Lecture on

Topological Semimetals

Andreas P. Schnyder

Max-Planck-Institut für Festkörperforschung, Stuttgart

Autumn School on Correlated Electrons, Jülich

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Contents

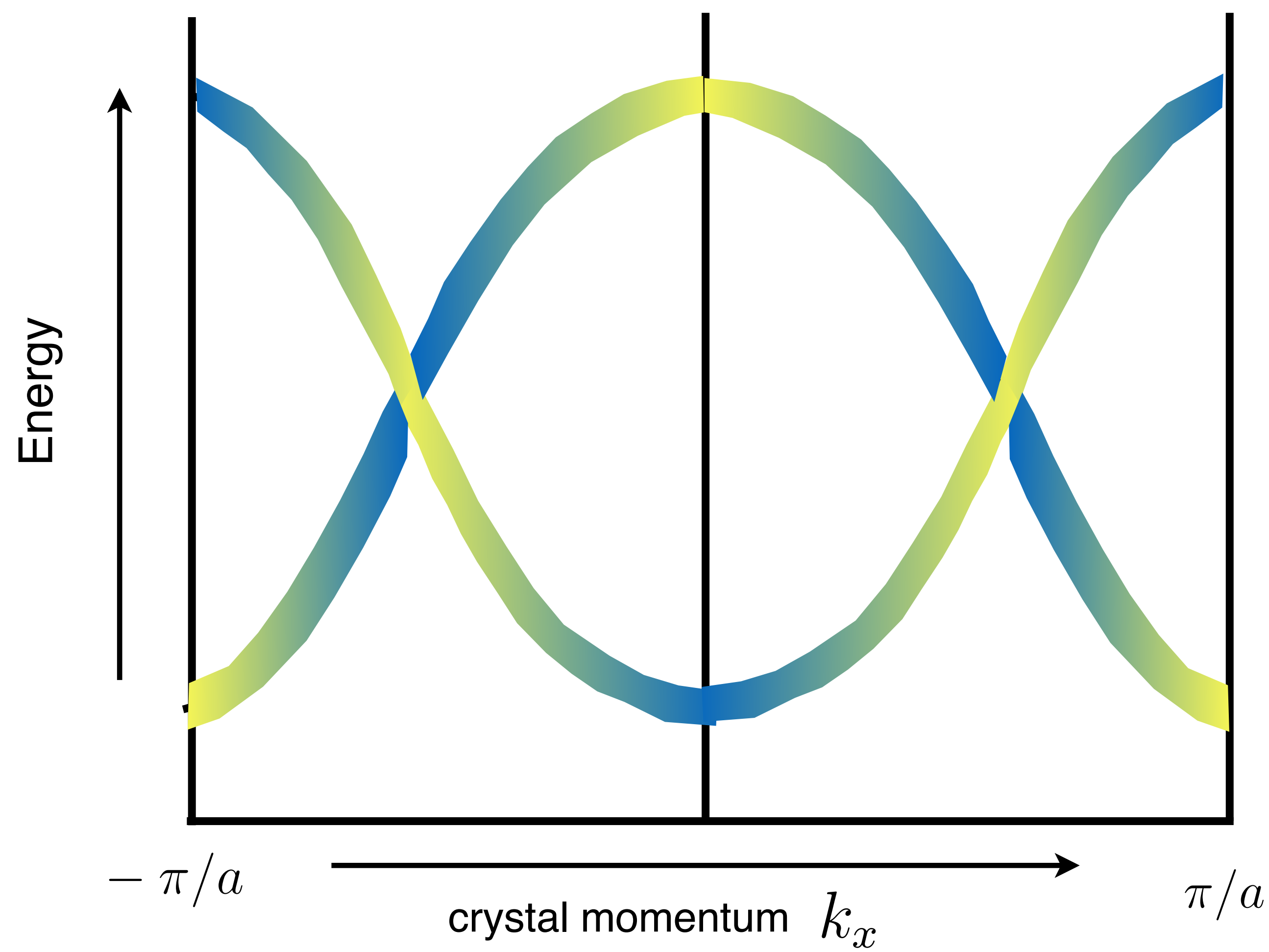
1. Introduction

$$H(\mathbf{k})\,|u_m(\mathbf{k})\rangle = E_m(\mathbf{k})\,|u_m(\mathbf{k})\rangle$$

- Bloch Hamiltonian $H(\mathbf{k})$
- Band structure of bloch bands $\{E_m(\mathbf{k})\}$
- Bloch wave functions $|u_m(\mathbf{k})\rangle$

? Under which conditions can the two $E_m(\mathbf{k})$ and $E_{m'}(\mathbf{k})$ become degenerate at points or lines in the BZ

2. Accidental band crossings



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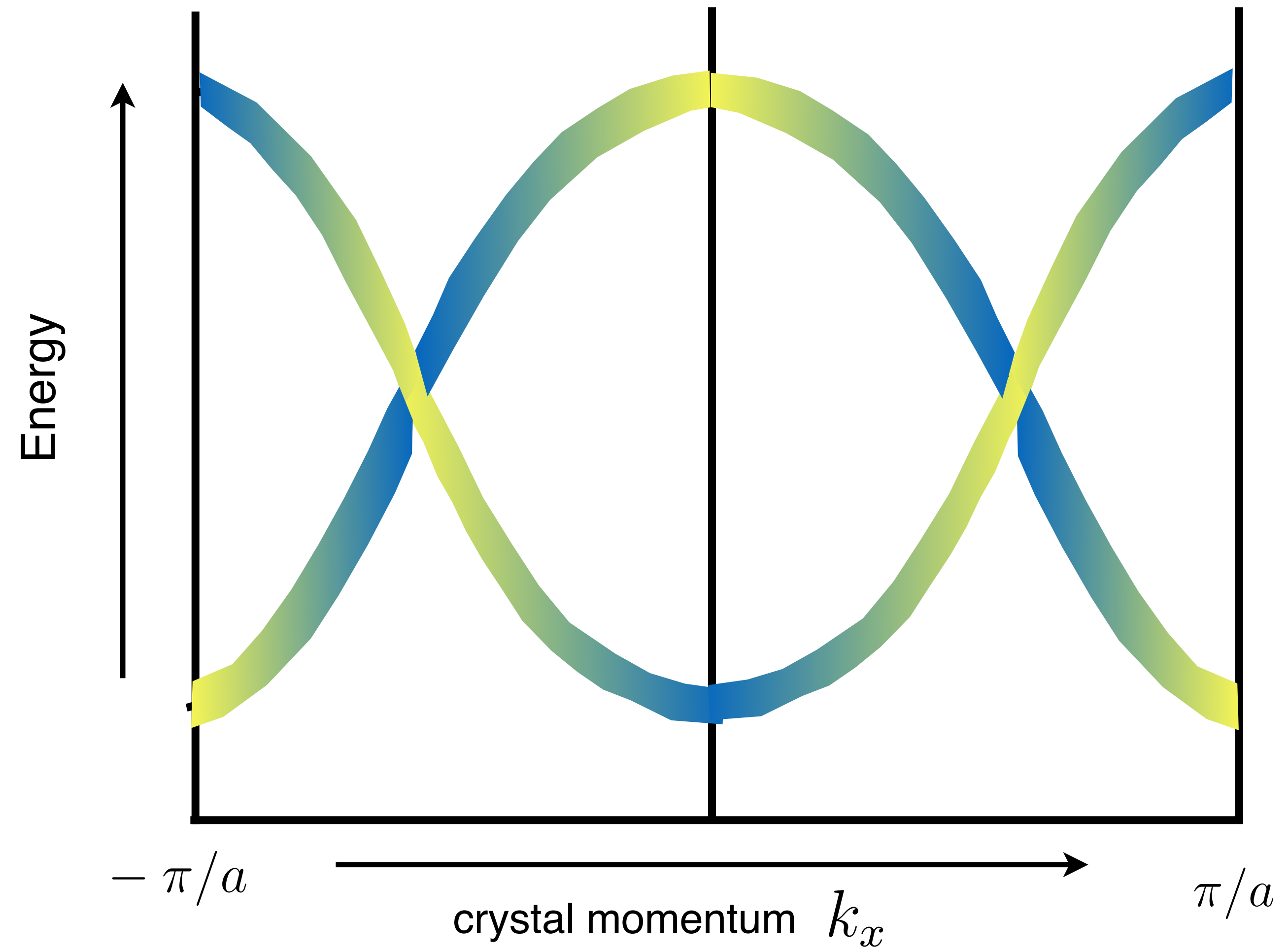

- (possibly) protected by *symmorphic* crystal symmetry and/or non-spatial symmetry
- exhibits a *local* topological charge $n_{\mathbb{Z}} = \frac{i}{2\pi} \oint \mathcal{F} d\mathbf{k} \in \mathbb{Z}$ ← topological invariant
- only perturbatively stable, removable by large deformation

$$\Longrightarrow \text{classification tells you that band crossing is } \textit{possible}$$

