From topological insulators to semimetals:

Some mathematical challenges

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Topological matter, strings, K-theory, and related areas

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Overview

Gapped phases, e.g. topological insulators, can be classified by bundle invariants $\rightarrow$ noncommutative/twisted/equivariant (KR)-cohomology invariants. Experiments: late 2000s.

Topological Weyl semimetals were experimentally realised in 2015/16, and advertised as the elusive "Weyl fermion". General mathematical characterisation still lacking.

[M+T, arXiv:1607.02242] Globally, topological semimetals realise invariants of "singular" bundles, connection to insulators is an extension problem. Tools: MV-principles, generalised degree theory, gerbes, Clifford modules...

Relativistic fermions and Clifford algebra

Convention. $Cl_{r,s}$ is real Clifford algebra, anticommuting $e_1, \ldots, e_r$ squaring to -1 and $e_{r+1}, \ldots, e_s$ squaring to $+1$. $\mathbb{C}l_n$ is complex Clifford algebra on n generators.

Elementary particles $\leftrightarrow$ unitary irreps of Poincaré group. Solutions to relativistic wave eqn provide examples, and can be built from irreps of $\mathrm{SL}(2, \mathbb{C}) \cong \mathrm{Spin}(3, 1) \xrightarrow{\text{2 to 1}} \mathrm{SO}_0(3, 1)$.

$\mathrm{Spin}(3, 1) \subset \mathrm{Cl}^+_{3,1} \subset \mathbb{C}\mathrm{l}_4$ and $\mathbb{C}\mathrm{l}_4 \cong M_4(\mathbb{C})$ has a unique irrep on $S \cong \mathbb{C}^4$ (Dirac spinor). Clifford multiplication is implemented by the 4×4 gamma matrices γ^μ satisfying $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$.

The chirality element $\gamma^5 := \mathrm{i}\gamma^0\gamma^1\gamma^2\gamma^3$ commutes with $\mathrm{Spin}(3, 1)$, decomposing $S = S^L \oplus S^R$, $\psi = (\psi_L, \psi_R)$ according to its ±1-eigenspaces. The spin irreps $S^{L/R}$ are the two-component left/right handed Weyl spinors.

Relativistic Dirac and Weyl equations

Massive Dirac equation is $(\not{D} - m)\psi = 0$ where $\not{D} = \mathrm{i}\gamma^\mu \partial_\mu$ is the Dirac operator. When $m = 0$, the massless Dirac equation decouples into two independent Weyl equations

$$\not{D}^L \psi_L = 0, \qquad \not{D}^R \psi_R = 0,$$

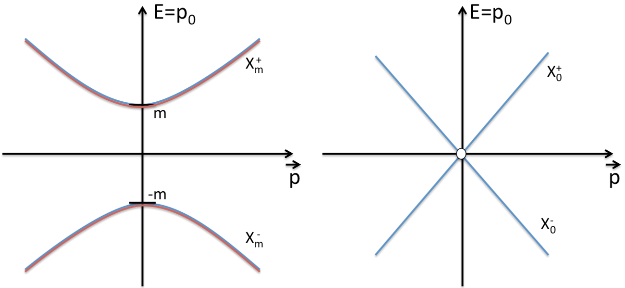
where $\not{D}^{L/R} := \mathrm{i}\partial_0 \underbrace{\mp \mathrm{i}\sum_{i=1}^{3} \sigma^i \partial_i}_{\text{Weyl Hamiltonian}}$ and σ^i are the Pauli matrices.

Fourier transform $\mathrm{i}\partial_\mu \mapsto p_\mu$ turns the Weyl Hamiltonians into

$$H^{L/R}(\vec{p}) = \pm p_i \sigma^i \in M_2(\mathbb{C}), \qquad \vec{p} = (p_1, p_2, p_3) \in \widehat{\mathbb{R}^3}.$$

Weyl Hamiltonian dispersion

Eigenvalues of $H^{L/R}(\vec{p})$ are $E(\vec{p}) = \pm|\vec{p}| \Rightarrow$ linear dispersion. Degenerate zero-energy mode at $|\vec{p}| = 0$. Symmetry of the spectrum — particle/antiparticle pairs.



