fig. IV.11(b) we plot the Wilson loop spectrum for an ellipsoid with radii $(1/a, 1/a, 1/c)$ centred at $k_c = \left(0, \frac{4\pi}{3\sqrt{3}a}, \frac{\pi}{4c}\right)$ which contains a single nodal loop. The spectrum has a non-trivial winding, thus exposing the non-trivial value of the $\pi_2$-charge.

Interestingly, a topological transition occurs for

$$1 = 2\frac{t_2^2}{t_1^2} \left(1 - \frac{m}{2t_3}\right) \quad \text{(IV.87)}$$

in which pairs of the doubly charged nodal loops merge together, thus forming nodal loops with a trivial value of the $\pi_2$-charge. For the values of $t_1, t_3, m$ listed in Eqs. (IV.86), the transition occurs for $t_{2c} = 1/\sqrt{2}$. Choosing $t_2 = 1.5 > t_{2c}$, we find the nearly circular nodal loops drawn in grey in Fig. IV.11(a). In Fig. IV.11(c), we plot the Wilson loop spectrum on an ellipsoid with radii $(3/2a, 3/2a, 3/2c)$ centred at $\tilde{k}_c = (0, 0, \pi/4c)$ which encloses a single such a nodal loop. The spectrum has a trivial winding, thus confirming the trivial value of the $\pi_2$-charge. Indeed, these loops disappear from the spectrum for $t_2 > 3/\sqrt{2}$, thus once again confirming their trivial (non-robust) nature.
Conclusions and outlook

The encompassing theme of this thesis is the interplay of symmetry and topology in nodal semimetals, with occasional digressions that are also applicable to nodal superconductors. We attempted to provide sufficient introduction and to organize the text in such a way, that it would serve as a practical exposition of the topic for non-experts. Especially, the entire chapter I serves as a summary of the mathematical tools frequently used in the study of topological aspects of band structures more generally, and were all developed elsewhere.

In chapter II, we considered the possible appearance of Weyl semimetals (WSM) due to a spontaneous structural phase transition in non-symmorphic Dirac semimetals (DSM). Such a transition may be energetically favourable in soft lattices at low temperatures, because the Dirac cone splitting decreases the kinetic energy of the electrons. However, opening a full insulator gap (INS) in the band structure leads to an even larger decrease of the electron energy. Consequently, we observed that only a very narrow WSM region exists in the phase diagram of the developed model between the DSM and INS phases. This suggests that, although the model allowed us to study interesting phenomena like the Weyl-Lifshitz transitions and the reentrant appearance of the symmetric phase at low temperatures, the setting is probably not of a direct experimental relevance. Furthermore, non-symmorphic DSMs which serve as the starting point of our reasoning have still not been found in real materials, even after five years since their original prediction [34]. The WSM phase has meanwhile been identified in tantalum arsenide (TaAs) [96–98], but the large number of exhibited Weyl points and the complicated nature of its surface states obscure many of the predicted phenomena characterizing this phase. The search for more ideal WSMs is still on.

We turned our attention to nodal line semimetals in chapter III. More
Conclusions and outlook

Specifically, we showed that non-centrosymmetric crystalline solids with a glide plane symmetry and strong enough spin-orbit interaction necessarily contain nodal lines in their band structure. Additionally, these nodal lines are automatically tuned to the Fermi level in materials with $4\nu + 2$ electrons per primitive unit cell, and with no additional Fermi surfaces. We explained that such species of nodal lines can be understood as perturbed non-symmorphic Dirac points, and we used this connection to predict a special anisotropy in magnetoresistance measurements. The presence of a pair of glide planes was argued to facilitate the appearance of a pair of touching nodal loops, which we call nodal chains.

While searching for such non-symmorphic nodal lines (NSNLs) by sifting through the very exhaustive material database ICSD [166], we noticed that the required $4\nu + 2$ filling is extremely disfavoured in crystals with the specified space group symmetry. This left us wondering whether there is some intrinsic instability associated with NSNL materials, e.g. a spontaneous structural distortion similar to the scenario we previously considered for non-symmorphic DSMs. In fact, we did not find any existing material exhibiting reasonably flat NSNLs at the Fermi level except the discussed compound iridium tetrafluoride (IrF$_4$) which hosts a nodal chain. Powder of IrF$_4$ has been first synthesized already four decades ago [165]. However, to probe the electron band structure using angle-resolved photoemission experiments, single crystals of IrF$_4$ are necessary and those seem to be challenging to grow. We are therefore still awaiting the experimental examination of our predictions. Our colleague, Dr. Quan-Sheng Wu, used first-principles calculations to predict the presence of nodal chains in a wider class of newly-predicted materials crystallizing in the same structure type as IrF$_4$ [40], which should be easier to grow.

We also left unanswered certain questions about the magnetoresistance (MR) of these materials. The adiabatic description of electrons occupying the Landau levels suggests the presence of the chiral anomaly, but only if the magnetic field is applied in the plane of the glide symmetry. A perpendicular component of the magnetic field is shown to open a gap in the Landau level spectrum. Furthermore, the semiclassical treatment for chemical potential away from the nodal line energy suggests a vanishing MR. These observations suggest a very complicated and anisotropic dependence of MR of NSNL materials on the direction of the applied magnetic field and on doping. Unfortunately, we did not have the time
Conclusions and outlook

to consider this problem more carefully. We also do not make specific predictions about MR of nodal chains. In this case, the main obstacle is the infinite extent of the node, which makes it impossible to describe by a finite-order $k \cdot p$ expansion. We hope to fill in these gaps in the future.

Finally, in chapter IV we discussed nodes protected solely by inversion symmetry and the global symmetries. We argued that such nodes can reach the very high degree of stability usually associated with Weyl points. Robust nodes carrying a pair of topological charges were shown to exist in four out of the ten centrosymmetrically extended Atland-Zirnbauer (AZ+) classes in 3D, and we indicated how such nodes may be relevant for various semimetallic as well as superconducting (SC) systems. Two of these possibilities have been previously reported [38, 39], while the other two are new. One of them, namely the robust nodal lines of the singlet SC order parameter in nodal-line metals, nicely supplements the list of recently predicted exotic SC phases that are only possible in topologically non-trivial Fermi surfaces [83, 191].

We made effort to provide the complete description of the topological protection of such doubly charged nodes, as well as of their relevance to realistic systems. On the other hand, we left out all the other possibly interesting aspects. Especially, we did not study whether the pair of charges lead to some novel type of topologically protected surface states, or whether they induce characteristic signatures in transport. For example, very recent Ref. [194] argued that a small inversion-breaking perturbation of class AI semimetallic nodal lines leads to an anomalous Hall response. Since the mathematical description of these nodes is similar that of the SC phase mentioned in the previous paragraph, we expect that an anomalous response to such a perturbation also exists in these SCs. Similarly, the nodal “Bogolyubov-Fermi” surfaces possible in time-reversal breaking multiorbital SCs act as sources of Berry phase quanta in $k$-space, similar to Weyl points. We are wondering whether phenomena related to chiral anomaly may also exist in such SC systems.

The complete classification of possible band structure nodes is still missing, although certain steps have recently been done in this direction [195]. On the other hand, the majority of the theoretically proposed nodes have not yet been observed experimentally. One of the obstacles is the need for time-consuming first-principles calculations for a large list of material candidates. We therefore greet with excitement the recent successful attempts at predicting stable new materials using machine
learning algorithms trained on databases such as ICSD [196]. Such algorithms, once properly trained, may provide computational shortcuts and allow for a high-throughput analysis of band structures. We believe that such endeavours will in the coming years greatly speed up the rate of discovering new topological materials.
Appendix

A Projective representations of space groups

Here, we provide a derivation of Eq. (II.47) that is heavily used to analyse the spectrum degeneracies of pyrochlore iridates in Sec. II.3. A more complete discussion can be found in Ref. [144]. For brevity, we write IR for an irreducible representation and nD IR for an n-dimensional IR throughout the appendix.

Every element of a space group $S$ can be expressed as a point operation $R$ followed by a uniform translation by some vector $t$, which we write compactly as $\{R | t\}$, i.e.

$$\{R | t\} : r \mapsto Rr + t$$  \hspace{1cm} (A.1a)

Action of this symmetry operation on functions in real space, including Bloch wave functions, is

$$\{R | t\} : f(r) \mapsto f[R^{-1}(r - t)]$$ \hspace{1cm} (A.1b)

and the composition rule is

$$\{R_2 | t_2\} \circ \{R_1 | t_1\} = \{R_2 \circ R_1 | R_2t_1 + t_2\}$$. \hspace{1cm} (A.1c)

The identity element is $\{E | 0\}$.