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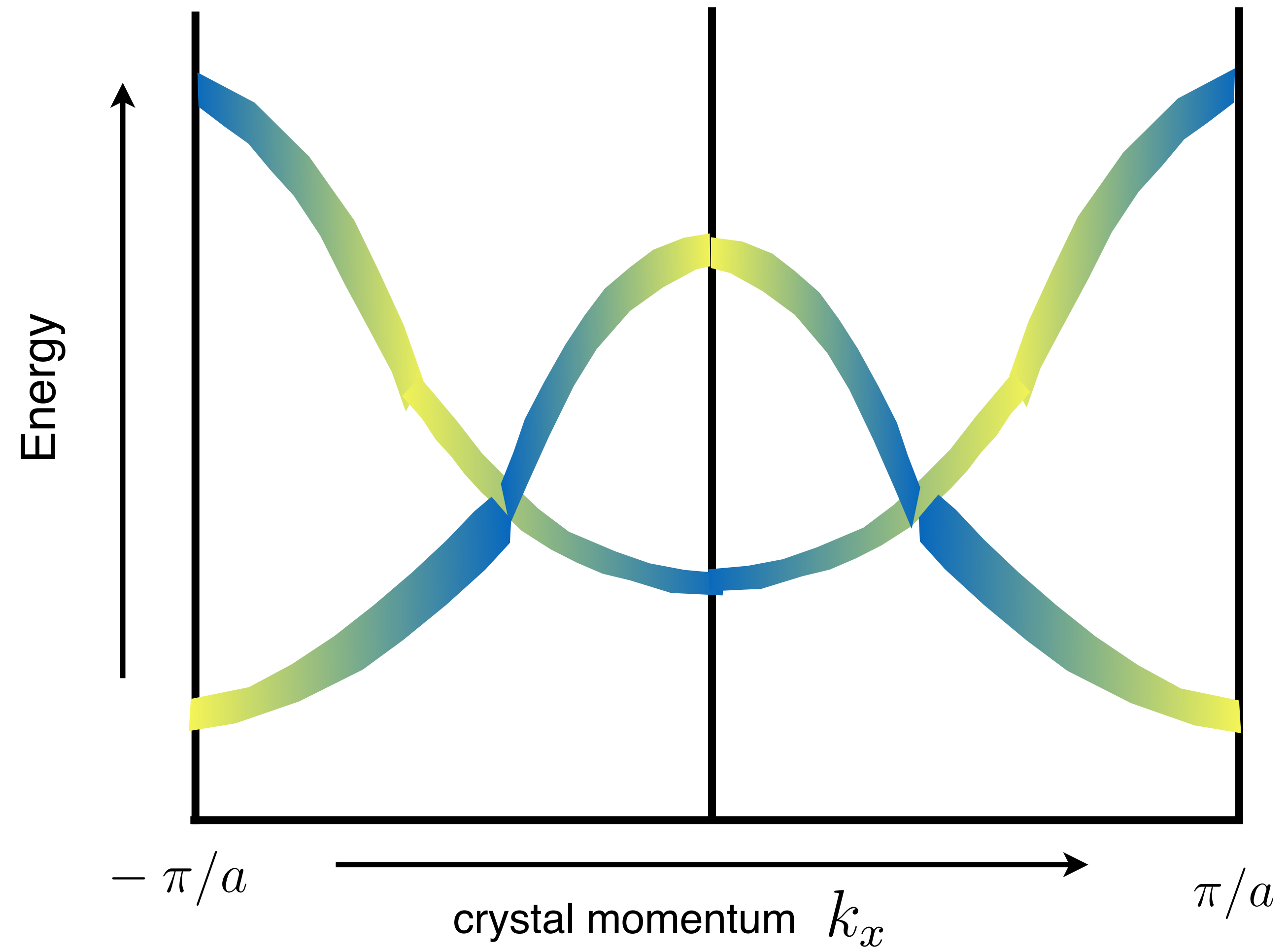

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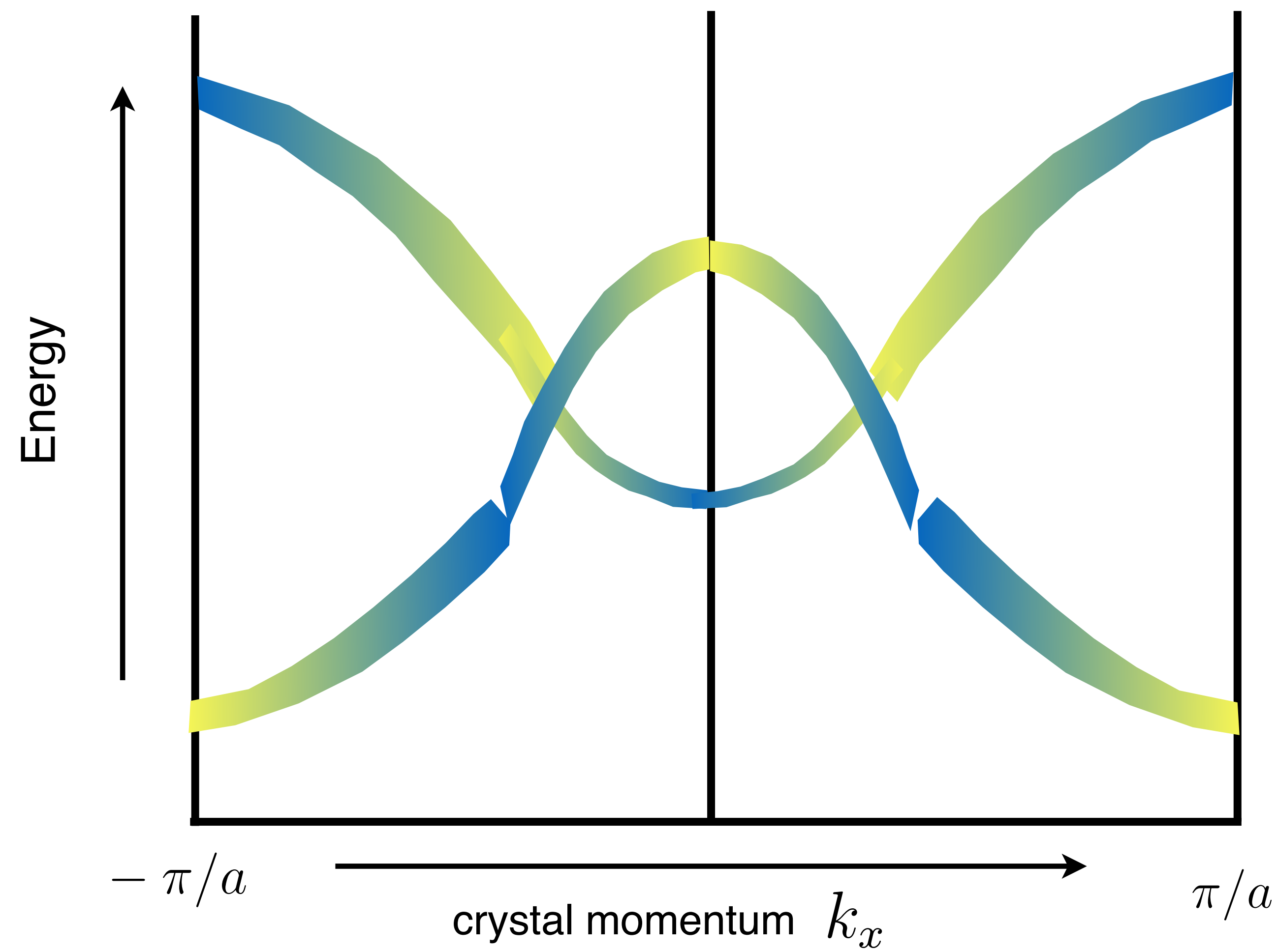