Condensed matter "Weyl fermions" come from H which look locally like $H^{L/R}$. Important differences: (1) quasi-momentum $k \in \mathbb{T}^3$ rather than $\vec{p} \in \widehat{\mathbb{R}^3}$, (2) non-isotropic dispersion, (3) Weyl charges annihilate instead of forming a Dirac spinor.

Condensed matter Weyl fermion

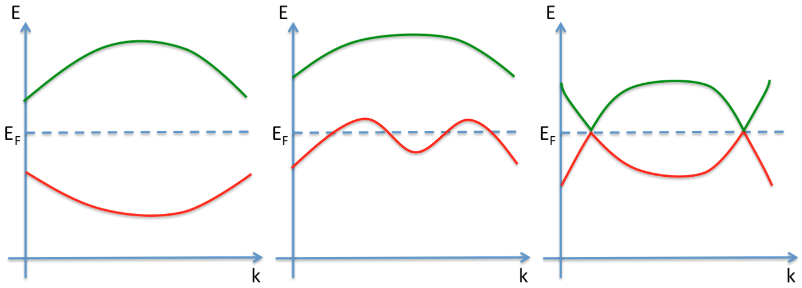
Electron motion in a crystalline material is described by a $\mathbb{Z}^d$-invariant Hamiltonian H acting on $L^2(\mathbb{R}^d)$. Brillouin zone of quasi-momenta in solid-state physics is topologically the Pontryagin dual torus $\mathbb{T}^d = \widehat{\mathbb{Z}^d}$.

Bloch–Floquet transform turns H into a (smooth/cts) family of of Bloch Hamiltonians $H(k)$ on a Hilbert bundle whose fibre at $k \in \mathbb{T}^d$ comprises the k-quasiperiodic Bloch wavefunctions.

One generally studies the restriction of $H(k)$ to a finite-rank low-energy subbundle $\mathcal{S}$ (or uses tight-binding model).

We're interested in (smooth/cts) families of finite-dimensional Hamiltonians. Could be Bloch, or just some parametrised family.

Bloch Hamiltonians

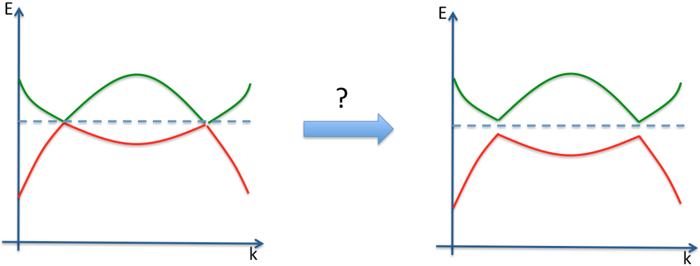


Spec(H) form energy bands, $E_{\text{Fermi}} \Rightarrow$ insulator/metal/semimetal (L to R). Energy dispersion near a two-band crossing looks linear, so the quasiparticle excitations $\sim$ Weyl fermions (allegedly).

Insulators: Fermi proj. onto $E < E_{\text{Fermi}}$ defines a valence subbundle $\mathcal{E}_F \subset \mathcal{S}$ (in a bundle category determined by symmetries).
Semimetals: $\mathcal{E}_F$ only defined on complement of crossings W.

Semi-metal or insulator?

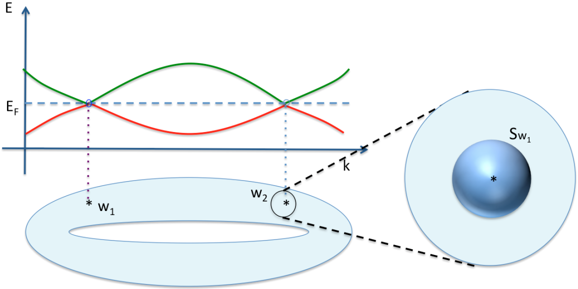
Can a semi-metal can be perturbed into an insulator?