The set $T$ of all pure translations by Bravais lattice vectors $R$ is a subset of $S$. It and can be used to list all elements of $S$ compactly as

$$S = T \circ \{R_1 | t_1\} \bigcup \ldots \bigcup T \circ \{R_n | t_n\}$$ \hspace{1cm} (A.2)

where the point operations $R_1, \ldots, R_n$ act with respect to the same point in real space and are all different, and for every point operation $R_i$ we
Appendix

fixed one possible translation vector \( t_i \). The pair \( \{ R_i \mid t_i \} \) is called a coset representative. If the vectors \( t_i \) can all be made zero by a proper choice of the point of symmetry, the lattice is called symmorphic. If this cannot be done, the lattice is dubbed non-symmorphic. Note also that the set

\[
\mathcal{F} = \{ R_1, \ldots, R_n \}
\]  

(A.3)
of the point operations is always a group, called the isogonal point group of \( \mathcal{S} \). On the other hand, the coset representatives \( \{ R_i \mid t_i \} \) form a group if and only if the space group \( \mathcal{S} \) is symmorphic, i.e. when all \( t_i \) can be removed by a proper choice of the point of symmetry.

If we take SOC into account, a \( 2\pi \)-rotation of a wave function in real space is accompanied by a \( 2\pi \)-rotation of the electron spin which results in a sign change of the wave function. This operation is not equivalent to identity and we denote it as \( \mathcal{E} \), but for a \( 4\pi \)-rotation \( \mathcal{E}^2 = \mathcal{E} \).

We adopt the periodic boundary conditions. Then the group \( \mathcal{T} \) is Abelian and as such it has only 1D IRs \( \rho_k \) labelled by momenta \( k \). Its representation space is spanned by (any) Bloch wave function at \( k \)

\[
\psi^\alpha_k(r) = \exp(i k \cdot r) u^\alpha_k(r)
\]  

(A.4)

where \( u^\alpha_k(r) \) is the cell-periodic part of the Bloch wave function. The representations of a pure translation by a Bravais vector \( R \) is

\[
\rho_k(\{ \mathcal{E} \mid R \}) = \exp(-i k \cdot R).
\]  

(A.5)

The IRs of the space group \( \mathcal{S} \) can be more than one-dimensional, but they decompose into the 1D IRs (A.5) on the subgroup \( \mathcal{T} \). Let us consider a representation \( \rho \) of \( \mathcal{S} \) that contains \( \rho_k \) in its decomposition on subgroup \( \mathcal{T} \), i.e. it contains \( \psi^\alpha_k(r) \) as one of the basis vectors in its representation space. Then according to Eq. (A.1b), element \( \{ R \mid t \} \) transforms a Bloch function at \( k \) into

\[
\{ R \mid t \} : \exp(i k \cdot r) u^\alpha_k(r) \mapsto \exp \left[ i k \cdot (R^{-1} r) - i k \cdot t \right] u^\alpha_k(R^{-1} r - t).
\]  

(A.6)

But since \( k \cdot (R^{-1} r) = (Rk) \cdot r \), this can be identified as a Bloch function at \( Rk \). This means that representation \( \rho \) necessarily also contains \( \rho_{Rk} \) in its decomposition on \( \mathcal{T} \).

---

\(^8\) Remember that if \( \{ R_i \mid t_i \} \) is a symmetry of the lattice, then for any Bravais vector \( R \) the operation \( \{ R_i \mid t_i + R \} \) is also a symmetry.
To find the allowed spectrum degeneracies at $k$ we have to consider only those symmetry operations that leave the momentum of a Bloch function invariant (modulo reciprocal lattice vectors). We construct it as follows. Let us denote the subgroup of point operations $\mathcal{F}$ that leave $k$ invariant (called the little co-group of $k$) as $\mathcal{F}^k$. Then the group we are looking for is

$$\mathcal{G}^k = \bigcup_i \mathcal{F} \circ \{ R_i \mid t_i \}, \quad R_i \in \mathcal{F}^k. \quad (A.7)$$

It is a subgroup of $\mathcal{F}$ called the little group of $k$.

The IRs $\tilde{\rho}_k$ of $\mathcal{G}^k$ reduce on the subgroup $\mathcal{F}$ to 1D IRs labelled by the same momentum $k$, so according to Eq. (A.5) for a Bravais vector $R$

$$\tilde{\rho}_k (\{ E \mid R \}) = \exp(-ik \cdot R) \mathbb{1} \quad (A.8)$$

where $\mathbb{1}$ is the unit matrix. This trivial form indicates that representations of Bravais translations commute with representations of all other elements of $\mathcal{G}^k$.

It is useful to perform a substitution

$$\tilde{\rho}_k (\{ R \mid t \}) = \exp(-ik \cdot t) \mathcal{D}_k (\{ R \mid t \}). \quad (A.9)$$

The composition rule (A.1c) and the representation of Bravais translations (A.8) imply that

$$\mathcal{D}_k (\{ R_i \mid t_i \}) \mathcal{D}_k (\{ R_j \mid t_j \}) = \exp(-ig_i \cdot t_j) \mathcal{D}_k (\{ R_k \mid t_k \}) \quad (A.10)$$

where $g_i = (R_i^{-1}k) - k$ is a reciprocal lattice vector, $R_k = R_i \circ R_j$ is a point group operation from $\mathcal{F}^k$, and $t_k$ is a vector appearing together with $R_k$ in a coset representative of expansion (A.2). Note that instead of considering the function $\mathcal{D}_k$ on elements of $\mathcal{G}^k$, we might restrict our attention to its values on elements of $\mathcal{F}^k$ by defining

$$\overline{\mathcal{D}}_k (R_i) := \mathcal{D}_k (\{ R_i \mid t_i \}), \quad (A.11)$$

such that

$$\overline{\mathcal{D}}_k (R_i) \overline{\mathcal{D}}_k (R_j) = \exp(-ig_i \cdot t_j) \overline{\mathcal{D}}_k (R_i \circ R_j). \quad (A.12)$$

This completes the derivation of equation (II.47).

The factors $\exp(-ig_i \cdot t_j)$ are completely fixed by the crystal symmetry and are referred to as the factor system of the projective representation.
The projective representations of group $\mathcal{G}^k$ can be found as ordinary representation of some larger group that we refer to as the extension group of $\mathcal{G}^k$. One only has to pick up those representations of the extension group that are compatible with the factor system. Ref. [144] goes through all high symmetry points and high-symmetry lines of all (non-magnetic) SGs, indicates the appropriate extension of the corresponding little co-group, provides a complete list of their representations, and picks up those that are compatible with the factor system.

## B Classifying spaces

In this appendix, we derive the classifying spaces $M_{CL}$ for the individual $AZ+I$ classes which are listed in Tab. IV.1 of the main text. The classifying spaces appeared in the context of the tenfold way classification of gapped band structures already in Refs. [21, 75]. However, we are not aware of a publication which provides their systematic derivation. We decided to satiate the curious reader by filling in the gap here.

For each symmetry class $CL$, we wish to identify a space of all the symmetry-compatible Hamiltonians $\mathcal{H}(k)$, i.e. those that fulfil criteria (IV.3), with a prescribed number of occupied ($n$) and unoccupied ($\ell$) states. However, if defined in this way, the space of Hamiltonians is unnecessarily too big. The standard procedure is to first perform the spectral decomposition (IV.5a), which can consequently be deformed into the flat-band Hamiltonian (IV.5b) without encountering a gap closing. In topological terms, the space of flat-band Hamiltonian corresponds to a deformation retraction of the original space of symmetry-preserving Hamiltonians, therefore maps $\mathcal{H}(k)$ and $Q(k)$ from any base-manifold are homotopy equivalent and no topological information has been lost [187]. We thus define the classifying space $M_{CL}$ as follows:

1. The classifying space $M_{CL}$ is a space of all symmetry-compatible flat-band Hamiltonians with a prescribed number of occupied and unoccupied states.