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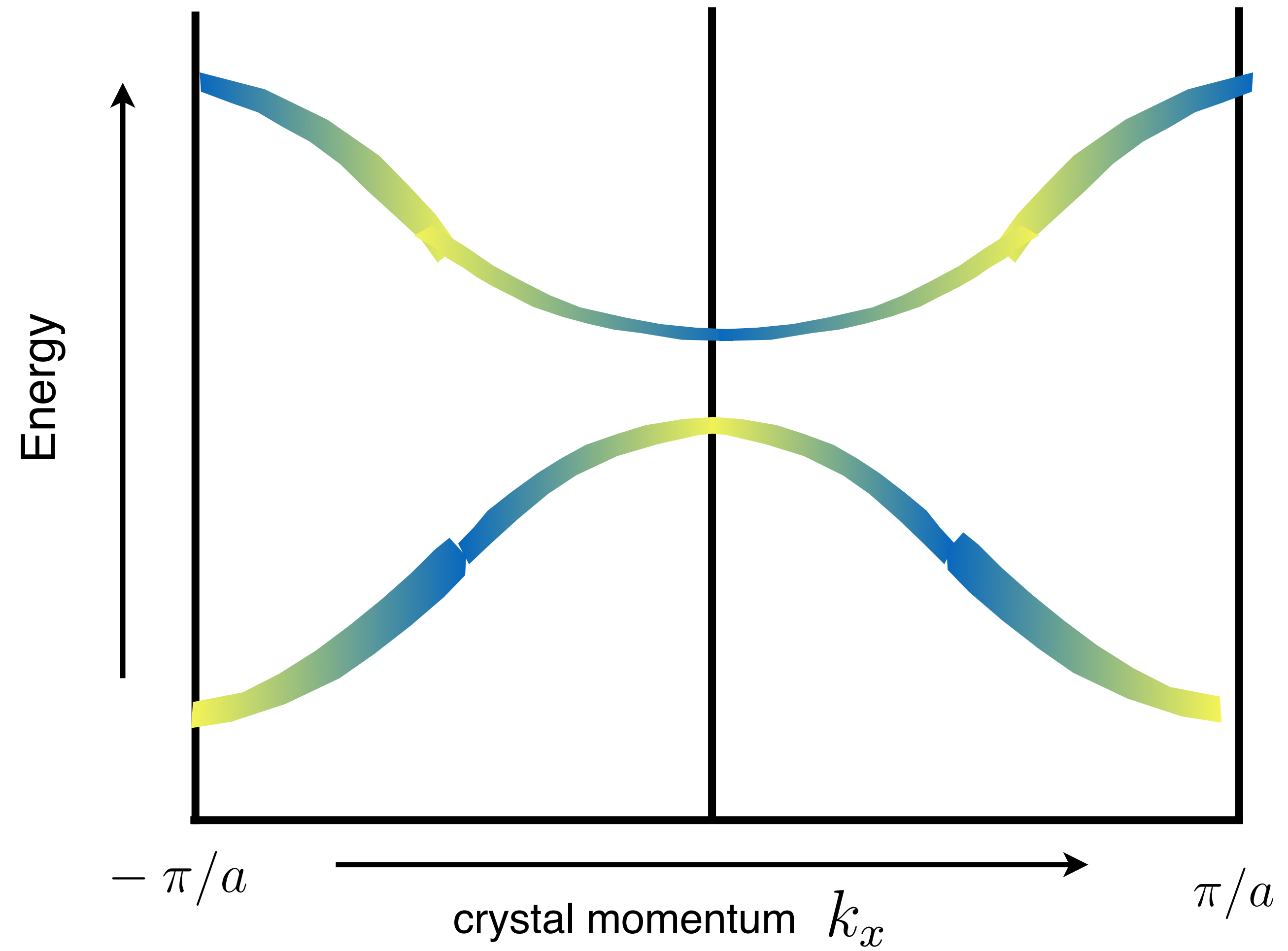

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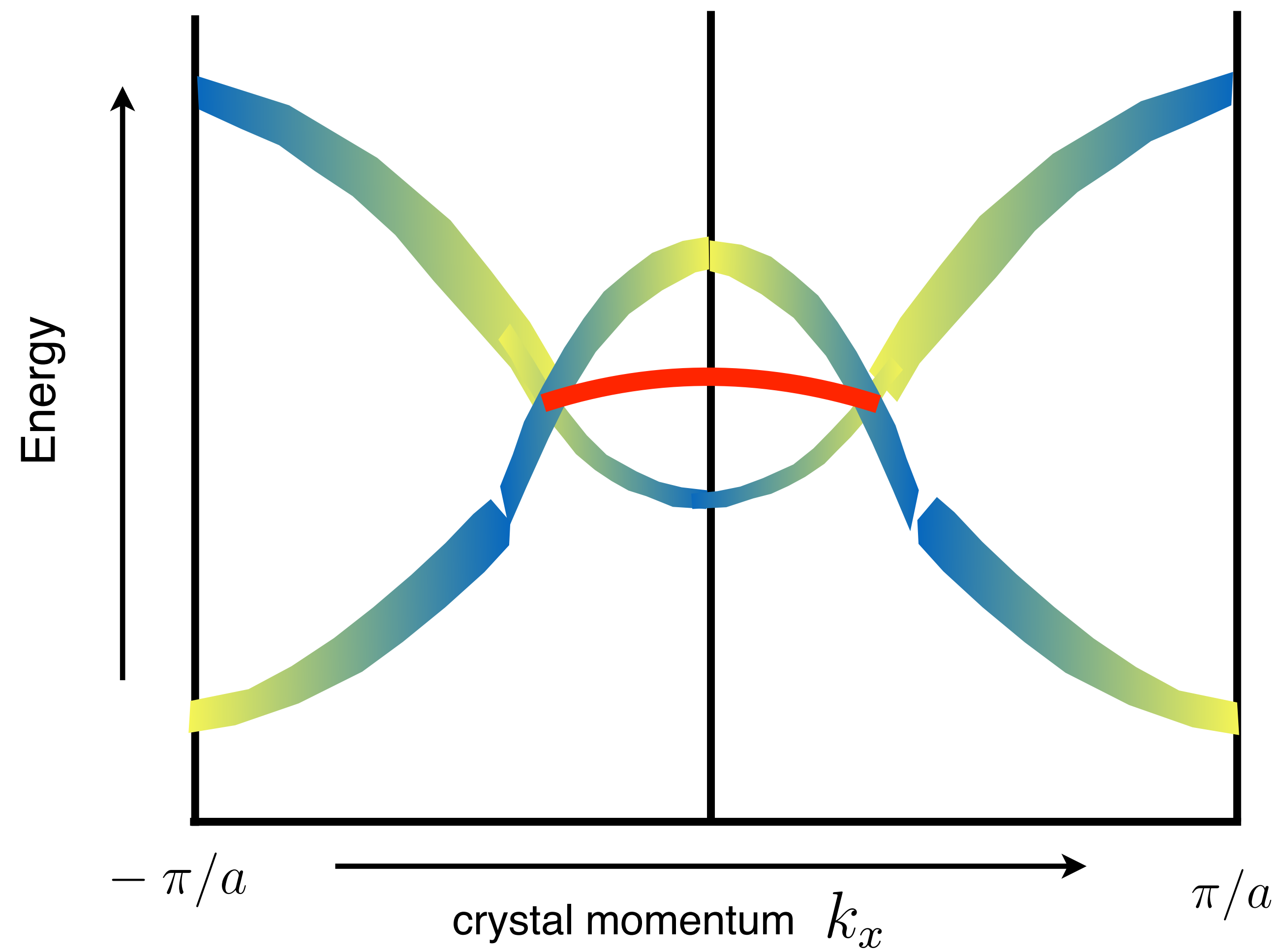


- (possibly) protected by *symmorphic* crystal symmetry and/or non-spatial symmetry
- exhibits a *local* topological charge $n_{\mathbb{Z}} = \frac{i}{2\pi} \oint \mathcal{F} d\mathbf{k} \in \mathbb{Z}$ ← topological invariant
- **Bulk-boundary correspondence:**

$$|n_{\mathbb{Z}}| = \# \text{ gapless edge states (or surface states)}$$

2.1 Classification of band crossings

- Approximate band crossing by Dirac Hamiltonian

$$H_D(\mathbf{k}) = \sum_{j=1}^{d} k_j \gamma_j$$

— gamma matrices: $\{\gamma_i, \gamma_j\} = 2\delta_{ij}\mathbb{1}, \qquad j = 0, 1, \ldots, d.$

— energy spectrum: $E = \pm\sqrt{\sum_{j=1}^{d} k_j^2},$

? are there symmetry preserving mass terms $m\gamma_0$ that open up a gap in the spectrum?

$$\{\gamma_0, \gamma_j\} = 0 \; (j = 1, 2, \ldots, d) \qquad E = \pm\sqrt{m^2 + \sum_{j=1}^{d} k_j^2}$$

NO: topologically non-trivial **YES:** topologically trivial

2.1 Classification of band crossings

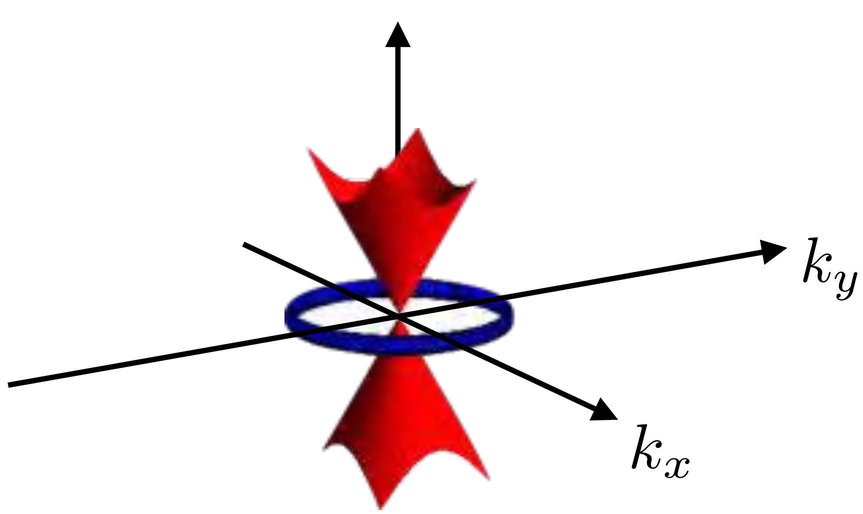
▶ Classification of topological semimetals depends on:

- symmetry of Hamiltonian (TRS, PHS, SLS)

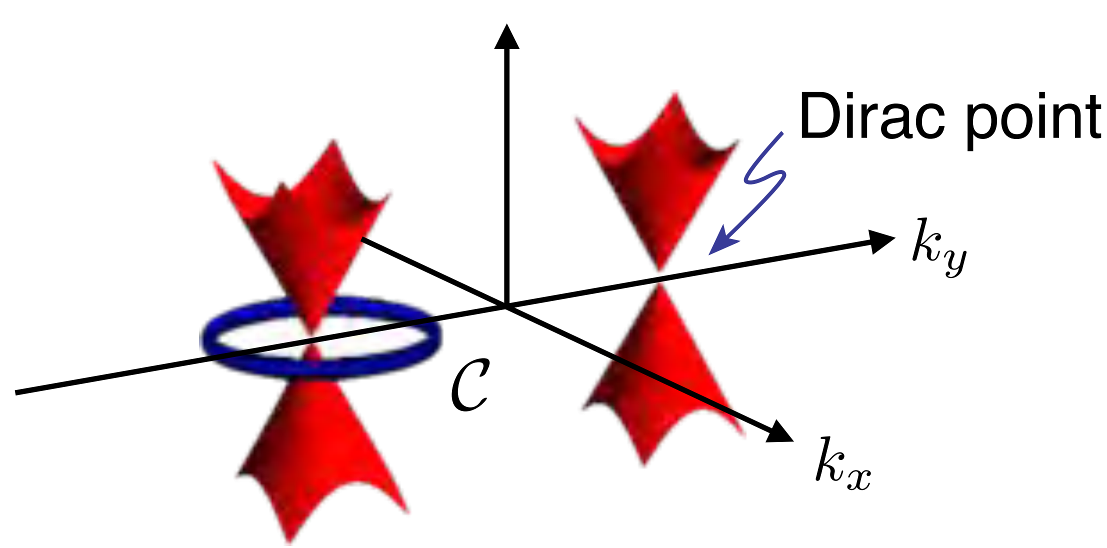
  $\Rightarrow$ **symmetry classes of ten-fold way, spatial symmetries**

- co-dimension $p = d - d_{\mathrm{FS}}$ of Fermi surface (d_{FS} : dimension of Fermi surface)
- how Fermi surface transforms under nonspatial symmetries

(i) Fermi surface is *invariant* under nonspatial symmetries



(ii) Fermi surfaces *pairwise related* by nonspatial symmetries



Classification of accidental band crossings

- Nonspatial symmetries:

★ time-reversal invariance: $T = U_T \mathcal{K}$

$$T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k}) \qquad T^2 = +1 \qquad T^2 = -1$$

★ particle-hole symmetry: $C = U_C \mathcal{K}$

$$C^{-1}\mathcal{H}(-\mathbf{k})C = -\mathcal{H}(\mathbf{k}) \qquad C^2 = +1 \qquad C^2 = -1$$

★ chiral symmetry / sublattice symmetry: $S \propto TC$

$$S\mathcal{H}(\mathbf{k}) + \mathcal{H}(\mathbf{k})S = 0$$

$$\{\gamma_i, \mathcal{T}\} = 0, \quad [\gamma_i, \mathcal{C}] = 0, \quad \{\gamma_i, \mathcal{S}\} = 0,$$

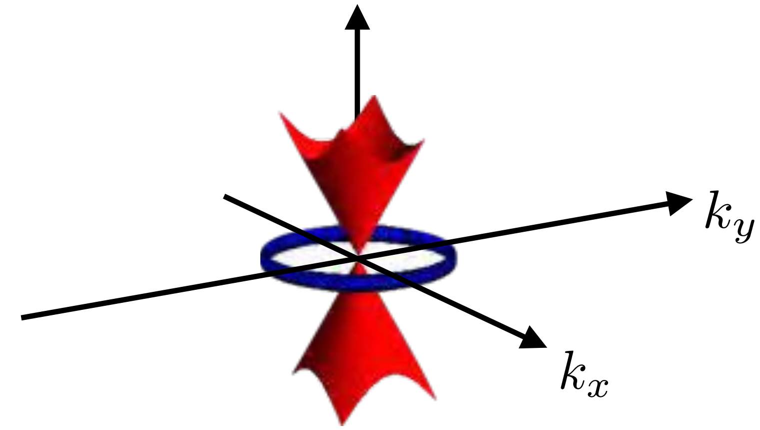
$$[\gamma_0, \mathcal{T}] = 0, \quad \{\gamma_0, \mathcal{C}\} = 0, \quad \{\gamma_0, \mathcal{S}\} = 0.$$

- Spatial symmetries:

★ reflection symmetry: $R^{-1}H(-k_1, \tilde{\mathbf{k}})R = H(k_1, \tilde{\mathbf{k}}),$

$$\{\gamma_1, R\} = 0, \quad [\gamma_j, R] = 0, \quad \text{where } j = 2, 3, \ldots, d, \qquad [\gamma_0, R] = 0.$$

2.1.2 Band crossings at high-symmetry points



1. write down d-dim Hamiltonian with minimal matrix dimension, that is invariant under the considered symmetries

$$H_D(\mathbf{k}) = \sum_{j=1}^{d} k_j \gamma_j$$

2. check whether there exist symmetry allowed mass terms $m\gamma_0$

$$\{\gamma_0, \gamma_j\} = 0 \; (j = 1, 2, \ldots, d) \qquad E = \pm\sqrt{m^2 + \sum_{j=1}^{d} k_j^2}$$

NO: topologically non-trivial **YES:** topologically trivial

3. to check whether single or multiple band crossings are protected, consider multiple copies of $H_D(\mathbf{k})$

$$H_D^{\mathrm{db}} = \sum_{i \in A} k_i \gamma_i \otimes \sigma_z + \sum_{i \in A^c} k_i \gamma_i \otimes \mathbb{1} \qquad A \subseteq \{1, 2, \ldots, d\}$$

Band crossings at high-symmetry points

- **Class A in 2D**

$$H^A_{2D} = k_x\sigma_x + k_y\sigma_y$$

– can be gapped out by $m\sigma_z \Rightarrow$ trivial

- **Class A in 3D**

$$H^A_{3D} = k_x\sigma_x + k_y\sigma_y + k_z\sigma_z$$

– no mass term exists $\Rightarrow$ topological

$$H^{A,\text{db1}}_{3D} = k_x\sigma_x \otimes \sigma_z + k_y\sigma_y \otimes \sigma_0 + k_z\sigma_z \otimes \sigma_0$$ (mass terms, e.g., $\sigma_x \otimes \sigma_x$ and $\sigma_x \otimes \sigma_y$)

$$H^{A,\text{db2}}_{3D} = k_x\sigma_x \otimes \sigma_0 + k_y\sigma_y \otimes \sigma_0 + k_z\sigma_z \otimes \sigma_0$$

– no mass term for $H^{A,db2}_{3D} \Rightarrow \mathbb{Z}$ classification

Band crossings at high-symmetry points

- **Class A + R in 2D**

$$H_{2D}^{A+R} = k_x \sigma_x + k_y \sigma_y$$

– reflection symmetric $R^{-1} H_{2D}^{A+R}(-k_x, k_y) R = H_{2D}^{A+R}(k_x, k_y) \qquad R = \sigma_y$

– mass term $m\sigma_z$ breaks reflection symmetry $\;(R^{-1}\sigma_z R = -\sigma_z)$

$\Rightarrow$ topological

- **Class AII in 2D**

$$H_{2D}^{\mathrm{AII}} = k_x \sigma_x + k_y \sigma_y$$

– time-reversal symmetric with $\mathcal{T} = i\sigma_y \mathcal{K}$

– mass term $m\sigma_z$ breaks time-reversal $(\mathcal{T}^{-1} m\sigma_z \mathcal{T} \neq m\sigma_z)$

$\Rightarrow$ topological

– doubled Hamiltonians: $\qquad H_{2D}^{\mathrm{AII,db}} = \begin{pmatrix} H_{2D}^{\mathrm{AII}} & 0 \\ 0 & H_{2D}^{\mathrm{AII}\prime} \end{pmatrix}$

$$H_{2D}^{\mathrm{AII}\prime} \in \{\pm k_x \sigma_x \pm k_y \sigma_y, \pm k_x \sigma_x \mp k_y \sigma_y\},$$

– for each $H_{2D}^{AII,db}$ there exist mass terms $\Longrightarrow \mathbb{Z}_2$ classification

Classification of accidental band crossings

Table 1: *Classification of stable band crossings in terms of the ten AZ symmetry classes [2], which are listed in the first column. The first and second rows give the co-dimensions $p = d - d_{BC}$ for band crossings at high-symmetry points [Fig. 2(a)] and away from high-symmetry points of the BZ [Fig. 2(b)], respectively.*

at high-sym. point off high-sym. point	p=8 p=2	p=1 p=3	p=2 p=4	p=3 p=5	p=4 p=6	p=5 p=7	p=6 p=8	p=7 p=1	T	C	S
A	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	0	0
AIII	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	0	0	1
AI	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	$+$	0	0
BDI	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$+$	$+$	1
D	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	0	$+$	0
DIII	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$-$	$+$	1
AII	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	$-$	0	0
CII	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	0^{a}	0	$-$	$-$	1
C	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	0^{a}	0	$-$	0
CI	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\mathrm{a,b}}$	$\mathbb{Z}_2^{\mathrm{b}}$	$\mathbb{Z}$	0	$+$	$-$	1

[a] For these entries there can exist bulk band crossings away from high-symmetry points that are protected by $\mathbb{Z}$ invariants inherited from classes A and AIII. (TRS or PHS does not trivialize the $\mathbb{Z}$ invariants.)