This is not simply a matter of modifying the spectrum $E(k)$. In fact, there are local and global topological obstructions to modifying $H(k)$ in order to "open a gap", so semimetal band structures can be very robust!

Basic two-band Weyl semimetal in 3D — Sketch

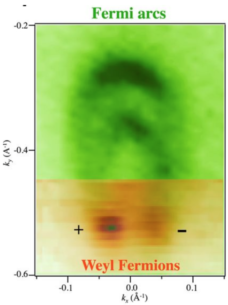
2×2 traceless $H(k) = \boldsymbol{h}(k) \cdot \boldsymbol{\sigma} \equiv \sum_{i=1}^{3} h_i(k)\sigma_i$ for some vector field $\boldsymbol{h}$ over $\mathbb{T}^3$, with spectrum $\pm|\boldsymbol{h}(k)|$. Bands cross precisely at zeroes of $\boldsymbol{h}$, generically a set W of isolated Weyl points.

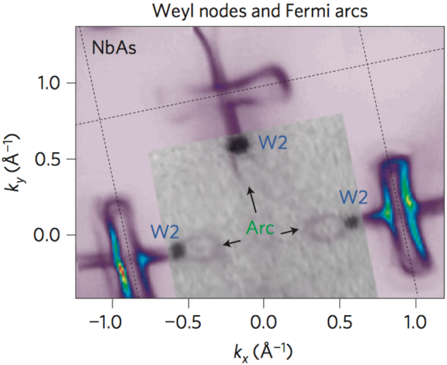


On $\mathbb{T}^3 \setminus W$, valence line bundle $\mathcal{E}_F$ is well-defined. Restricted to a small 2-sphere $S^2_{w_i}$ surrounding $w_i \in W$, its Chern class in $H^2(S^2_{w_i}, \mathbb{Z}) \cong \mathbb{Z}$ is equal to the local index of $\boldsymbol{h}$ at w_i (deg. of $\hat{\boldsymbol{h}} \equiv \frac{\boldsymbol{h}}{|\boldsymbol{h}|} : S^2_{w_i} \to S^2 \subset \mathbb{R}^3$).

Weyl semimetal in 3D and Fermi arcs

Globally, $\sum_i \mathrm{Ind}(w_i) = 0$ by Poincaré–Hopf. Weyl points come in pairs with local index ± 1. Experimental signature is a "Fermi arc" connecting Weyl points, and was found in 2015/16.





(L) S.-Y. Xu et al, Discovery of a Weyl Fermion semimetal and topological Fermi arcs, Science **349** 613 (2015);
(R) [—] Discovery of a Weyl fermion state with Fermi arcs in niobium arsenide, Nature Phys. **11** 748 (2015).

Abstract semimetal

$H(k) = \boldsymbol{h}(k) \cdot \boldsymbol{\sigma}$ is a local, basis-dependent expression. More generally, the Bloch bundle $\mathcal{S}$ is a complex Hermitian U(2)-bundle over a compact 3-manifold T (of momenta).

Bundle of traceless Hermitian endomorphisms of $\mathcal{S}$ is a real oriented rank-3 bundle $\mathcal{F}$ with metric $g(H_1, H_2) = \frac{1}{2}\mathrm{tr}(H_1 H_2)$. Structure group is $\mathrm{PU}(2) = \mathrm{SO}(3)$ under adjoint action, liftable to $\mathrm{Spin}^c(3) = \mathrm{U}(2)$.