Often it is convenient to express a flat-band Hamiltonian using the pro-
jectors onto the occupied and unoccupied bands as

\[ Q = - \sum_{a=1}^{n} |u^a\rangle \langle u^a| + \sum_{b=1}^{\ell} |u^b\rangle \langle u^b| \]

\[ \equiv -U_{\text{occ}} U_{\text{occ}}^\dagger + U_{\text{un}} U_{\text{un}}^\dagger = 1 - 2U_{\text{occ}} U_{\text{occ}}^\dagger \]  

(B.1)

where matrices \( U_{\text{occ}} \) and \( U_{\text{un}} \) are formed by stacking the occupied or the unoccupied states, respectively, in a row. In the last step we used the completeness relation \( U_{\text{occ}} U_{\text{occ}}^\dagger + U_{\text{un}} U_{\text{un}}^\dagger = 1 \). Hence, relation (B.1) leads us to an equivalent definition of the classifying space:

2. The classifying space \( \mathcal{M}_{\text{CL}} \) is a space of all symmetry-preserving projectors \( U_{\text{occ}} U_{\text{occ}}^\dagger = \mathbb{P} \) with a prescribed number of bands.

Importantly, it follows from the form (IV.5b) that \( Q^2 = 1 \), which in combination with the hermiticity \( Q^\dagger = Q \) leads to unitarity

\[ Q^\dagger Q = QQ^\dagger = 1. \]  

(B.2)

We can therefore reformulate the definition as follows:

3. The classifying space \( \mathcal{M}_{\text{CL}} \) is a space of all symmetry-compatible Hermitian unitary matrices with a prescribed number of +1 and −1 eigenvalues.

Finally, note that by stacking matrices \( U_{\text{occ}} \) and \( U_{\text{un}} \) next to each other we obtain a unitary matrix \( U \) of all eigenstates of \( Q \). The flat-band Hamiltonian is uniquely determined by this unitary matrix via Eq. (B.1). However, the converse is not true, because there are gauge transformations of \( U \) which keep \( Q \) invariant, leading to a fiber-bundle structure. Furthermore, sometimes symmetries constrain \( U \) to lie within some subgroup of unitary matrices. This leads us to our last definition:

4. The classifying space \( \mathcal{M}_{\text{CL}} \) is a fiber bundle of all matrices \( U = (U_{\text{occ}}, U_{\text{un}}) \) such that Hamiltonian \( Q \) as defined in (B.1) preserves all symmetries, with a fiber defined by gauge transformations that leave \( Q \) invariant.

In the rest of the appendix we go individually through all ten symmetry classes and derive the classifying space for each. Since the four definitions of \( \mathcal{M}_{\text{CL}} \) are all equivalent, we will use them interchangeably.
Class A: We apply definition (4). Because of the orthogonality of the eigenstates, matrices $U_{\text{occ.}}$ and $U_{\text{un.}}$ taken together form a matrix $U \in \mathbb{U}(n+\ell)$. However, relabelling the occupied (or the unoccupied) states corresponds to the same system. More generally, one can mix the occupied states by any $X_{\text{occ.}} \in \mathbb{U}(n)$ and the unoccupied states by any $X_{\text{un.}} \in \mathbb{U}(\ell)$, while preserving the flat-band Hamiltonian, explicitly

$$\tilde{Q} = -\tilde{U}_{\text{occ.}} \tilde{U}_{\text{occ.}}^\dagger + \tilde{U}_{\text{un.}} \tilde{U}_{\text{un.}}^\dagger = -U_{\text{occ.}} X_{\text{occ.}} X_{\text{occ.}}^\dagger U_{\text{occ.}}^\dagger + U_{\text{un.}} X_{\text{un.}} X_{\text{un.}}^\dagger U_{\text{un.}}^\dagger = -U_{\text{occ.}} U_{\text{occ.}}^\dagger U_{\text{un.}} U_{\text{un.}}^\dagger = Q.$$ (B.3)

This implies, that every flat-band Hamiltonian $Q$ can be perceived as a $\mathbb{U}(n) \times \mathbb{U}(\ell)$ fiber within the larger group $\mathbb{U}(n+\ell)$, i.e. the flat-band Hamiltonians are elements of the fiber bundle

$$\mathbb{M}_A = \mathbb{U}(n+\ell)/\mathbb{U}(n) \times \mathbb{U}(\ell) \equiv \text{Gr}_\mathbb{C}(n,\ell).$$ (B.4)

The resulting manifold is also called the complex Grassmanian.

Class AIII: We apply definition (4). We argued in Subsec. IV.4.3 that in the presence of chiral symmetry $C = \sigma_z \otimes 1_n$ (class AIII), the matrices of (un)occupied states take the form

$$U_{\text{occ.}} = \frac{1}{\sqrt{2}} \begin{pmatrix} U_1 & \ \ \ \ \ -U_2 \\ \end{pmatrix} \quad \text{and} \quad U_{\text{un.}} = \frac{1}{\sqrt{2}} \begin{pmatrix} U_1 \\ U_2 \end{pmatrix}$$ (B.5)

where $U_{1,2} \in \mathbb{U}(n)$, meaning that $U_{\text{occ.}}$ and $U_{\text{un.}}$ are specified by an element in $\mathbb{U}(n) \times \mathbb{U}(n)$. But we have to take care of gauge transformations again, which in this case take the form

$$\tilde{U}_{\text{occ.}} = U_{\text{occ.}} X \quad \text{and} \quad \tilde{U}_{\text{un.}} = U_{\text{un.}} X$$ (B.6)

with $X \in \mathbb{U}(n)$ rotating both occupied and unoccupied states, because we fix $U_{\text{un.}} = C U_{\text{occ.}}$ as implemented in (B.5). Factoring out the fibers, we obtain

$$\mathbb{M}_{\text{AIII}} = \mathbb{U}(n) \times \mathbb{U}(n)/\mathbb{U}(n) \cong \mathbb{U}(n).$$ (B.7)

Equivalently, starting with definition (1) we find that the most general symmetry-compatible flat-Hamiltonian is

$$Q = \begin{pmatrix} \ 0 \ 
\ q \ q^\dagger 
\ 0 \ \end{pmatrix} \quad \text{with} \quad q = U_1 U_2^\dagger \in \mathbb{U}(n),$$ (B.8)

thus leading to result (B.10) again.
Class AI: This class is characterized by the presence of $\mathcal{T}^2 = +1$. We can represent $\mathcal{T} = 1_{n+\ell}K$, which presents a reality condition on the Hamiltonian, as well as on the eigenstates. As a consequence, the matrices $U_{\text{occ.}}$ and $U_{\text{un.}}$ taken together form an element of $O(n + \ell)$, i.e. of the orthogonal (real) subgroup of $U(n + \ell)$. Similarly, the gauge transformations compatible with the reality condition are $X_{\text{occ.}} \in O(n)$ and $X_{\text{un.}} \in O(\ell)$, such that according to definition (4)

$$M_{\text{AI}} = O(n + \ell)/O(n) \times O(\ell) \equiv \text{Gr}_{\mathbb{R}}(n, \ell)$$

which is also called the real Grassmanian.

Class BDI: Assuming $n = \ell$ and the additional presence of chiral symmetry $C = \sigma_z \otimes 1_{n}$ (class BDI) in a class AI Hamiltonian, we can repeat the arguments presented for classes A/AIII above to find

$$M_{\text{BDI}} = O(n) \times O(n)/O(n) \cong O(n)$$

using either definition (1) or (4).