[b] $\mathbb{Z}_2$ invariants protect only band crossings of dimension zero at high-symmetry points.

Classification of accidental band crossings

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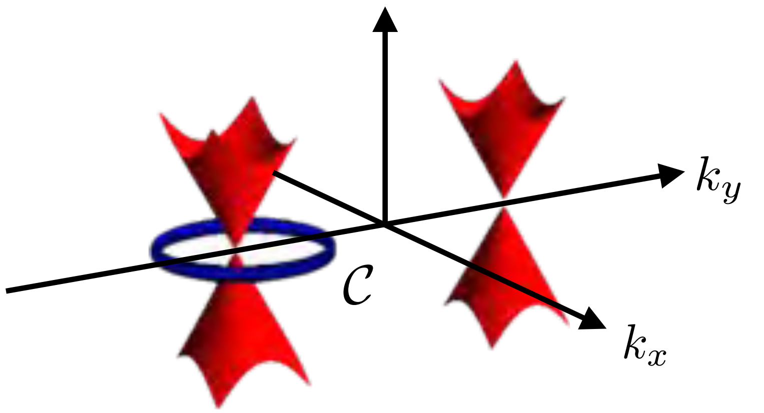
at high-sym. point	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7	T	C	S
off high-sym. point	p=2	p=3	p=4	p=5	p=6	p=7	p=8	p=1			
A	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	0	0
AIII	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	0	0	1
AI	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	$+$	0	0
BDI	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$+$	$+$	1
D	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	0	$+$	0
DIII	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	0	$-$	$+$	1
AII	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	0^{a}	0	$2\mathbb{Z}$	$-$	0	0
CII	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	0^{a}	0	$-$	$-$	1
C	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	0^{a}	0	$-$	0
CI	0^{a}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{a,b}$	$\mathbb{Z}_2^{b}$	$\mathbb{Z}$	0	$+$	$-$	1

[a] For these entries there can exist bulk band crossings away from high-symmetry points that are protected by $\mathbb{Z}$ invariants inherited from classes A and AIII. (TRS or PHS does not trivialize the $\mathbb{Z}$ invariants.)

[b] $\mathbb{Z}_2$ invariants protect only band crossings of dimension zero at high-symmetry points.

2.1.3 Band crossings off high-symmetry points



1. write down d-dim Hamiltonian with $p = d - d_{BC}$,
that is invariant under the considered symmetries

$$H_D = \sum_{i=1}^{p-1} \sin k_i \gamma_i + (p - 1 - \sum_{i=1}^{p} \cos k_i) \tilde{\gamma}_0$$

2. check whether there exists

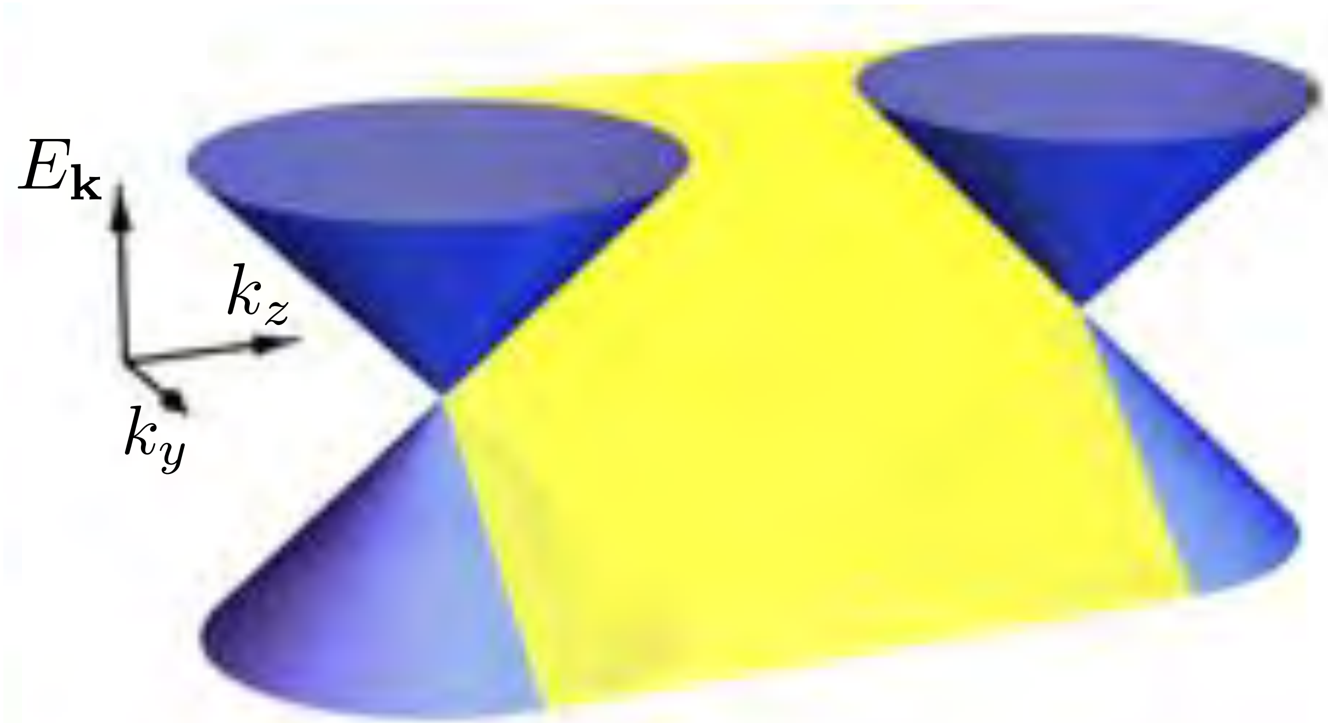
— momentum independent mass term $\tilde{\Gamma}$

— momentum dependent kinetic term $\sin k_p \gamma_p$

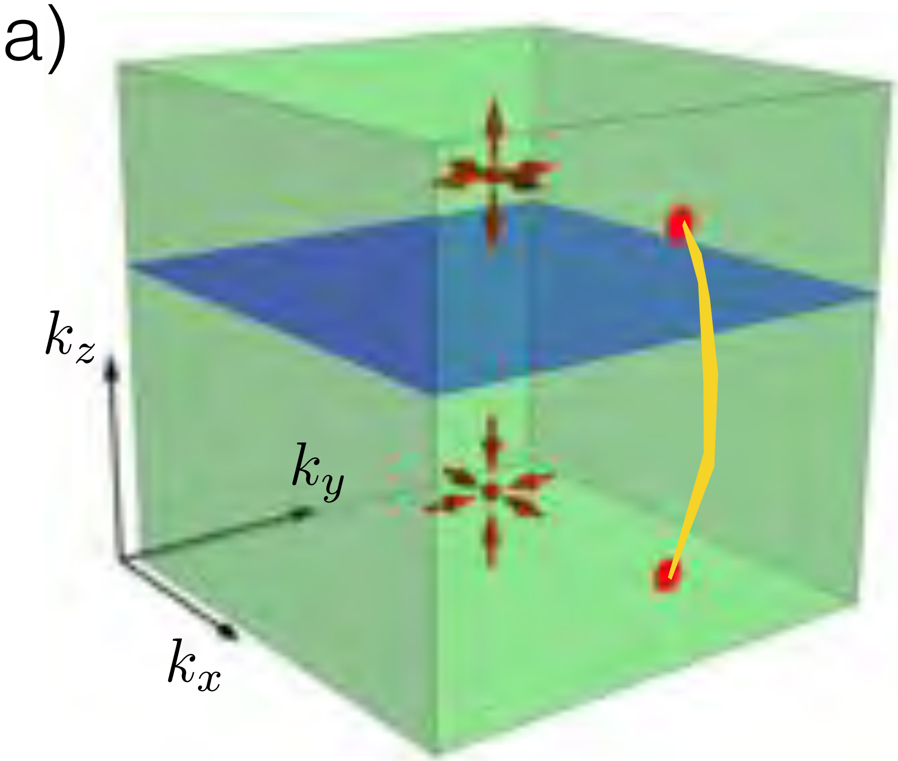
NO: topologically non-trivial **YES:** topologically trivial

3. To check whether multiple band crossings are protected, consider doubled Hamiltonian

2.2 Weyl semimetal



Weyl semimetal



- 2 x 2 Hamiltonian:

$$H^A_{3D} = \sin k_x \sigma_x + \sin k_y \sigma_y + (2 - \cos k_x - \cos k_y - \cos k_z)\sigma_z$$

