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

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Topological states of matter & symmetries

Sources: [Akh+; AOP16; BH13; SA17]
Topo phases occur in nature: [Geh+13]
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 2×2 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

We will take the approach of deriving the Su–Schrieffer–Heeger (SSH) model by beginning with a generic one-dimensional crystal, and trying to make it topologically interesting the simplest way we can.

To begin with, we assume that the crystal extends infinitely in both directions. We will introduce a boundary later, but its relevant properties will turn out to be determined by the crystal's bulk topology. Concretely, we have a one-dimensional chain of unit cells indexed by $n \in \mathbb{Z}$; at this point, we do not make any assumptions on the internal structure of these unit cells. We require that the real-space Hamiltonian of the system is periodic in these unit cells, so that by Bloch's theorem, two crystal momenta k and k' are equivalent if they differ by an integer multiple of 2π. This means we can take our Brillouin zone B to be the interval $[-\pi, \pi]$ with the points $-\pi$ and π identified, which is homeomorphic to S^1.

We might begin with a simple 2 band Bloch Hamiltonian $H(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma}$, with

$$\mathbf{h} : B \cong S^1 \to \mathbb{R}^3, \quad k \mapsto \begin{pmatrix} h_x(k) \\ h_y(k) \\ h_z(k) \end{pmatrix}.$$

Such a Hamiltonian describes a gapped phase precisely when the map $\mathbf{h}$ is nowhere vanishing, so that the topological classification of these phases is given by classes of maps from S^1 to $\mathbb{R}^3$ minus the origin—that is, homotopy classes of loops in $\mathbb{R}^3 \setminus \{0\}$. But this space has a trivial fundamental group $\pi_1\big(\mathbb{R}^3 \setminus \{0\}\big) \cong 0$, meaning all such loops can be

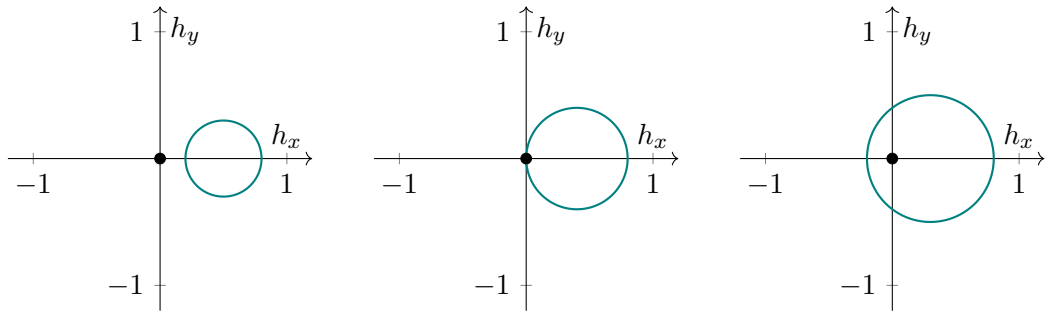
contracted to a point; in other words, all gapped phases are adiabatically connected, and there are no topologically interesting phases.

To remedy this situation, we impose a constraint on the Hamiltonian: we require that $h_z(k) = 0$, so that we effectively have a map $S^1 \to \mathbb{R}^2$. The gapped phases are now classified by the group $\pi_1\big(\mathbb{R}^2 \setminus \{\,0\,\}\big) \cong \mathbb{Z}$, indexed by winding number: loops that wind around the origin $a \in \mathbb{Z}$ times cannot be deformed into those with a different winding number $b \neq a$. In particular, loops with a non-zero winding number cannot be contracted to a point, and the associated phases are considered topological. Note that imposing a constraint on the Hamiltonian has made this system topologically interesting; once we move to the physical picture, we will see that this really amounts to imposing a certain symmetry on the system.

