Non-symmorphic symmetry protected topological phases

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Topological Quantum Matter, KITP 2016

Agenda

1. Topological Dirac insulator
2. Beyond Dirac and Weyl fermions

Theme: non-symmorphic symmetries

Collaborators

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(Max Planck Institute
Chem. Phys of Solids)

Non-symmorphic symmetries: screws/glides w *fractional* lattice translation

C_{6z} screw:
$2\pi/6$ rot.
$z \rightarrow z+1/2$

g_x glide:
$x \rightarrow -x$
$z \rightarrow z+1/2$

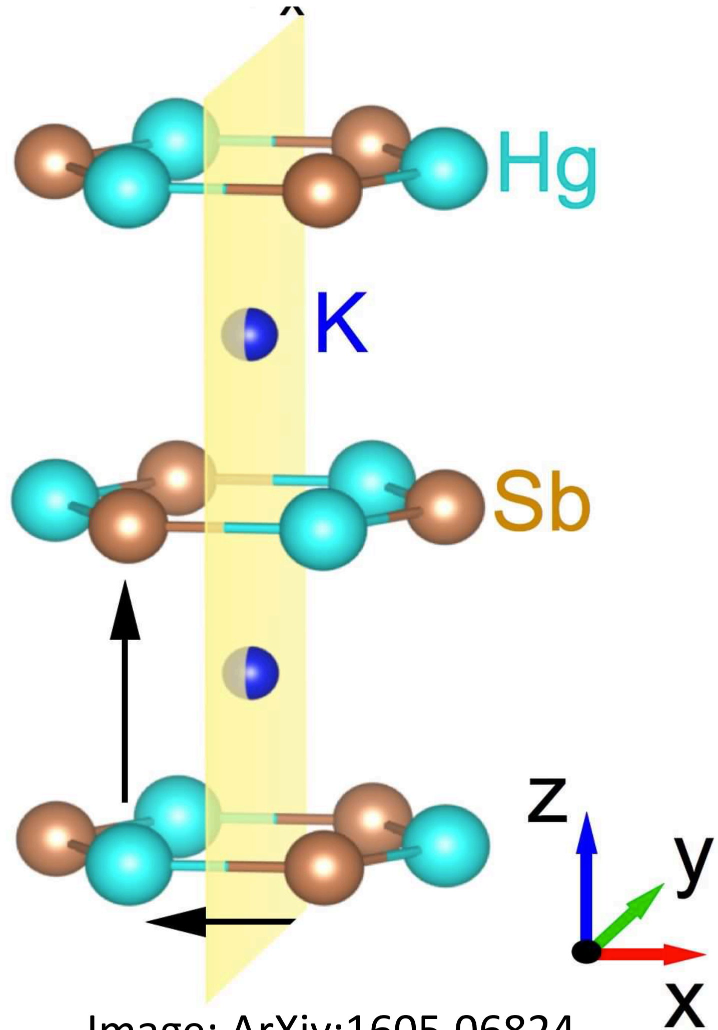
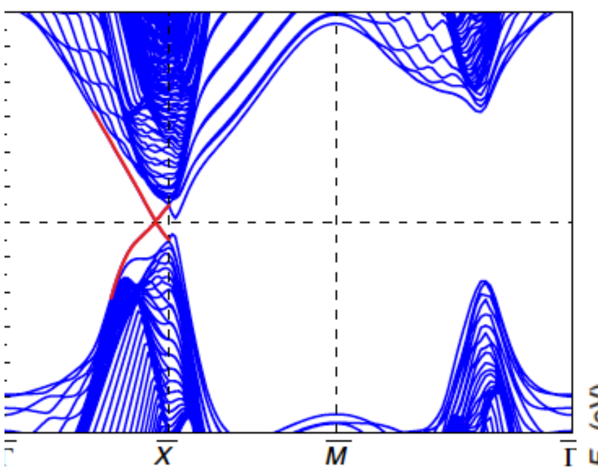


Image: ArXiv:1605.06824

Crystal symmetries yield topological invariants

- Mirror Chern number (Teo, Fu, Kane)
- Topological crystalline insulator (Fu)

Hourglass fermions (Wang, Alexandradinata, Cava, Bernevig)

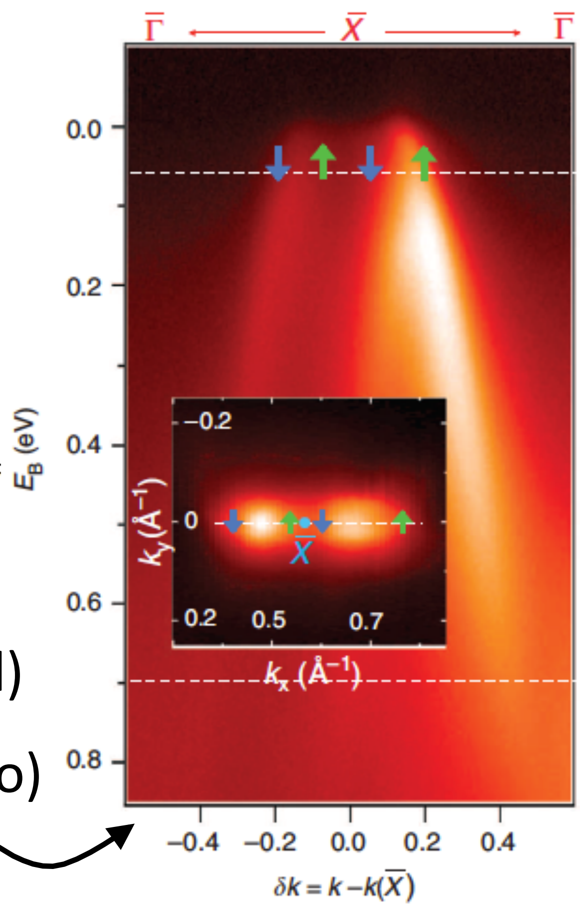


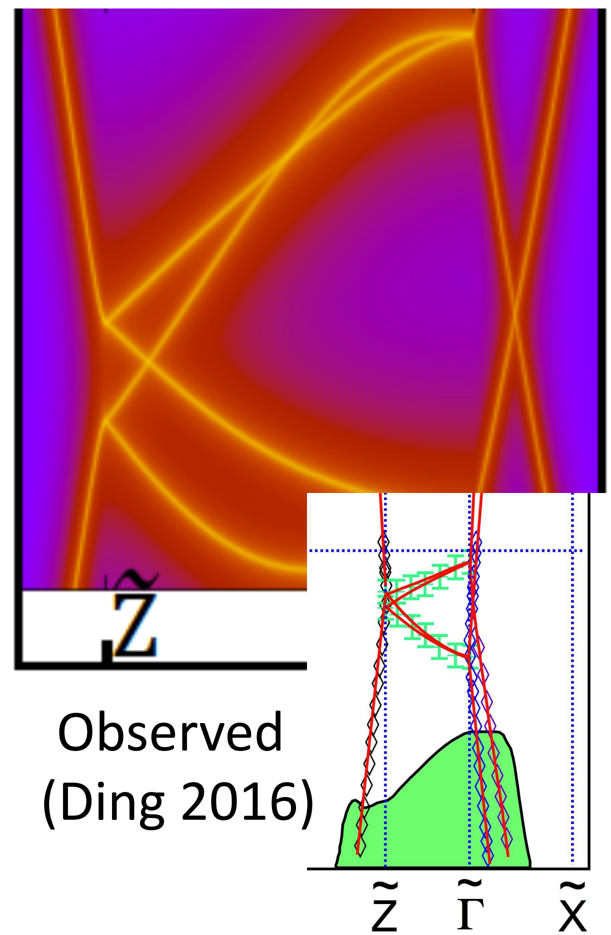
SnTe

Predicted (Hsieh, et al)

Observed (Hasan, Ando)