Class AII: In systems with $\mathcal{T}^2 = -1$, we represent $\mathcal{T} = -1_{n+\ell}K$ where the real antisymmetric matrix

$$U_{n+\ell} = \text{i} \sigma_y \otimes 1_{n+\ell}$$

is the so-called symplectic form. Note that Kramers theorem implies there is an even number of both the occupied and the unoccupied bands, hence we denote these as $2n, 2\ell$. To derive the classifying space $M_{\text{AII}}$, we start with definition (4). However, we organize the eigenstates of $Q$ slightly differently, namely we first take $n + \ell$ (both occupied and unoccupied) states without their Kramers partners, and then their $n + \ell$ Kramers partners in the same order. Then

$$U = \begin{pmatrix} M & -N^* \\ N & M^* \end{pmatrix} \in U(2n + 2\ell)$$

where the second column is obtained by acting with $\mathcal{T}$ on the first one, and both $M, N$ are $(n + \ell) \times (n + \ell)$ matrices over $\mathbb{C}$ (not necessarily elements of any interesting group). From the unitarity of $U$

$$U^\dagger U = \begin{pmatrix} M^\dagger M + N^\dagger N & -M^\dagger N^* + N^\dagger M^* \\ -N^\dagger M + M^\dagger N & N^\dagger N^* + M^\dagger M^* \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
we directly obtain

$$U^\top \mathcal{U}_{n+\ell} U = \begin{pmatrix} -\mathcal{N}^\top \mathcal{M} + \mathcal{M}^\top \mathcal{N} & \mathcal{N}^\top \mathcal{N}^* + \mathcal{M}^\top \mathcal{M}^* \\ -\mathcal{M}^\top \mathcal{M} - \mathcal{N}^\top \mathcal{N} & \mathcal{M}^\top \mathcal{N}^* - \mathcal{N}^\top \mathcal{M}^* \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathcal{U}_{n+\ell}$$

meaning that $U$ is an element of symplectic group $\text{Sp}(2n + 2\ell, \mathbb{C})$ [197]. But since $U$ is also unitary, it is an element of the compact symplectic group [197]

$$U \in \text{Sp}(n + \ell) = \text{Sp}(2n + 2\ell, \mathbb{C}) \cap U(2n + 2\ell). \quad (B.14)$$

We further need to identify the set of all unitary transformations that keep the form (B.12) as well as the Hamiltonian $Q$ invariant. To do so, we split $M = (M_{\text{occ.}}, M_{\text{un.}})$ (and similarly for the $\mathcal{N}$ matrix). The gauge transformation cannot mix the occupied and the unoccupied states, hence we need to find all $\chi_{\text{occ.}} \in U(2n)$ such that

$$\begin{pmatrix} M_{\text{occ.}} & -\mathcal{N}_{\text{occ.}}^* \\ \mathcal{N}_{\text{occ.}} & M_{\text{occ.}} \end{pmatrix} \chi_{\text{occ.}} = \begin{pmatrix} \tilde{M}_{\text{occ.}} & -\tilde{\mathcal{N}}_{\text{occ.}}^* \\ \tilde{\mathcal{N}}_{\text{occ.}} & \tilde{M}_{\text{occ.}} \end{pmatrix}$$

and similarly for the unoccupied states. From the first line

$$\begin{pmatrix} M_{\text{occ.}} & -\mathcal{N}_{\text{occ.}}^* \end{pmatrix} \chi_{\text{occ.}} = \begin{pmatrix} \tilde{M}_{\text{occ.}} & -\tilde{\mathcal{N}}_{\text{occ.}}^* \end{pmatrix}$$

we obtain that

$$\begin{pmatrix} \mathcal{N}_{\text{occ.}} & M_{\text{occ.}}^* \end{pmatrix} \chi_{\text{occ.}} = \begin{bmatrix} \mathcal{K} \begin{pmatrix} \mathcal{N}_{\text{occ.}}^* & M_{\text{occ.}} \end{pmatrix} \end{bmatrix} \chi_{\text{occ.}} = \begin{bmatrix} \mathcal{K} \begin{pmatrix} M_{\text{occ.}} & -\mathcal{N}_{\text{occ.}}^* \end{pmatrix} \end{bmatrix} \mathcal{U}_n \chi_{\text{occ.}} = \begin{bmatrix} \mathcal{K} \begin{pmatrix} \tilde{M}_{\text{occ.}} & -\tilde{\mathcal{N}}_{\text{occ.}}^* \end{pmatrix} \end{bmatrix} \mathcal{U}_n \chi_{\text{occ.}} = \begin{bmatrix} \tilde{M}_{\text{occ.}}^* & -\tilde{\mathcal{N}}_{\text{occ.}} \end{pmatrix} \mathcal{U}_n^{\top} \chi_{\text{occ.}} = \begin{bmatrix} \tilde{\mathcal{N}}_{\text{occ.}} & \tilde{M}_{\text{occ.}}^* \end{pmatrix} \mathcal{U}_n \chi_{\text{occ.}}.$$

where now $\mathcal{U}_n = i\sigma^y \otimes \mathbb{1}_n$. For the second line of (B.15) to be true, $\chi_{\text{occ.}}$ must fulfil

$$\chi_{\text{occ.}}^{\top} \mathcal{U}_n \chi_{\text{occ.}} = \mathcal{U}_n.$$

Taking into account the unitary, we are led to conclude that $\chi_{\text{occ.}} \in \text{Sp}(n)$. Analogous arguments can be presented for the unoccupied states, such that the fiber leading to an invariant value of $Q$ is homeomorphic to $\text{Sp}(n) \times \text{Sp}(\ell)$. Therefore, the classifying space is

$$\mathbb{M}_{\text{All}} = \text{Sp}(n + \ell) / \text{Sp}(n) \times \text{Sp}(\ell) \equiv \text{Gr}_{\|}(n, \ell) \quad (B.19)$$

also called the quaternion Grassmanian.
B. Classifying spaces

Class CII: We apply definition (1). Gapped systems belonging to this symmetry class must have $4n$ bands – one doubling comes from the Kramers theorem, while the other is a consequence of the particle-hole symmetry. We represent $\mathcal{C} = \sigma_z \otimes 1_{2n}$ such that the flat-band Hamiltonian takes the block-off-diagonal form

$$
Q = \begin{pmatrix}
0 & q \\
q^\dagger & 0
\end{pmatrix}
$$

with $q \in U(2n)$, \hspace{1cm} (B.20)

We further represent time-reversal symmetry as $T = -1_{\sigma} \otimes U_n K$ with the symplectic form $\mathcal{U}_n$. The condition $[\mathcal{S}, Q] = 0$ constrains $q$ by

$$
q^\dagger U_n = U_n q^\top \implies q^\top U_n q = U_n
$$

where we used the unitary of $q$. Conditions (B.20) and (B.21) together mean that the space of Hamiltonians $Q$ is homeomorphic to the compact symplectic group,

$$
\mathbb{M}_{\text{CII}} = \text{Sp}(n).
$$

Class CI: We use definition (3). Because of the particle-hole symmetry, gapped Hamiltonians of this symmetry class have $2n$ bands. For the purpose of this derivation, we represent $\mathcal{C} = \sigma_z \otimes 1_n$ and $\mathcal{T} = \sigma_x \otimes 1_n K$. Note that their composition $\mathcal{C} \mathcal{T} = i \sigma^y \otimes 1_n K$ squares to $-1$ while $\mathcal{T}^2 = 1$, as required. Because of the chiral symmetry, $Q$ takes form (B.8) with $q \in U(n)$, while time-reversal symmetry leads to

$$
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
0 & q^* \\
q^\top & 0
\end{pmatrix}
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix} = \begin{pmatrix}
0 & q \\
q^\dagger & 0
\end{pmatrix}
$$

from where $q = q^\top$. Hence $q$ is a symmetric unitary matrix. We will label the space of such matrices as $U_S(n)$. Following [198, p. 58], we prove

$$
U_S(n) \cong U(n) / O(n)
$$

where on the right-hand side two elements $u_{1,2} \in U(n)$ are deemed equivalent ($u_1 \sim u_2$) if $u_1 = u_2 o$ for some $o \in O(N)$. To show (B.24), we first demonstrate that

$$
u_1 \sim u_2 \iff u_1 u_1^\top = u_2 u_2^\top.
$$

The “$\implies$” part follows from $u_1 u_1^\top = u_2 o u_2^\top = u_2 u_2^\top$. For the “$\iff$” part we use the unitarity of $u_{1,2}$ to express the right-hand side of (B.25) as
(u_2^\dagger u_1)(u_2^\dagger u_1)^\top = 1. This implies that u_2^\dagger u_1 \in O(N) such that indeed u_1 = u_2 s for some s \in O(n), and therefore u_1 \sim u_2. We have thus shown that matrices uu^\top build up \mathbb{U}(n)/O(n). Furthermore, uu^\top is clearly unitary and symmetric, meaning that uu^\top \in \mathbb{U}_S(N). It only remains to be shown that every element of \mathbb{U}_S(N) can be expressed in the form uu^\top. To achieve this, we consider the spectral decomposition of a symmetric unitary matrix q is [199, Prop. 4.4.13]

\[ q = m \Lambda m^\top \]  

(B.26)

where m \in O(n) is the matrix of eigenvectors of q and \Lambda = \text{diag}\{e^{i\varphi_j}\}_{\varphi=1}^n is the corresponding matrix of its unimodular eigenvalues. Clearly, the decomposition q = uu^\top is achieved with u = m \text{diag}\{e^{i\varphi_j}/2\}_{\varphi=1}^n, thus completing the proof of homeomorphism (B.24). Therefore,

\[ \text{IM}_{CI} = \mathbb{U}(n)/O(n) \]  

(B.27)

which is also called the real Lagrangian Grassmanian.

