New Frontiers for Topological Semimetals

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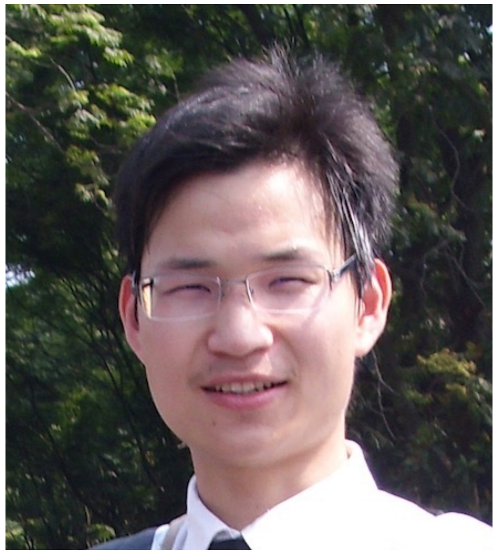

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arXiv:1603.03093

Outline

- Review - crystal symmetries, Weyl semimetals
- Symmetry protected topological metals - beyond Weyl and Dirac fermions
- Outlook - topological band theory

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Review - Non-symmorphic Symmetries

- Structure of crystal symmetry group (space group) G

1. Bravais lattice translations $\sim \mathbb{Z}^3$
2. Point group $\bar{G} \equiv G/\mathbb{Z}^3$
   - Rotation & reflection symmetries of a crystal
   - 32 in 3D

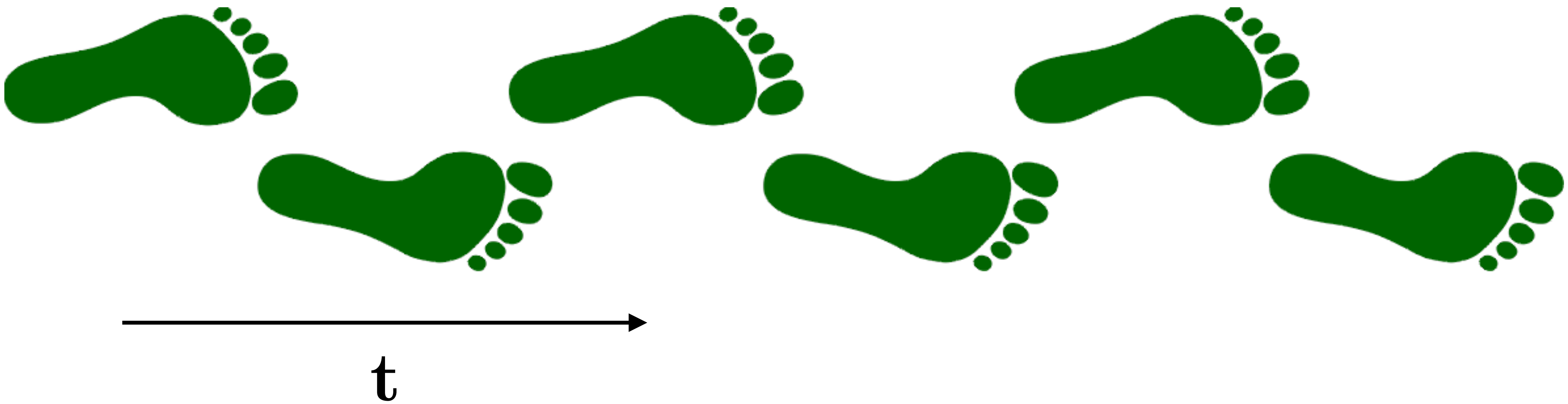
- How many ways can we put $\bar{G}$ and $\mathbb{Z}^3$ together (group extension problem)?

Review - Non-symmorphic Symmetries

- General element of a crystalline symmetry group: $\mathcal{G} = \{R|\vec{d}\}$
- $\{R_1|\vec{d}_1\}\{R_2|\vec{d}_2\} = \{R_1 R_2|\vec{d}_1 + R_1\vec{d}_2\}$
- All space groups contain $\{E|\vec{t}_i\}$ where $\vec{t}_i$ are Bravais lattice vectors
- Symmorphic group (73) - Extension splits: Every element can be written as $\mathcal{G} = \{E|n_i\vec{t}_i\}\{R|\vec{0}\}$
- Otherwise, non-symmorphic: elements with *fractional lattice translations* (157)

Review - Non-symmorphic Symmetries

- Example:

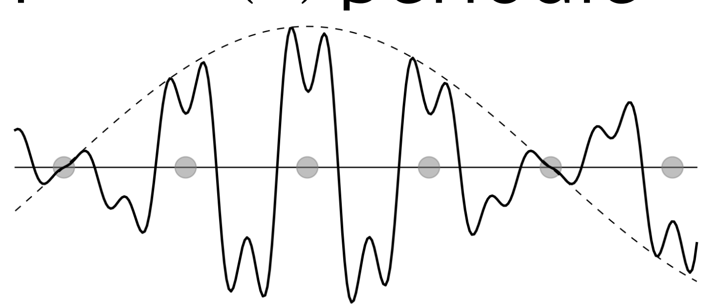


Non-symmorphic glide mirror $\{m_y|\frac{1}{2}\mathbf{t}\}$

- This is the *frieze group* p11g

Review - $\mathbf{k}\cdot\mathbf{p}$ Hamiltonains

- Recall Bloch's theorem: $H(\mathbf{r}+\mathbf{t}_a) = H(\mathbf{r}) \implies H(\mathbf{r})\psi_n(\mathbf{k},\mathbf{r}) = \epsilon_n(\mathbf{k})\psi_n(\mathbf{k},\mathbf{r})$
- $\psi_n(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}$ with $u_{n\mathbf{k}}(\mathbf{r})$ periodic



- Assume the solutions are known at some high-symmetry point $\mathbf{k}_0$ with symmetry group $G^{\mathbf{k}_0}$

1. Solutions fall into irreducible representations Δ of $G^{\mathbf{k}_0}$
2. We can expand $\psi(\mathbf{k},\mathbf{r}) = \sum_n c_n(\mathbf{k})\left[e^{i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{r}}\psi_n(\mathbf{k}_0,\mathbf{r})\right]$

What is a Weyl Semimetal?

Two-band crossing in 3 dimensions:

$$H(\vec{k}) = d_i(\vec{k})\sigma_i;\; d_i(k_x, k_y, k_z) = 0, \quad i = 1, 2, 3$$

3 functions, 3 variables - solution set is 0-dimensional (points);

Berry curvature:

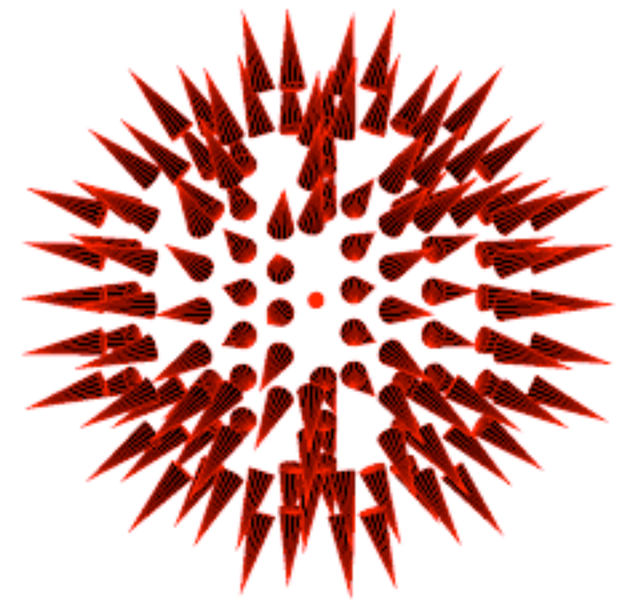
$$H(k) = \vec{k} \cdot \vec{\sigma}$$

$$H(k) \left| \vec{k} \right\rangle = \mu \left| \vec{k} \right\rangle$$

$$a_i = -i \left\langle \vec{k} \right| \frac{\partial}{\partial k_i} \left| \vec{k} \right\rangle$$

$$\vec{\Omega} = \nabla \times \vec{a} = \frac{\vec{k}}{2k^3}$$

$$\frac{1}{2\pi} \oint d\vec{S} \cdot \vec{\Omega} = 1$$



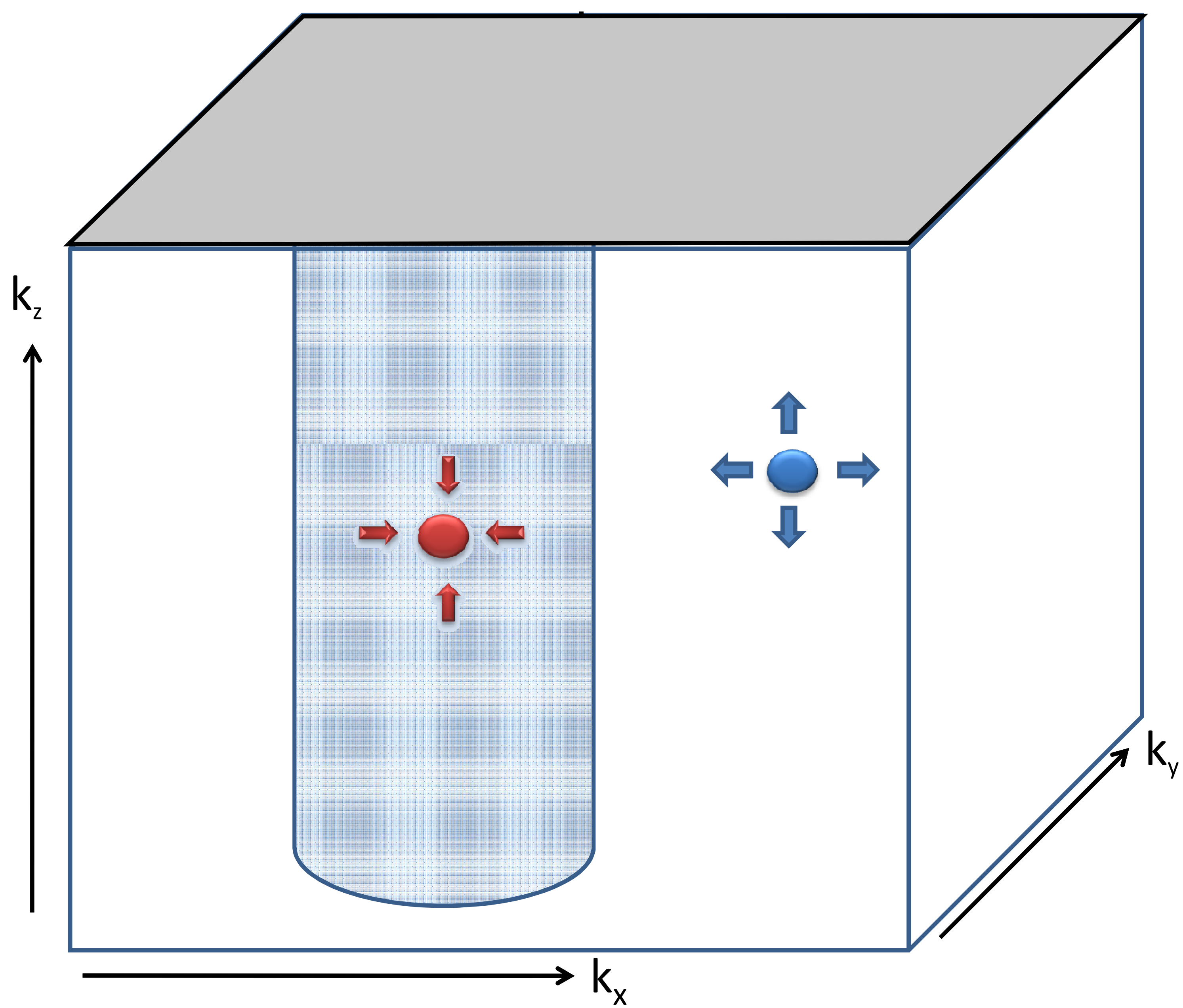
Monopole of Berry Curvature

c.f. Volovik

What is a Weyl Semimetal

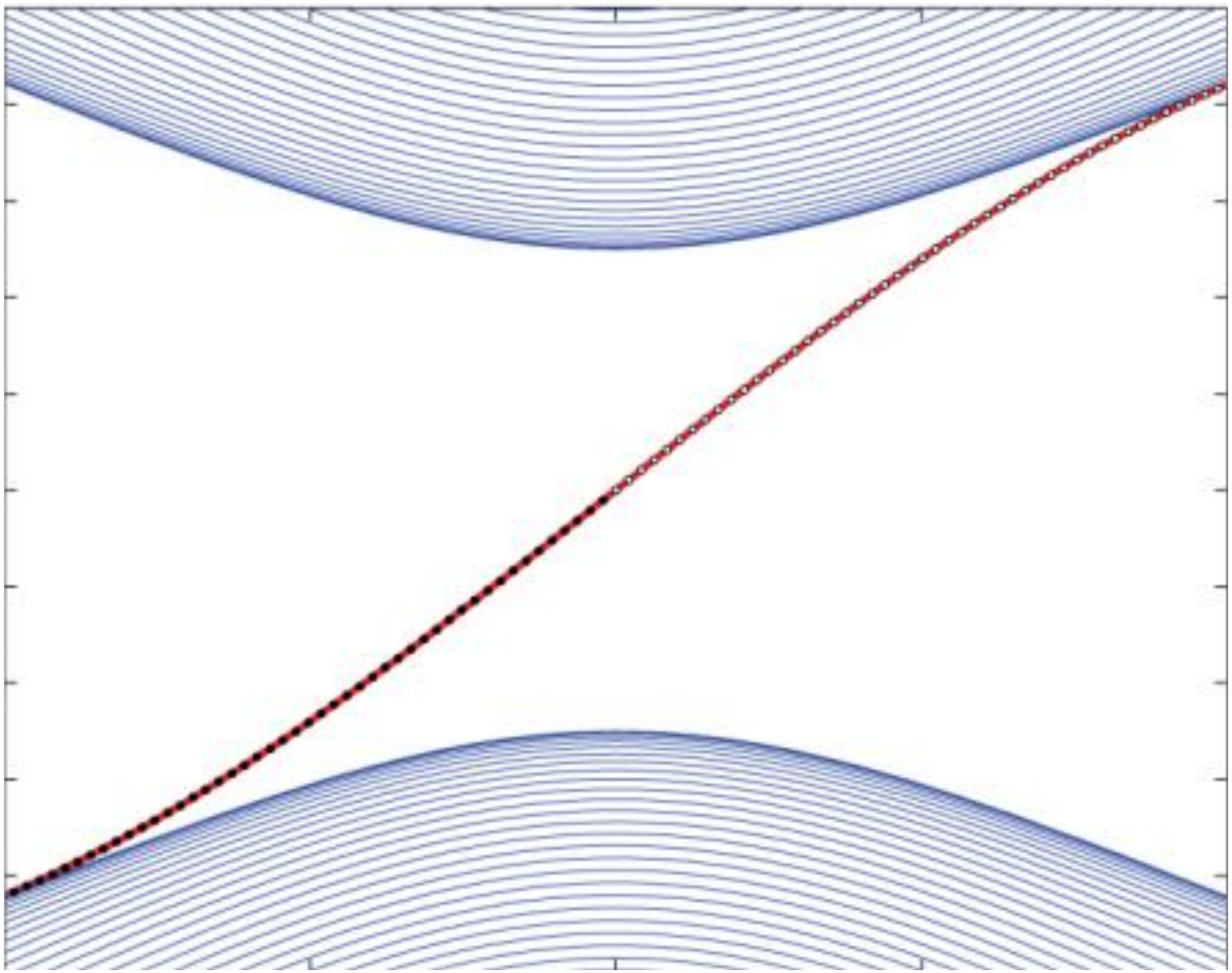
- Weyl nodes cannot be removed by small perturbations
- Gapped only through pairwise annihilation
- Nielsen-Ninomiya: Weyl points come in pairs of opposite chirality
- Must break either time-reversal or inversion symmetries; otherwise, can only get Dirac semimetals
- What are the observable consequences?