2012





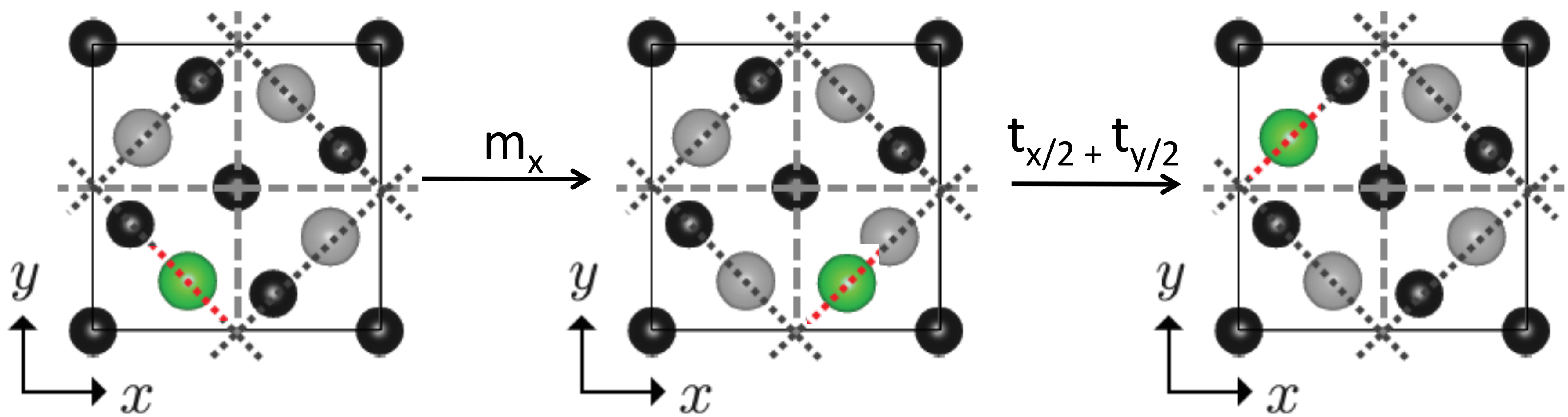
Observed (Ding 2016)

Topological Dirac Insulator

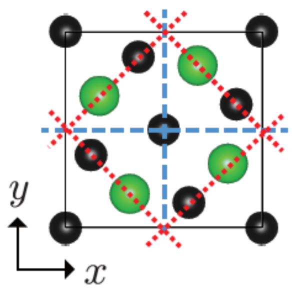
$$g_{x,y} = \{m_{x,y}|\frac{1}{2}\frac{1}{2}0\} \quad \Rightarrow g_x^2 = -e^{ik_y} \quad , \quad g_x g_y = -g_y g_x e^{ik_x - ik_y}$$

$$g_y^2 = -e^{ik_x}$$

$$\mathcal{T}^2 = -1$$



Topological Dirac Insulator



$$\mathcal{T}^2 = -1 \qquad g_{x,y}^2 = -e^{ik_{y,x}}, \quad g_x g_y = -g_y g_x e^{ik_x - ik_y}$$

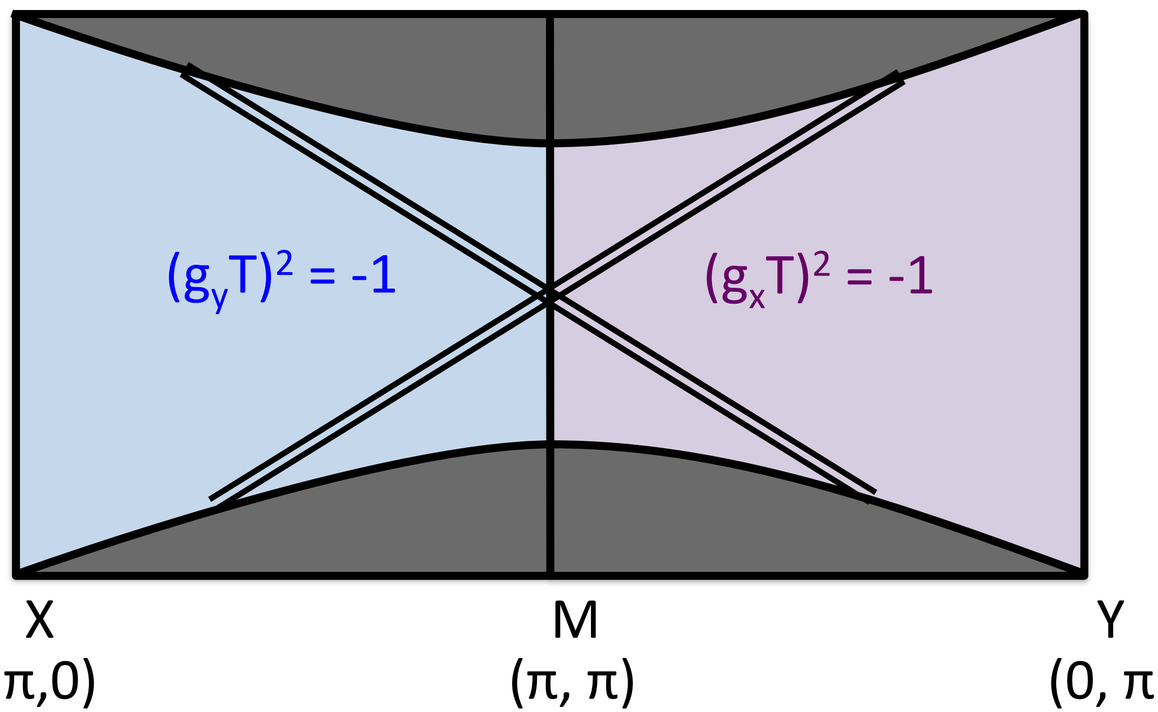
At M: $\{g_x, g_y\} = 0$, TR

Given $g_x \Psi = \lambda \Psi$

→ Ψ, $T\Psi$, $g_y\Psi$, $Tg_y\Psi$ are orthonormal

→ 4-fold degeneracy

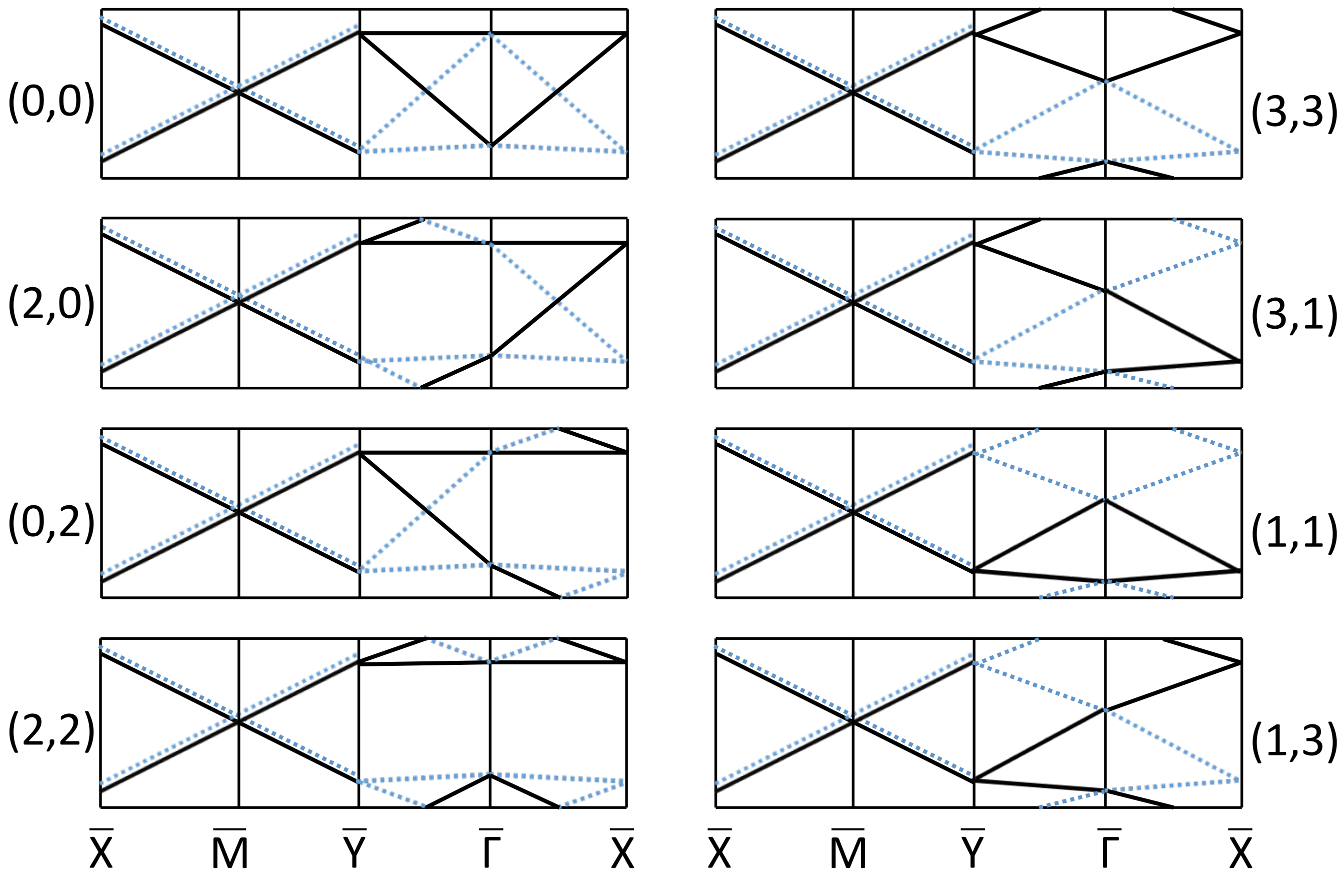
Slab band structure



Topological Dirac Insulator

$Z_4 \times Z_2$ classification of topologically distinct states

(generalize Shiozaki, et al, PRB 93, 195413 (2016))