– no third Pauli matrix → topologically stable

- Energy spectrum:

$$E_{\mathbf{k}} = \pm\sqrt{(\sin k_x)^2 + (\sin k_y)^2 + (2 - \cos k_x - \cos k_y - \cos k_z)^2}$$

$\Rightarrow$ two Weyl points at $(0, 0, \pm\pi/2)$

- Chern number:

$$C(k_z) = \frac{1}{4\pi} \oint_{\mathcal{C}_{k_z}} dk_x dk_y \, \hat{\mathbf{d}}_{\mathbf{k}} \cdot \left[\partial_{k_x} \hat{\mathbf{d}}_{\mathbf{k}} \times \partial_{k_y} \hat{\mathbf{d}}_{\mathbf{k}}\right], \qquad \text{with} \quad \hat{\mathbf{d}}_{\mathbf{k}} = \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|},$$

$d_x(\mathbf{k}) = \sin k_x$, $d_y(\mathbf{k}) = \sin k_y$, and $d_z(\mathbf{k}) = (2 - \cos k_x - \cos k_y - \cos k_z)$

— guarantees stability of the Weyl points

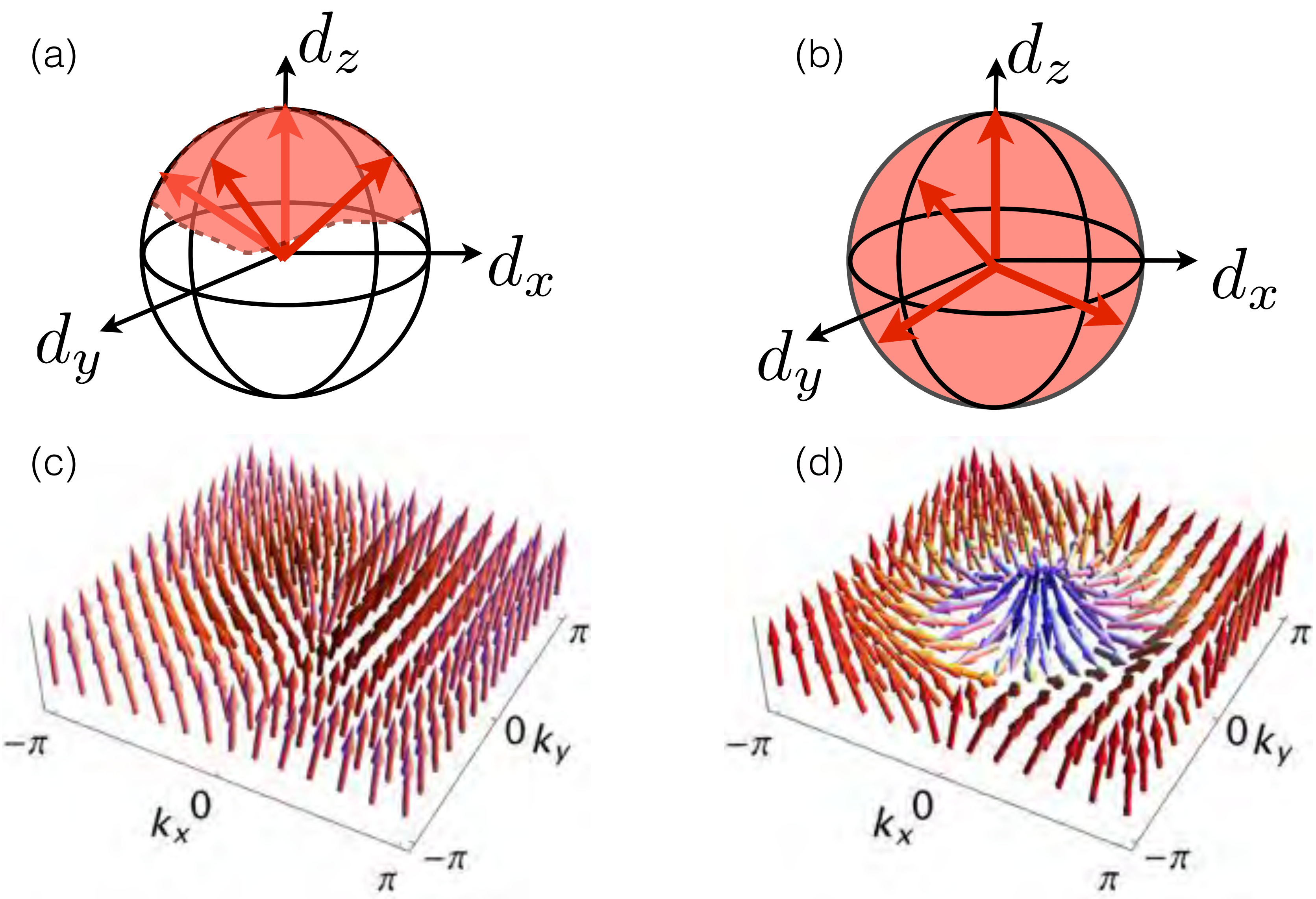
— leads to Fermi arc surface state

Weyl semimetal

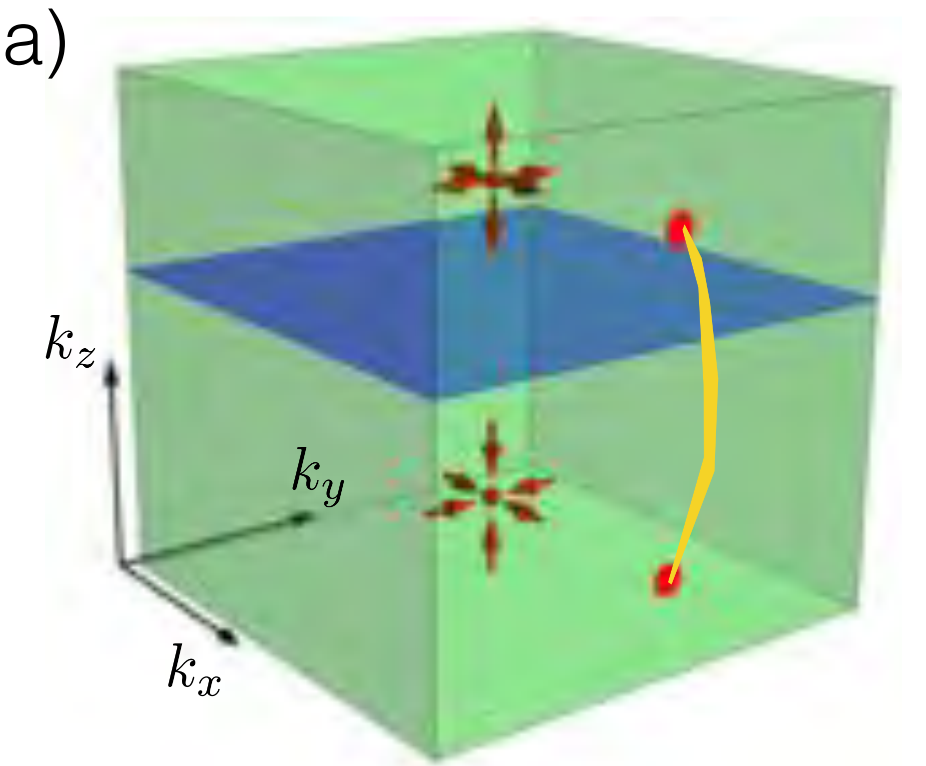
- Chern number: $$C(k_z) = \frac{1}{4\pi} \oint_{\mathcal{C}_{k_z}} dk_x dk_y \, \hat{\mathbf{d}}_{\mathbf{k}} \cdot \left[\partial_{k_x} \hat{\mathbf{d}}_{\mathbf{k}} \times \partial_{k_y} \hat{\mathbf{d}}_{\mathbf{k}} \right], \qquad \text{with} \quad \hat{\mathbf{d}}_{\mathbf{k}} = \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|},$$

$$d_x(\mathbf{k}) = \sin k_x, \; d_y(\mathbf{k}) = \sin k_y, \text{ and } d_z(\mathbf{k}) = (2 - \cos k_x - \cos k_y - \cos k_z)$$

$|k_z| > \frac{\pi}{2}$ $\qquad$ $|k_z| < \frac{\pi}{2}$



(a)