$\mathcal{S}$ is a Clifford module bundle for $\mathrm{Cliff}(\mathcal{F}, g)$. Thus an orthonormal frame $\{e_1, e_2, e_3\}$ of $\mathcal{F}$ is quantized to a set of Pauli operators $\{\sigma_1, \sigma_2, \sigma_3\}$. Similarly, a section $\boldsymbol{h} \in \Gamma(\mathcal{F})$ is quantized to $c(\boldsymbol{h})$, which on $\mathcal{S}$ looks locally like $c(\boldsymbol{h})(k) = \boldsymbol{h}(k) \cdot \boldsymbol{\sigma}$.

Abstract semimetal

The square of $\boldsymbol{h}$ in the Clifford algebra is its length-squared, so $\mathrm{Spec}(c(\boldsymbol{h})) = \pm|\boldsymbol{h}|$ in any Clifford module bundle such as $\mathcal{S}$, e.g. can twist $\mathcal{S}$ by some line bundles. The local Weyl charge information is in $\boldsymbol{h}$ and its zeroes.

This abstraction is useful for constructing and analysing generalizations of "Dirac-type Hamiltonians" in higher dimensions, which condensed matter physicists are quite fond of.

Furthermore, the (real) representation theory of Clifford algebras can already suggest which antiunitary symmetries (time-reversal / particle-hole) could be present; reciprocally, such symmetries can isolate the Dirac-type Hamiltonians as the compatible ones[1]

[1] E.g. traceless 2×2 Hamiltonians are precisely particle-hole symmetric ones.

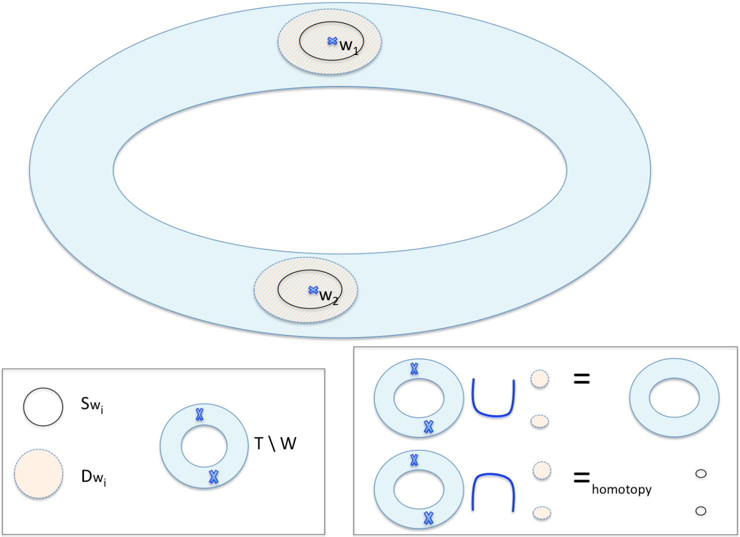
Semimetal $\to$ insulator extension problem

The local charge at $H^2(S^2_{w_i}, \mathbb{Z}) \cong \mathbb{Z}$ measures the obstruction to opening a gap at w_i. These are "monopoles of Berry curvature" for the line bundle $\mathcal{E}_F$.

These local obstructions are not independent — globally there is an extension problem for $\mathcal{E}_F$, from $\mathbb{T}^3 \setminus W$ to all of $\mathbb{T}^3$. This global obstruction to "opening up all the crossings" (semimetal $\to$ insulator) is captured by a Mayer–Vietoris sequence.

Notation: write T for $\mathbb{T}^3$, and $W = \coprod_i W_i \subset T$. Its tubular neighbourhood is $D_W = \coprod_i D_{w_i}$, whose boundary is a bunch of 2-spheres $S_W = \coprod_i S_{W_i}$.