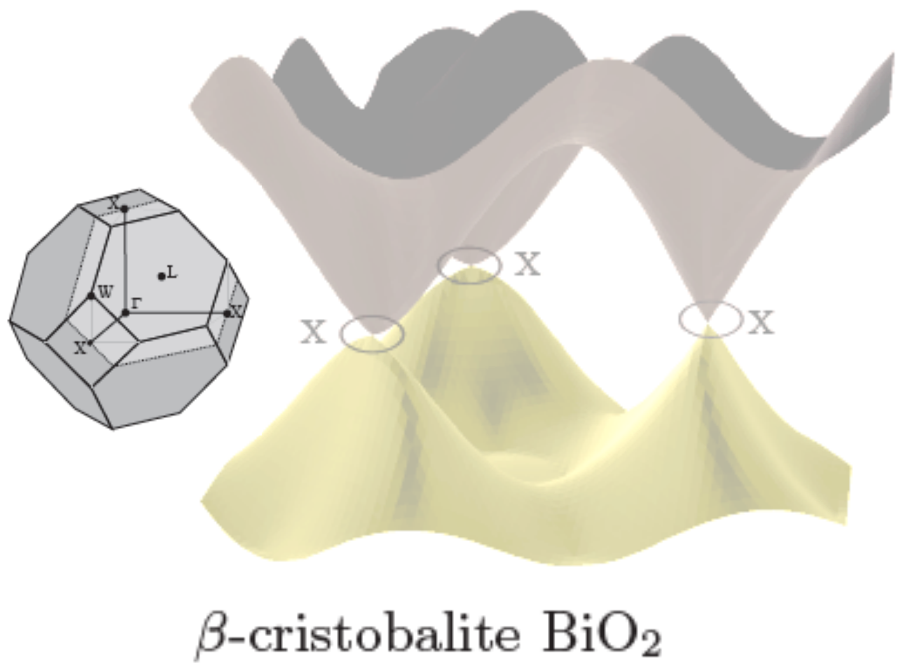


"Weak" TIs

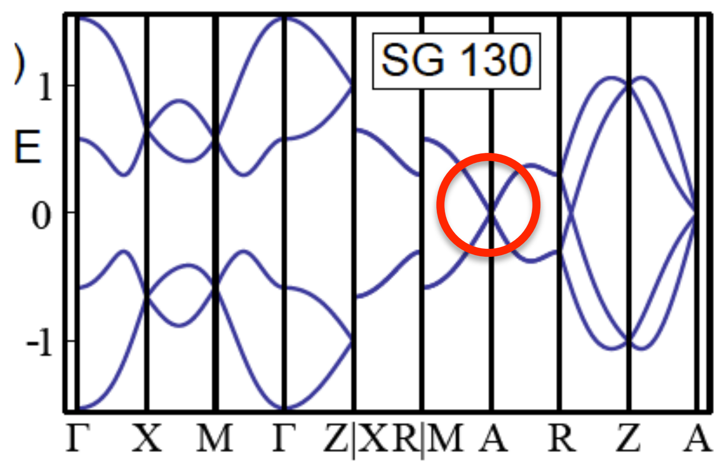
"Strong" TIs

Non-symmorphic symmetries protect semi-metals

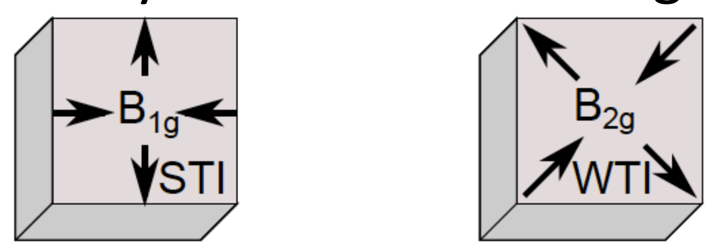
Diracs at BZ corners
(Young, et al, PRL 2012)



Double Dirac points
(Wieder, Kim, Rappe, Kane 2015)



Strain yields weak or strong TI



What other semimetals are protected by crystal symmetry?

In addition to: Weyl, Dirac, Nodal line, Double Dirac

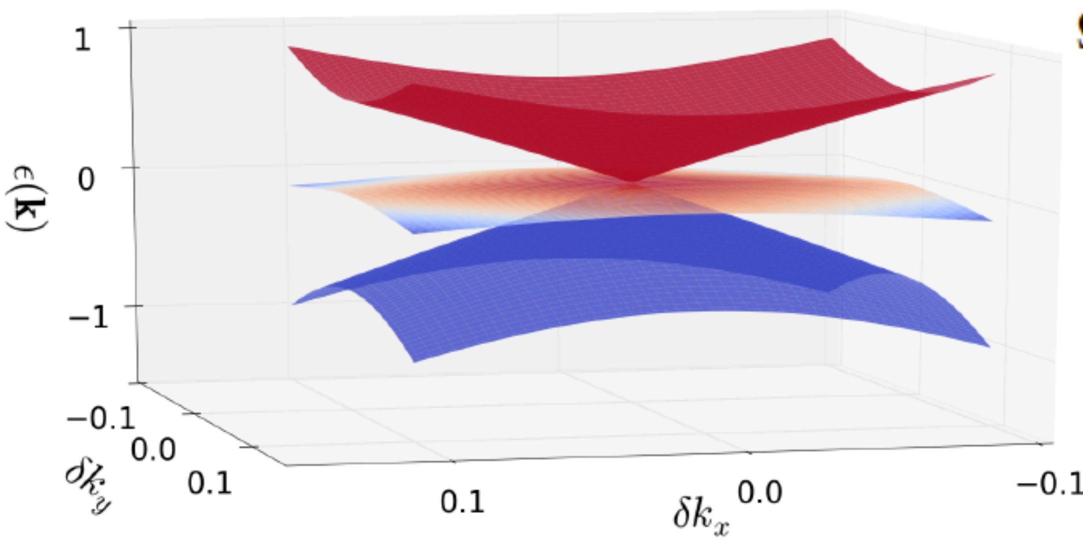
- 2-,3-, 4-, 6-, and 8-fold degeneracies
- Generalized Weyl and Dirac points
- Complete classification w TR and SOC

Beyond Weyl and Dirac Semimetals:
Unconventional quasiparticles in conventional crystals
Science 343, 6299 (2016)

"Spin-1 Weyl"

Definition: $H = \mathbf{k} \cdot \mathbf{S}$ $\qquad E = 0, \pm\sqrt{\sum k_i^2}$

(S_i are spin-1 matrices)



$$\Omega_\pm = i\nabla \times \langle \psi_\pm | \nabla \psi_\pm \rangle = \pm \frac{\delta \mathbf{k}}{|\delta \mathbf{k}|^3}$$

$$\Omega_0 = i\nabla \times \langle \psi_\pm | \nabla \psi_\pm \rangle = 0.$$

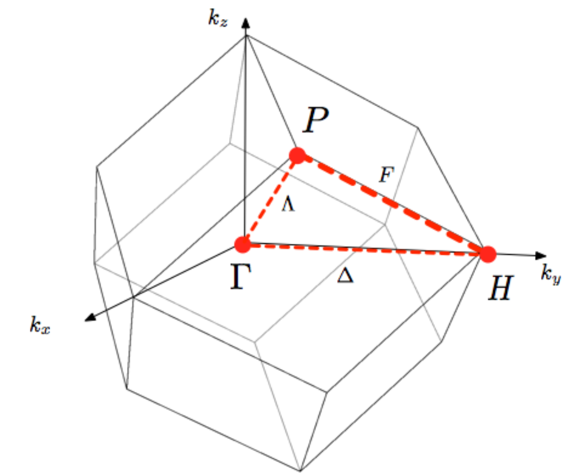
⬇

$$\nu_\pm = \frac{1}{2\pi} \oint \Omega_\pm \cdot d\mathbf{a} = \pm 2,$$

Charge-2 monopole of Berry curvature!

Also: Orlita, et al, Nat. Phys. 10, 233–238 (2014) (critical point)
D. Bercioux, et al, PRA 80, 063603 (2009) (2D realization)

“Spin-1 Weyl”



Occurs in space groups 199 and 214 (bcc) at P = (¼, ¼, ¼)

Not time-reversal invariant point!