**Class DIII:** We apply definition (3). Due to Kramers theorem and particle-hole symmetry, the minimal number of bands in symmetry class DIII is 4n. We represent \( C = \sigma_z \otimes 1_{2n} \) and \( \mathcal{K} = i \sigma_y \otimes 1_{2n} \mathcal{K} \). Because of the chiral symmetry, \( \mathcal{Q} \) takes form (B.20) with \( q \in \mathbb{U}(2n) \). Time-reversal symmetry further constrains

\[
\begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}
\begin{pmatrix}
0 & q^* \\
q^\top & 0
\end{pmatrix}
\begin{pmatrix}
0 & -1 \\
1 & 0
\end{pmatrix} =
\begin{pmatrix}
0 & q \\
q^\top & 0
\end{pmatrix}
\]  

(B.28)

from where \( q = -q^\top \), meaning that q is an antisymmetric unitary matrix. We denote the space of such matrices as \( \mathbb{U}_A(2n) \). We prove that

\[ \mathbb{U}_A(2n) \cong \mathbb{U}(2n)/\text{Sp}(n). \]  

(B.29)

where two elements \( u_{1,2} \in \mathbb{U}(2n) \) are deemed equivalent if \( u_1 = u_2 s^\top \) for some \( s \in \text{Sp}(n) \).\(^9\) To prove isomorphism (B.29), first note that

\[ u_1 \sim u_2 \iff u_1 \mathcal{U}_n u_1^\top = u_2 \mathcal{U}_n u_2^\top \]  

(B.30)

where \( \mathcal{U}_n = i \sigma_y 1_n \) is the symplectic form. The “\( \Rightarrow \)” part follows from \( u_1 \mathcal{U}_n u_1^\top = u_2 s^\top \mathcal{U}_n s u_2^\top = u_2 \mathcal{U}_n u_2^\top \). For the “\( \Leftarrow \)” part, we use the unitarity of \( u_{1,2} \) to rewrite the right-hand side of (B.30) as \((u_2^\dagger u_1)\mathcal{U}(u_2^\dagger u_1)^\top = \mathcal{U},\)  

\(^9\)Since any two unitary matrices are automatically related by a unitary matrix, we really only need to request that \( s \in \text{Sp}(2n, \mathbb{C}) \), cf. relation (B.14).
meaning that \( u_2^\dagger u_1 \in \text{Sp}(2n, \mathbb{C}) \). However, \( u_1 u_2^\dagger \) is also unitary, hence \( u_2^\dagger u_1 \in \text{Sp}(n) \) and therefore \( u_1 \sim u_2 \). As the next step of the proof, note that \( u \tilde{\Omega}_n u^\dagger \) is unitary and antisymmetric, i.e. an element of \( U_A(2N) \). It remains to be shown, that every element \( q \) of \( U_A(2N) \) can be written in such a form. To that end, note that every antisymmetric unitary matrix \( q \) has a spectral decomposition \([199, \text{p. 217}]^{10}\)

\[
q = m \Sigma m^\dagger \tag{B.31}
\]

where \( m \in O(2n) \) and \( \Sigma \) is an antisymmetric matrix that can be expressed as a direct sum of \( 2 \times 2 \) blocks as

\[
\Sigma = \bigoplus_{i=1}^{N} \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix} \equiv \bigoplus_{i=1}^{N} \Sigma_i \tag{B.32}
\]

where \( \lambda_i = e^{i \varphi_i} \) are unimodular. We can rewrite

\[
\Sigma_i = \left( e^{i \varphi_i/2} \mathbb{1}_2 \right) \tilde{\Omega}_1 \left( e^{-i \varphi_i/2} \mathbb{1}_2 \right) . \tag{B.33}
\]

We observe that \( q \) can be written in the form \( u \tilde{\Omega}_n u^\dagger \) with

\[
u = m \left( \bigoplus_{i=1}^{N} e^{i \varphi_i/2} \mathbb{1}_2 \right) \in U(2n). \tag{B.34}
\]

This completes the proof of (B.29). We therefore conclude that

\[
\mathbb{M}_{DIII} = U(2n) / \text{Sp}(n). \tag{B.35}
\]

**Class D:** We apply definition (3). We consider a system with \( n \) occupied and \( n \) unoccupied states. We represent the particle-hole operator as \( \tilde{\Psi} = \mathcal{K} \), such that \( \tilde{\Psi}^* = -\tilde{\Psi} \) is purely imaginary. However, it is more convenient to work with real matrix \( \tilde{\Psi} = i \tilde{Q} \). Then the Hermiticity and the unitarity of \( \tilde{Q} \) imply antisymmetry and orthogonality of \( \tilde{\Psi} \), i.e. the classifying space \( \mathbb{M}_D \) is homeomorphic to the space of antisymmetric orthogonal matrices \( O_A(2n) \). We prove that

\[
O_A(2n) \cong O(2n) / U(n). \tag{B.36}
\]

---

\(^{10}\)In Ref. [199], the space \( M_n \) stands for the space of \( n \times n \) matrices with values in \( \mathbb{C} \), i.e. \( \mathbb{C}^{n \times n} \). Furthermore, normal matrix \( A \) is a matrix fulfilling \([A, A^\dagger] = AA^\dagger - A^\dagger A = 0\). The space of normal matrices includes all unitary, Hermitian and antiHermitian matrices.
This relation may seem strange at first, because $U(n)$ does not look like a subgroup of $O(2n)$. However, by writing the representation space $\mathbb{C}^n$ of unitary matrices as $\mathbb{R}^{2n}$, it is possible to show that

$$M \in U(n) \iff \begin{pmatrix} \Re[M] & \Im[M] \\ -\Im[M] & \Re[M] \end{pmatrix} \in O(2n)$$

(B.37)

meaning that $U(n)$ matrices can be represented as $O(2n)$ matrices with a special block structure. We will denote the space of such orthogonal $2n \times 2n$ matrices [right-hand side of (B.37)] as $U_R(n)$. Importantly,$^{11}$

$$U_R(n) = O(2n) \cap \text{Sp}(2n, \mathbb{R}).$$

(B.38)

which will come in handy in a moment. Then by (B.36) two elements $o_{1,2} \in O(2n)$ are equivalent if $o_1 = o_2 u$ for some $u \in U_R(n)$. We show that this is equivalent to

$$o_1 \sim o_2 \iff o_1 \mathcal{O}_n o_1^\top = o_2 \mathcal{O}_n o_2^\top.$$ 

(B.39)

The ”$\Rightarrow$” part follows easily from the symplectic property (B.38) of $U_R(n)$. For the ”$\Leftarrow$” part, we rewrite the left-hand side of (B.39) as

$$(o_2^\top o_1) \mathcal{O}_n (o_2^\top o_1)^\top = \mathcal{O}_n,$$

(B.40)

implying that $o_2^\top o_1 \in \text{Sp}(2n, \mathbb{R})$. But by construction $o_2^\top o_1$ is also orthogonal, such that by (B.38) we have $o_2^\top o_1 \in U_R(n)$. This completes the proof of (B.39). Furthermore, matrices $o \mathcal{O}_n o^\top$ with $o \in O(2n)$ are easily shown to be antisymmetric orthogonal, i.e. elements of $O_A(2n)$. The converse is also true, i.e. any antisymmetric orthogonal matrix can be expressed as $o \mathcal{O}_n o^\top$ with $o \in O(2n)$. This is because antisymmetric orthogonal matrices can be spectrally decomposed as $[200]$

$$\mathcal{Q} = m \Sigma m^\top$$

(B.41)