To arrive at a concrete physical system, let us begin with the simplest possible* distinct states, one trivial and one topologically interesting:

$$\mathbf{h}_{\text{triv}}(k) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{h}_{\text{top}}(k) = \begin{pmatrix} \cos(k) \\ \sin(k) \\ 0 \end{pmatrix}.$$

To characterise a phase transition between these two states, we look at the linear combination $\mathbf{h}(k) = v\mathbf{h}_{\text{triv}}(k) + w\mathbf{h}_{\text{top}}(k)$, with $v, w \geq 0$. The phase described by the resulting Bloch Hamiltonian is trivial when $v > w$, gapless (i.e. conducting) when $v = w$, and topological when $v < w$; see Figure 2.1.



(a) $v = 0.5$, $w = 0.3$ (b) $v = w = 0.4$ (c) $v = 0.3$, $w = 0.5$

Figure 2.1: Contours in Hamiltonian space for (a) trivial, (b) conducting and (c) topological phases.

Now that we have a simple setup, it's time to analyse the physics. Concretely, the momentum space Hamiltonian is given by

$$H(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma} = \big(v + w\cos(k)\big)\sigma_x + w\sin(k)\sigma_y = \begin{pmatrix} 0 & v + w\,\mathrm{e}^{-ik} \\ v + w\,\mathrm{e}^{ik} & 0 \end{pmatrix}.$$

*Of course, our choice of x, y, and z coordinates very conveniently sets us up to arrive at the SSH model. However, mathematically speaking, all similar models are related by a simple change of basis.

We can set up a Fourier transform to real space by rewriting this suggestively in terms of the unit cell index n:

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

I need to work out the details of this Fourier transform later, my calculations aren't working out. Transforming from a periodic Brillouin zone to (discrete or infinite) real space is breaking my brain. I imagine it needs to look something like this (where $M_{0/\pm1}$ are the three matrices above):

$$\begin{aligned}
\hat{H} &= \int_B H(k) \left|k\right\rangle \left\langle k\right| \\
&= \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \left(\sum_{a\in\{0,\pm1\}} \mathrm{e}^{-ika} M_a \right) \left(\sum_n \mathrm{e}^{-ikn} \left|n\right\rangle \right) \left(\sum_{n'} \left\langle n'\right| \mathrm{e}^{ikn'} \right) \\
&= \sum_{a,n,n'} \left(\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{-ik(a+n-n')} \right) M_a \left|n\right\rangle \left\langle n'\right| \\
&= \sum_{a,n,n'} \delta_{n+a,n'} M_a \left|n\right\rangle \left\langle n'\right| \\
&= \sum_{a,n} M_a \left|n\right\rangle \left\langle n+a\right|
\end{aligned}$$

But I don't fully understand the first step, the sign of a is wrong and normalization is broken. Maybe it's easier to discretize first and do a DFT?

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

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

- Mention tight binding somewhere around this point

It's clear that we have a term parametrized by v which acts within the unit cells, and terms depending on w which act between neighbouring unit cells. To further elucidate the structure of these interactions, we go to a finite chain of length N; the Hamiltonian then becomes

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

where we've introduced open boundary conditions on the ends of the chain, allowing us to study the boundary behaviour in a moment. We can then expand the tensor product

in order to cast the Hamiltonian into a full $2N \times 2N$ matrix:

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

A clear interpretation of this system presents itself to us immediately: it describes a chain of $2N$ sites, with alternating hopping amplitudes v and w between neighbouring sites. The unit cells now consist of two of these sites, and v and w are referred to as the *intra-cell* and *inter-cell* hoppings, respectively. In particular, the gapless phase $v = w$ corresponds to a chain where all hoppings are equal; intuitively, this allows electrons to move around freely along the chain, whereas they are confined around the stronger hoppings in the insulating cases.