Derive 3-fold degeneracy: irreps of the “little group” at P

$$\{C_{2x}|\frac{\bar{1}}{2}\frac{1}{2}0\}^2 = \{C^{-1}_{3,111}|101\}^3 = 1$$

Rules:

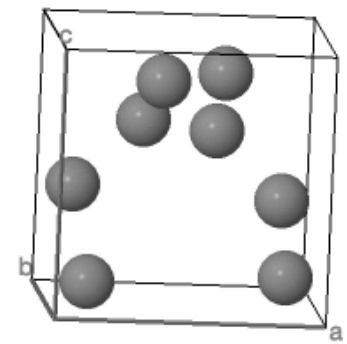
- 2π rotations represented by -1
- Translation t represented by $e^{iP.t}$

Result: 3d and 1d irreps

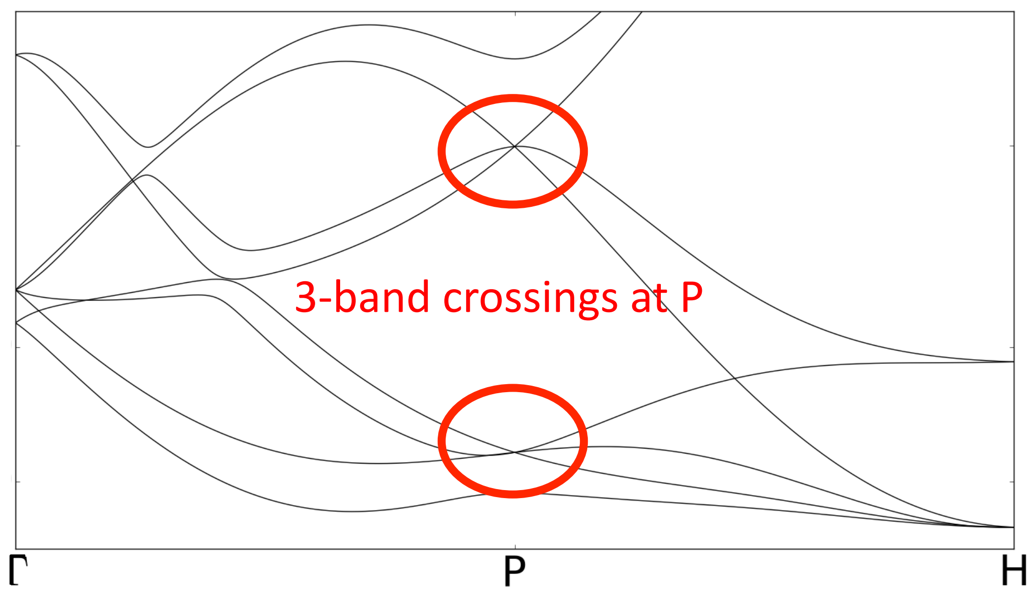
"Spin-1 Weyl"

Ex: tight-binding model for SG 214

- 4 atoms/unit cell
- 3 p orbitals/atom



Conv. unit cell (ICSD)

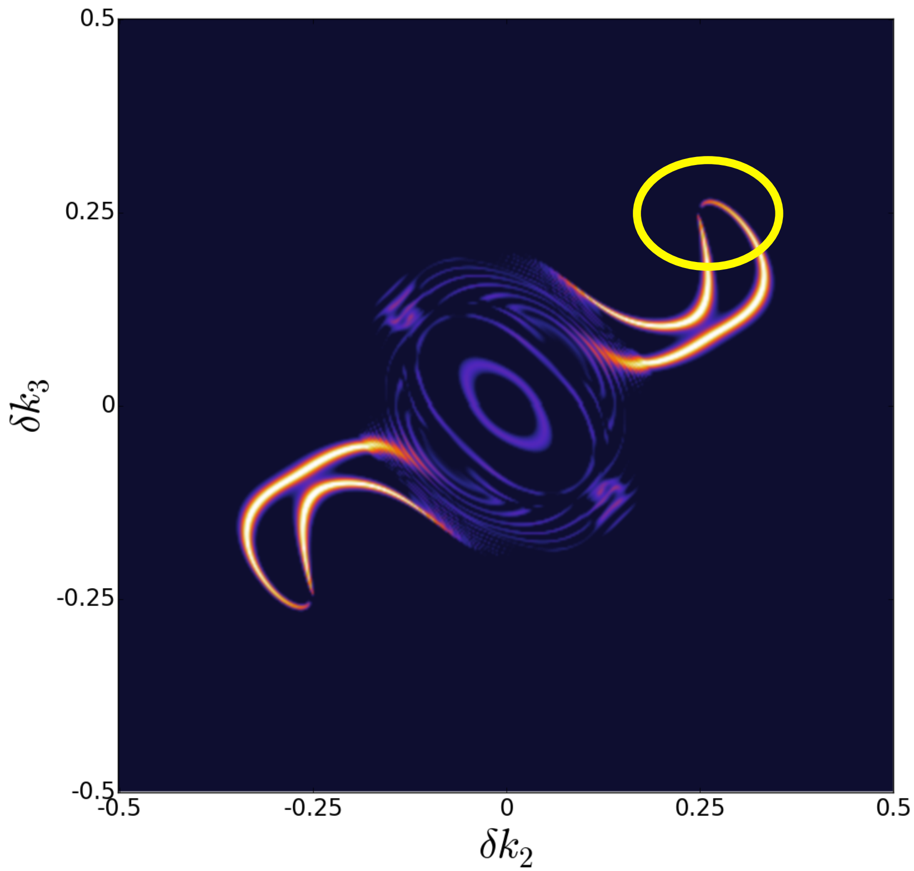


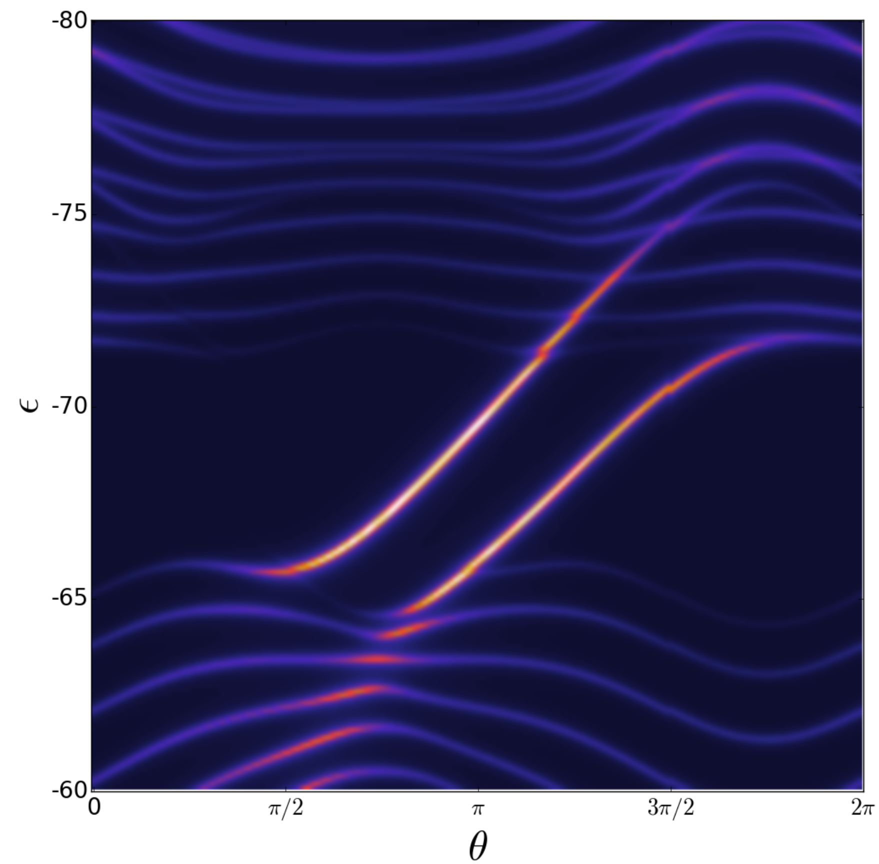
“Spin-1 Weyl”

Experimental signature: surface Fermi arc

Wan, Turner, Vishwanath, Savrasov (2011)