---

$^{11}$We have already argued that $U_R(n) \subset O(2n)$. It is further easy to check that for $u \in U_R(n) : u^\top \mathcal{O}_n u = \mathcal{O}_n$ such that $U_R(n) \subset \text{Sp}(2n, \mathbb{R})$ too. To prove equality in (B.38), we also need to show the subset relation in the opposite direction. To that end, let us assume that $u$ belongs to both $O(2n)$ (such that $u^\top u = \mathbb{1}$) and $\text{Sp}(2n, \mathbb{R})$ (such that $u^\top \mathcal{O}_n u = \mathcal{O}_n$). A combination of these two conditions leads to $\mathcal{O}_n u = u \mathcal{O}_n$, which implies a block structure identical to the right-hand side of (B.37), implying that $O(2n) \cap \text{Sp}(2n, \mathbb{R}) \subset U_R(n)$. We have thus proved equality (B.38).
with \( m \in O(2n) \) and \( \Sigma \) as in Eq. (B.32). Repeating the same steps as for class DIII, we find that \( \tilde{Q} = o\tilde{\delta}_n o^\top \) with \( o \) as in Eq. (B.34). In summary, we showed that \( O_\Lambda(2n) \) matrices can be represented as equivalence classes of orthogonal matrices up to an element of \( U_R(n) \cong U(n) \), therefore

\[
\mathcal{M}_D = O(2n)/U(n). \tag{B.42}
\]

**Class C:** We finally consider class C with \( n \) occupied and \( n \) unoccupied bands. We use closely related definitions (2) and (3), and represent \( P = -\bar{Q}_n K \). Then the occupied and unoccupied states can be collected into two \( 2n \times n \) matrices

\[
U_{\text{occ.}} = \begin{pmatrix} M \\ \mathcal{N} \end{pmatrix} \quad \text{and} \quad U_{\text{un.}} = P U_{\text{occ.}} = \begin{pmatrix} -\mathcal{N}^* \\ M^* \end{pmatrix} \tag{B.43}
\]

i.e. the latter is completely specified by the first. The space of projectors \( \mathcal{P} = U_{\text{occ.}} U_{\text{occ.}}^\dagger \) is therefore homeomorphic to the space of \( U(2n) \) matrices of the form

\[
U = \begin{pmatrix} U_{\text{occ.}} & U_{\text{un.}} \end{pmatrix} = \begin{pmatrix} M & -\mathcal{N}^* \\ \mathcal{N} & M^* \end{pmatrix} \tag{B.44}
\]

up to gauge transformations. Note that \( \mathcal{Q}_n U = U^* \mathcal{Q}_n \), from where by the unitarity \( U^T U^* = 1 \) follows \( U^T \mathcal{Q}_n U = \mathcal{Q}_n \), therefore

\[
U \in U(2n) \cap \text{Sp}(2n, \mathbb{C}) = \text{Sp}(n). \tag{B.45}
\]

However, we have to factor out gauge transformations that preserve both \( Q = 1 - 2U_{\text{occ.}} U_{\text{occ.}}^\dagger \) as well as the relation between matrices (B.43). This corresponds to a simultaneous rotation \( \tilde{U}_{\text{occ.}} = U_{\text{occ.}} \chi \) and \( \tilde{U}_{\text{un.}} = \tilde{U}_{\text{un.}} \chi^* \) with \( \chi \in U(n) \). Therefore

\[
\mathcal{M}_C = \text{Sp}(n)/U(n) \tag{B.46}
\]

which is also called the complex Lagrangian Grassmanian. Note that for \( U(n) \) in relation (B.46) to be a subgroup of \( \text{Sp}(n) \), we need to understand the latter as the unitary matrices with values in \( \mathbb{H}^{n \times n} \). Then \( U(n) \) is a subgroup of such matrices in which two of the three imaginary units happen to be absent. In this regards, result (B.46) is analogous to (B.27) obtained for class CI.
Notations

∅  empty set
★ Hodge dual operator
* complex conjugation
⊤ matrix transpose
† Hermitian conjugation
|0⟩ vacuum for ladder operators
. indicates time derivative
~ indicates gauge-transformed or rotated variables
|...| absolute value of a scalar, or the order of a group
||...|| vector norm
[.,.] commutator
{.,} anticommutator
⟨.,⟩ nearest neighbor sites in a lattice
⟨⟨.,⟩⟩ next-to-nearest neighbor sites in a lattice
∧ exterior product
⊕ direct sum
⊗ direct/tensor/Kronecker product
∪ union of sets
0 trivial one-element group
1, 1n unit matrix (identity operator) of a given dimension
a, b, α, β band indices
a, b, c unit cell dimensions
a†, a raising and lowering ladder operator
a(k), b(k) (vector) functions used to decompose $\mathcal{H}(k)$ into basis
Å Ångstrom $10^{-10}$ m
A antiunitary operator
$\mathcal{A}, \mathcal{A}^{ab}$ Berry-Wilczek-Zee connection and its components
Notations

\( A, A_i^a \) single-band Berry connection and its components
\( A, A_i \) EM vector potential and its components
\( b \) rescaled magnetic field
\( B, B_i \) magnetic field
\( \mathcal{B} \) sewing matrix between two gauge choices
\( c \) a generic complex number
\( c \) value of topological invariant (charge)
\( c_{\text{CL}}(M) \) charge value in symmetry class CL on manifold \( M \)
\( c^\dagger, c \) fermionic creation and annihilation operator
\( C_{ni} \) operator of n-fold rotation around coordinate \( i \)
\( \mathbb{C} \) complex numbers
\( C \) chiral symmetry
\( \mathfrak{c} \) class of a group
\( \gamma \) path in parameter space
\( d \) exterior derivative
\( d \) superconducting triplet order parameter (changed!!)
\( d \) differential
\( \delta_{ij}, \delta^{ab} \) Kronecker symbol
\( \delta(x) \) Dirac delta function
\( \delta \) variation of a parameter
\( \mathfrak{d} \) codimension
\( D \) number of spatial dimensions
\( \mathcal{D} \) domain (e.g. of integration)
\( D \) dimension of a group representation
\( \mathcal{D}_k \) projective (ray) representation of little group \( \mathcal{G}^k \)
\( \overline{\mathcal{D}}_k \) projective (ray) representation of little co-group \( \overline{\mathcal{G}}^k \)
\( \Delta_k \) gap function of a superconducting state
\( \partial_i \) partial derivative with respect to coordinate \( i \) or \( k_i \)
\( \partial \) boundary operator
\( \nabla, \nabla_k \) del (nabla) operator in real/momentum space
\( e \) Euler’s number \( 2.71828182 \ldots \)
\( e \) charge of a proton, \( e > 0 \)
\( e_i \) unit vector along coordinate axis \( i \)
\( \exp \) path-ordered exponential
\( E, E_i \) electric field and its components
\( \varepsilon_{ijk} \) Levi-Civita symbol
\( \varepsilon, \varepsilon^a(k) \) band energy
\( \varepsilon \) infinitesimal small positive number
Notations