Fermi Arcs

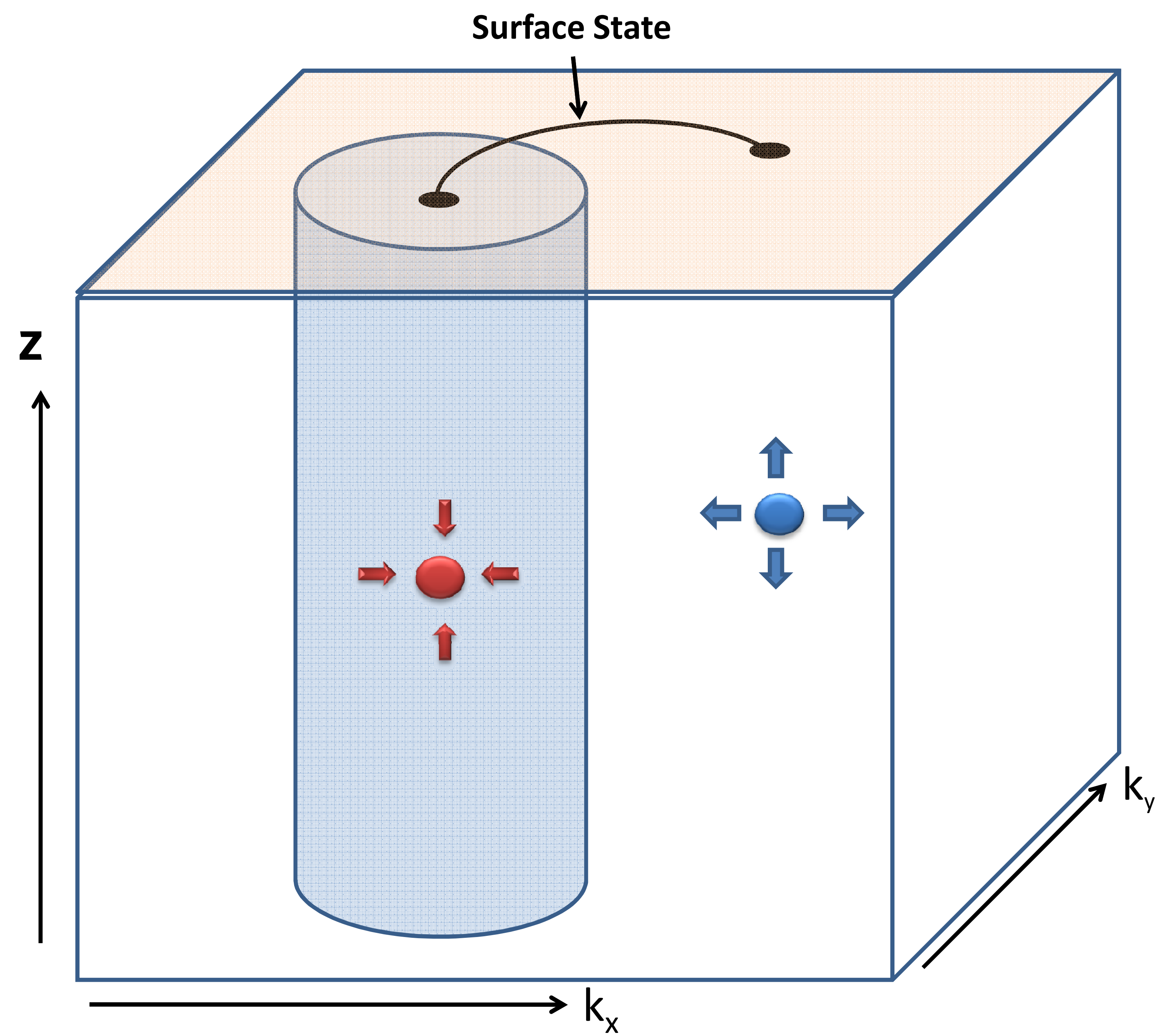


Wan, Turner, Vishwanath (2011)

Fermi Arcs

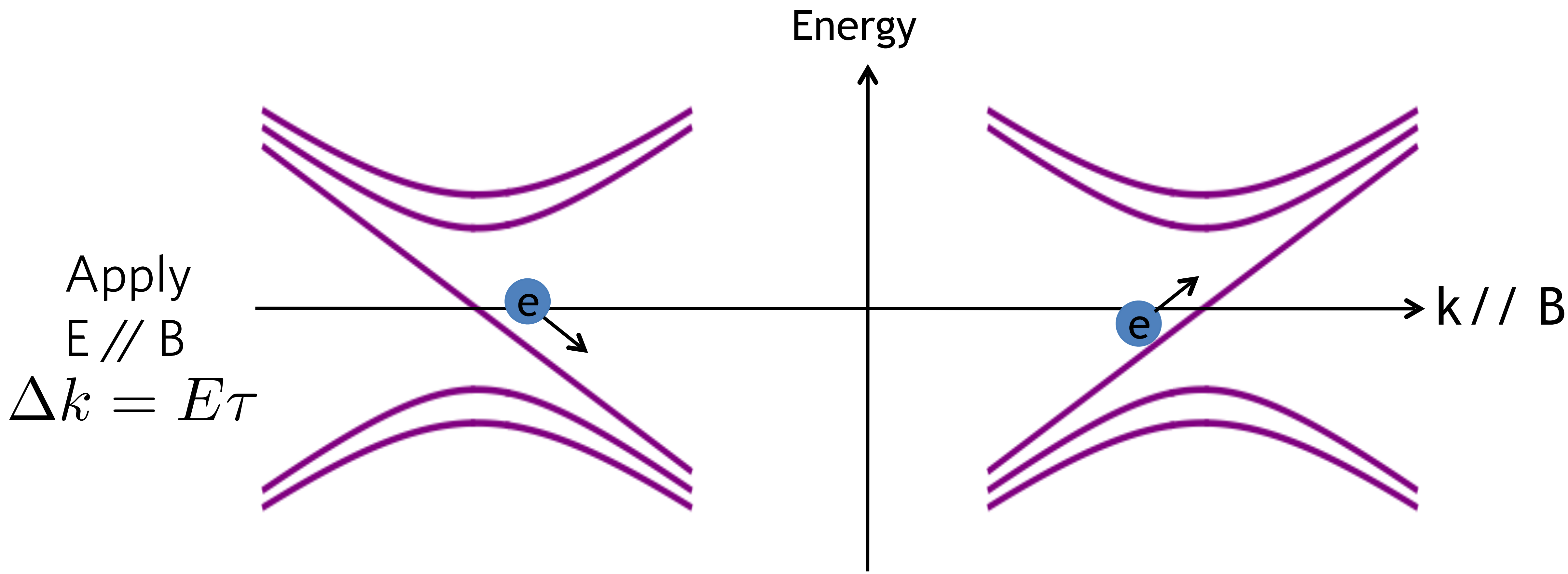


Fermi Arcs



Wan, Turner, Vishwanath (2011)

Chiral Anomaly in Condensed Matter



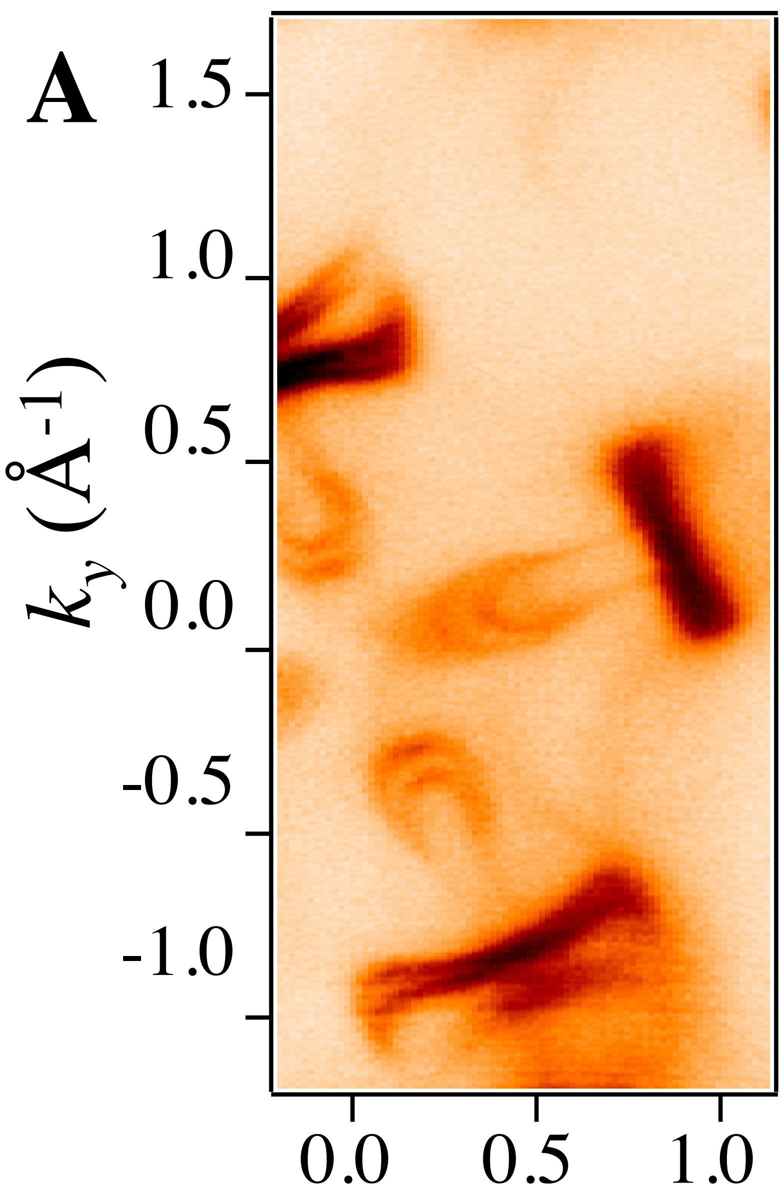
Electric field pumps charge between Weyl points:

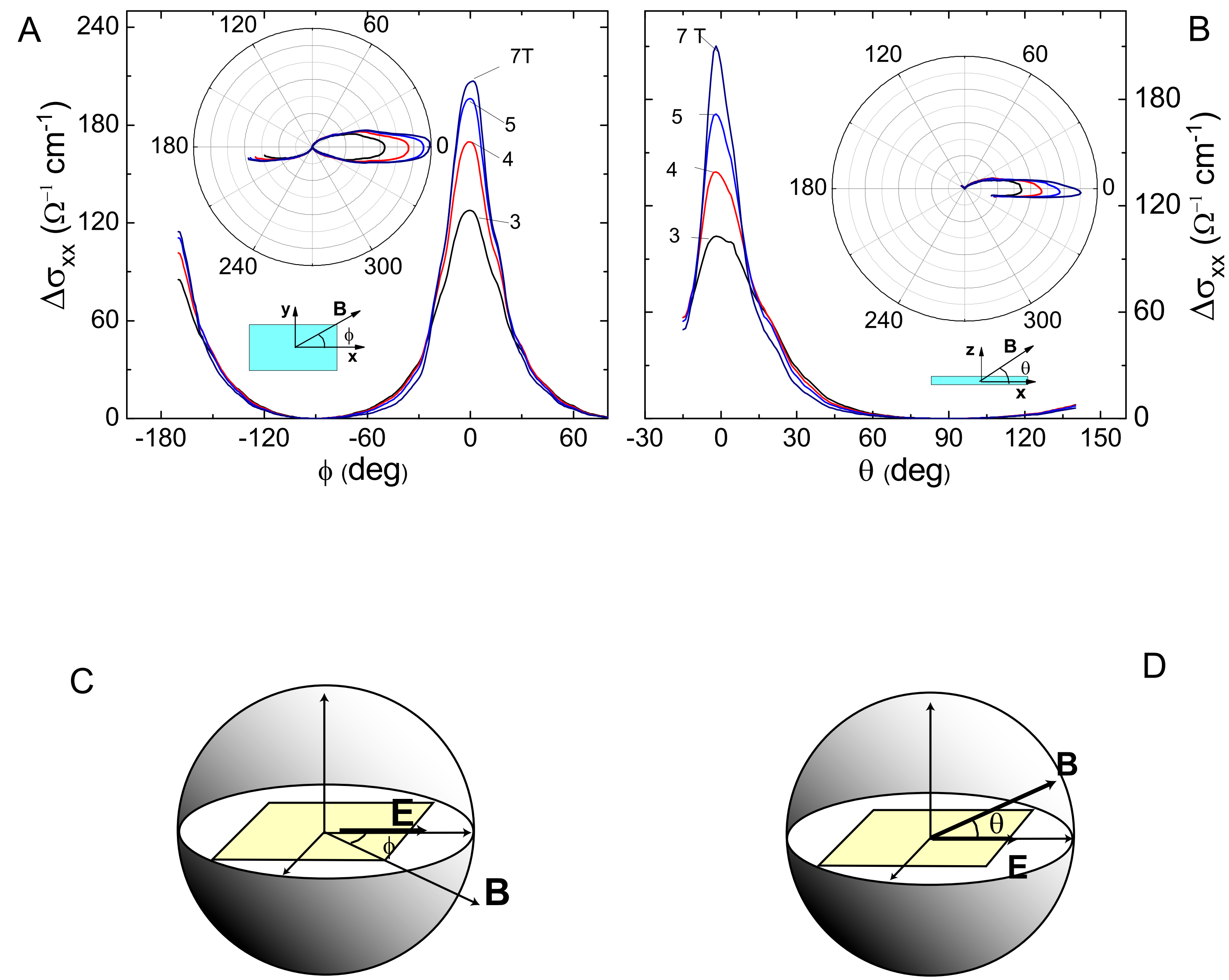
$$\Delta N_R - \Delta N_L \propto E \cdot B$$

Manifestation of Adler-Bell-Jackiw anomaly

Cond. mat. perspective: Nielsen + Ninomiya, Vafek + Vishwanath

Experimental Observation - TaAs, Na3Bi





Hasan, Ong, IOP group

Outline

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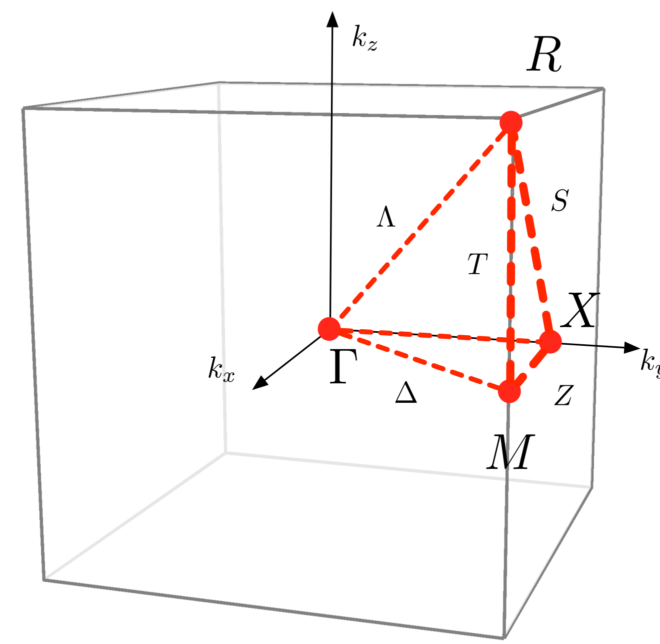
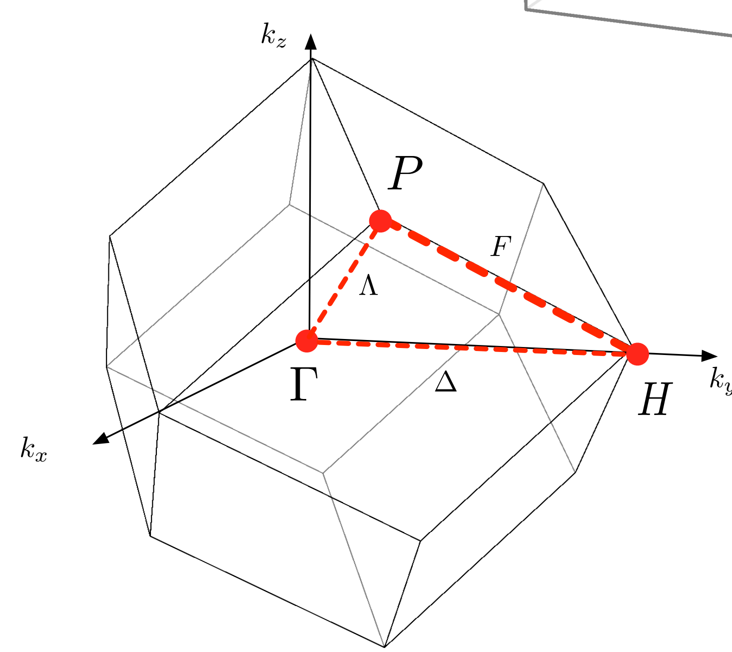
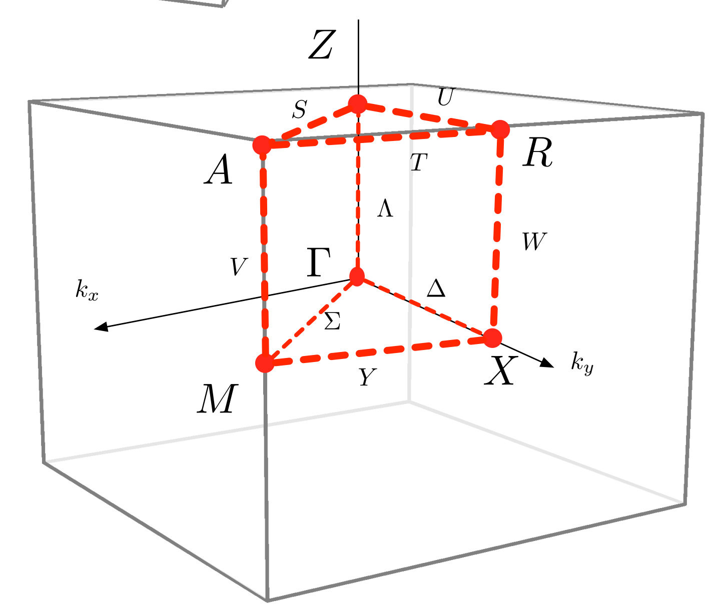
- Symmetry protected topological metals - beyond Weyl and Dirac fermions
- Outlook - topological band theory