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

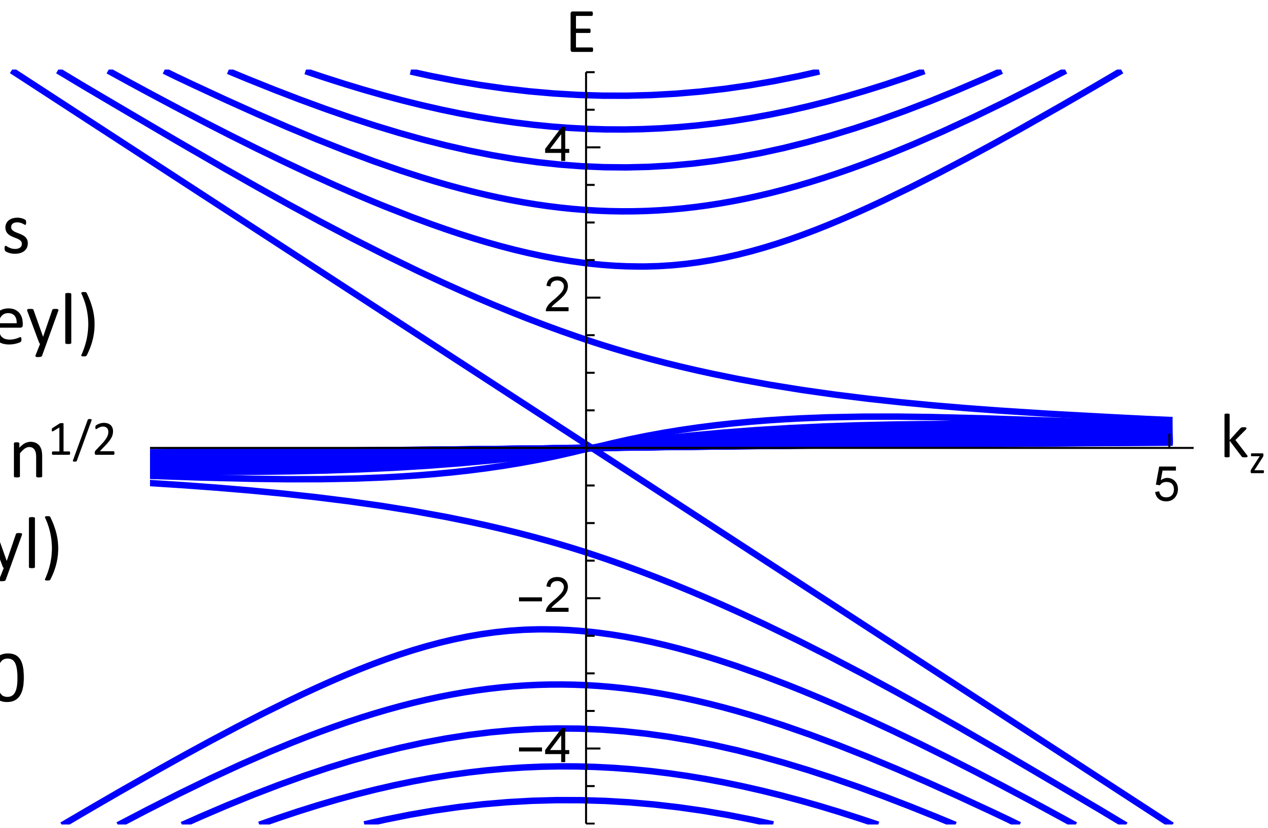




“Spin-1 Weyl”

Experimental signature: Landau levels

- Two chiral modes
  (like double Weyl)
- Level spacing → $n^{1/2}$
  (like single Weyl)
- High d.o.s. at E=0

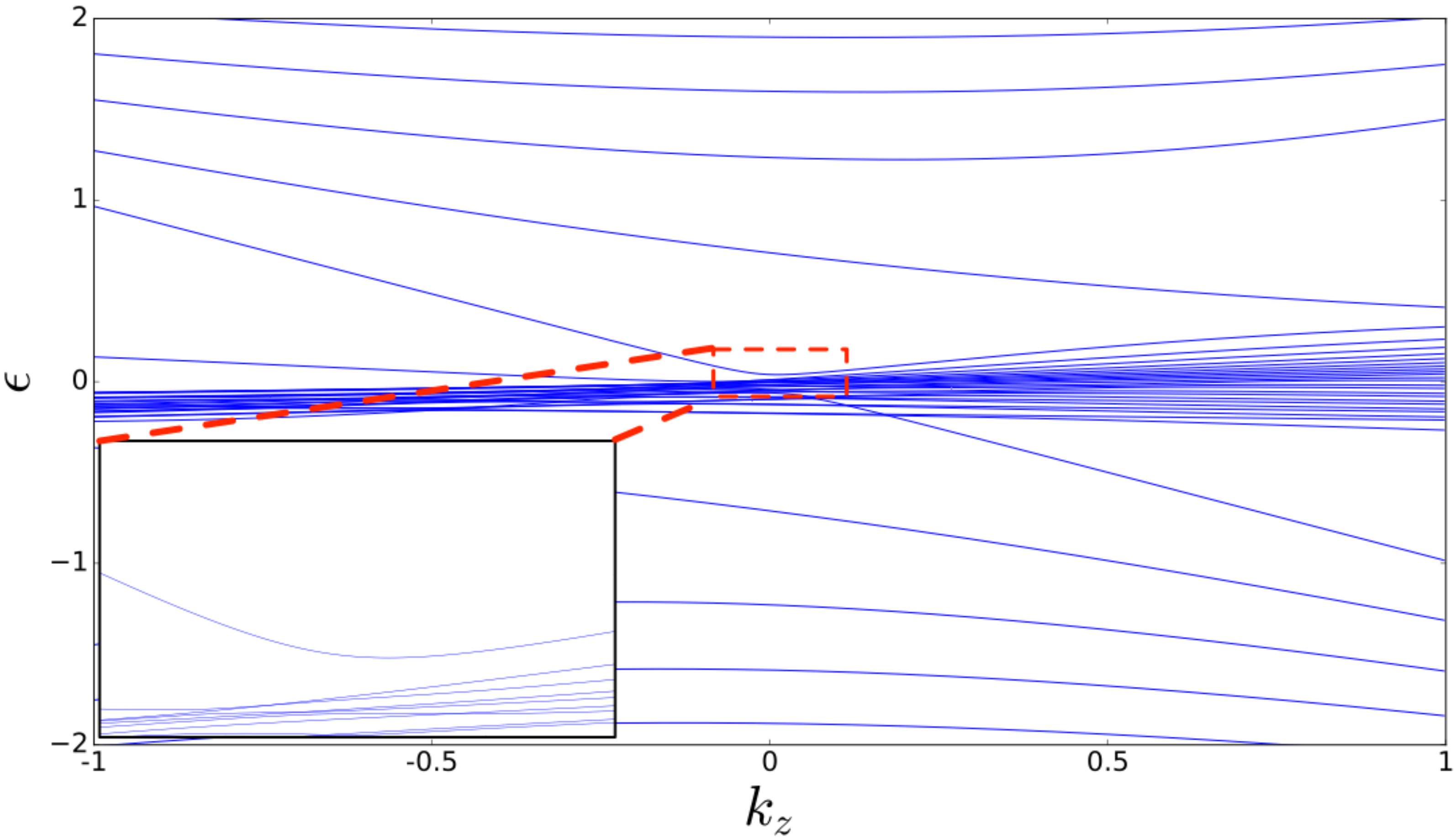


Exact spectrum when H=k.S

“Spin-1 Weyl”