The division of our unit cells into two sites allows us to distinguish two *sublattices* of the crystal, which we label A and B. We then simplify our notation by labelling quantum states according to the sublattice that they are localized to:

$$|n, A\rangle \equiv |n\rangle \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |n, B\rangle \equiv |n\rangle \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In this notation, our Hamiltonian becomes

$$\hat{H} = \left(\sum_{n=0}^{N} v \, |n, B\rangle \langle n, A| + \sum_{n=0}^{N-1} w \, |n+1, A\rangle \langle n, B| \right) + \text{h.c.} \tag{2.1}$$

The picture of alternating hoppings that we have arrived at is precisely the original motivation for this model: it was first introduced in 1979 by Wu-Pei Su, John Robert Schrieffer, and Alan J. Heeger in order to study the properties of polyacetylene (Figure 2.2), a polymer chain which features alternating single and double covalent bonds [SSH79; SSH80]. This material displays unexpectedly high conductivity when doped with halogen impurities, and the SSH model helps explain this behaviour.

To understand how this conductive behaviour comes about, we need to examine the differences between the trivial and the conductive phase somewhat more closely. At a first glance, the two phases appear to be identical: if we choose the unit cell in polyacetylene in such a way that the stronger double bond represents the intra-cell hopping v, then we are in the trivial phase $v > w$, and if we center the unit cell around a single bond, we have $v < w$ and the phase is topological. In either case we expect valence electrons to remain localized around the double bonds, leading to the same insulating bulk behaviour.[†]

[†]The attentive reader might wonder why the conductive $v = w$ phase does not occur naturally in this

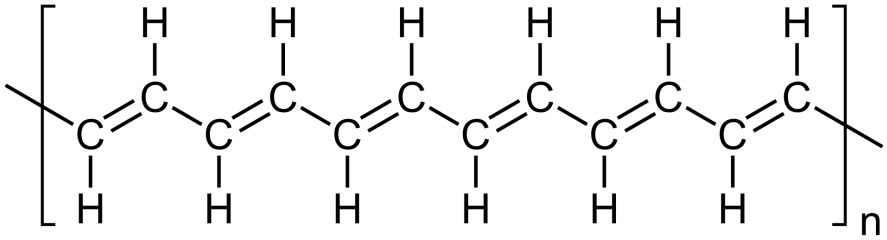


Figure 2.2: Structural diagram of polyacetylene. Electrons are transported more readily along the double bonds, which is modelled using a larger hopping potential.

The difference between the two phases only becomes apparent when we look at the endpoints of the chain. For example, the leftmost atom is not subject to any inter-cell hopping, and it is only connected to the other atom in its unit cell. In the trivial case this connection is strong and the two atoms share their valence electrons. On the other hand, in the topological phase the second atom from the left prefers to share electrons with its right-hand neighbour, and the leftmost atom becomes isolated. In the limit where v goes to zero, this isolation becomes complete and the edge sites carry zero-energy eigenstates: in this case only the second term in the Hamiltonian (2.1) survives, and we have

$$\hat{H}\,|1, A\rangle = \hat{H}\,|N, B\rangle = 0.$$

Even for non-zero v the topological phase has edge modes, which can be shown to become highly localized and approach zero energy in the $N \to \infty$ limit. The exact mechanics of this are beyond the scope of this review; the interested reader is referred to e.g. [AOP16]. The salient point is that the boundary modes of the chain are gapless: their energy eigenvalues have a degeneracy at the Fermi level $\varepsilon_F = 0$.

Something remarkable has happened: we have started from a topological description of a gapped bulk phase, and the resulting physical effects appear as gapless edge modes on the boundary of the material. As we will see, this is a fairly[‡] general feature of topological phases of matter, called the *bulk-boundary correspondence*. We can think of it as being a result of the inability to go continuously from a topological gapped phase to a trivial one in real space; in particular, the outside boundary of an idealised material connects to the vacuum, which is also considered a trivial gapped phase.

- Discuss physics of polyacetylene (solitons on trivial/topological interface) and experimental observations of solitons + berry phase [MAG16; Ata+13]

system. This is a result of the so-called Peierls transition: in a nutshell, introducing a band gap locally lowers the energy of the (filled) valence band and raises that of the (empty) conduction band. This makes it energetically favourable for atoms in the chain to pair up, in a process referred to as dimerisation.