Crystal Symmetry Protection

- More exotic fermions are allowed in crystalline systems
- New degeneracies protected by (non-symmorphic) crystal symmetries
- We focus on high symmetry points in the BZ
- Demand TR symmetry, allow for SOC
- Strategy - construct irreps of these symmetry groups, and the most general Hamiltonian consistent with each







Review - $\mathbf{k} \cdot \mathbf{p}$ Hamiltonains

- Recall Bloch's theorem: $H(\mathbf{r} + \mathbf{t}_a) = H(\mathbf{r}) \implies H(\mathbf{r})\psi_n(\mathbf{k}, \mathbf{r}) = \epsilon_n(\mathbf{k})\psi_n(\mathbf{k}, \mathbf{r})$
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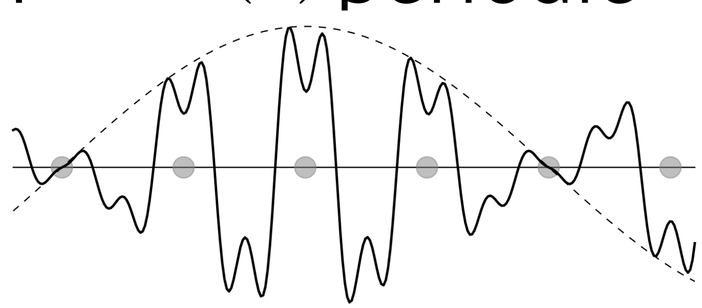

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1. Solutions fall into irreducible representations Δ of $G^{\mathbf{k}_0}$
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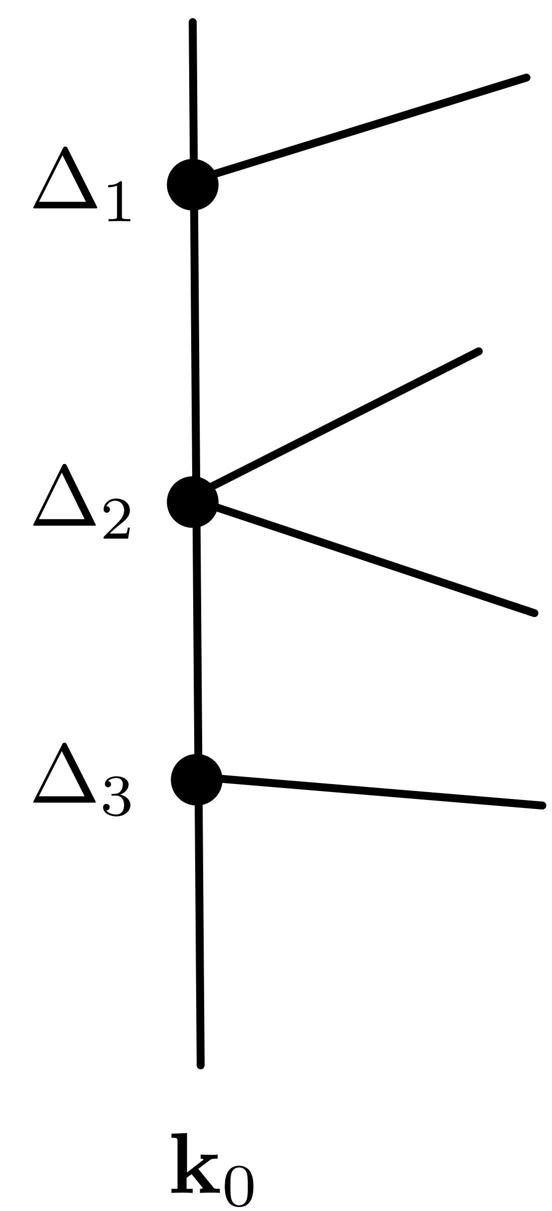
Review - $\mathbf{k} \cdot \mathbf{p}$ Hamiltonains

- Symmetry contrains the Bloch Hamiltonian

$$\Delta(\mathcal{G})H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$$

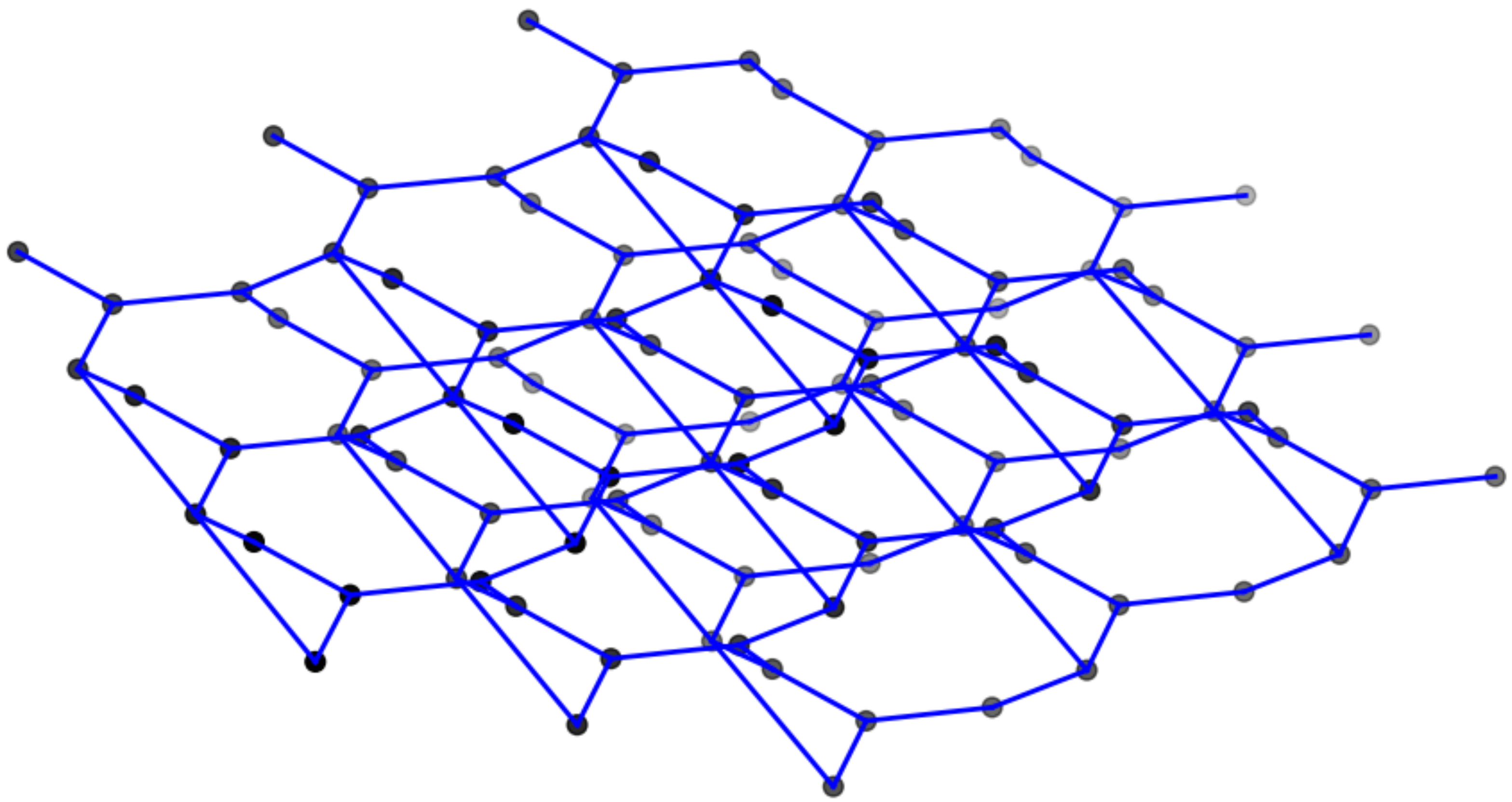
- Schur's Lemma: $H(\mathbf{k}_0) = \bigoplus_{\text{irreps}} E_\Delta \mathbb{1}_\Delta$

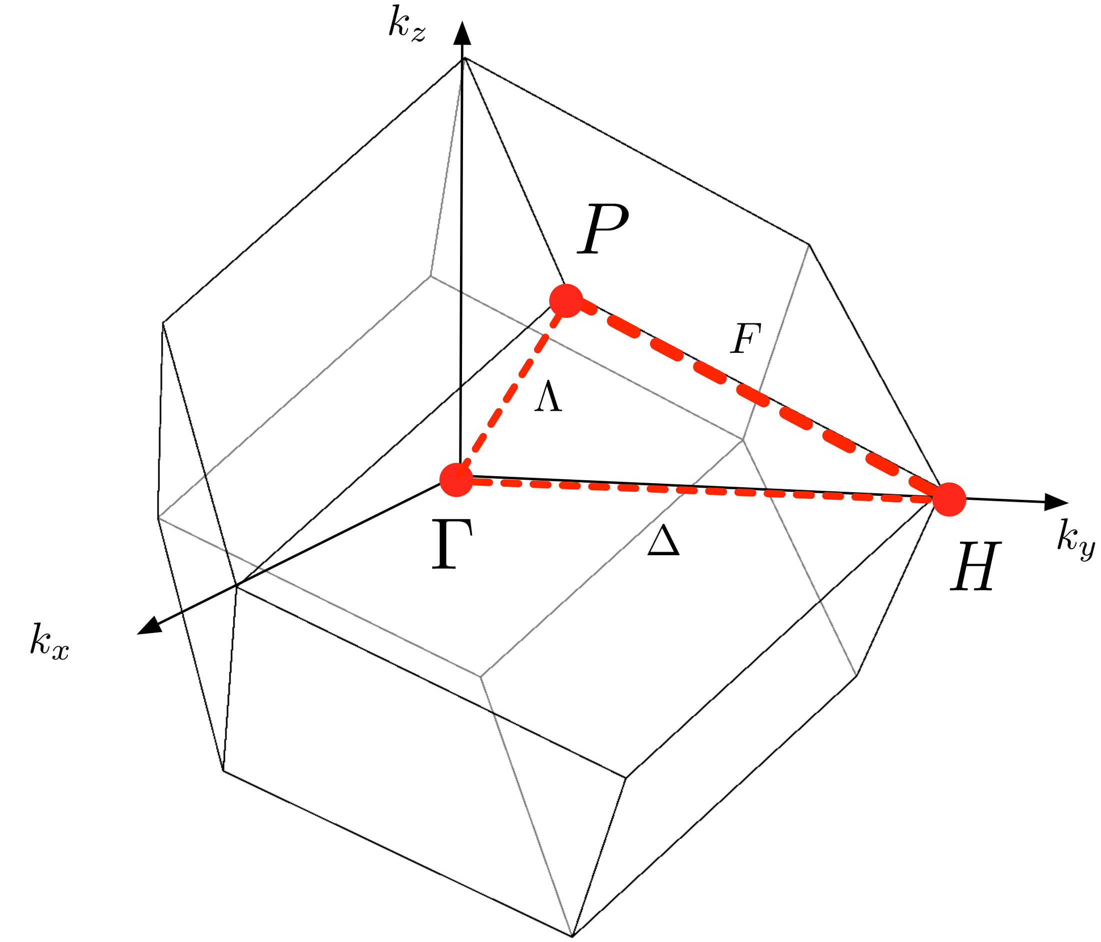
- For $\delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0$ small, $H(\mathbf{k}) \approx \bigoplus_{\text{irreps}} H_\Delta(\mathbf{k})$



“Spin-1 Weyl” Fermions

- Space groups 199 and 214 at the P point $\mathbf{k}_0 = (\pi, \pi, \pi)$

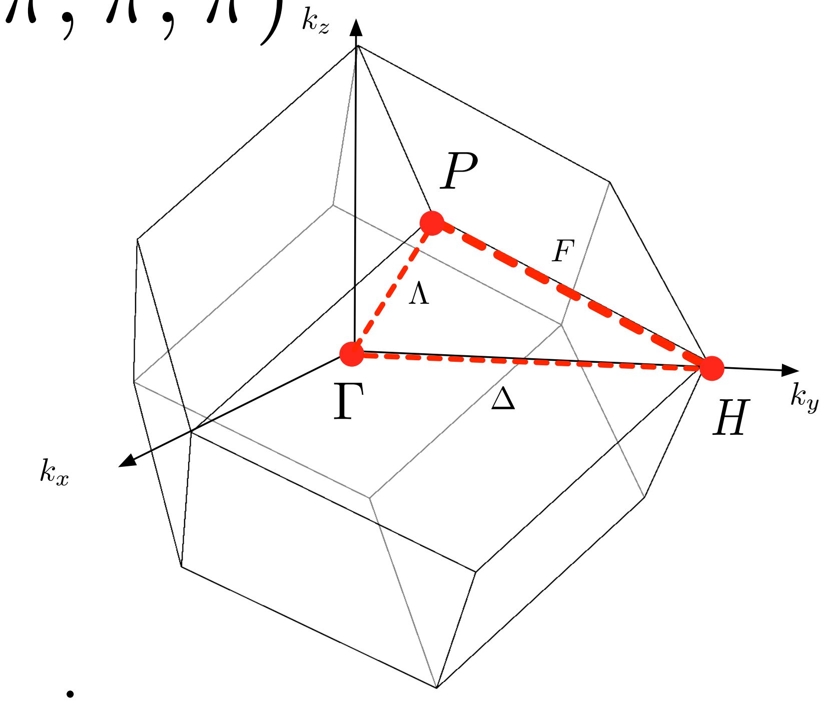




"Spin-1 Weyl" Fermions

- Space groups 199 and 214 at the P point $\mathbf{k}_0 = (\pi, \pi, \pi)$
- Symmetries: $\{C_{3,111}^{-1}|101\}$ $\{C_{2x}|\frac{\bar{1}}{2}\frac{1}{2}0\}$
- We seek representations Δ compatible with

$$\Delta(\{E|\mathbf{d}\}) = e^{-i\mathbf{k}_0\cdot\mathbf{d}}$$



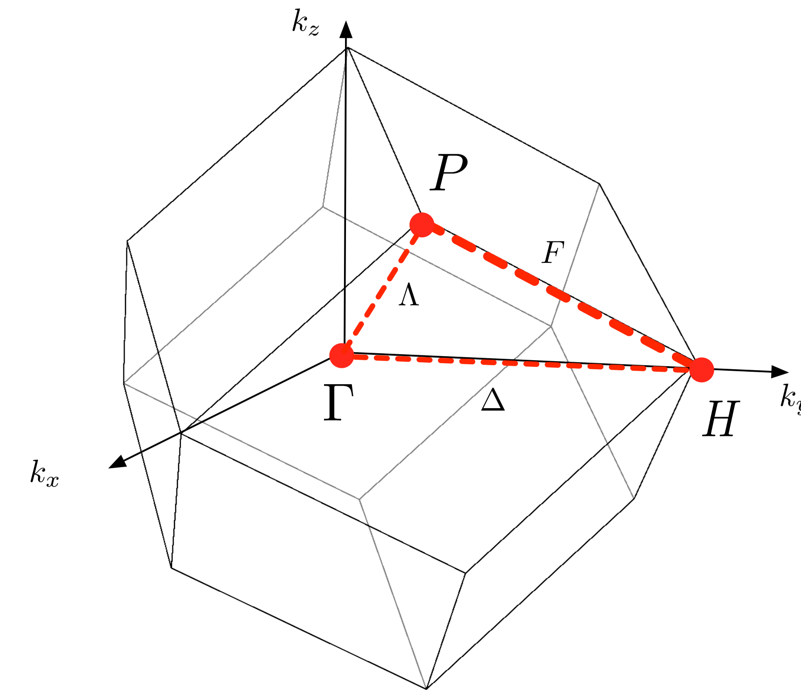
- Spin-1/2 particles - 2π rotation must give overall minus
- 3-dimensional irrep:

$$\Delta(\{C_{31}^{-1}|101\}) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad \Delta(\{C_{2x}|\frac{\bar{1}}{2}\frac{1}{2}0\}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

“Spin-1 Weyl” Fermions

- Linearized Hamiltonian

$$H = \begin{pmatrix} 0 & a\delta k_x & a^*\delta k_y \\ a^*\delta k_x & 0 & a\delta k_z \\ a\delta k_y & a^*\delta k_z & 0 \end{pmatrix}$$