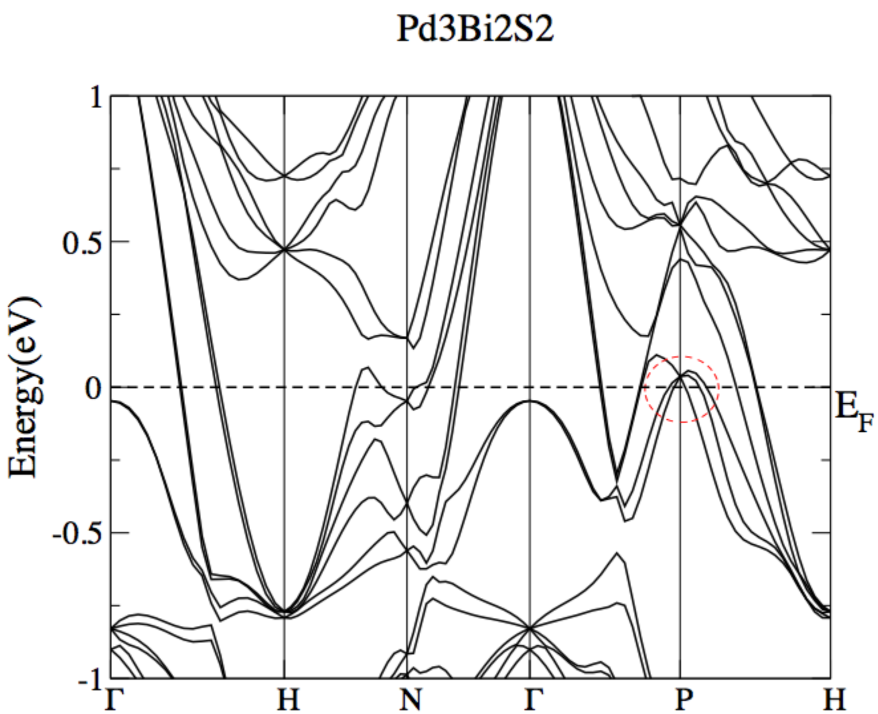
Experimental signature: Landau levels

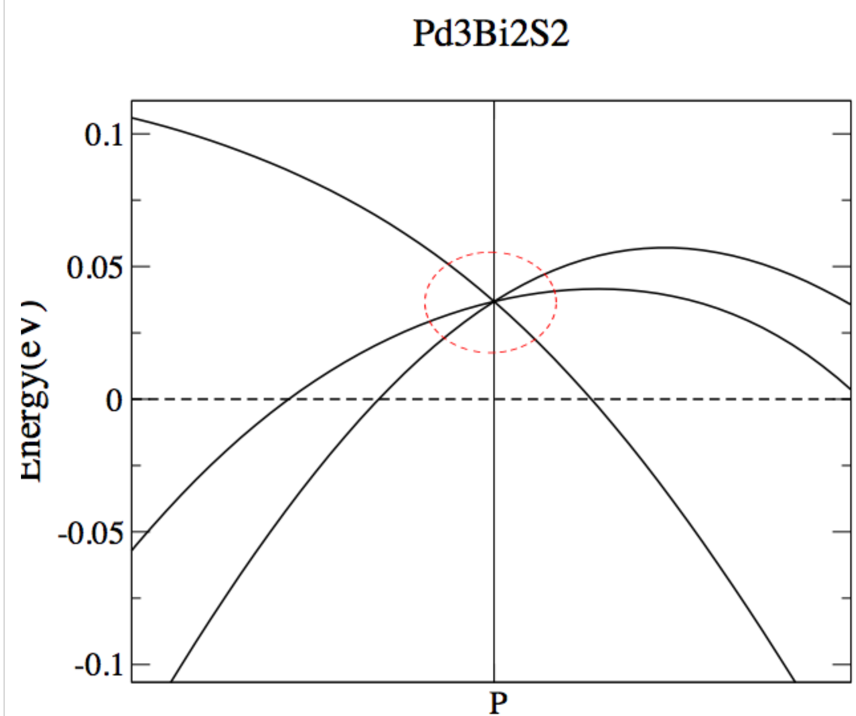
Numerical solution with higher-order terms: degeneracy is not protected



“Spin-1 Weyl”

Candidate materials

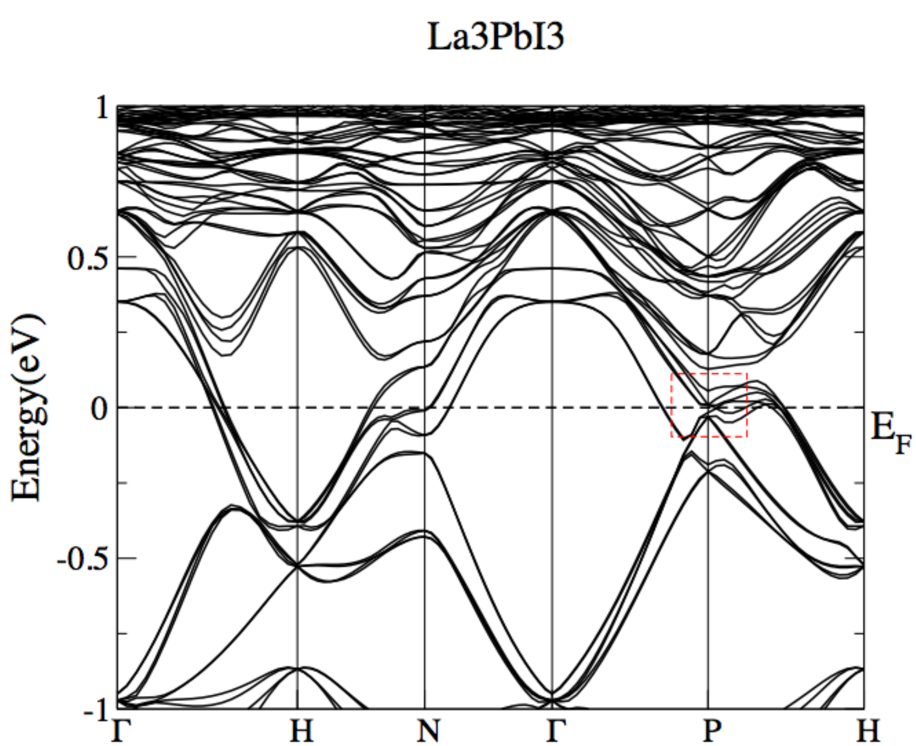


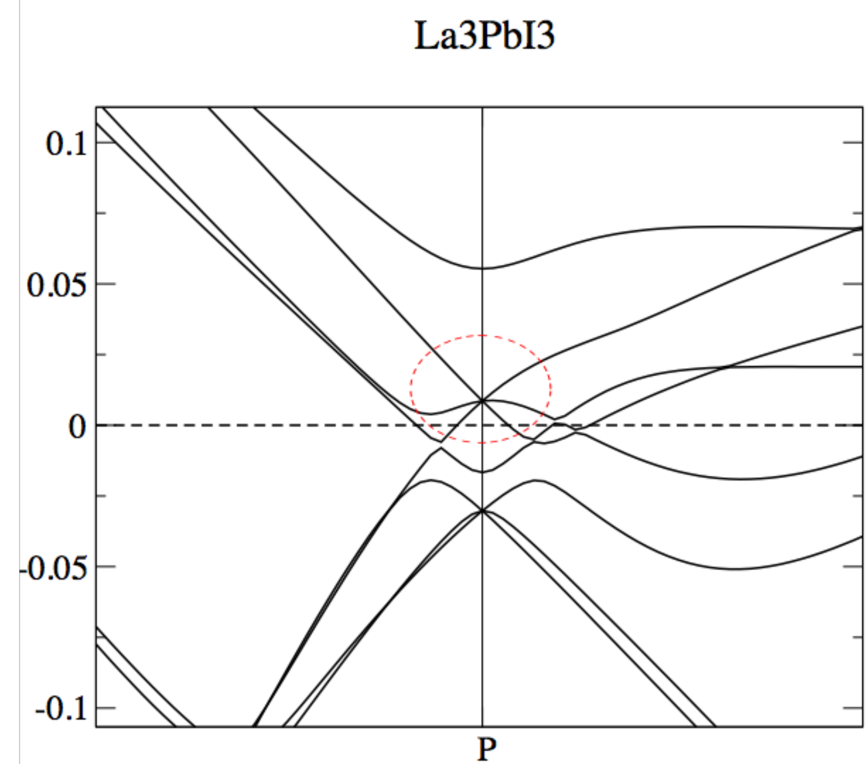


SG 199

“Spin-1 Weyl”

Candidate materials

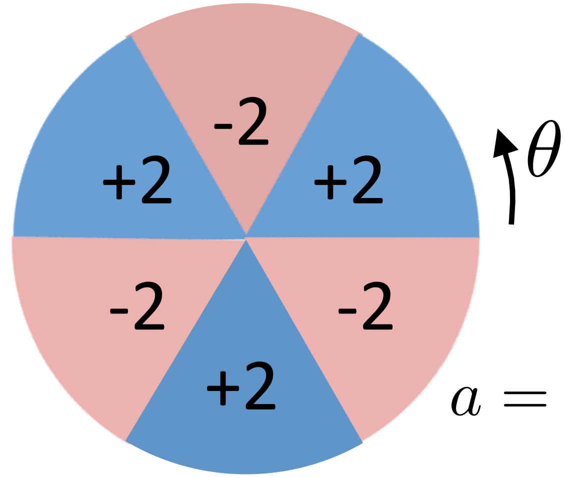




SG 214

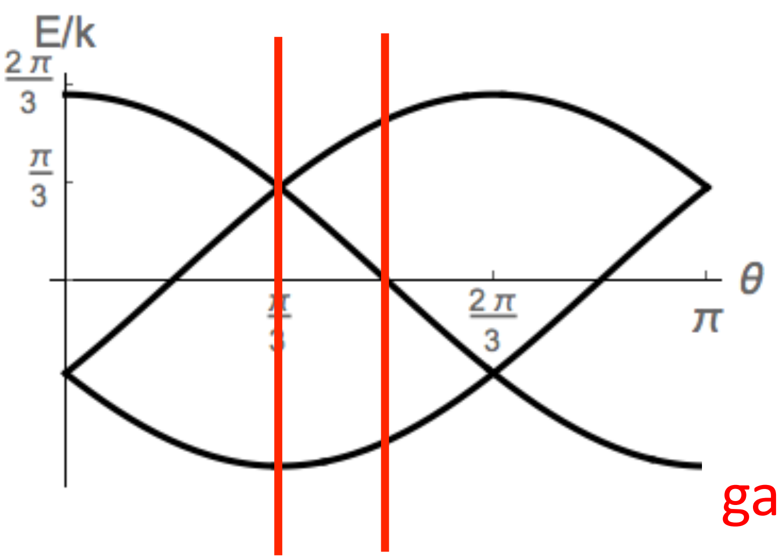
Critical spin-1 Weyl is generic in SG 220

