Utrecht University

# Topology of Weyl semimetals
## with non-orientable Brillouin zones

by

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A thesis

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# Abstract

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# Chapter 1

# Introduction

Example citation.[Fon+24] Example expanded citation.[MT17, Remark 3.8]

## 1.1 Main results

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## 1.4 Notational conventions

# Chapter 2

# Topological states of matter & symmetries

Sources:[Akh+][AOP16][BH13]

Finish intro when chapter is more complete

## 2.1 Basic definitions

- Conductive properties of materials are understood in terms of band structure → Fermi energy. Conductance means Fermi level lies inside one of the bands. [picture]
- $N$-band system has hilbert space $\mathcal{H} \cong \mathbb{C}^N$, Hamiltonian represented by $N \times N$ matrix. Static system: $H\psi = E\psi$, eigenvalues are energy bands.
- Mostly interested in 2-band systems since only valence/conduction bands are relevant. Then $H$ is a $2 \times 2$ Hermitian (for now) matrix. These are given by $H = h_0\mathbb{I} + \mathbf{h} \cdot \boldsymbol{\sigma}$ in general; $h_0$ corresponds to the Fermi level and can be normalized to 0. [understand this better] → Bloch Hamiltonian [higher dimensional systems: Clifford algebra]
- For a Bloch Hamiltonian, eigenvalues are $\pm|\mathbf{h}|$, so conductance occurs when $\mathbf{h} = 0$.
- Insulating Hamiltonians are adiabatically connected if they can be continuously deformed into each other without band crossings. Insulators are considered topological if they are not adiabatically connected to a reference trivial phase; then these inhabit different regions of the phase diagram → existence of edge states (not always[BH13], footnote)

### 2.1.1 Bloch theory

- We work with crystalline materials which are composed of periodically repeating unit cells.

- In the bulk, we assume the Hamiltonian is periodic in the unit cell. This enables use of Bloch's theorem[Blo29] $\psi(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$.
- Different values of crystal momentum may yield identical eigenstates, the set of equivalence classes is the Brillouin zone
- Brillouin zone usually has $\mathbb{T}^n$ topology, but internal symmetries etc. may alter this[Fon+24] [other sources]

## 2.2 One-dimensional models

- SSH is usually introduced "physics first", but we would like to work backwards in a sense, to see how bulk topology gives rise to physical properties of a system.

### 2.2.1 The Su–Schrieffer–Heeger model

- Start with an infinite 1D chain of unit cells; then the Brillouin zone has $S^1 \cong [-\pi, \pi] / \{ -\pi \sim \pi \}$ topology
- Parametrizing the Hamiltonian by $\mathbf{h}(k)$ gives a map $\mathbf{h} : S^1 \to \mathbb{R}^3$, and restricting to insulators gives $\mathbf{h} : S^1 \to \mathbb{R}^3 \setminus \{ 0 \}$.
- However, $\pi_1(\mathbb{R}^3 \setminus \{ 0 \}) = 0$ and so all insulating Hamiltonians are adiabatically connected
- We can fix this by imposing $h_z = 0$, so that effectively $\mathbf{h} : S^1 \to \mathbb{R}^2 \setminus \{ 0 \}$, with fundamental group $\mathbb{Z}$ indexed by winding number around the origin. We will see that this amounts to imposing a physical symmetry.
- Start with the simplest topologically trivial state $\mathbf{h}_{\mathrm{triv}}(k) = (1, 0, 0)^{\mathsf{T}}$ and the simplest topologically interesting state $\mathbf{h}_{\mathrm{top}}(k) = \big(\cos(k), \sin(k), 0\big)^{\mathsf{T}}$. We choose these combinations of $x$, $y$, $z$ conveniently to arrive at the SSH but in principle any similar model would be equivalent by change of basis.
- Now make a linear combination $\mathbf{h}(k) = v\mathbf{h}_{\mathrm{triv}}(k) + w\mathbf{h}_{\mathrm{top}}(k)$. This is trivial when $v > w$, conducting when $v = w$ and topological when $v < w$. [picture]
- The momentum-space Hamiltonian is now

$$H(k) = \begin{pmatrix} 0 & v + w\mathrm{e}^{-ik} \\ v + w\mathrm{e}^{ik} & 0 \end{pmatrix}.$$

  For FT we can suggestively rewrite as

$$H(k) = \mathrm{e}^{-ik(n-n)} \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix} + \mathrm{e}^{-ik\big((n+1)-n\big)} \begin{pmatrix} 0 & w \\ 0 & 0 \end{pmatrix} + \mathrm{e}^{-ik\big(n-(n+1)\big)} \begin{pmatrix} 0 & 0 \\ w & 0 \end{pmatrix}$$

  where $n$ is the unit cell index.