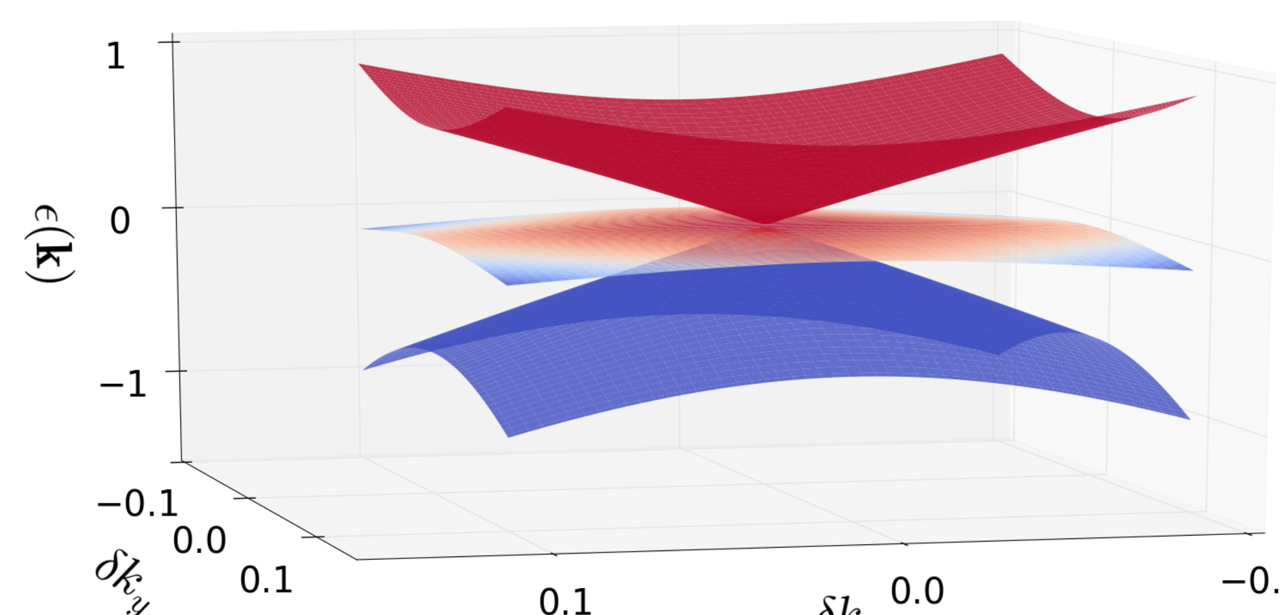


- Topological properties: $a = i|a|$

$$H \to |a|\delta\mathbf{k}\cdot\mathbf{L}$$

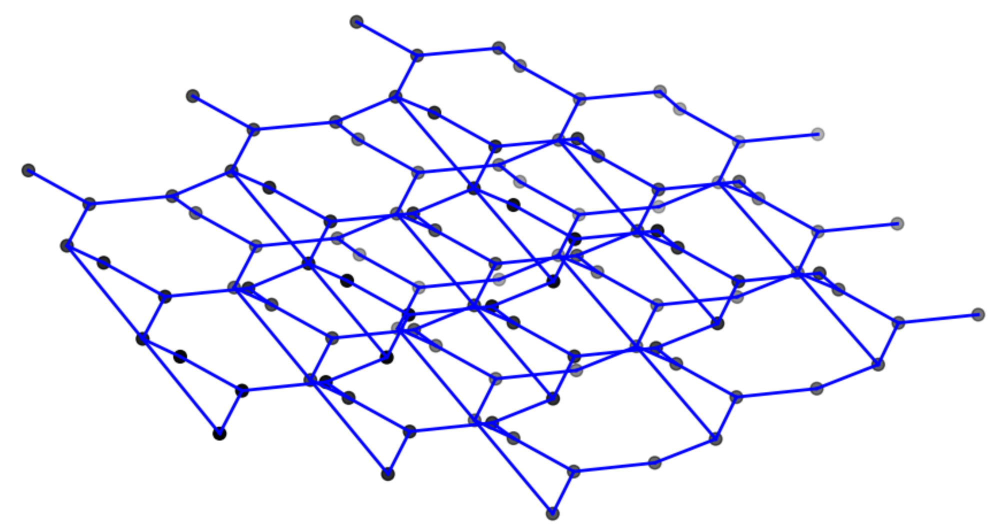
- Nontrivial Berry curvature ± 2 , 0

- (c.f. $H = \mathbf{B}\cdot\mathbf{L}$)

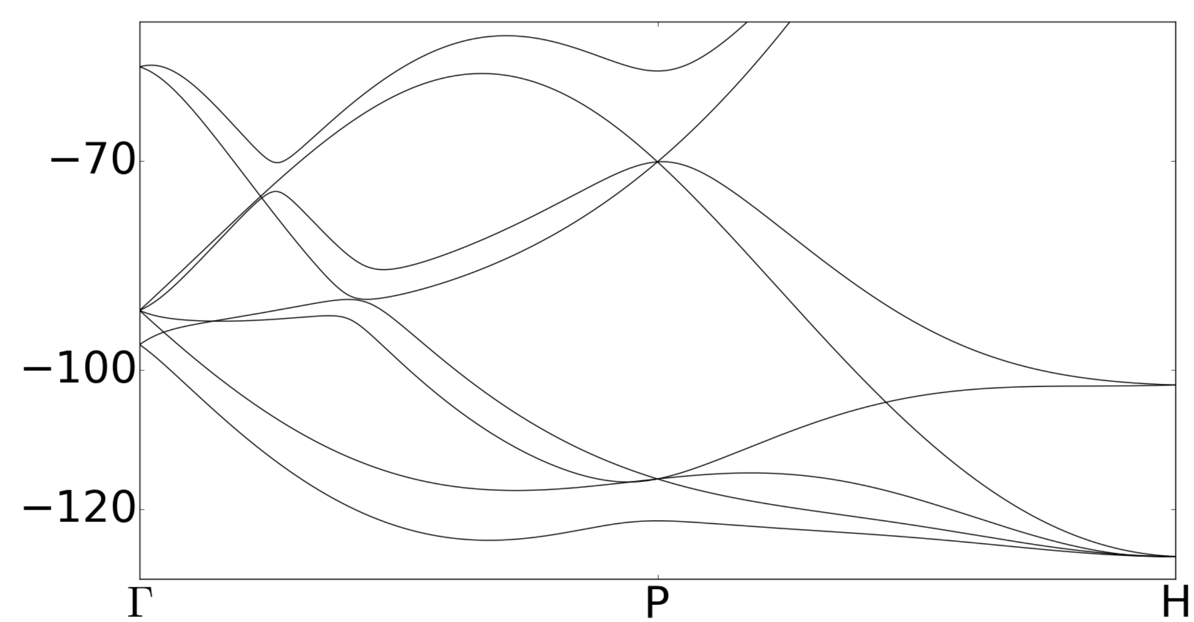


Consequences - Surface Fermi Arcs

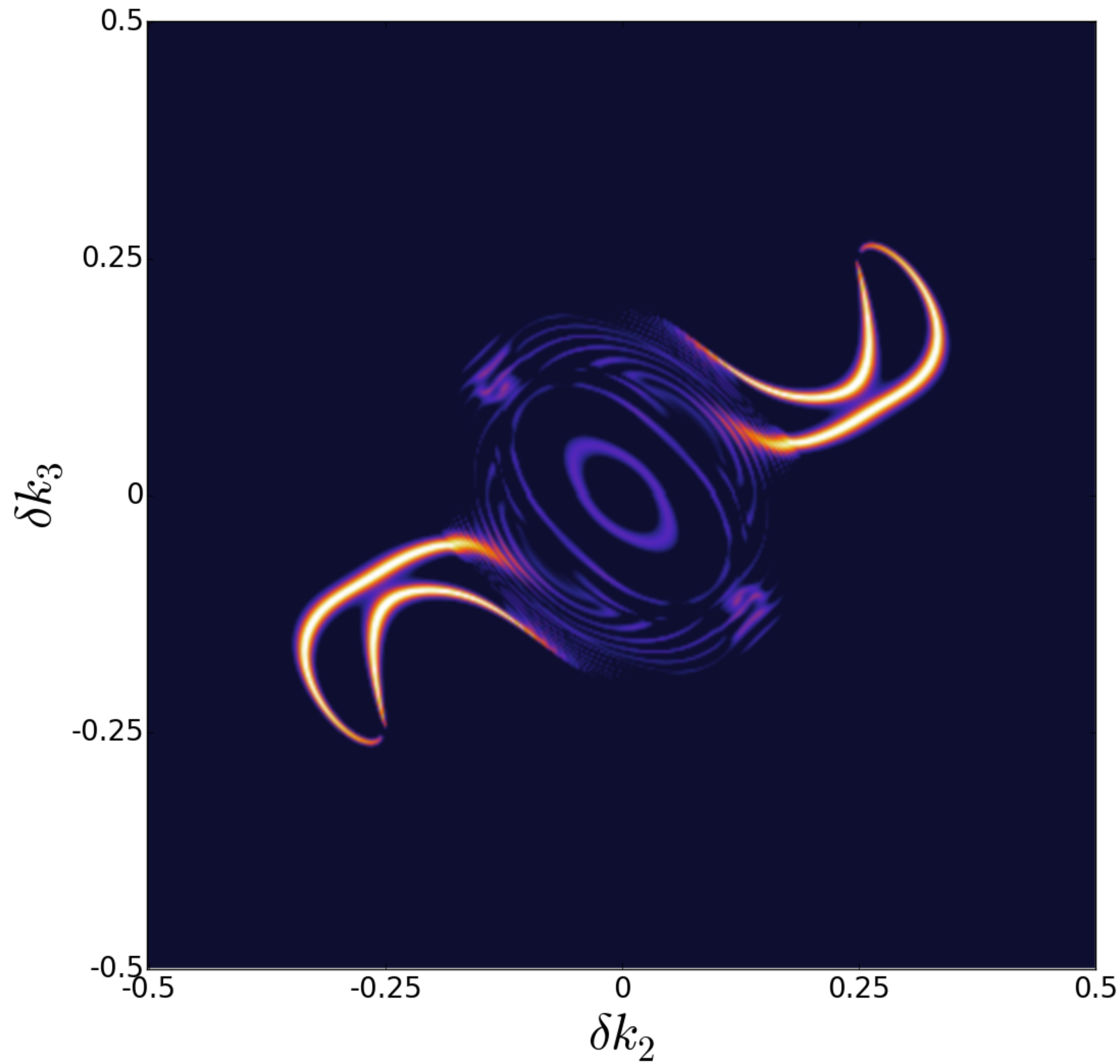
- Numerical check: tight-binding model for SG 214
- 4 atoms/unit cell, 3 p-orbitals per atom, 2NN hoppings
- Slab geometry, compute surface spectral function



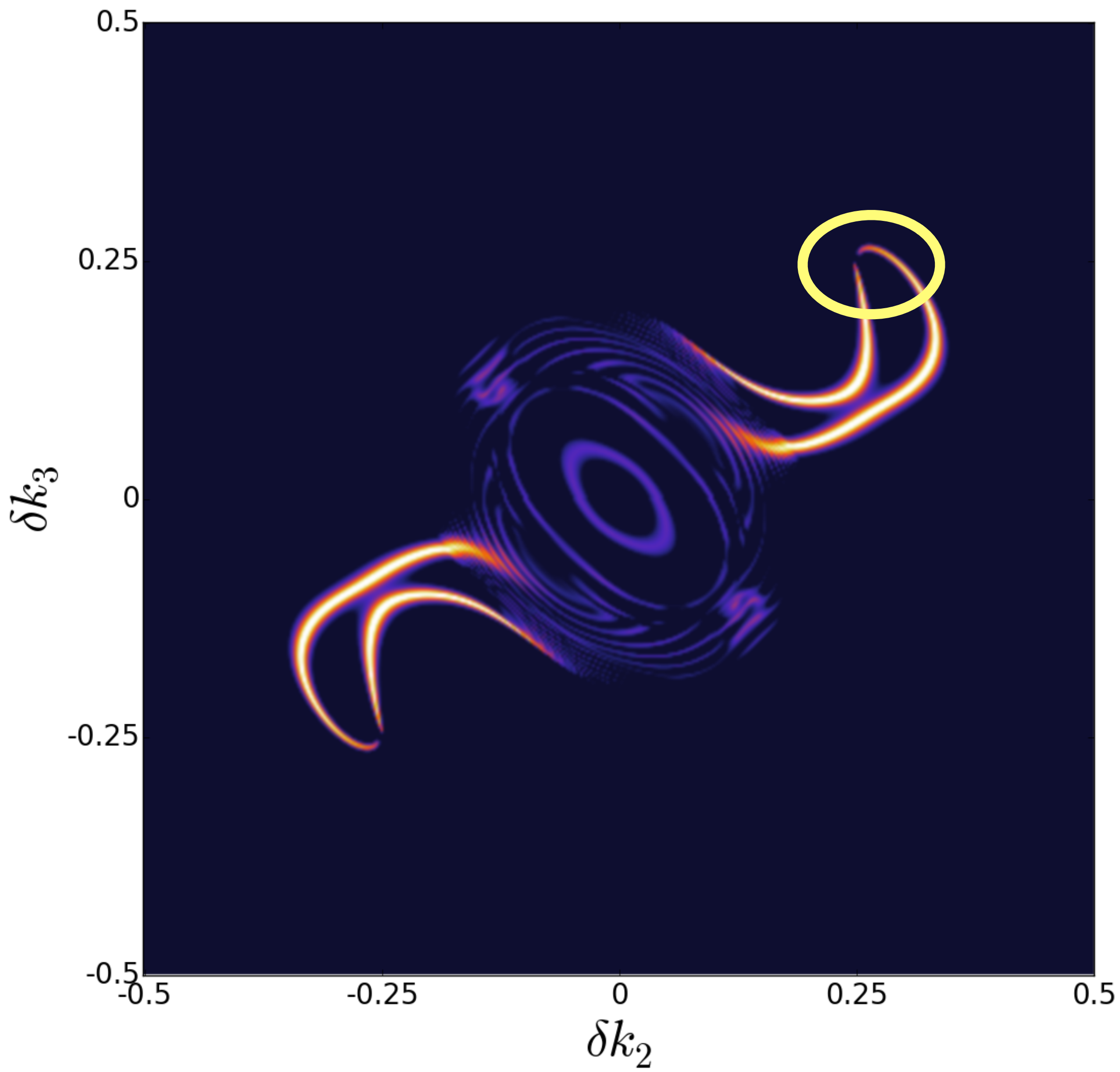
$$A(k_1, k_2) = -\frac{1}{\pi}\mathrm{Im}\left[\mathrm{tr}_{\mathrm{orb}}\left(\frac{1}{E + i\delta - H}\right)_{00}\right]$$