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



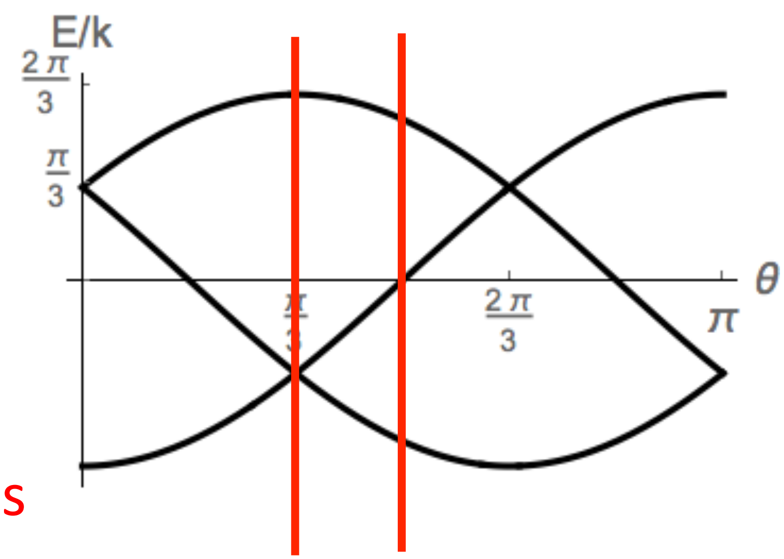
$a = |a|e^{i\theta}$

Energy along (k,k,k)



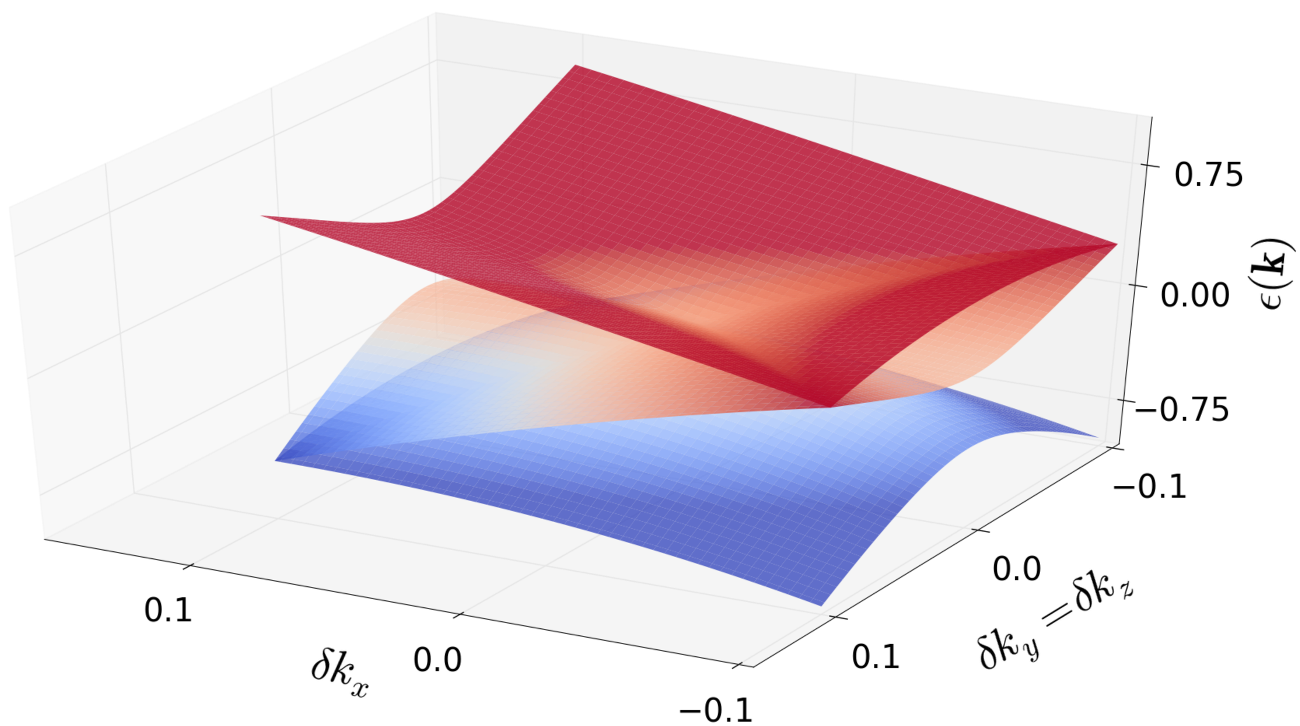
gapless

Energy along (k,-k,k)



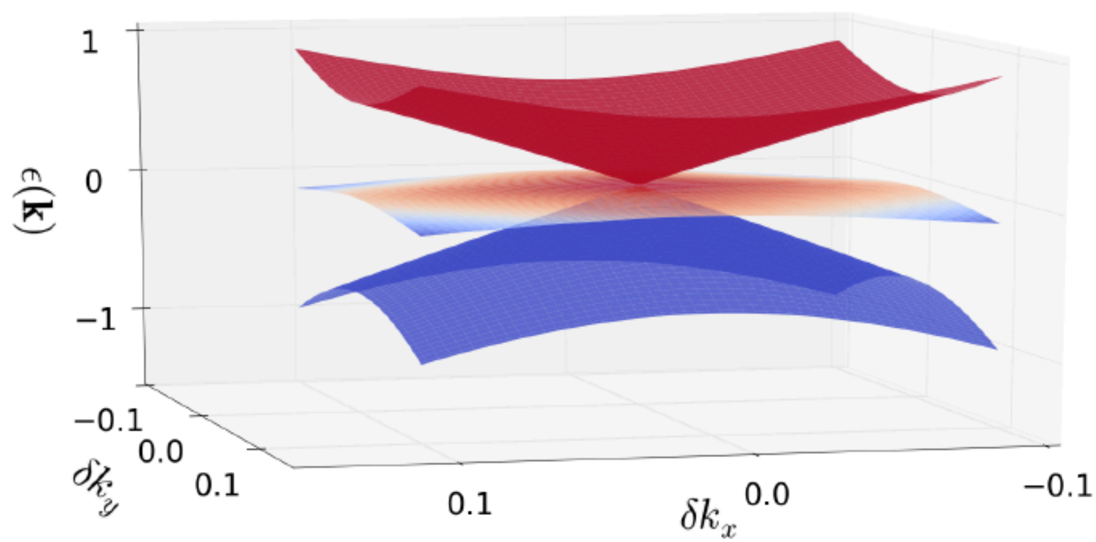
Critical spin-1 Weyl is generic in SG 220

Protected by product of inversion and C_4 screw

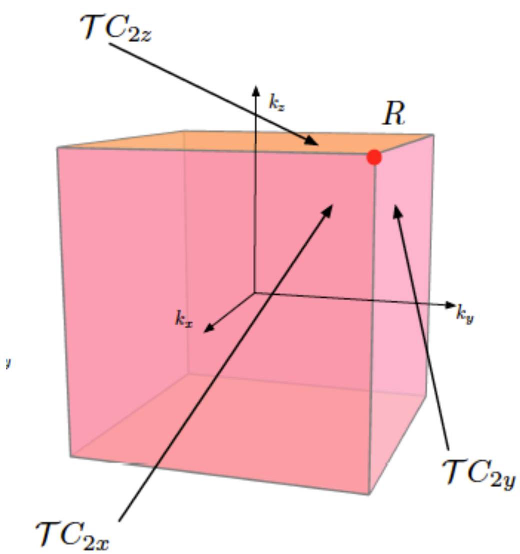


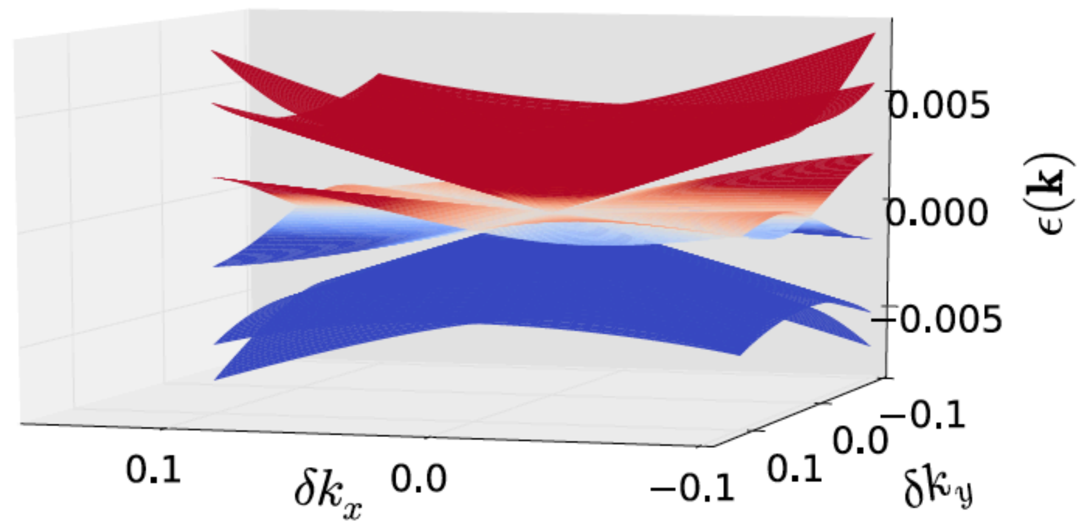
"Spin-1 Dirac"