Mayer–Vietoris principle



Mayer–Vietoris principle

Apply MV to the cover $T = (T \setminus W) \cup D_W$, whose intersection is S_W. Possibly singular line bundles $\leftrightarrow H^2(T \setminus W, \mathbb{Z})$:

$$\cdots 0 \to \underbrace{H^2(T)}_{\text{insulators}} \xrightarrow{\text{restr.}} \underbrace{H^2(T \setminus W)}_{\text{insulator/semimetal}} \xrightarrow{\text{restr.}} \underbrace{H^2(S_W)}_{\text{local charges}} \xrightarrow{\Sigma} H^3(T) \to 0$$

- Exactness $\Rightarrow \Sigma$ local charges of a candidate semimetal in $H^2(T \setminus W)$ must cancel.
- A candidate semimetal which comes from $H^2(T)$ can be gapped into an insulator ($\mathcal{E}_F$ extends across W). Exactness $\Rightarrow$ insulators contribute no local charge.
- Need ≥ 2 points in W so that $H^2(T \setminus W)$ contains elements which don't come from $H^2(T)$ — "topological semimetal".

Gerbes from semimetals — sketch

Gerbes had been used [Gawedzki '15] to study topological insulators. They also appear in semimetals:

Let w be a (Weyl) point in T. Cover T with the complement $U_1 = T \setminus \{w\}$, and neighbourhood $U_0 = D_w \cong \mathbb{R}^3$ of w. Then $U_0 \cap U_1 \cong S^2 \times \mathbb{R} \sim_h S_w = S^2$. Take the line bundle $\mathcal{L}_{01} \to U_0 \cap U_1$ pulled back from the generator of $H^2(S^2_w, \mathbb{Z})$. The corresponding gerbe generates $H^3(T, \mathbb{Z}) = \mathbb{Z}$.

The "semimetal gerbe" has at least two Weyl points and is trivial.

In higher d, a semimetal has a codim-3 "Weyl submanifold" $W = \coprod W_i$. For the corresponding gerbe, each W_i contributes to $H^3(T, \mathbb{Z})$ the Poincaré dual of W_i, and these must sum to zero.

Insulator bulk-boundary correspondence – Heuristics

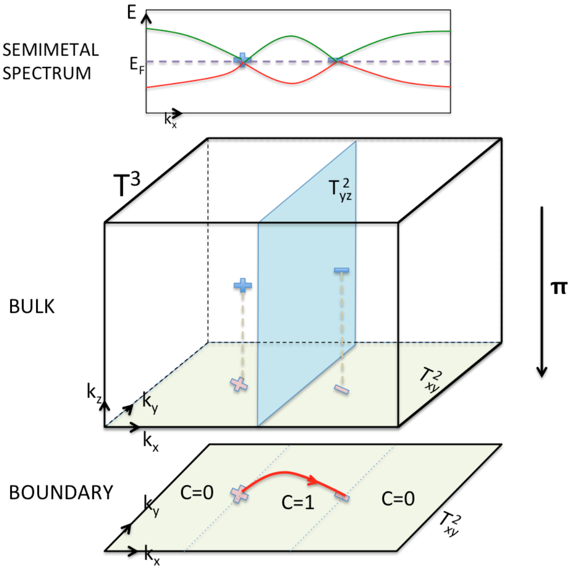
For insulators, non-trivial $\mathcal{E}_F$ is detected through metallic behaviour at the material boundary. Heuristic: interpolating $\mathcal{E}_F$ to vacuum requires violation of the insulating condition on the boundary. Furthermore, the boundary states inherits some topological data from the bulk.

Example: 2D Quantum Hall Effect is characterised by a Chern number. Boundary states are chiral with quantised conductivity.

Mathematically, there is a push-forward under the map π which projects out the direction orthogonal to boundary,

$$\pi_! : \underbrace{H^2(\mathbb{T}^2)}_{\text{Invariant for 2D insulator}} \longrightarrow \underbrace{H^1(\mathbb{T}^1)}_{\text{1D boundary invariant}}$$

Semimetal bulk-boundary correspondence — Heuristics



For each k_x away from $W = \{+,-\}$, $\mathcal{E}_F$ has a first Chern number C on the 2D subtorus in the y-z direction (blue). C remains constant as k_x is varied, unless a Weyl point is traversed, whence C jumps by an amount equal to the local charge. Whenever k_x is such that C is non-zero, a boundary state appears — these form the (red) Fermi arc.