\( E \) identity element of a group
\( \mathcal{E} \) 2\( \pi \)-rotation in half-integer spin systems
\( \mathcal{E} \) staggered strain
\( f \) function, map
\( \mathcal{F}_{\text{FD}} \) Fermi-Dirac distribution function
\( F \) free energy
\( \mathcal{F}, \mathcal{F}^{a}_{ij} \) single-band Berry curvature for non-degenerate bands
\( \mathcal{F}, \mathcal{F}^{ab}_{ij} \) Berry curvature (2-form) and its components
\( \mathbb{F} \) algebraic field (we encounter \( \mathbb{Z}_2, \mathbb{Z}, \mathbb{R}, \mathbb{C} \) and \( \mathbb{H} \))
\( \mathcal{P} \) isogonal point group of a given space group
\( \text{fin.} \) for "final"
\( g \) group element
\( g \) reciprocal lattice vector
\( G \) a group
\( G_i \) operator of glide plane perpendicular to coordinate \( i \)
\( \gamma^k, \bar{\gamma}^k \) little group and little co-group of \( k \)
\( \text{Gr}_\mathbb{F}(n, \ell) \) Grassmannian space over field \( \mathbb{F} \)
\( \Gamma \) time-reversal invariant momenta (TRIMs)
\( \Gamma_{i}, \Gamma_{ij} \) Dirac matrices, \( \{ \Gamma_{i}, \Gamma_{j} \} = 2\delta_{ij} \) and \( \Gamma_{ij} = -\frac{i}{2}[\Gamma_{i}, \Gamma_{j}] \)
\( h(k) \) (vector) function used to decompose \( \mathcal{H}(k) \) into basis
\( h(k) \) off-diagonal block of a chiral-symmetric Hamiltonian
\( H \) Hamiltonian in second quantization form
\( \mathbb{H} \) quaternions
\( \mathcal{H} \) Hamiltonian matrix
\( \mathcal{h} \) (reduced) Planck constant \( 1.0545718 \times 10^{-35} \text{ J.s} \)
\( \eta_{k,\pm} \) glide eigenvalues
\( h \) chirality of a Weyl point
\( \Theta \) factor system of a projective representation
\( \theta \) azimuthal angle in spherical coordinates
\( i, j, k, l \) enumerate elements of something
\( i, j, k, \ell \) generic vector and tensor indices
\( i \) imaginary unit, \( i^2 = -1 \)
\( \mathcal{I} \) spatial inversion operator
\( I_{\text{coll.}} \) collision integral
\( \Im \) imaginary part of a complex expression
\( \text{in.} \) for "initial"
\( j \) current density
\( j_{i}^{s} \) spin \( s \) rotation matrices, \( i \in \{ x, y, z \} \)
\( k = (k_x, k_y, k_z) \) momentum space coordinates
\( \mathcal{K} \) operator of complex conjugation
\( \mathcal{H} \) 2D cut in 3D momentum space
\( \ell \) number of unoccupied bands
\( \lambda \) mean free path of an electron
\( L_i \) length of the crystal in direction \( i \)
\( m \) mass, tunable parameter in tight-binding model
\( m \) eigenvalues (and labels of states) of \( J_z \) spin operator
\( m \) a generic point of a manifold \( M \)
\( M_i \) mirror reflection with respect to coordinate \( i \)
\( \mathcal{M}, \mathcal{N} \) generic matrices
\( \mathcal{M} \) manifold
\( \mu \) Fermi level (chemical potential at zero temperature)
\( \mu, \nu, \rho, \sigma \) enumerate irreducible representations of a group
\( n \) number of occupied bands
\( n \) any integer, \( n \in \mathbb{Z} \)
\( n \) occupation function
\( n \) unit vector
\( N \) a generic large integer
\( \xi \) energy with respect to Fermi level, \( \xi = \varepsilon - \mu \)
\( \Xi_k \) normal state kinetic matrix in BdG Hamiltonian
\( o \) a generic orthogonal matrix
\( O(n) \) orthogonal Lie group
\( \mathcal{O} \) a generic operator on Hilbert space
\( \mathcal{O} \) big \( \mathcal{O} \) notation to describe limiting behavior
\( \hat{p}, \hat{p}_i \) momentum operator and its components
\( p \) order of a differential form
\( \mathcal{P} \) point group
\( \mathcal{P} \) particle-hole symmetry
\( \mathcal{P} \) composition of particle-hole with inversion, \( \mathcal{P} = \mathcal{P}I \)
\( \chi \) eigenvalues of various operators in Subsec. II.3
\( \mathcal{P}(k) \) projector onto occupied bands at \( k \)
\( \psi \) character of a group representation
\( \pi \) Ludolph’s number 3.14159265 \ldots
\( \pi_D(M) \) \( D \)th homotopy group of manifold \( M \)
\( \varpi \) solid angle in three spatial dimensions
\( \prod \) path-ordered product
\( \Pi, \Pi_i \) canonical momentum in EM fields and its components
\( q = (q_x, q_y, q_z) \) momentum displacement
\( q \) off-diagonal component of \( Q \) in the presence of \( C \)
\( Q_e \) electric charge
\( Q \) flat-band Hamiltonian
\( r = (x, y, z) \) real-space coordinates
\( \hat{r} = (\hat{x}, \hat{y}, \hat{z}) \) position operator and its components
\( r = (r_x, r_y, r_z) \) additional set of orbital Pauli matrices
\( R \) point group operation (rotation)
\( \{ R | t \} \) affine transformation with rotation \( R \) and shift \( v \)
\( R \) Bravais vectors in 1D
\( R \) Bravais vectors in 2D and higher
\( \mathbb{R} \) real numbers
\( \mathbb{R} \) real part of a complex expression
\( \varrho = (\varrho_x, \varrho_y, \varrho_z) \) layer Pauli matrices
\( \rho \) group representation
\( \varrho \) density of states
\( \rho \) electrical resistance
\( s = (s_x, s_y, s_z) \) particle-hole Pauli matrices
\( s \) sign, \( s = \pm 1 \)
\( s \) spin magnitude, \( 2s \in \mathbb{Z} \)
\( S_{n,i} \) operator of \( n \)-fold screw rotation around coordinate \( i \)
\( S_{\xi}^{p,x} (k) \) functional in the description of SrPtAs lattice
\( S \) space group
\( SO(n) \) special orthogonal Lie group
\( Sp(2n, \mathbb{F}), Sp(n) \) symplectic group over \( \mathbb{F} \), and compact symplectic group
\( SU(n) \) special unitary Lie group
\( S^D \) \( D \)-dimensional sphere
\( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) spin Pauli matrices
\( \zeta = (\zeta_x, \zeta_y, \zeta_z) \) reduced particle-hole spin Pauli matrices
\( \sigma \) electrical conductivity
\( t \) time
\( t \) spin-independent hopping amplitude in a TB model
\( t = \{ t_1, t_2, t_3 \} \) set of vectors used in the description of SrPtAs lattice
\( t \) translation associated with non-symmorphic symmetry
\( T \) spin-dependent hopping amplitude (SOC) in a TB model
\( T = \{ T_i \}_{i=1}^3 \) set of vectors used in the description of SrPtAs lattice
\( T^D \) \( D \)-dimensional torus
\( \mathcal{T} \) time-reversal symmetry
Notations

\( \mathcal{T} \) composition of time-reversal with inversion, \( \mathcal{T} = \mathcal{T} \mathcal{I} \)

\( \mathcal{I} \) translation group of a crystalline lattice

\( \tau = (\tau_x, \tau_y, \tau_z) \) Pauli matrices of orbital degree of freedom

\( \tau \) relaxation time

\( u \) a generic unitary matrix

\( |u^a_k\rangle, u^a_k(r) \) cell-periodic part of Bloch ket-state in band \( a \) at \( k \)

\( \langle u^a |, u^a_k^*(r) \) the corresponding bra-state

\( u(n) \) Lie algebra of skew-Hermitian matrices

\( U \) \( (n + \ell) \times n \) matrix of occupied states (form columns)

\( U(n) \) Lie group of unitary matrices

\( \mathcal{U} \) a generic unitary matrix or operator, \( \mathcal{U} \in U(n) \)

\( \mathcal{U} \) matrix permuting Pauli matrices

\( \phi \) polar angle of spherical/polar coordinates

\( v \) velocity

\( v, w \) vectors of basis matrices for various symmetry classes

\( V \) phase space volume

\( \mathcal{V} \) (real space) volume

\( \phi_B, \phi_{\text{Zak}} \) geometric Berry/Zak phase

\( \Phi \) magnetic flux

\( \Phi_0 \) magnetic flux quantum, \( \Phi_0 = 2\pi\hbar/e \)

\( w \) winding number

\( \mathcal{W} \) Wilson loop operator

\( W \) Wannier orbitals

\( \mathcal{X} \) element of a Lie algebra

\( \mathcal{X} \) gauge transformation matrix, element of \( U(n) \)

\( \chi \) susceptibility, Lindhard function

\( Y \) Young modulus

\( \psi \) wave function

\( |\psi^a_k\rangle, \psi^a_k(r) \) Bloch wave function in band \( a \) with momentum \( k \)

\( \psi \) superconducting singlet order parameter

\( z_2 \) value of a \( \mathbb{Z}_2 \) invariant

\( \mathbb{Z} \) integers

\( \mathbb{Z}_p \) cyclic group of order \( p \) with binary operation \( "+" \)

\( \mathbb{Z}^+, \mathbb{Z}_0^+ \) positive integers, and non-negative integers

\( \omega_n \) special complex numbers in the description of SrPtAs

\( \Omega, \Omega^{ab}_i \) dual Berry curvature for \( D = 3 \) systems

\( \Omega, \Omega^a_i \) dual single-band Berry curvature in \( D = 3 \)