- Two copies of spin-1 Weyl with opposite chirality
- Protected by inversion symmetry
- Occurs in SGs 206 and 230



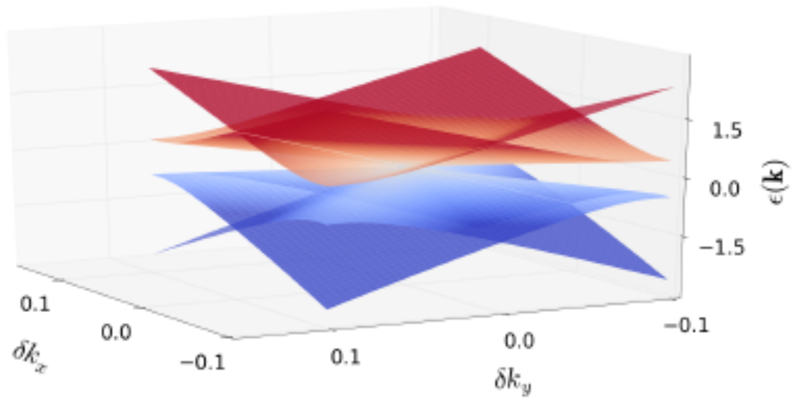
6-fold degeneracy without inversion





“Plane nodes”: 2-fold degenerate bands along faces of BZ

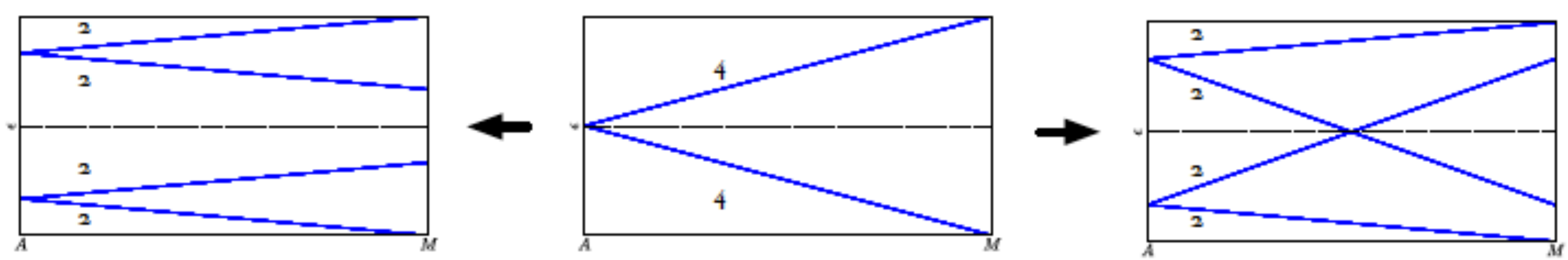
A parent phase for topological semimetals: 8-fold band crossings



TR + inversion → bands doubly-degenerate

4-fold degenerate "Dirac line nodes"

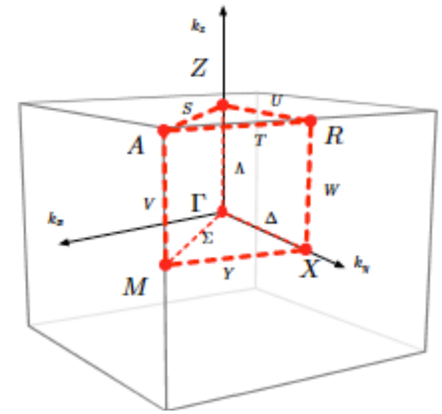
Applied magnetic field: line node splits into Dirac point

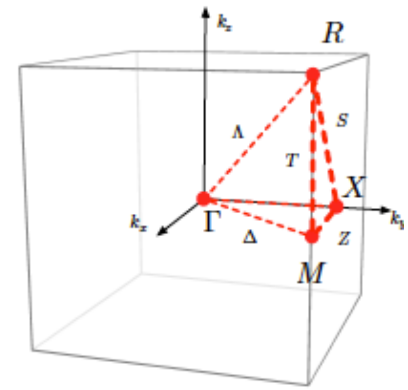


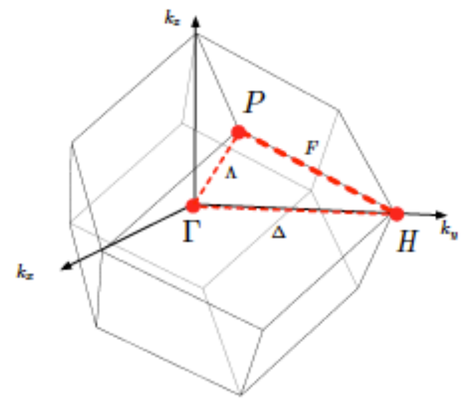
Recall: Wieder, et al: strain gaps into weak/strong TI

Space groups with 3-, 6-, 8- band crossing

SG	La	k	d	Generators
198	cP	R	6	$\{C_{3,111}^{-}\|010\}$, $\{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}$, $\{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}$
199	cB	P	3	$\{C_{3,111}^{-}\|101\}$, $\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, $\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$
205	cP	R	6	$\{C_{3,111}^{-}\|010\}$, $\{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}$, $\{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}$, $\{I\|000\}$
206	cB	P	6	$\{C_{3,111}^{-}\|101\}$, $\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, $\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$
212	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$,$\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{3,111}^{-}\|000\}$,$\{C_{2,1\bar{1}0}\|\frac{1}{4}\frac{1}{4}\frac{1}{4}\}$
213	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$,$\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{3,111}^{-}\|000\}$,$\{C_{2,1\bar{1}0}\|\frac{3}{4}\frac{3}{4}\frac{3}{4}\}$
214	cB	P	3	$\{C_{3,111}^{-}\|101\}$, $\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, $\{C_{2y}\|0\frac{1}{2}\frac{\bar{1}}{2}\}$
220	cB	P	3	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\}$,$\{IC_{4x}^{-}\|\frac{1}{2}11\}$
230	cB	P	6	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$,$\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\}$,$\{IC_{4x}^{-}\|\frac{1}{2}11\}$
130	tP	A	8	$\{C_{4z}\|000\}$, $\{\sigma_{\bar{x}y}\|00\frac{1}{2}\}$, $\{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
135	tP	A	8	$\{C_{4z}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$, $\{\sigma_{\bar{x}y}\|00\frac{1}{2}\}$, $\{I\|000\}$
218	cP	R	8	$\{C_{2x}\|001\}$, $\{C_{2y}\|000\}$, $\{C_{3,111}^{-}\|001\}$, $\{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
220	cB	H	8	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}$, $\{C_{2y}\|0\frac{1}{2}\frac{3}{2}\}$, $\{C_{3,111}^{-}\|001\}$, $\{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
222	cP	R	8	$\{C_{4z}^{-}\|000\}$, $\{C_{2x}\|000\}$, $\{C_{3,111}^{-}\|010\}$, $\{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
223	cP	R	8	$\{C_{4z}^{-}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$, $\{C_{2x}\|000\}$, $\{C_{3,111}^{-}\|010\}$, $\{I\|000\}$
230	cB	H	8	$\{C_{4z}\|0\frac{1}{2}0\}$, $\{C_{2y}\|1\frac{1}{2}\frac{1}{2}\}$, $\{C_{3,111}\|111\}$, $\{I\|000\}$

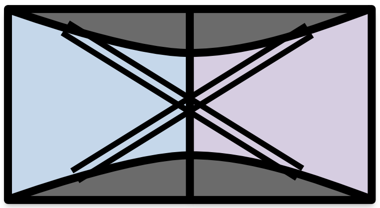


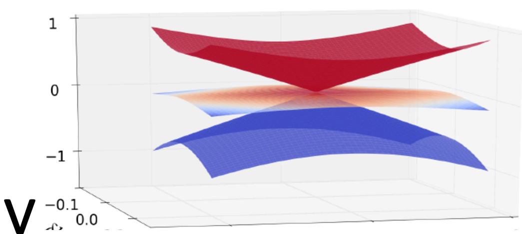




(c)

Non-symmorphic symmetries protect novel topological phases





Materials growth: underway

Challenge: isolated bands at Fermi level

Are there other observable signatures?
(topological phases w/o surface states??)

New features in magnetic space groups?

What is the role of interactions?