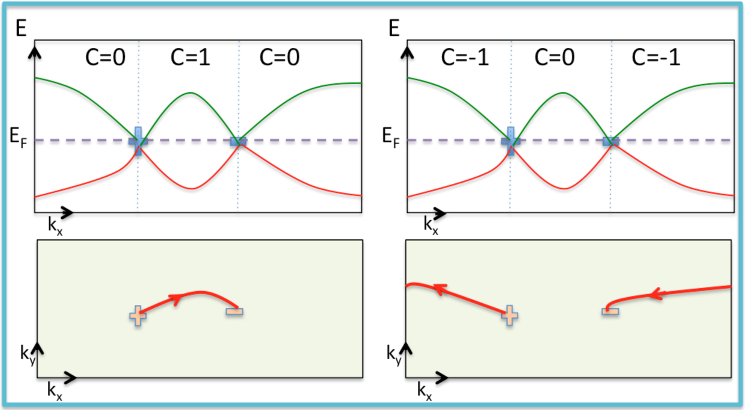
Poincaré duality and boundary Fermi arcs

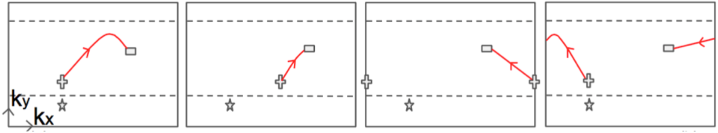
Let $T = \mathbb{T}^3$. Mathematically, the bulk-boundary homomorphism for semimetals is most conveniently defined via Poincaré (Lefschetz/Alexander) duality, i.e. $H^2(T \setminus W) \cong H_1(T, W)$.

Let π be projection of T onto a 2-subtorus $\widetilde{T}$, and $\widetilde{W} := \pi(W)$ be the projected Weyl submanifold. We define $\pi_!$ by the diagram

$$\begin{array}{ccc} H^2(T \setminus W) & \xrightarrow[\text{PD}]{\sim} & H_1(T, W) \\ \downarrow \pi_! & & \downarrow \pi_* \\ H^1(\widetilde{T} \setminus \widetilde{W}) & \xleftarrow[\sim]{\text{PD}} & H_1(\widetilde{T}, \widetilde{W}) \end{array}$$

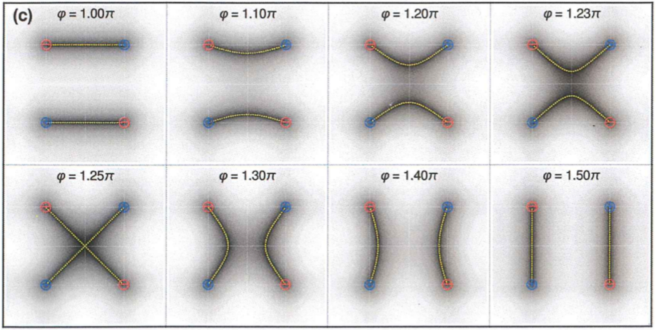
Boundary Fermi arcs are precisely the new relative cycles in $H_1(\widetilde{T}, \widetilde{W})$ compared to the usual torus cycles in $H_1(\widetilde{T})$!





Fermi arcs are global objects — not simply labelled by local charges at their end points (clarified in [M+T'16]). E.g. a Dehn twist takes the left config. to the right config. in the blue box, inducing a non-identity map on $H_1(\widetilde{T}, \widetilde{W})$.