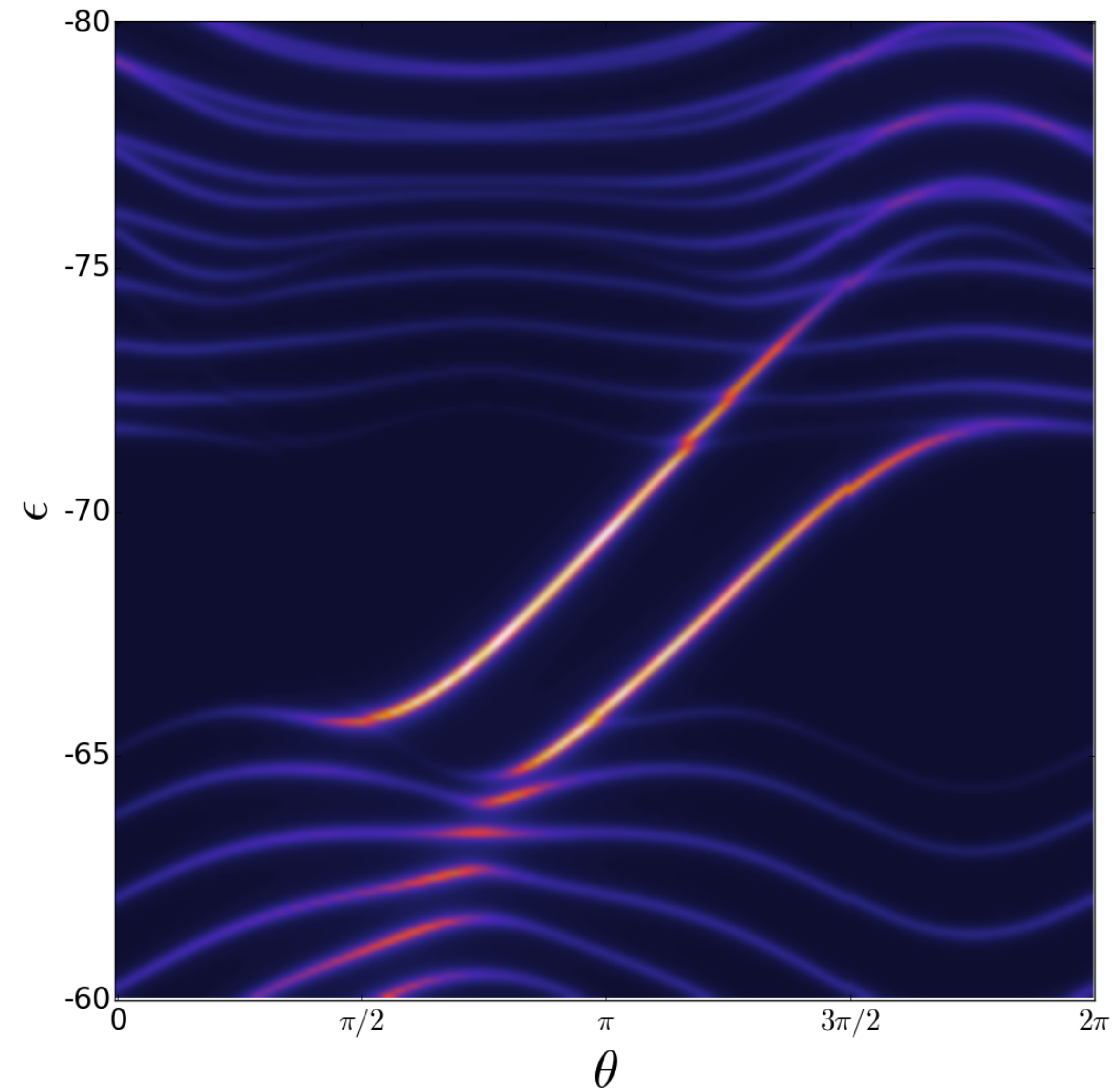


Consequences - Surface Fermi Arcs



Consequences - Surface Fermi Arcs





Consequences - Landau Levels

- Introduce magnetic field $k_{x,y} \to \Pi_{x,y} \equiv k_{x,y} + eA_{x,y}$

- Landau level creation/annihilation operators

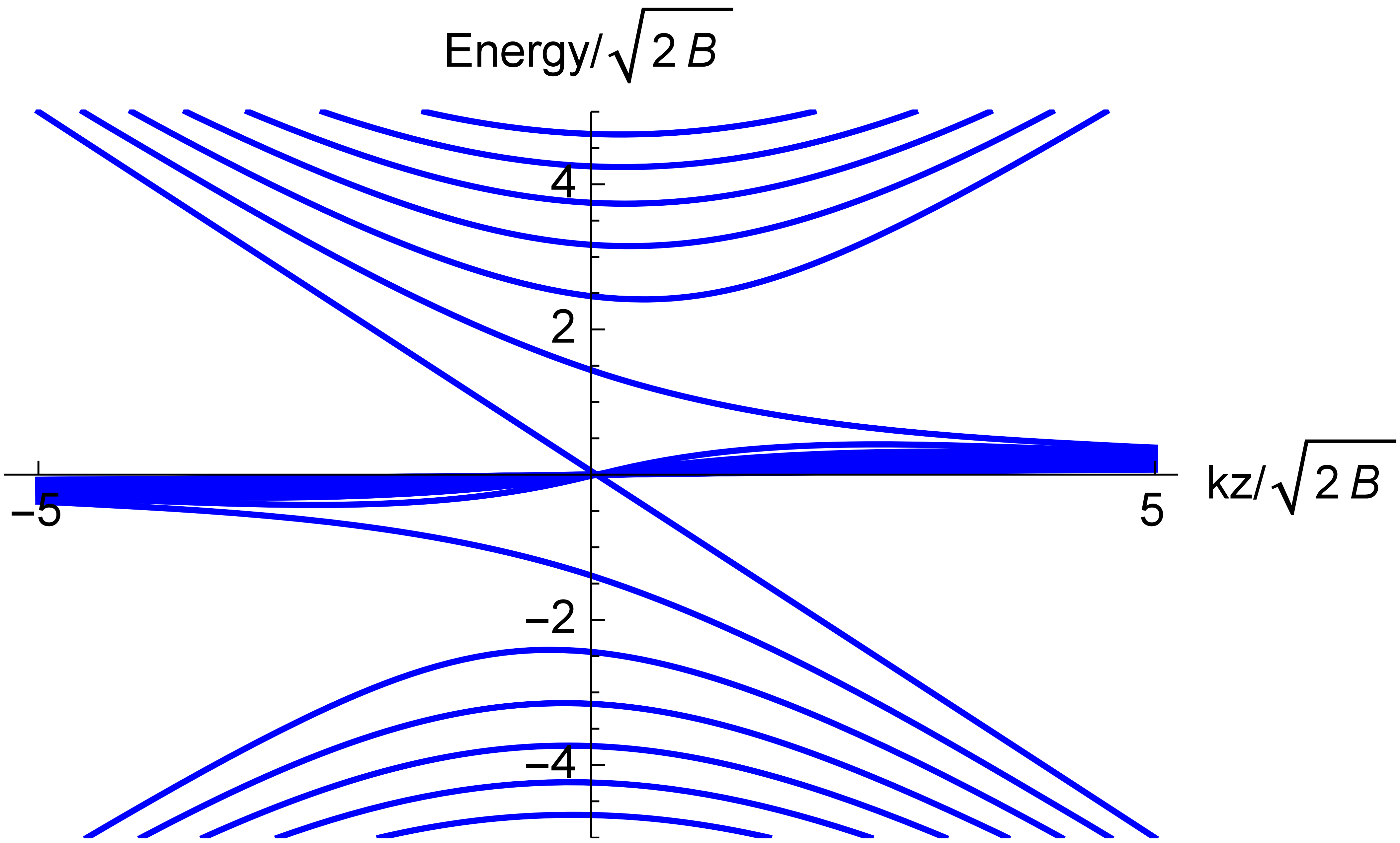
$$a = \frac{1}{\sqrt{2B}} \left(\Pi_x - i\Pi_y \right), \quad a^\dagger = \frac{1}{\sqrt{2B}} \left(\Pi_x + i\Pi_y \right)$$

- Linear Hamiltonian

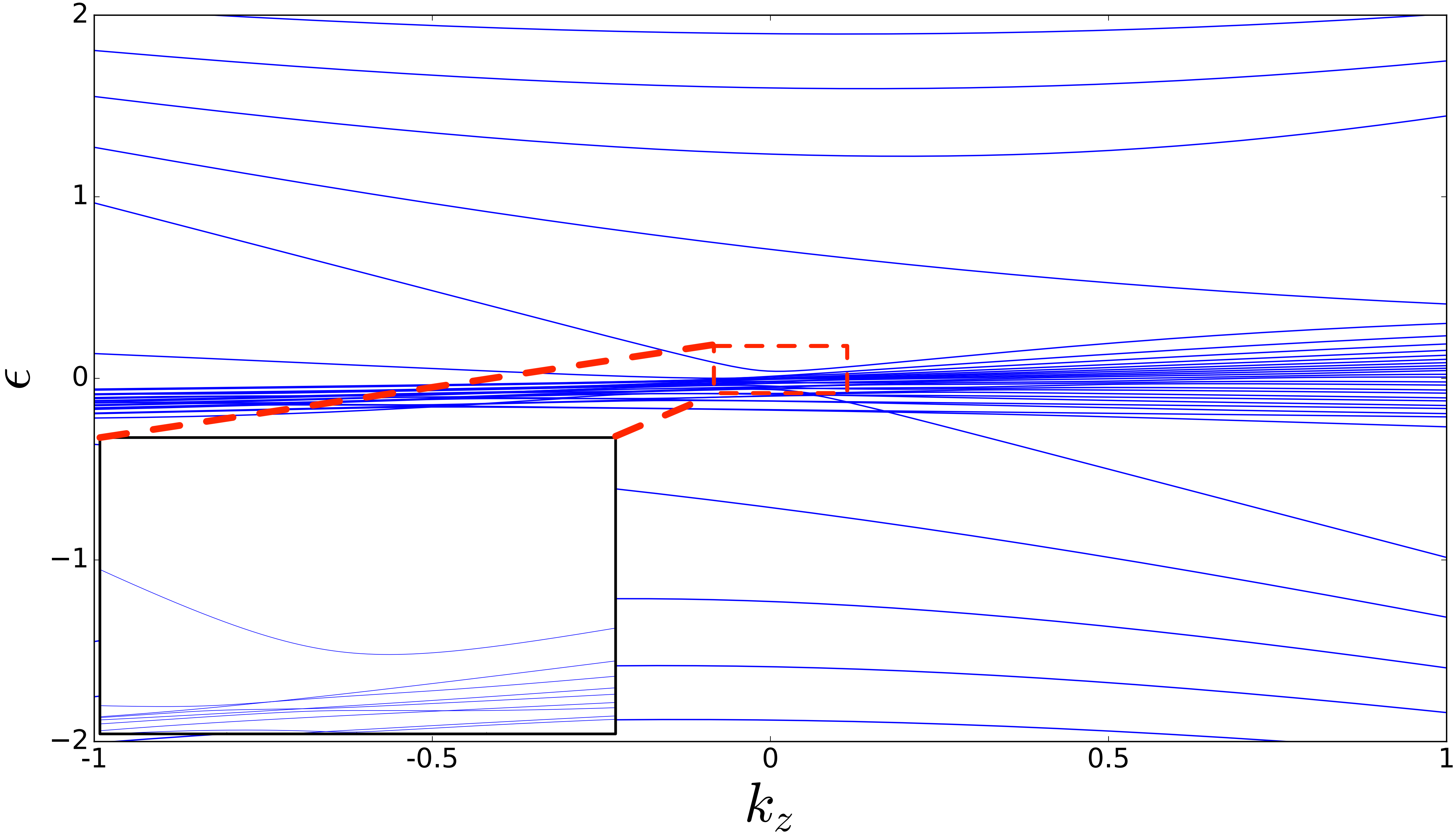
$$H(B, k_z) = \sqrt{\frac{B}{2}} \begin{pmatrix} 0 & e^{i\phi}(a + a^\dagger) & ie^{-i\phi}(a - a^\dagger) \\ e^{-i\phi}(a + a^\dagger) & 0 & e^{i\phi}\bar{k}_z \\ ie^{i\phi}(a - a^\dagger) & e^{-i\phi}\bar{k}_z & 0 \end{pmatrix}$$

- Exactly solvable when $\phi = \pi/2$

Consequences - Landau Levels (Exact)

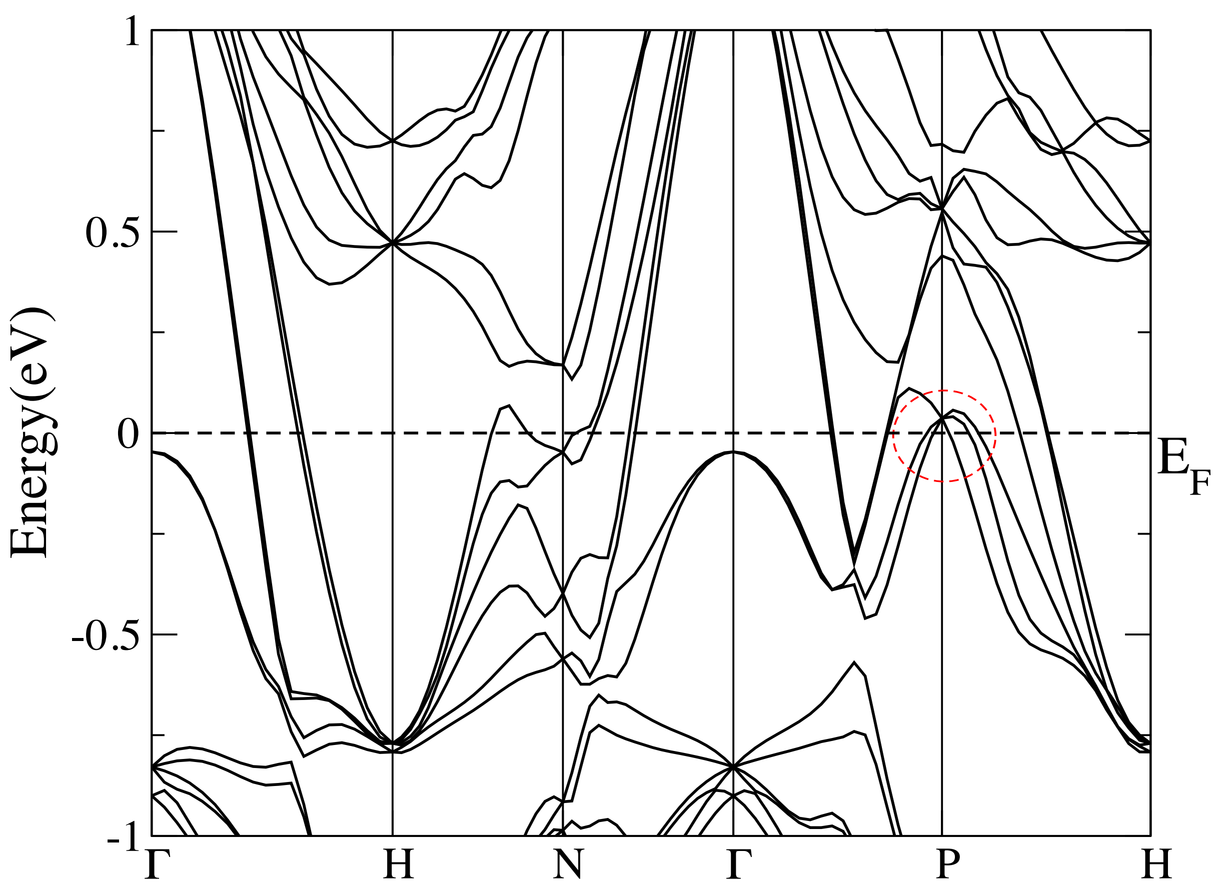


Consequences - Landau Levels (Higher order)