- It follows [how exactly?] that we can write the Hamiltonian in a unit cell basis as

$$\hat{H} = \sum_{n=-\infty}^{\infty} \left[ |n\rangle\langle n| \otimes \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix} + \left( |n+1\rangle\langle n| \otimes \begin{pmatrix} 0 & w \\ 0 & 0 \end{pmatrix} + \text{h.c.} \right) \right]$$

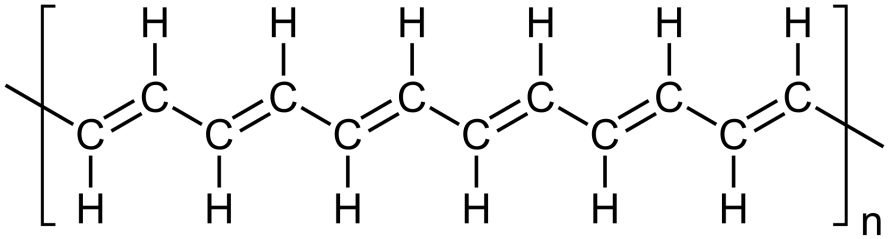
- We can introduce a boundary by setting finite $N$ with open BC:

$$\hat{H} = \sum_{n=0}^{N} |n\rangle\langle n| \otimes \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix} + \sum_{n=0}^{N-1} \left( |n+1\rangle\langle n| \otimes \begin{pmatrix} 0 & w \\ 0 & 0 \end{pmatrix} + \text{h.c.} \right)$$

- This case can be represented as

$$\hat{H} = \begin{pmatrix} 0 & v & 0 & 0 & & & & & & \\ v & 0 & w & 0 & & & & & & \\ 0 & w & 0 & v & & & & & & \\ 0 & 0 & v & 0 & & & & & & \\ & & & & \ddots & & & & & \\ & & & & & 0 & 0 & & & \\ & & & & & w & 0 & & & \\ & & & & & 0 & w & 0 & v & \\ & & & & & 0 & 0 & v & 0 & \end{pmatrix}$$

- This looks like a chain of length 2N with alternating hopping amplitudes, meaning we can realize the system in terms of unit cells with two atoms, intra-cell hopping $v$ and inter-cell hopping $w$. This is realised in e.g. polyacetylene:




- The trivial $v > w$ case has strong hopping within the cells, including to and from the edge modes. The conducting $v = w$ phase is just a chain of equal hoppings, and the topological $v < w$ has weaker hopping inside the cells so that the edge modes become isolated.

- We can now physically interpret the meaning of setting $h_z = 0$: it ensures that hopping only occurs between the two sublattices $A$ and $B$, and not within them (i.e. there are only off-diagonal elements in the internal degrees of freedom). If we define the sublattice projection operators

$$\hat{P}_A = \mathbb{I} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{P}_B = \mathbb{I} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

then the Hamiltonian obeys

$$\hat{P}_A \hat{H} \hat{P}_A = \hat{P}_B \hat{H} \hat{P}_B = 0$$

and so since $\hat{P}_A + \hat{P}_B$ is the identity we have

$$\begin{aligned} \hat{H} &= (\hat{P}_A + \hat{P}_B)\hat{H}(\hat{P}_A + \hat{P}_B) \\ &= \hat{P}_A \hat{H} \hat{P}_B + \hat{P}_B \hat{H} \hat{P}_A \\ &= (\hat{P}_A - \hat{P}_B)\hat{H}(\hat{P}_B - \hat{P}_A) \\ &\equiv -\hat{\Gamma} \hat{H} \hat{\Gamma} \end{aligned}$$

with $\hat{\Gamma} \equiv \hat{P}_A - \hat{P}_B$ having the property that $\hat{\Gamma} = \hat{\Gamma}^{-1} = \hat{\Gamma}\dagger$; this is called sublattice symmetry and it also applies to the momentum space Hamiltonian $H(k)$.

- An immediate consequence of our setup is that the trivial and topological phase become adiabatically connected if we allow for sublattice symmetry breaking ($h_z \neq 0$).

Expand more on boundary states

### 2.2.2 The Kitaev chain

## 2.3 Two-dimensional models

### 2.3.1 The Kane–Mele model

### 2.3.2 Quantum Hall effect

# Chapter 3

# Weyl semimetals

## 3.1 Physics perspective

## 3.2 Mathematics perspective

# Chapter 4

# Non-orientable manifolds

## 4.1 Mathematical exploration

Concepts explored in personal notes so far:

- Calculations of (co)homology and semimetal MV sequence for manifolds in $\geq 2$ dimensions:
  - All compact surfaces without boundary, i.e. the surfaces $M_g$ and $N_g$
  - All spaces of the form $M = K^2 \times \mathbb{T}^{d-2}$
- The map $\Sigma : H^{d-1}(\bigsqcup_k S^{d-1}) \to H^d(M)$ in the semimetal MV has a clear interpretation in terms of total charge in the (orientable) $d = 3$ case. This would provide a clear picture of the total charge cancellation in the orientable case ($H^d(M) = \mathbb{Z}$ in general) vs. the mod 2 charge cancellation in the non-orientable case ($H^d(M) = \mathbb{Z}_2$ in general).
- However, $\Sigma$ and the other maps in the MV sequence are difficult to interpret in the $\chi \neq 0$ case (maybe even generally for odd dimensions). Taking the oriented case as an example, the MV sequence ends as

$$H^{d-1}(M \setminus \Delta) \;\to\; H^{d-1}\left(\bigsqcup_k S^{d-1}\right) \cong \mathbb{Z}^k \;\xrightarrow{\Sigma}\; H^d(M) \cong \mathbb{Z}$$

  so that the "charge configuration" in $\mathbb{Z}^k$ must map to 0 by $\Sigma$ in order to descend from the semimetal, regardless of whether $\chi = 0$.
- This may imply that the Bloch vector field carries more topological information about the total charge than the MV sequence (which makes sense since it generates *all* homology groups of the valence bundle, and all Betti numbers factor into $\chi$). As a concrete example, consider $M = S^2$ with a single puncture of charge $+2$. The punctured sphere is topologically a disc, so that the valence bundle must be trivial, while the Bloch vector field is topologically non-trivial in the sense that it has an

index +2 singularity. In addition, all relevant $H_n(A) \oplus H_n(B)$ are zero, so that the semimetal MV reduces to the statement that $H_2(S^2) \cong H_1(S^1)$.

- It may even be the case that the valence bundle cannot be generated from the Bloch vector field in the $d = 2$ case; it's probably worth studying the $d \in \{3, 4, 5\}$ cases (pullback of some universal bundle) to learn more about this. The $d = 3$ case should be especially helpful in understanding how the valence bundle arises from the vector field.

- A complicating factor in the non-orientable case is that the homology groups are different from the cohomology groups, since the torsion moves up one dimension. This makes the homological semimetal MV different from the cohomological one (it's a short exact sequence in $d \geq 3$!), and this leads to additional challenges in interpretation.

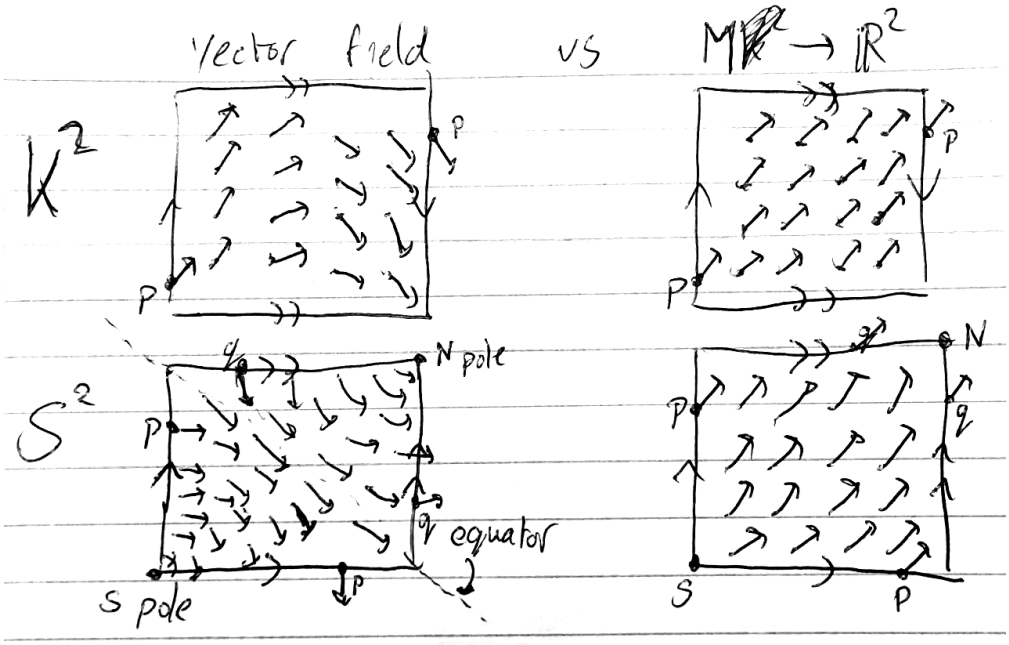
- The map $H : \mathbb{R}^3 \to \mathfrak{su}(2)$, $\vec{h} \mapsto \vec{h} \cdot \vec{\sigma}$ is an isomorphism of Lie algebras, with the cross product as a Lie bracket on $\mathbb{R}^3$. Still the vector field is discontinuous on a non-orientable manifold, while $H$ is not. This suggests an alternative approach for constructing the valence bundle: consider $h$ as a map $M \to \mathbb{R}^d$ instead of an element of $\mathfrak{X}(M)$, and then pull back the universal bundle along the unit map $\hat{h} : M \setminus \Delta \to S^{d-1}$. That is, we detach $\vec{h}$ from the tangent bundle and consider it a more abstract map. An added "benefit" of this is that we lose all coordinate dependence. However, this may also be a downside in the sense that the map will not be subject to the same constraints (Poincaré–Hopf etc.) that the vector field is; for example, $S^2 \to \mathbb{R}^2$, $x \mapsto (1, 0)$ is a perfectly valid map that would violate the hairy ball theorem as a vector field (and this is a result of being unable to cover $S^2$ by a single chart). At this point the question may become more about which description is more physical in nature, and the non-orientable Weyl point paper[Fon+24] seems to imply there may be more to the $h : M \to \mathbb{R}^3$ story. It also seems to agree better with the intuition of an applied external potential removing all Weyl nodes – something that's impossible for $\chi \neq 0$ if charge corresponds to vector field index. It also explains how the valence bundle can be trivial on the once punctured $S^2$.