Tunable Fermi arcs



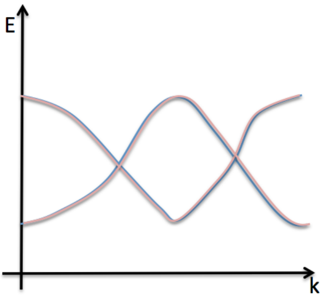
Fermi arcs for model Hamiltonians in [Dwivedi+Ramamurthy, arXiv:1608:01313] with tuning parameter φ. Also [Liu+Fang+Fu, 1604:03947]. Easy to analyse in our framework: horizontal and vertical configurations are homologous rel W ("rewirable"); arcs differing by some torus cycle cannot be "rewired" continuously.

Generalisations to more bands and higher dimensions

Take $d = 5, n = 4$, so the Bloch Hamiltonians $H(k), k \in \mathbb{T}^5$ are 4×4 matrices. Consider Dirac-type Hamiltonians

$$H(k) = \boldsymbol{h}(k) \cdot \boldsymbol{\gamma}, \qquad \{\gamma^i, \gamma^j\} = 2\delta^{ij}, \gamma^i = (\gamma^i)^\dagger, i = 1, \ldots, 5.$$

Spectrum of $H(k)$ is $\pm|\boldsymbol{h}(k)|$. Doubly degenerate e-values, which become 4-fold degen. at zeros of $\boldsymbol{h}$ (generically at points in $\mathbb{T}^5$).



A crossing at w is protected by the local index of $\boldsymbol{h}$, equal to the degree of $\hat{\boldsymbol{h}} = \frac{\boldsymbol{h}}{|\boldsymbol{h}|} : S^4_w \to S^4 \subset \mathbb{R}^5$. Globally the $\sum_i \mathrm{Ind}(w_i) = 0$ by Poincaré–Hopf. Generically, dispersion near w is linear looks like that of 4-component massless Dirac fermion with both particle/antiparticle d.o.f. (red herring).

Generalisations to more bands and higher dimensions

Dirac-type 4×4 Hamiltonians $H(k) = \boldsymbol{h}(k) \cdot \gamma$ in are convenient, but not generic, and again local, basis-dependent.

Actually, they are distinguished by compatibility with fermionic T-symmetry[2] (quaternionic structure $\mathcal{Q}$). Globally, this is a reduction of a U(4) Bloch bundle $\mathcal{S}$ to a Sp(2) = Spin(5) bundle (not all U(4) gauge trans. preserve $H = \boldsymbol{h} \cdot \gamma$ form).

Abstractly, we can consider a rank-5 oriented real vector bundle $\mathcal{F}$ over a compact 5-manifold T, with fibre metric g. A section $\boldsymbol{h} \in \Gamma(\mathcal{F})$ is quantized to $c(\boldsymbol{h}) \in \text{Cliff}(\mathcal{F}, g)$.

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[2] Actually a TP symmetry.

Higher n, d generalisations

On a spinor bundle $\mathcal{S}$ (or any Clifford module bundle), the analysis of the $\mathrm{Spec}(c(\boldsymbol{h}))$ is the same as before. In particular, a four-band crossing at w is protected by the local index of $\boldsymbol{h}$ at w.

Away from W, there is a rank-2 valence subbundle $\mathcal{E}_F$, which is really a quaternionic line bundle. We can regard $\hat{\boldsymbol{h}}$ (locally) as a map to $S^4 \sim \mathbb{HP}^1$ (c.f. $S^2 \sim \mathbb{CP}^1$ in the two-band case).

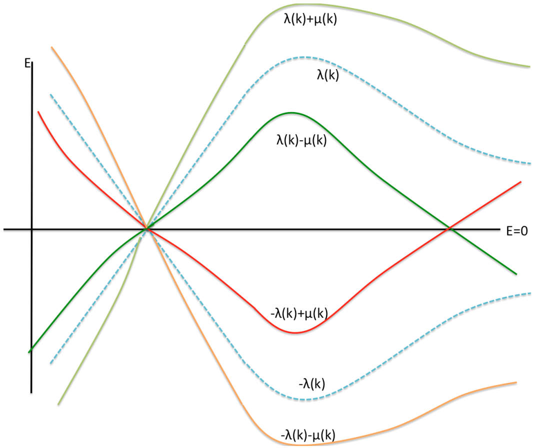
There is again an extension problem of $\mathcal{E}_F$ from $T \setminus W$ to T. In $d = 5$, quaternionic line bundles are stable, and we can use the MV-sequence in $\widetilde{KSp}$ to study the semi-metal $\rightarrow$ insulator problem.