Material Candidates

Pd3Bi2S2



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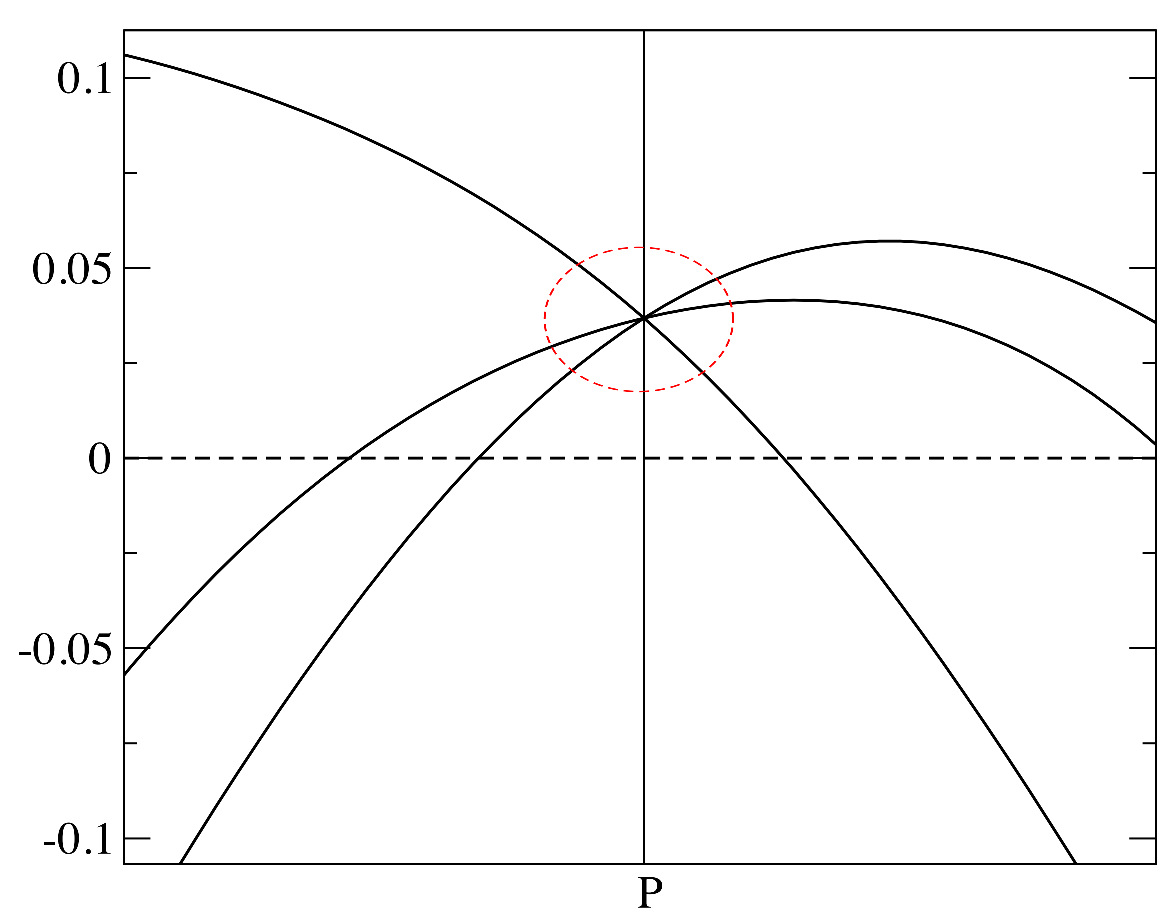
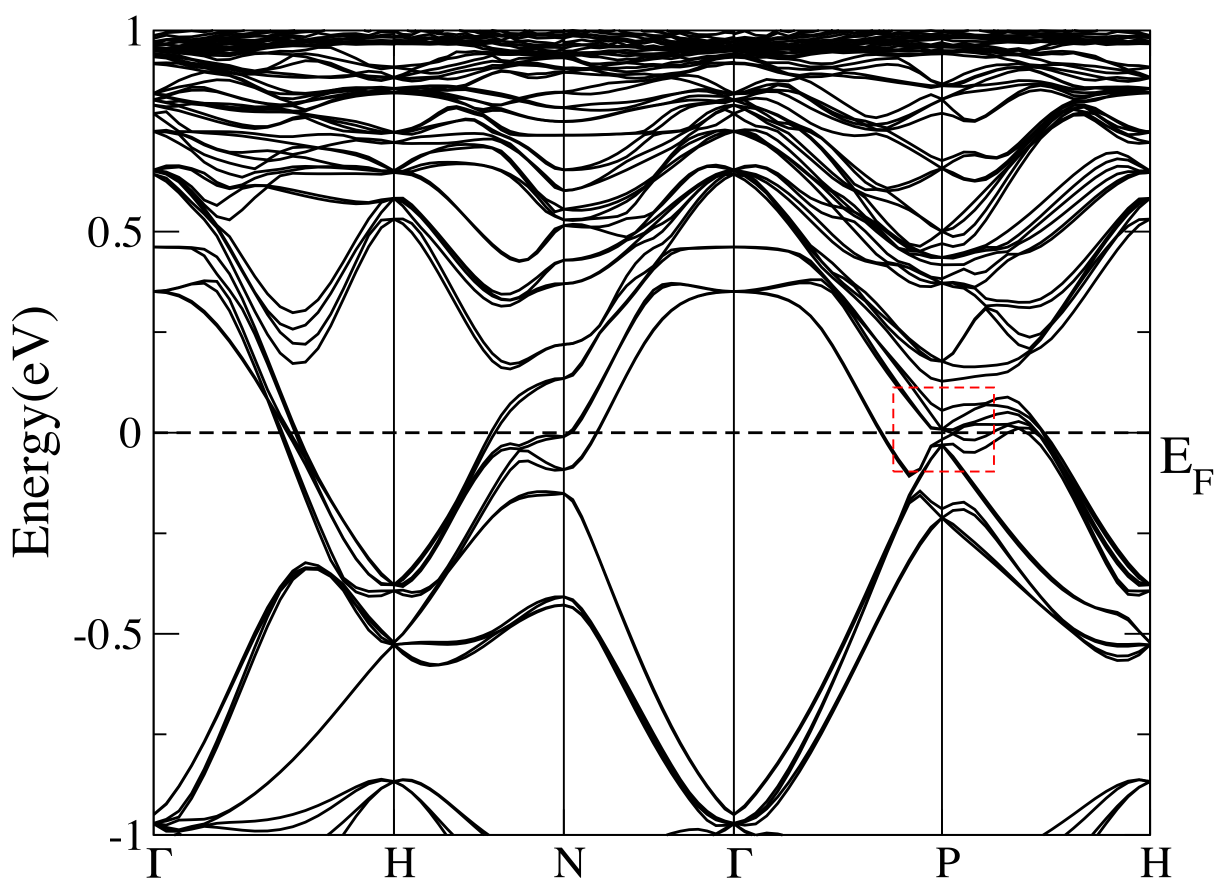
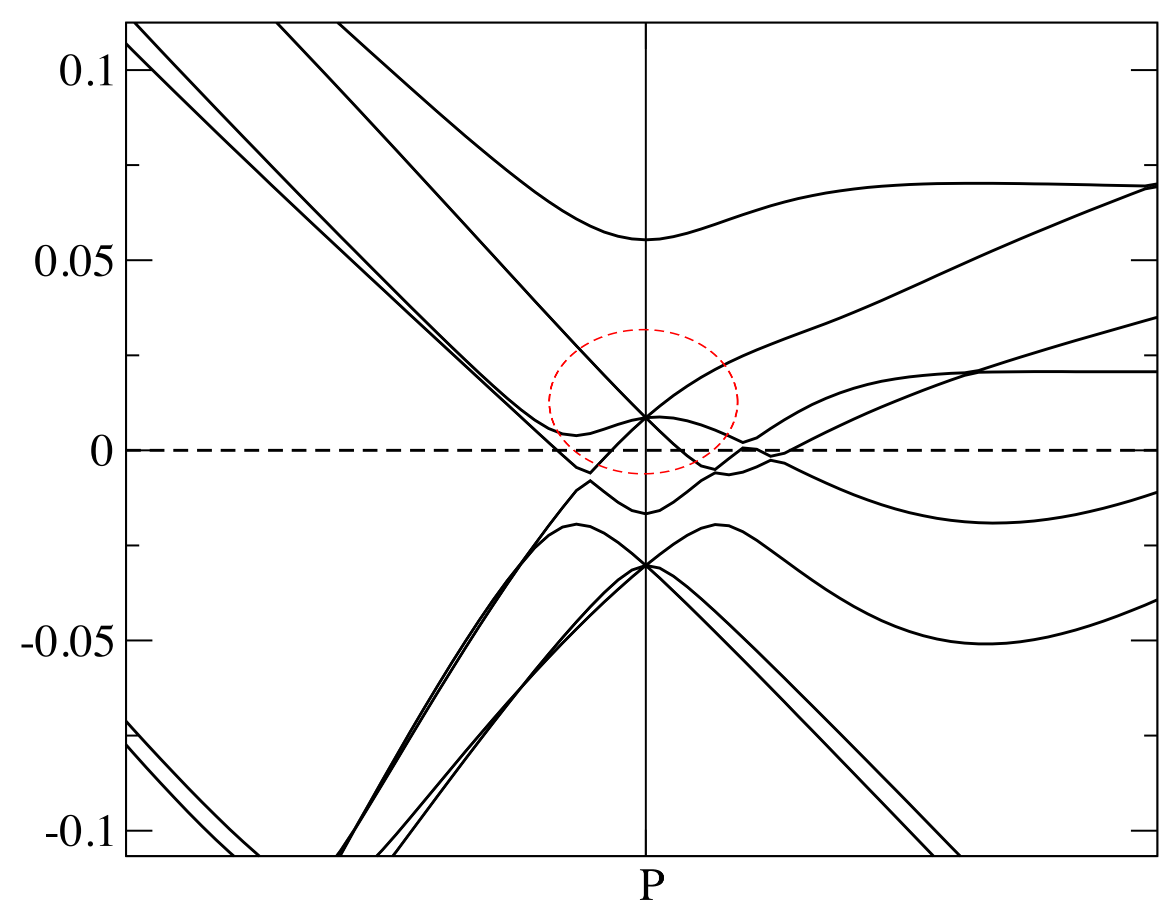


Material Candidates

La3PbI3



La3PbI3

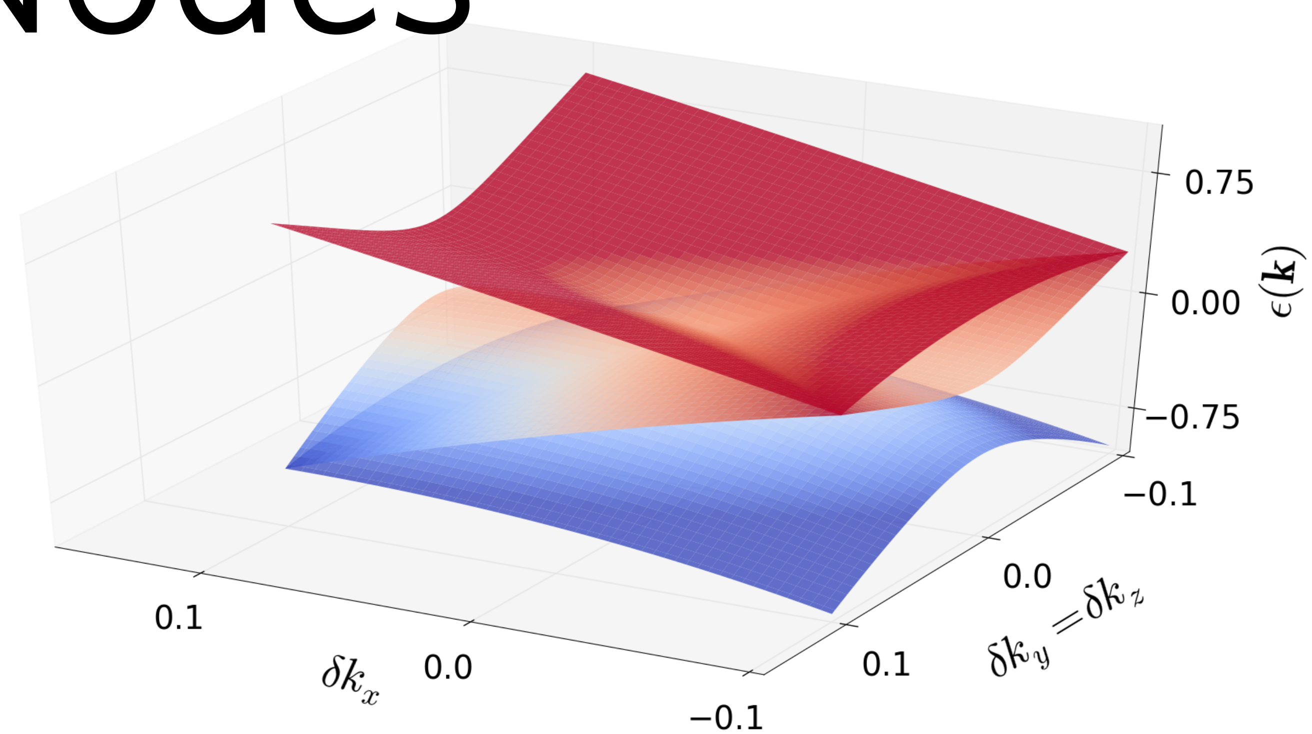


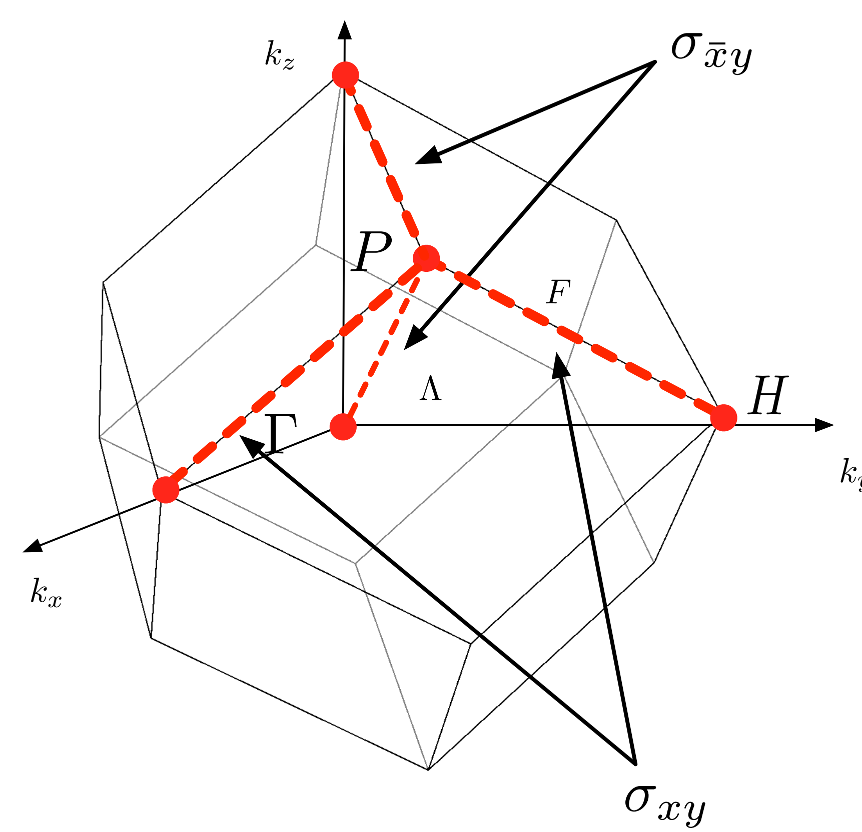
3-fold Degeneracy with Line Nodes

- Space group 220 at the P point
- Symmetries $\{C_{3,111}|000\}$
  $\{C_{2y}|0\frac{1}{2}\frac{1}{2}\}$ $\{IC_{4x}^{-1}|\frac{1}{2}11\}$
- Linearized Hamiltonian

$$H = a\begin{pmatrix} 0 & \delta k_x & \delta k_y \\ \delta k_x & 0 & \delta k_z \\ \delta k_y & \delta k_z & 0 \end{pmatrix}$$

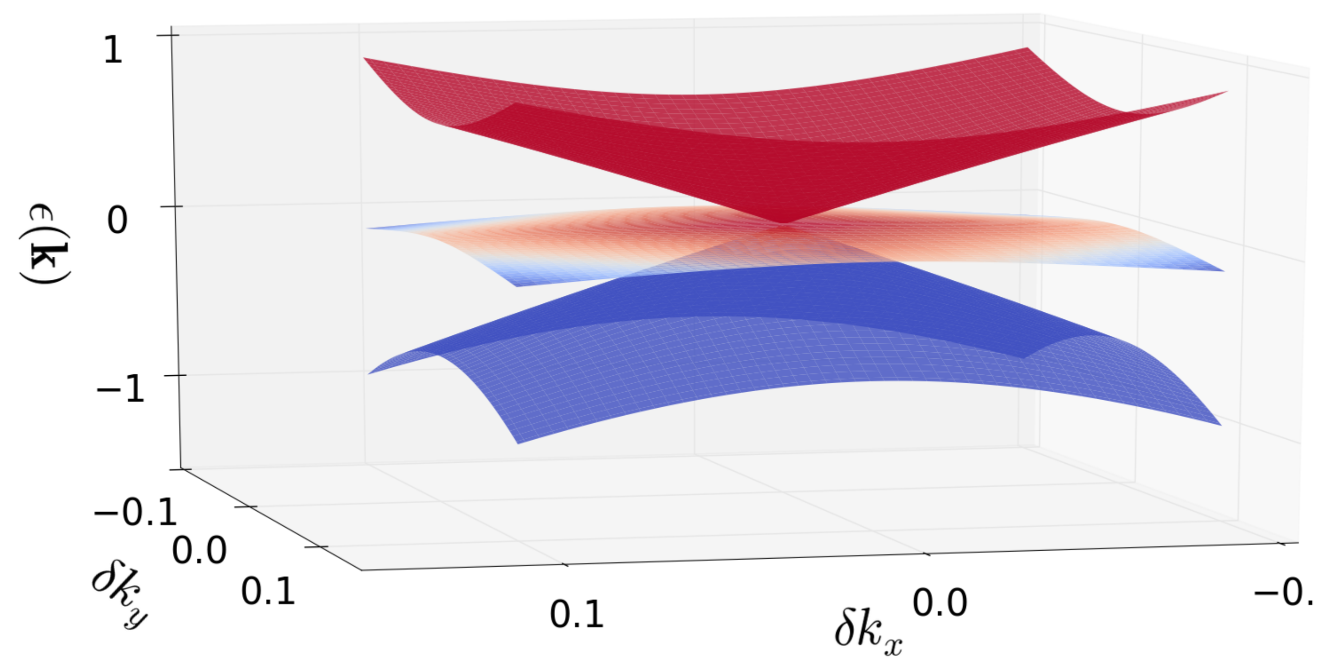
- Spin-1 Weyl at a phase transition
  - protected line nodes