- In light of the previous point, this may be an important observation: every $d$-manifold $M$ with $\chi(M) = 0$ admits a nowhere-vanishing vector field (link). ~~This may imply that the vector field description is equivalent to the map to $\mathbb{R}^d$ in these cases, though one needs to be careful about charts. It would be good to find or write a (dis)proof for something like $\mathfrak{X}(M) \cong C^\infty(M, \mathbb{R}^d)$ (or similar for non-vanishing maps) in this case. Or more specifically:~~

$$~~\left[M \setminus \Delta, S^{d-1}\right] \overset{?}{\cong} \left\{ \vec{h} \in \mathfrak{X}(M \setminus \Delta) \,\middle|\, \vec{h} \text{ is non-vanishing} \right\}~~$$

Update: I think the real requirement for equivalence is that the base manifold $M$ is parallelisable (i.e. has a trivial tangent bundle), since we're essentially using a trivial $\mathbb{R}^d$-bundle in this construction.

- Any smooth $d$-manifold can be given a CW complex structure with one $d$-cell (link). On this $d$-cell there is an exact correspondence between vector fields and maps to $\mathbb{R}^d$, since it can be embedded in $\mathbb{R}^d$. What distinguishes the two is how points on the boundary of the $d$-cell are identified with each other; this determines whether the "vectors" need to change orientation. To illustrate:




- On any orientable manifold, the Stokes' theorem argument shows that the total charge must be zero regardless of Euler characteristic:

$$\sum_\alpha w(S_\alpha) = \sum_\alpha \int_{S_\alpha} c_1(E) = \sum_\alpha \int_{S_\alpha} \frac{\operatorname{Tr}\mathcal{F}}{2\pi} = \int_{B'} \mathrm{d}\frac{\operatorname{Tr}\mathcal{F}}{2\pi} = 0$$

  where the last equality holds by the Bianchi identity for the trace. This means the valence bundle cannot be a pullback along a tangent vector field for $\chi \neq 0$.

  On a non-orientable manifold, this argument doesn't hold since the integral over $B'$ isn't well defined.

## 4.2 Physical implications

# Appendix A

# Homology and cohomology

# Bibliography


[Akh+] Anton Akhmerov et al. *Online course on topology in condensed matter*. URL: https://topocondmat.org/ (visited on 10/07/2024).

[AOP16] János K. Asbóth, László Oroszlány, and András Pályi. *A Short Course on Topological Insulators*. Springer International Publishing, 2016. ISBN: 9783319256078. DOI: 10.1007/978-3-319-25607-8. URL: http://dx.doi.org/10.1007/978-3-319-25607-8.

[BH13] B. Andrei Bernevig and Taylor L. Hughes. *Topological insulators and topological superconductors*. Princeton University Press, 2013. ISBN: 978-0-691-15175-5.

[Blo29] Felix Bloch. "Über die Quantenmechanik der Elektronen in kristallgittern". In: *Zeitschrift für Physik* 52.7–8 (July 1929), pp. 555–600. DOI: 10.1007/bf01339455.

[Fon+24] André Grossi Fonseca et al. "Weyl Points on Nonorientable Manifolds". In: *Phys. Rev. Lett.* 132 (26 June 2024), p. 266601. DOI: 10.1103/PhysRevLett.132.266601. URL: https://link.aps.org/doi/10.1103/PhysRevLett.132.266601.

[MT17] Varghese Mathai and Guo Chuan Thiang. "Differential Topology of Semimetals". In: *Communications in Mathematical Physics* 355.2 (July 2017), pp. 561–602. ISSN: 1432-0916. DOI: 10.1007/s00220-017-2965-z. URL: http://dx.doi.org/10.1007/s00220-017-2965-z.