[‡]This is not a completely general statement: topological phases with gapped edge modes have been shown to be theoretically feasible [Fre+04]. For our purposes, it will do to restrict our attention to the gapless edge modes.

- 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 ($h_z \neq 0$).

- Talk more about $\mathbb{Z}$ invariant (next nearest neighbour hopping etc.)

2.2.2 The Kitaev chain

- Introduce Majorana modes
- Talk about superconductivity
- Discuss $\mathbb{Z}_2$ invariant vs. $\mathbb{Z}$ for SSH topologically

2.3 Two-dimensional models

2.3.1 Quantum Hall effect

2.3.2 The Kane–Mele model

2.4 Classification of symmetries

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 ≥ 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, Σ 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 Σ 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 χ). 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.

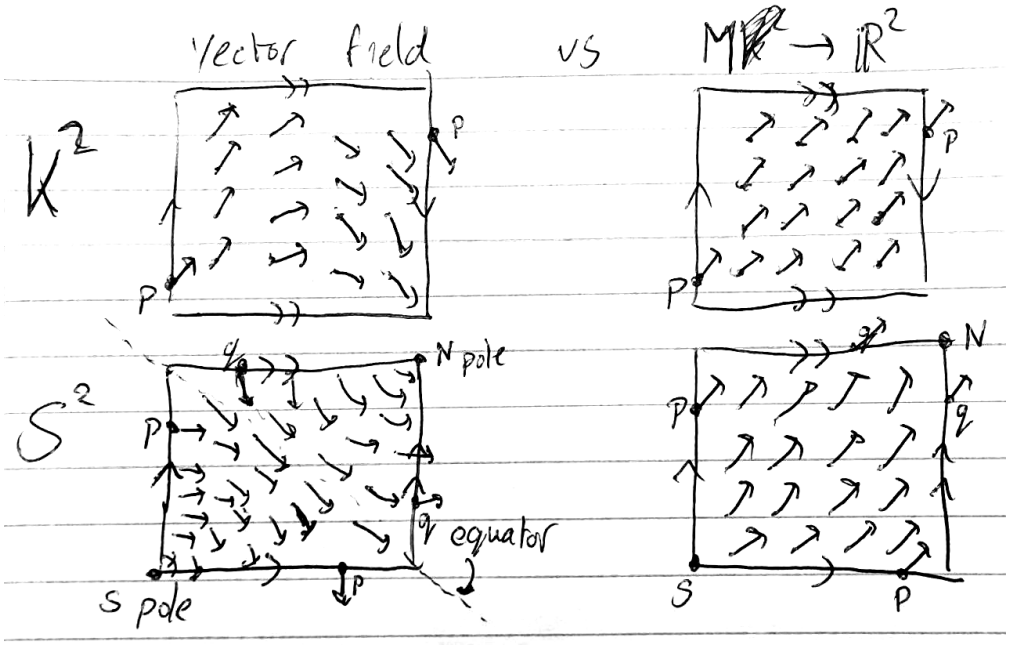
- The map $H : \mathbb{R}^3 \to \mathfrak{su}(2)$, $\vec{h} \mapsto \vec{h} \cdot \vec{\sigma}$ is an isomorphism of Lie algebras, with the cross product as a Lie bracket on $\mathbb{R}^3$. Still the vector field is discontinuous on a non-orientable manifold, while H is not. This suggests an alternative 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.

- Total chirality isn't well defined on a non-orientable manifold (at least in odd dimensions, not sure how to interpret even dimensions). Still there is charge cancellation in the form of Fermi arcs etc.; it may take moving to a different homology system to get the full picture, such as homology with local coefficients or equivariant homology. (See e.g. [TSG17])

- It may be worth classifying which manifolds are candidates for physical material Brillouin zones; I have a feeling that this might be restricted to those manifolds for which the n-torus is a covering space. In this case a full classification of symmetries

on the torus (and e.g. their related equivariant homologies) would be sufficient to classify all material topologies.

4.2 Physical implications

Appendix A

Homology and cohomology

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