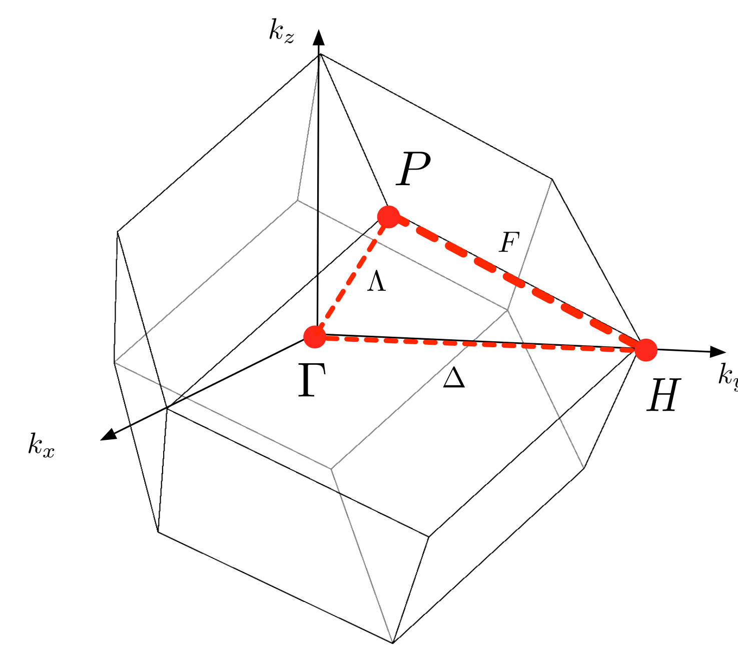




“Spin-1 Dirac” Fermions

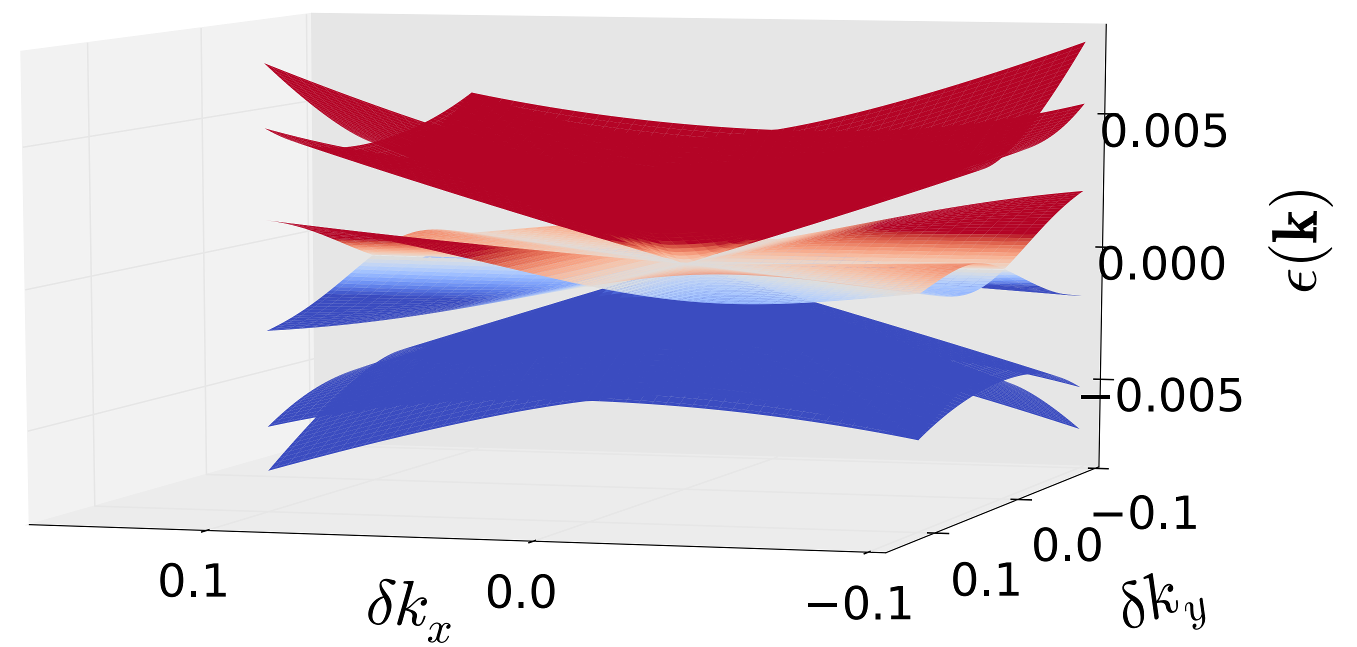
- Space groups 206 and 230 at the P point
- Same symmetries as the spin-1 Weyl, but now also respects $I\mathcal{T}$
- Two superimposed copies of a spin-1 Weyl
- No protected surface states (a la Dirac nodes at high symmetry points)

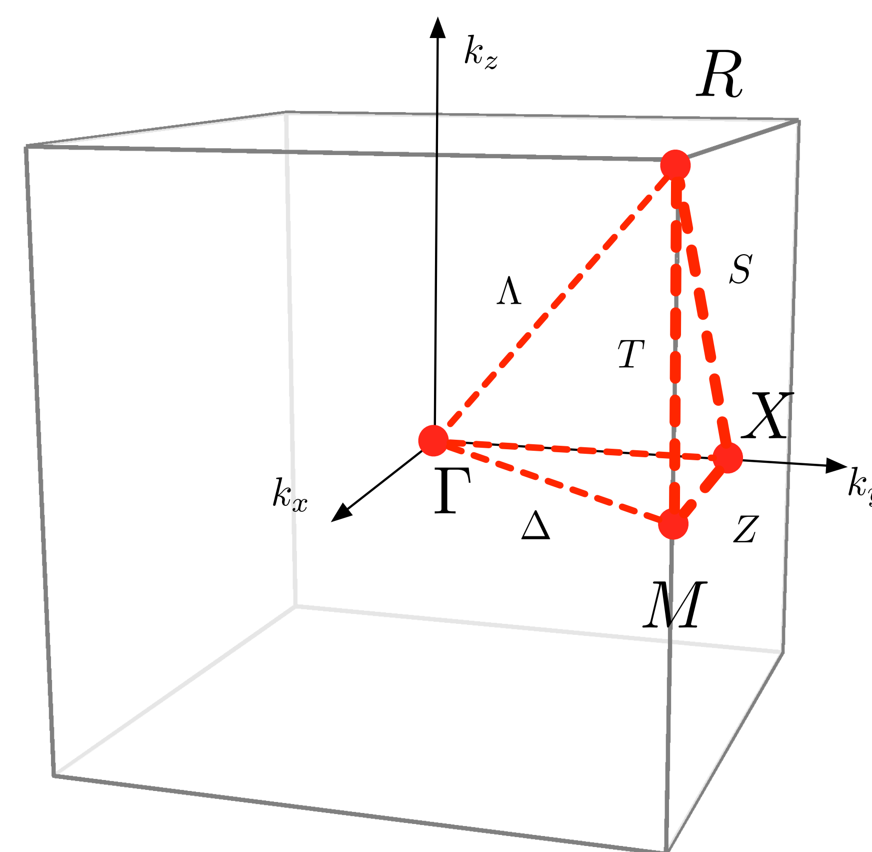




"Double Spin-1"

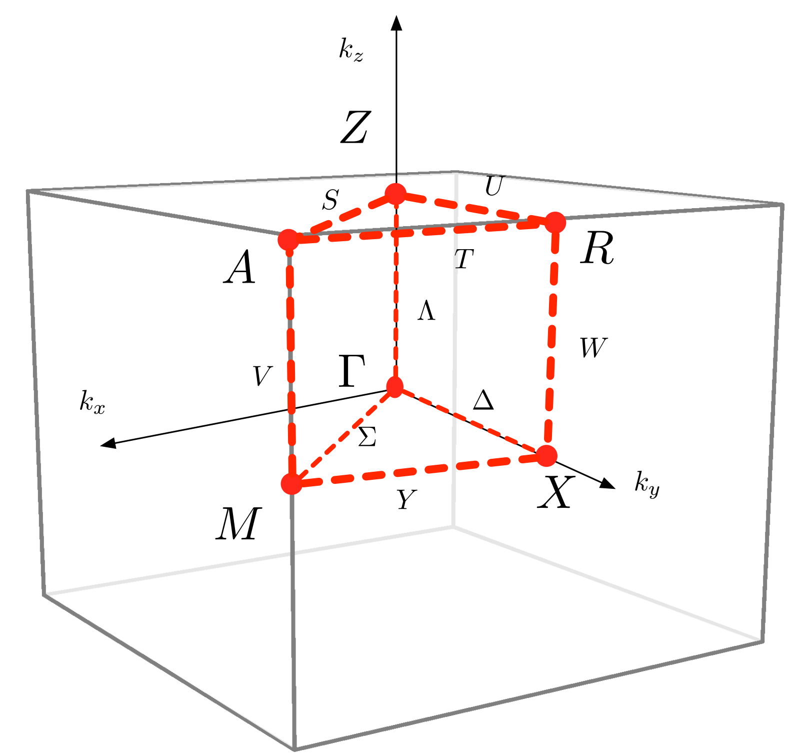
- Space groups 198, 212, 213
- Primitive cubic version of 199 - TR pairs two spin-1 Weyls
- No mirrors - these both have the same monopole charge
- c.f. Chang et al., arXiv: 1706.04600

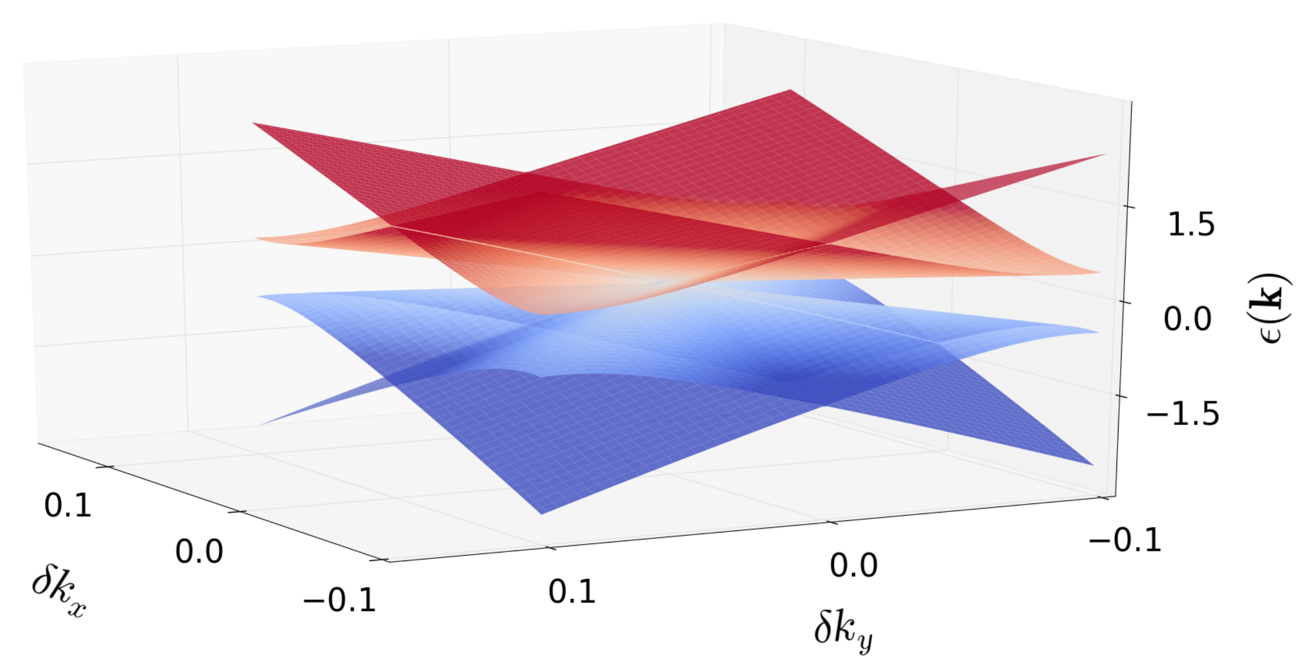




Eightfold Degeneracy - Dirac Lines

- SG 130 and 135 at the A point
- **Only one** allowed representation of the symmetry group - 8-fold degeneracy required
- Can appear as an isolated feature at the Fermi level
- Mirror symmetry along BZ edges -> fourfold *Dirac* line nodes
- Zeeman splitting / Strain splitting -> Dirac, Weyl, and line-node semimetals, strong/weak TIs



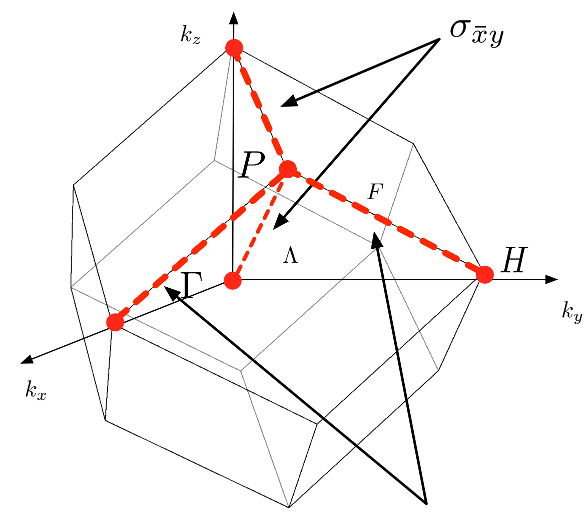


Full Classification: Surface/Line Degeneracies

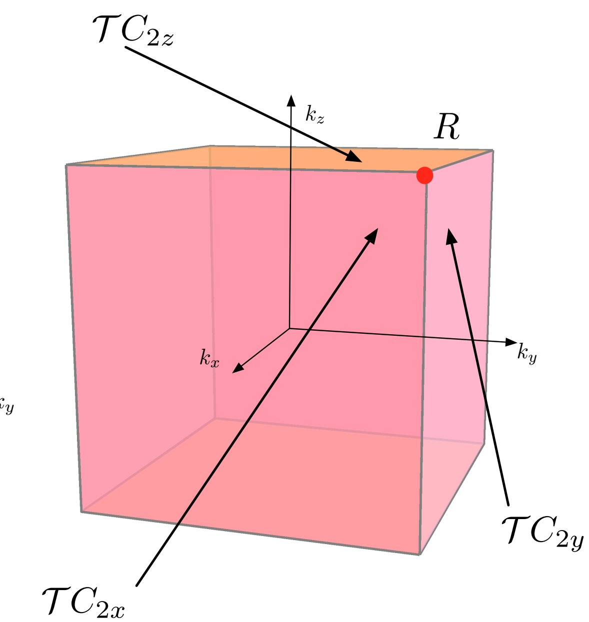
Due to nonsymmorphicity, T C2 squares to -1

Bravais lattice	Lattice vectors	Reciprocal lattice vectors
Primitive cubic	$(a,0,0),(0,a,0),(0,0,a)$	$\frac{2\pi}{a}(1,0,0),\frac{2\pi}{a}(0,1,0),\frac{2\pi}{a}(0,0,1)$
Body-centered cubic	$\frac{a}{2}(-1,1,1),\frac{a}{2}(1,-1,1),\frac{a}{2}(1,1,-1)$	$\frac{2\pi}{a}(0,1,1),\frac{2\pi}{a}(1,0,1),\frac{2\pi}{a}(1,1,0)$
Primitive tetragonal	$(a,0,0),(0,a,0),(0,0,c)$	$\frac{2\pi}{a}(1,0,0),\frac{2\pi}{a}(0,1,0),\frac{2\pi}{c}(0,0,1)$

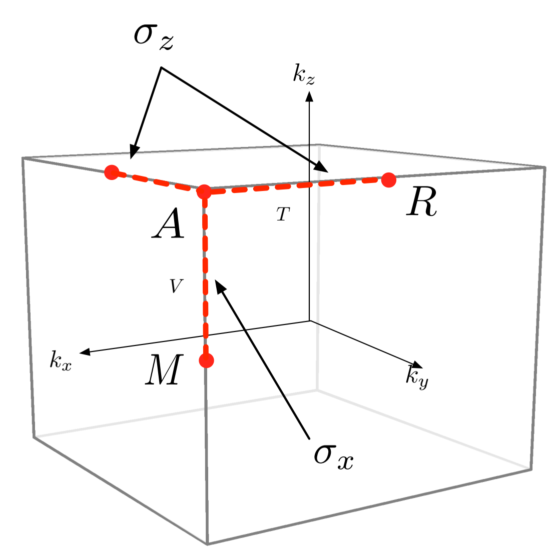
SG	La	k	d	Generators
198	cP	R	6	$\{C^-_{3,111}\|010\},\{C_{2x}\|\frac12\frac32 0\},\{C_{2y}\|0\frac32\frac12\}$
199	cI	P	3	$\{C^-_{3,111}\|101\},\{C_{2x}\|\frac12\frac12 0\},\{C_{2y}\|0\frac12\frac12\}$
205	cP	R	6	$\{C^-_{3,111}\|010\},\{C_{2x}\|\frac12\frac32 0\},\{C_{2y}\|0\frac32\frac12\},\{I\|000\}$
206	cI	P	6	$\{C^-_{3,111}\|101\},\{C_{2x}\|\frac12\frac12 0\},\{C_{2y}\|0\frac12\frac12\}$
212	cP	R	6	$\{C_{2x}\|\frac12\frac12 0\},\{C_{2y}\|0\frac12\frac12\},\{C^-_{3,111}\|000\},\{C_{2,1\bar10}\|\frac14\frac14\frac14\}$
213	cP	R	6	$\{C_{2x}\|\frac12\frac12 0\},\{C_{2y}\|0\frac12\frac12\},\{C^-_{3,111}\|000\},\{C_{2,1\bar10}\|\frac34\frac34\frac34\}$
214	cI	P	3	$\{C^-_{3,111}\|101\},\{C_{2x}\|\frac{\bar1}{2}\frac12 0\},\{C_{2y}\|0\frac12\frac{\bar1}{2}\}$
220	cI	P	3	$\{C_{3,\bar1\bar11}\|0\frac12\frac12\},\{C_{2y}\|0\frac12\frac12\},\{C_{2x}\|\frac32\frac32 0\},\{IC^-_{4x}\|\frac12 11\}$
230	cI	P	6	$\{C_{3,\bar1\bar11}\|0\frac12\frac12\},\{C_{2y}\|0\frac12\frac12\},\{C_{2x}\|\frac32\frac32 0\},\{IC^-_{4x}\|\frac12 11\}$
130	tP	A	8	$\{C_{4z}\|000\},\{\sigma_{\bar xy}\|00\frac12\},\{I\|\frac12\frac12\frac12\}$
135	tP	A	8	$\{C_{4z}\|\frac12\frac12\frac12\},\{\sigma_{\bar xy}\|00\frac12\},\{I\|000\}$
218	cP	R	8	$\{C_{2x}\|001\},\{C_{2y}\|000\},\{C^-_{3,111}\|001\},\{\sigma_{\bar xy}\|\frac12\frac12\frac12\}$
220	cI	H	8	$\{C_{2x}\|\frac12\frac12 0\},\{C_{2y}\|0\frac12\frac32\},\{C^-_{3,111}\|001\},\{\sigma_{\bar xy}\|\frac12\frac12\frac12\}$
222	cP	R	8	$\{C^-_{4z}\|000\},\{C_{2x}\|000\},\{C^-_{3,111}\|010\},\{I\|\frac12\frac12\frac12\}$
223	cP	R	8	$\{C^-_{4z}\|\frac12\frac12\frac12\},\{C_{2x}\|000\},\{C^-_{3,111}\|010\},\{I\|000\}$
230	cI	H	8	$\{C_{4z}\|0\frac12 0\},\{C_{2y}\|1\frac12\frac12\},\{C_{3,111}\|111\},\{I\|000\}$