\( \mathcal{U}_n \) symplectic form of dimensions \( 2n \times 2n \)
Bibliography


# List of acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
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<tbody>
<tr>
<td>1D, 2D, 3D, 4D</td>
<td>1-dimensional, 2-dimensional, etc.</td>
</tr>
<tr>
<td>ANL</td>
<td>accidental nodal line/loop</td>
</tr>
<tr>
<td>AZ</td>
<td>Atland-Zirnbauer</td>
</tr>
<tr>
<td>AZ+I</td>
<td>centrosymmetrically extended AZ symmetry class</td>
</tr>
<tr>
<td>BdG</td>
<td>Bogolyubov-de-Gennes</td>
</tr>
<tr>
<td>BZ</td>
<td>Brillouin zone</td>
</tr>
<tr>
<td>CHS</td>
<td>chiral symmetry</td>
</tr>
<tr>
<td>CL</td>
<td>Cartan label</td>
</tr>
<tr>
<td>DFT</td>
<td>density functional theory</td>
</tr>
<tr>
<td>DOS</td>
<td>density of states</td>
</tr>
<tr>
<td>DSM</td>
<td>Dirac semimetal</td>
</tr>
<tr>
<td>FCC</td>
<td>face-centred cubic</td>
</tr>
<tr>
<td>HEP</td>
<td>high energy physics</td>
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<tr>
<td>INS</td>
<td>insulator</td>
</tr>
<tr>
<td>IPR</td>
<td>irreducible projective representation</td>
</tr>
<tr>
<td>IR</td>
<td>irreducible representation</td>
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<tr>
<td>Abbreviation</td>
<td>Full Form</td>
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<td>--------------</td>
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<tr>
<td>LHS</td>
<td>left-hand side</td>
</tr>
<tr>
<td>LL</td>
<td>Landau level</td>
</tr>
<tr>
<td>MR</td>
<td>magnetoresistance</td>
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<tr>
<td>NI</td>
<td>normal (non-topological) insulator</td>
</tr>
<tr>
<td>NL</td>
<td>nodal line/loop</td>
</tr>
<tr>
<td>NN</td>
<td>nearest neighbour</td>
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<tr>
<td>NNN</td>
<td>next-to-nearest neighbour</td>
</tr>
<tr>
<td>NSNL</td>
<td>non-symmorphic nodal line/loop</td>
</tr>
<tr>
<td>PHS</td>
<td>particle-hole symmetry</td>
</tr>
<tr>
<td>QHE</td>
<td>quantum Hall effect</td>
</tr>
<tr>
<td>SBZ</td>
<td>surface Brillouin zone</td>
</tr>
<tr>
<td>SC</td>
<td>superconductor/superconducting</td>
</tr>
<tr>
<td>SG</td>
<td>space group</td>
</tr>
<tr>
<td>SLS</td>
<td>sublattice symmetry</td>
</tr>
<tr>
<td>SOC</td>
<td>spin-orbit coupling</td>
</tr>
<tr>
<td>SRS</td>
<td>spin-rotation symmetry</td>
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<tr>
<td>TI</td>
<td>topological insulator</td>
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<tr>
<td>TRIM</td>
<td>time-reversal invariant momentum</td>
</tr>
<tr>
<td>TRS</td>
<td>time-reversal symmetry</td>
</tr>
<tr>
<td>WCC</td>
<td>Wannier charge center</td>
</tr>
<tr>
<td>WSM</td>
<td>Weyl semimetal</td>
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Philosophical Magazine 95, 609 (2015)
Acknowledgements

This work would not have reached its full blossom, were it not for the great many people that I interacted with during the four years I spent at ETH Zürich. This includes the group members that contributed to the stimulating atmosphere at the Institute for Theoretical Physics, my active collaborators, the frequent discussion partners, numerous visitors, and importantly all the people that “nudged” me in the right direction when I wondered what problems to tackle next.

First of all, I am grateful to my supervisor Manfred Sigrist for giving me the opportunity to enter this inspiring environment. Apart from sharing his knowledge on a variety of topics in superconductivity, solid state theory and group theory, he granted me much freedom to work on any problem I found interesting – even if it went outside the scope of physics. Manfred as a teacher served as a great role model, and, importantly, he always cared about a healthy work-life balance of his students. Manfred taught me to think of the academic network as of another kind of family.

Further words of gratitude belong to my collaborators. During the first two years of my PhD studies, Andreas Rüegg played a prominent role and strongly influenced the choice of problems that I worked on. Even after he left ETH for a job in a company, he kept regularly visiting our institute and spent his time critically assessing my ideas and results. His expertise in correlation effects and topological aspects of condensed matter systems was just too solid to wear off after leaving academia.

The later half of my studies was greatly nurtured by a collaboration with Alexey Soluyanov and Quan-Sheng Wu from the computational physics group of Matthias Troyer. Alexey had an excellent intuition about topological invariants, while Quan-Sheng was a wizard
with a wide range of numerical techniques. Their qualifications perfectly complemented my understanding of group theory and of tight-binding models. We often spent hours of fruitful discussions together, which eventually culminated in our publication in Nature. I want to remark that I admire Alexey’s affable attitude and his good sense of humour, which didn’t break after he was diagnosed the terrible health condition. I am indebted to Oded Zilberberg for bringing me in touch with Alexey. In addition, my research at various stages also significantly benefited from discussions with Alexander Balatsky, Chen Fang, Sebastian Huber, Sergej Moroz, Titus Neupert, Andreas Schnyder and the many visitors we had over the years.

Many of my colleagues took great care in keeping me from working too much on my projects. I would especially like to mention here Adrien Bouhon who taught me a great deal of group theory, Sarah Etter who explained me all there is about Ginzburg-Landau functionals and much else, Michael Fergusson for organizing plentiful free-time activities, Mark Fischer whose curiosity and talkativeness always led to a reason to procrastinate just a little bit more, Ye-Hua Liu for the discussions about machine learning, Evert van Nieuwenburg for teasing me with a multitude of riddles and bringing Project Euler to my attention, and Roland Willa who had a special interest in musical theory. Furthermore, Jonathan Buhmann helped me significantly to get around Zürich and ETH during the first few months of my PhD studies, and Markus Legner was repeatedly my favourite colleague for co-organizing exercise classes for students.

I very much enjoyed all the little discussions with Luca Papariello, Murad Tovmasyan, and Roman Süssstrunk who started their doctoral studies at the condensed-matter theory division at about the same time as me. Matteo Biondi and David Oehri were the best pals at the irregularly organized glass of beer (or two) after work. From the computational physics side, I very much enjoyed interactions with Dominik Gresch, Jakub Imriška, Juan Osorio, Kiryl Pakrouski, Hiroshi Shinaoka, Maryam Tahirinejad, Lei Wang, and Georg Winkler. The unique atmosphere in the condensed matter theory cluster would not be the same without its numerous further members, especially Adel Benlagra, Wei Chen, Rama Chitra, Dima Ivanov, Maciej Koch-Janusz, Andrei Lebedev, David Möckli, Paolo Molignini, Daniel Müller, Tudor Pahomi, Ioannis Petrides, Aline Ramirez, Sebastian Schmidt, Antonio Štrkalj, Tobias
Wolf, Nobuyuki Yoshioka, Sina Zeytinoglu, Bastian Zinkl and professors Gianni Blatter, Dima Geshkenbein, and Maurice Rice.

Of course, I would not have been at ETH without the many people that influenced my life along the way. My special thanks go to my parents, Vladimír and Anna, who taught me to value education above all else. My physics training was greatly nurtured especially by Ivo Čáp, Vlado Černý, Marián Fecko, Tomáš Kulich, Milan Maro, Peter Maták, Martin Mojžiš, Lubomír Mucha, Juraj Tekel, and Jakub Závodný. Professor Richard Hlubina was my advisor at the Comenius University in Bratislava for four years, and suggested me to spend some time at ETH Zürich as a visiting student, which had a profound impact on the way I perceive science and education today.

Finally, I am greatly indebted to my wife, Karolína. She has never stopped supporting my childish curiosity for physics, even when it led me to spend long nights at work or weeks on conferences away from home. Karolína, you played the most important role of all.

Tomáš Bzdušek
Zürich, 9 June 2017