γ-quadratic Hamiltonians

In a spinor bundle, $\boldsymbol{a} \wedge \boldsymbol{b}$ determines the concrete Hamiltonian $H_{\boldsymbol{a},\boldsymbol{b}}(k) := \frac{\mathrm{i}}{2} \left(\boldsymbol{a}(k) \wedge \boldsymbol{b}(k)\right)_I \gamma^I$, where I is a 2-multi-index.

$\mathrm{Spec}(H_{\boldsymbol{a},\boldsymbol{b}}(k)) = \pm|\boldsymbol{a} \wedge \boldsymbol{b}|(k)$ — two-fold degenerate eigenvalues becoming 4-fold degenerate at zeroes of $\boldsymbol{a} \wedge \boldsymbol{b}$. Looks identical to γ-linear case, but as we will see, topological protection of crossings is very different!

In fact, we can easily find the spectrum of the general $c(\boldsymbol{a} \wedge \boldsymbol{b} + \boldsymbol{c} \wedge \boldsymbol{d}) = H_{\boldsymbol{a},\boldsymbol{b}} + H_{\boldsymbol{c},\boldsymbol{d}}$. Writing $\lambda = |\boldsymbol{a} \wedge \boldsymbol{b}|$, $\mu = |\boldsymbol{c} \wedge \boldsymbol{d}|$, the spectrum is $\pm(\lambda \pm \mu)$.



Spectrum of γ-quadratic Hamiltonians. We are interested in 4-band crossings, which occur at $\lambda = \mu = 0$, and whether they can be gapped. Might as well take $\mu \to 0$.

γ-quadratic Hamiltonians

[E. Thomas '67] There is a subtle local index for vector 2-fields $\boldsymbol{a}, \boldsymbol{b}$ over a 5-manifold, for points where $\boldsymbol{a} \wedge \boldsymbol{b} = 0$ (linearly dependent), and an analogue of Poincaré–Hopf. This invariant is given by the homotopy class of the map $(\hat{\boldsymbol{a}}, \hat{\boldsymbol{b}}) : S^4_w \to \mathcal{V}_{5,2}$ (Stiefel manifold), and $\pi_4(\mathcal{V}_{5,2}) \cong \mathbb{Z}_2$.

Recall the fibration $S^3 = \mathcal{V}_{4,1} \to \mathcal{V}_{5,2} \to \mathcal{V}_{5,1} = S^4$, where the S^4 base parametrises the choice of e_1, and the fiber parametrises the choice of e_2 orthonormal to e_1. $\pi_4(\mathcal{V}_{5,2}) = \mathbb{Z}_2$ comes from the famous $\pi_4(S^3) = \mathbb{Z}_2$.

This suggests a subtle topological $\mathbb{Z}_2$-semimetallic phase.

Summary + Outlook

Abstracted semimetal topological invariant in Clifford algebraic language, paving the way for generalizations to semimetallic "Dirac-type Hamiltonians".

Analysed semimetal/insulator relationship globally, as an extension problem, using MV.

Identified Fermi arc topological invariant, whence the problem of "tuning/rewiring" Fermi arcs is easy to analyse.

Point symmetries such as P imposes an equivariance condition on vector fields $\boldsymbol{h}$ (whose quantizations are Dirac-type Hamiltonians). An equivariant index captures local gap-opening obstructions — relevant in experiments where H has P-symmetry.

Noncommutative/C^*-algebraic treatment of semimetals?