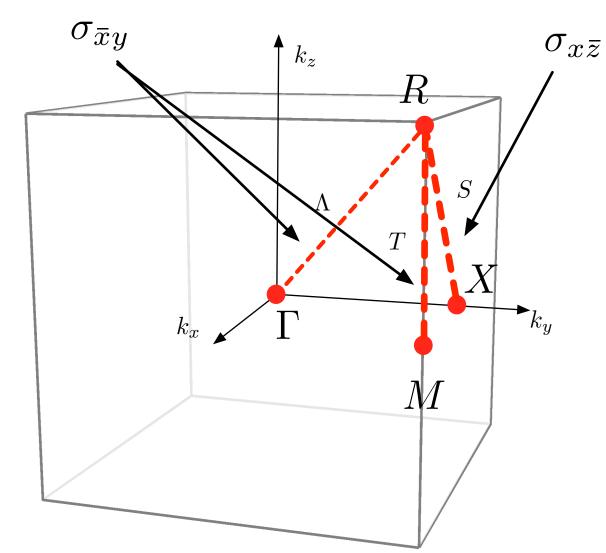
(a) Line Nodes in SG 220



(b) Surface Nodes in SGs 198,212, and 213



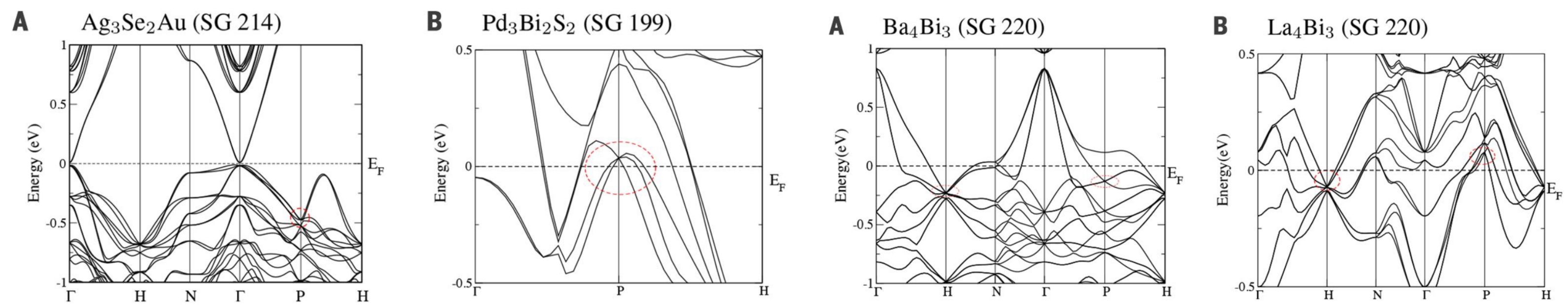
(c) Dirac line nodes in SGs 130 and 135

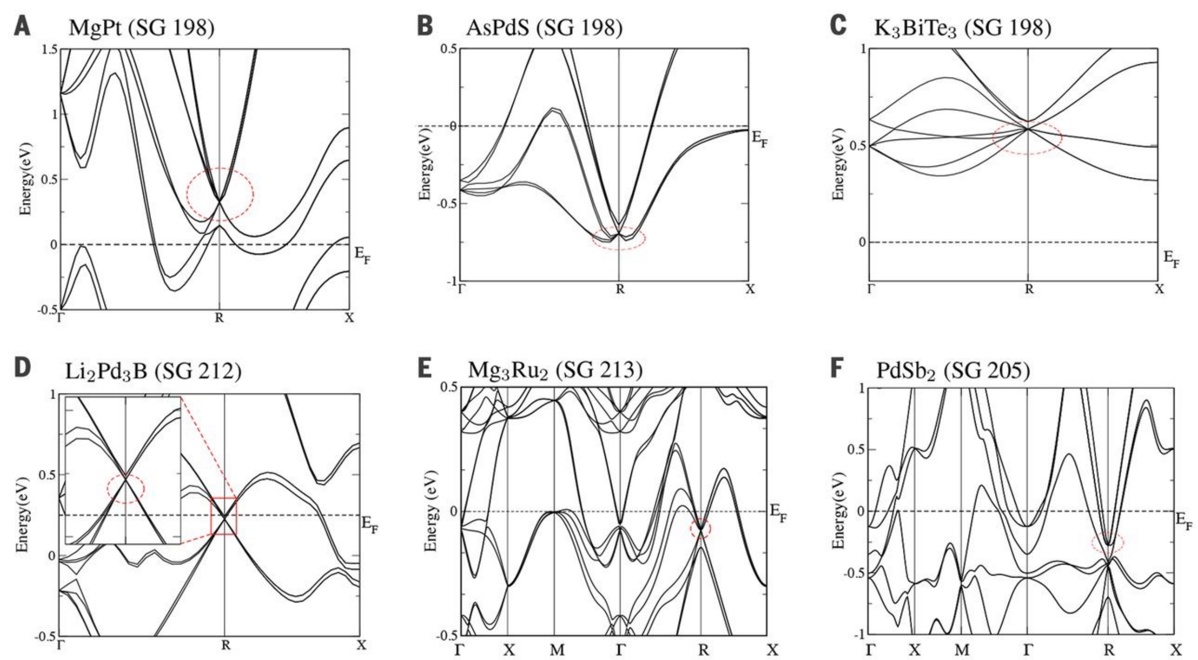


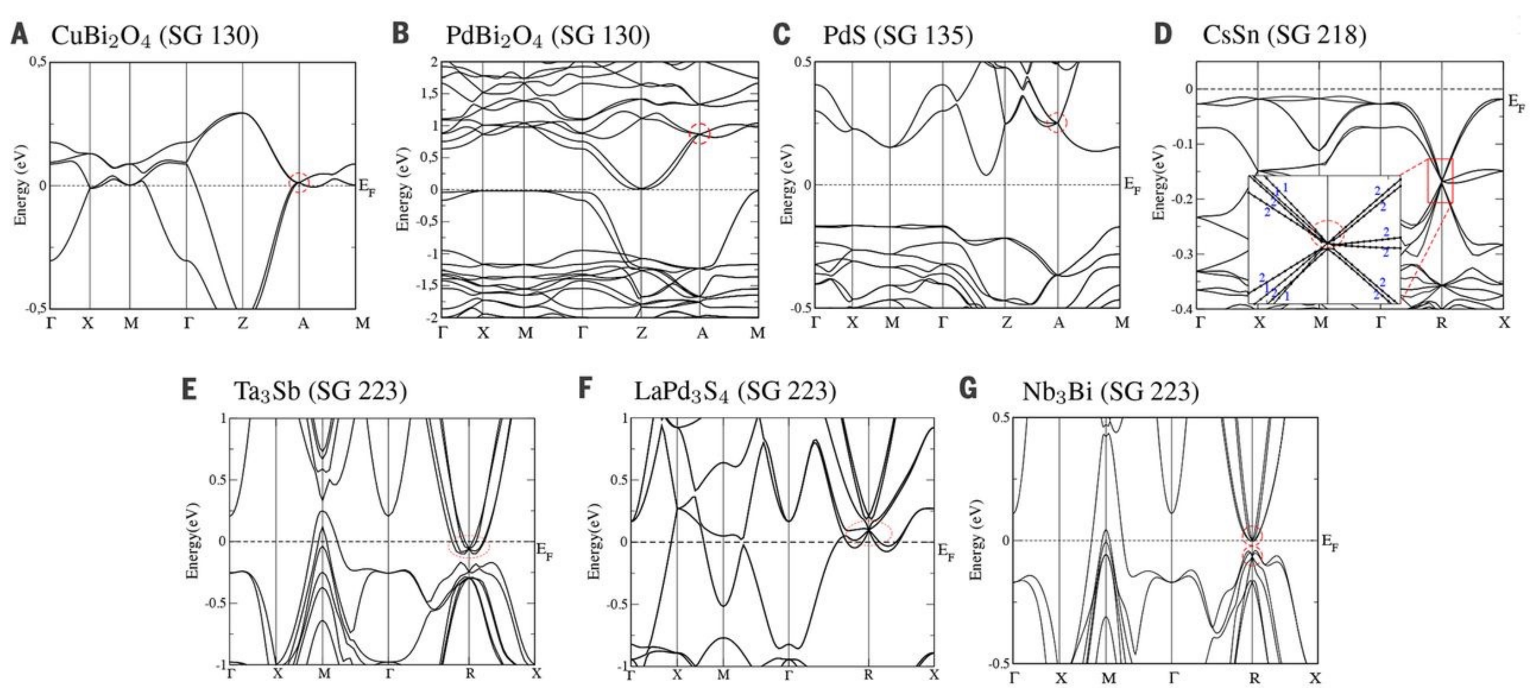
(d) Line nodes in SG 218

For 8-fold see also Wieder et al., PRL 116, 186402 (2016)

Material Candidates







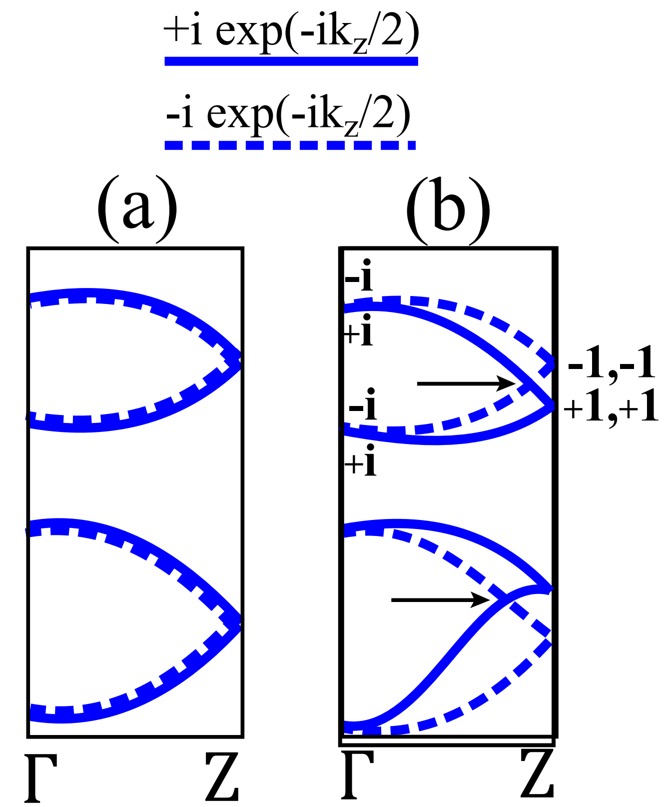
Outline

- Review - crystal symmetries, Weyl semimetals
- Symmetry protected topological metals - beyond Weyl and Dirac fermions
- Outlook - topological band theory

Band Connectivity

- Why are there so many bands?
- Momentum space perspective: Non-symmorphic symmetries force bands to stick together along high symmetry **lines**
  - Ex: Glide Symmetry $g_x = \{m_x|00\tfrac{1}{2}\}, g_x^2 = -e^{-ik_z}$

With time-reversal symmetry, bands must come in groups of 4



Alexandradinata, Wang, Bernevig (2016)

Review - $\mathbf{k}\cdot\mathbf{p}$ Hamiltonains

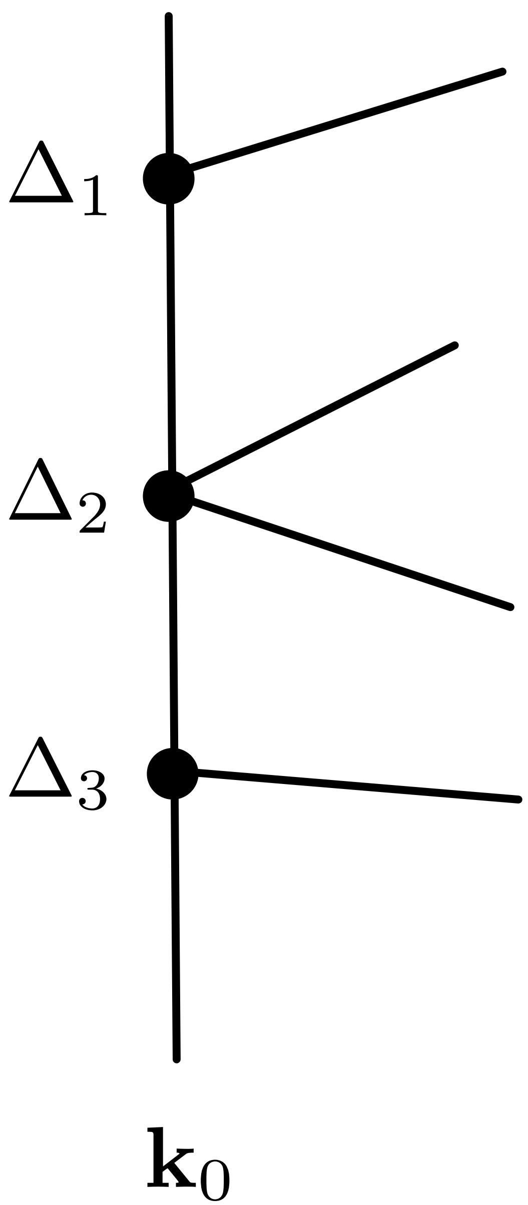
- Symmetry contrains the Bloch Hamiltonian

$$\Delta(\mathcal{G})H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$$

- Schur's Lemma: $H(\mathbf{k}_0) = \bigoplus_{\text{irreps}} E_\Delta \mathbb{1}_\Delta$

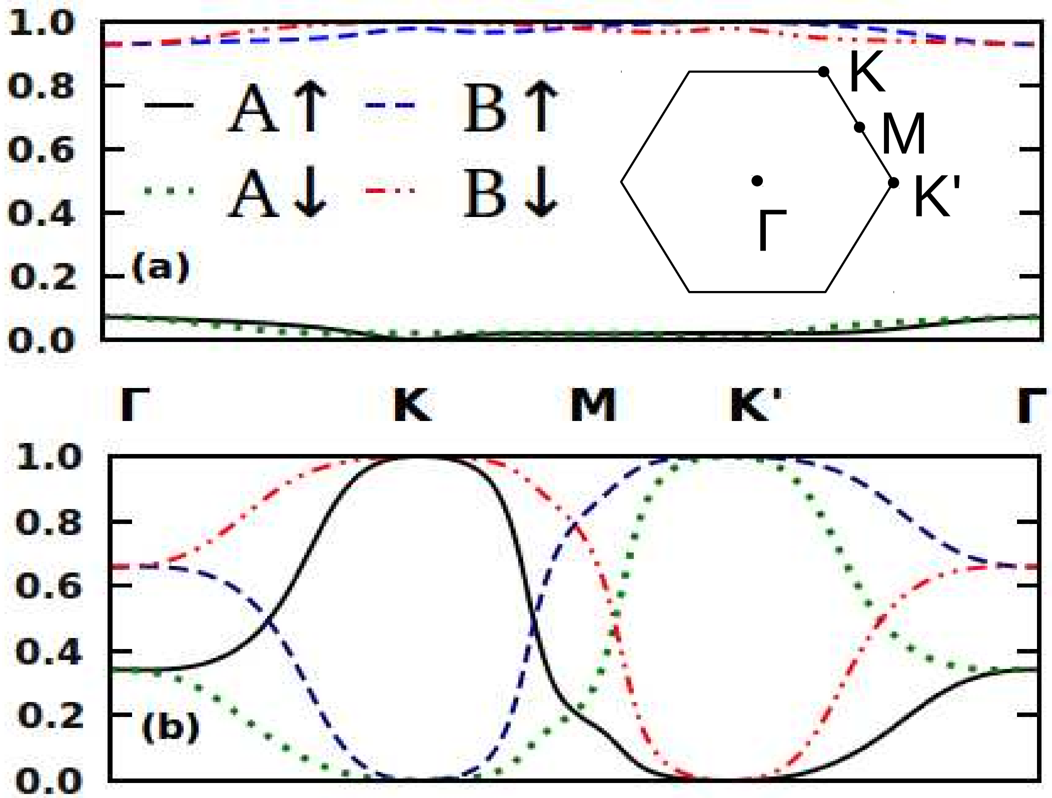
- For $\delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0$ small, $H(\mathbf{k}) \approx \bigoplus_{\text{irreps}} H_\Delta(\mathbf{k})$

- Local in momentum space -> Misses connectivity and topology



Bigger Picture

- Global band topology (and geometry!) determines a set of Wannier functions for each gapped band
- Topologically trivial -> these Wannier functions are smoothly deformable to atomic orbitals while preserving symmetries



Ex: Graphene
[Soluyanov & Vanderbilt (2011)]

Bigger Picture

- By combining representation theory with band topology, **we have applied this logic to all 230 space groups**.
- *Predictive* classification of non-interacting TCIs
- See next talk for more details