Weyl semimetal

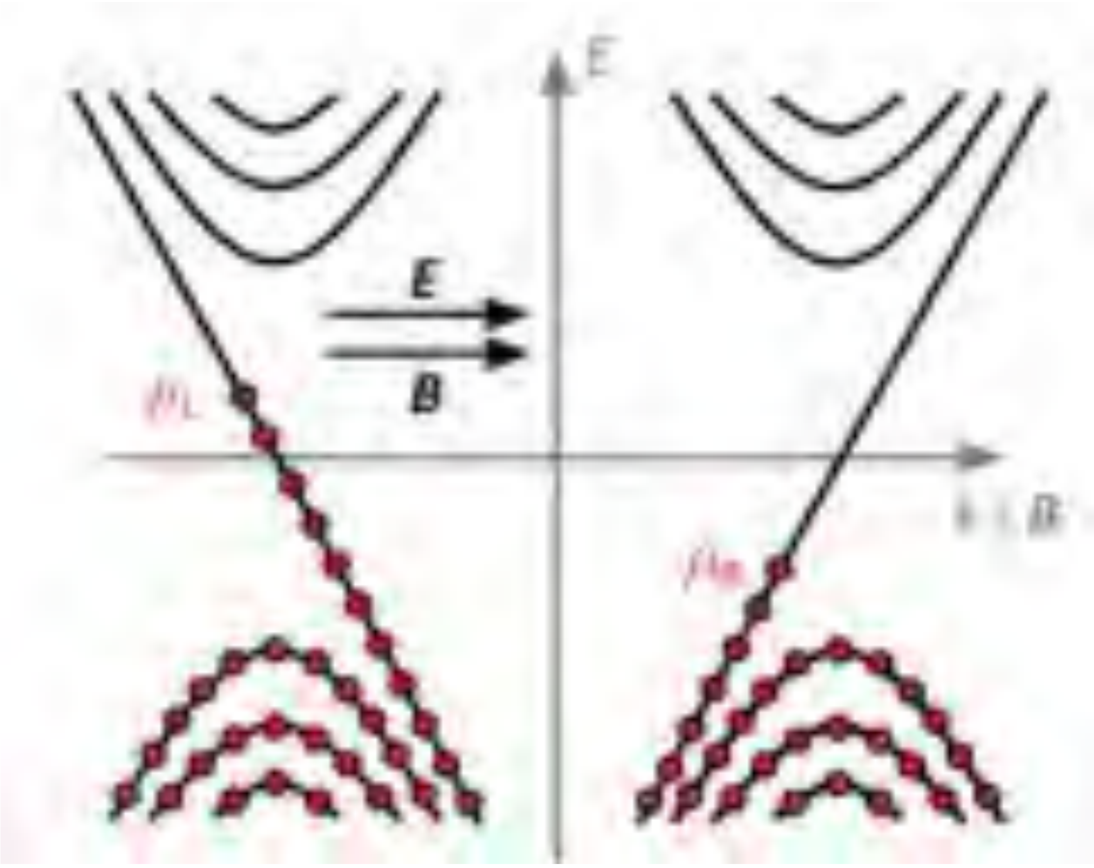
Quantum Anomaly:

Symmetry of classical action broken by regularization of quantum theory

- chiral charge $e(n_+ - n_-)$ is not conserved at the quantum level

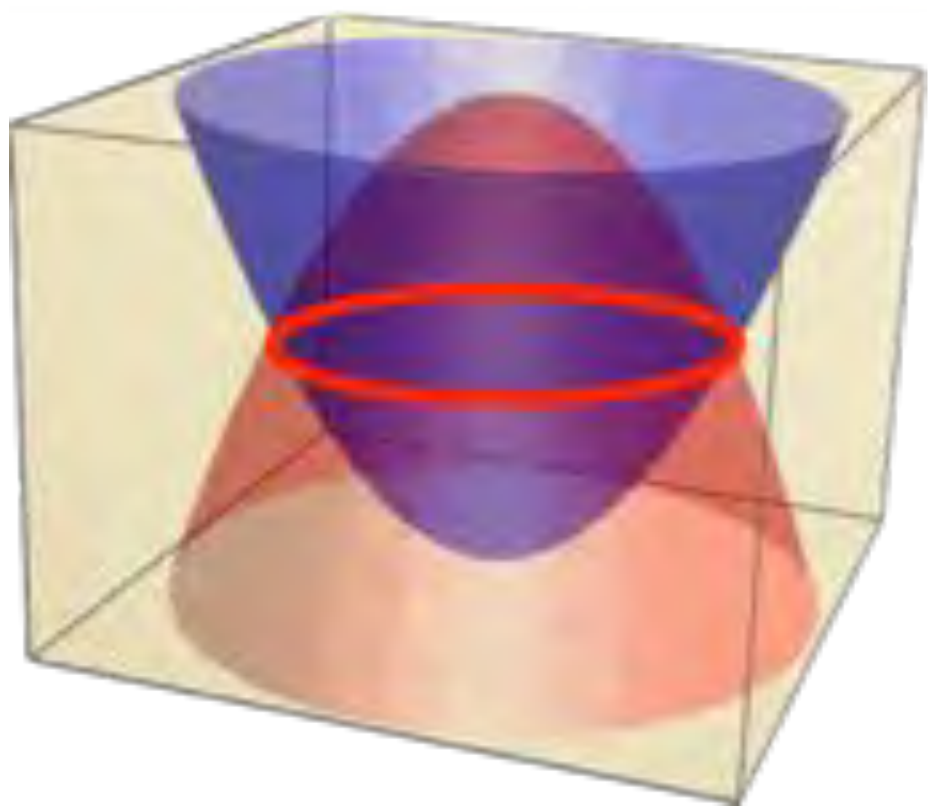
- presence of electric and magnetic field changes number of electrons as

$$\frac{d}{dt}n_{\pm} = \pm\frac{e^2}{h^2}\mathbf{E}\cdot\mathbf{B}$$

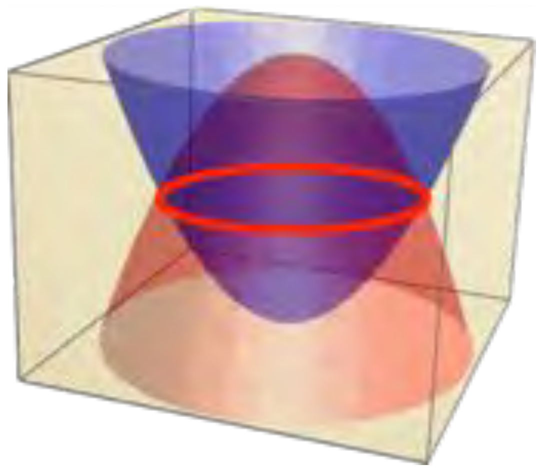


2.1 Dirac nodal-line semimetal

Ca_3P_2



Dirac nodal-line semimetal



- low-energy effective Hamiltonian:

$$H_{3D}^{AI+R} = \sin k_z \sigma_2 + [2 - \cos k_x - \cos k_y - \cos k_z]\, \sigma_3$$

- symmetry operators:

  – reflection: $R = \sigma_3$ – time-reversal: $T = \sigma_0 \mathcal{K}$ – inversion: $P = \sigma_3$

- Gap-opening term $m\sigma_1$ is symmetry forbidden:

  – breaks reflection symmetry: $R^{-1} m \sigma_1 R = -m\sigma_1$

  – breaks PT symmetry: $(PT)^{-1} m \sigma_1 (PT) = -m\sigma_1$

  $\Rightarrow$ nodal line is stable

- $\mathbb{Z}$ versus $\mathbb{Z}_2$ classification:

$$H_{3D}^{AI+R,\mathrm{db}} = \sin k_z \sigma_2 \otimes \sigma_0 + [2 - \cos k_x - \cos k_y - \cos k_z]\, \sigma_3 \otimes \sigma_0$$

  – consider gap opening term $\hat{m} = \sigma_1 \otimes \sigma_2$:

  - (PT)-symmetric:

$$(\sigma_3 \otimes \sigma_0 \mathcal{K})^{-1} \hat{m} (\sigma_3 \otimes \sigma_0 \mathcal{K}) = \hat{m} \qquad \Rightarrow \mathbb{Z}_2 \text{ classification}$$

  - but breaks R:

$$(\sigma_3 \otimes \sigma_0)^{-1} \hat{m} (\sigma_3 \otimes \sigma_0) \neq \hat{m} \qquad \Rightarrow \mathbb{Z} \text{ classification}$$

Dirac nodal-line semimetal

- Berry phase:

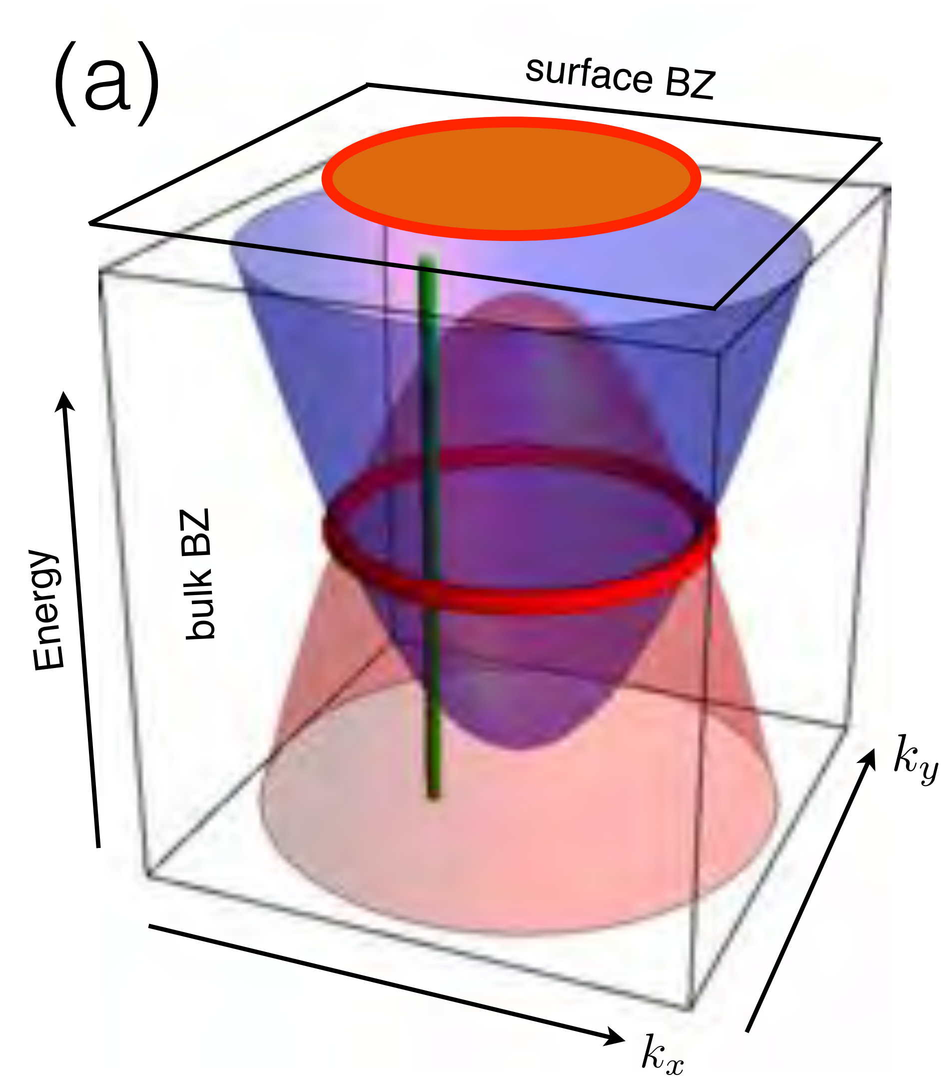
$$P_{\mathcal{L}} = -i \oint_{\mathcal{L}} dk_l \left\langle u_-(\mathbf{k}) \right| \nabla_{k_l} \left| u_-(\mathbf{k}) \right\rangle$$

– In Ca_3P_2 Berry phase is quantized due to:

(i) reflection symmetry $z \to -z$

(ii) inversion + time-reversal symmetry

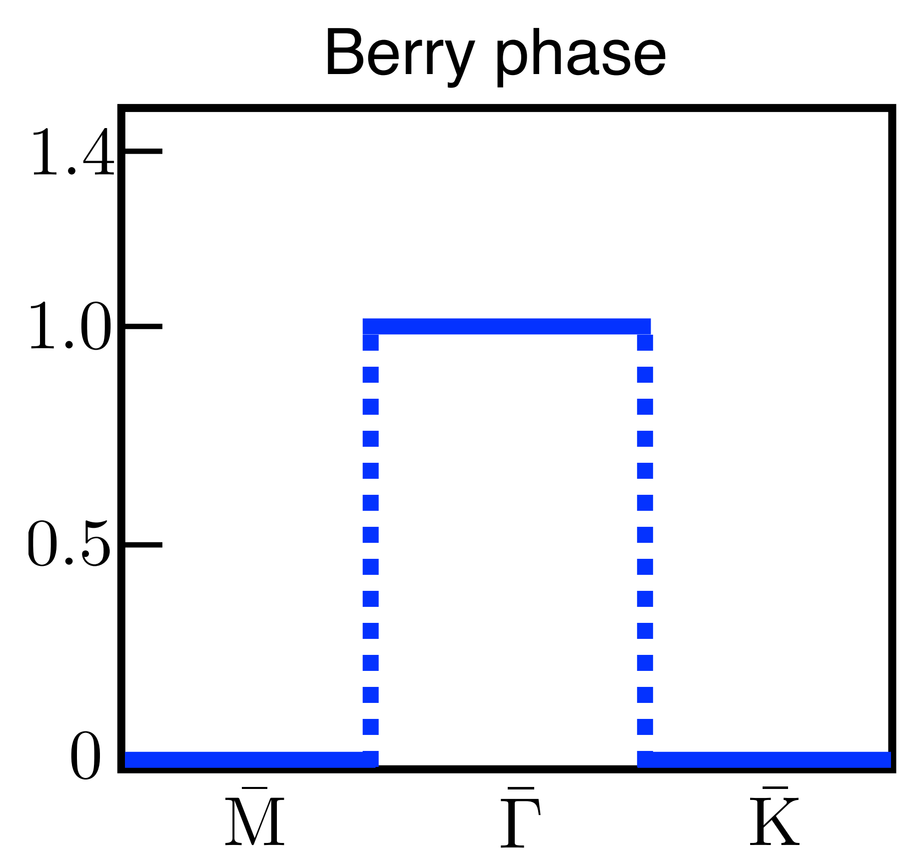
– $\mathcal{P}(k_{\|})$ quantized to $\pi \Rightarrow$ stable line node



Bulk-boundary correspondence:

– surface charge: $\sigma_{\text{surf}} = \dfrac{e}{2\pi}\mathcal{P} \bmod e$

$\Rightarrow$ **Nearly flat 2D surface states connecting Dirac ring**



Dirac nodal-line semimetal

Quantum Anomaly:

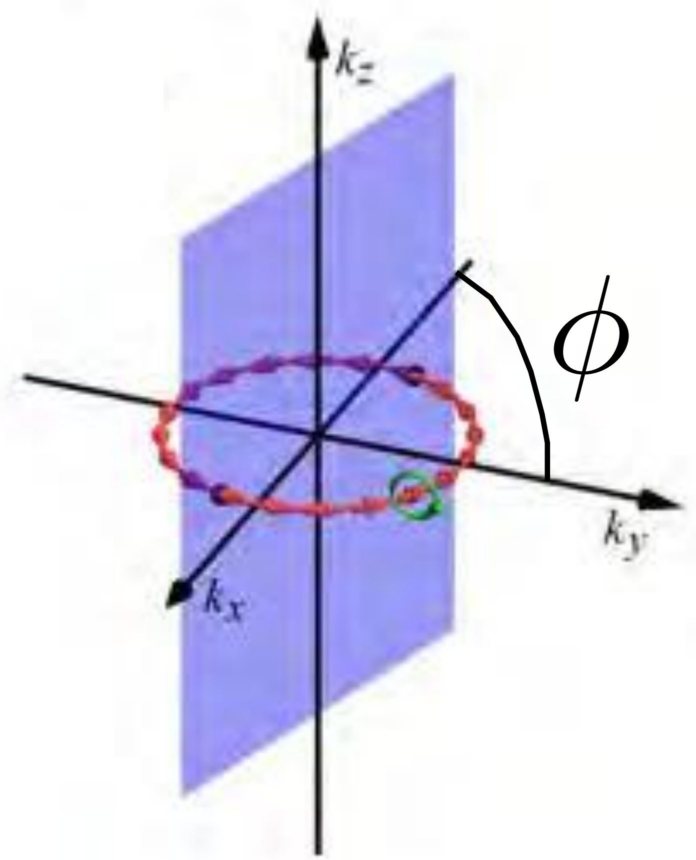
Symmetry of classical action broken by regularization of quantum theory

Anomaly in topological semimetals:

Top. semimetals with FS of co-dimension p, generally, exhibit (p+1)-dim anomaly:

- $\mathbf{p=3}$: (3+1)D chiral anomaly in Weyl semi-metals
- $\mathbf{p=2}$: (2+1)D parity anomaly in graphene

? Is there an anomaly in nodal-line semimetals?



$\Longrightarrow$ consider family of 2D subsystems

$\Longrightarrow$ study (2+1)D parity anomaly as a function of angle ϕ

Dirac nodal-line semimetal

Parity anomaly for a 2D subsystem:

Action for (2+1)D Dirac fermions coupled to gauge field A_μ

breaks PT symmetry

$$S^\phi = \int d^3x \, \bar{\psi} \, [i\gamma^\mu(\partial_\mu + ieA_\mu) + m] \, \psi$$

$\Longrightarrow$ effective action $S^\phi_{\text{eff}}[A, 0]$ with $m = 0$ is UV divergent

$\Longrightarrow$ Pauli-Villars regularization of theory breaks PT symmetry

$$S^{\text{R}}_{\text{eff}}[A] = S_{\text{eff}}[A] - \lim_{M \to \infty} S_{\text{eff}}[A, M]$$

- Pauli-Villars mass term remains finite for $M \to \infty$, yielding Chern-Simons term:

Berry phase

$$S_{CS} = \frac{\mathcal{P}}{8\pi} \int d^3x \, \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda$$

- anomalous current from one Dirac point: $j^\mu = \dfrac{\mathcal{P}}{4\pi} \epsilon^{\mu\nu\lambda} \partial_\nu A_\lambda$

→ transverse charge response to applied electric field

Dirac nodal-line semimetal

Anomalous transport within semi-classical response theory:

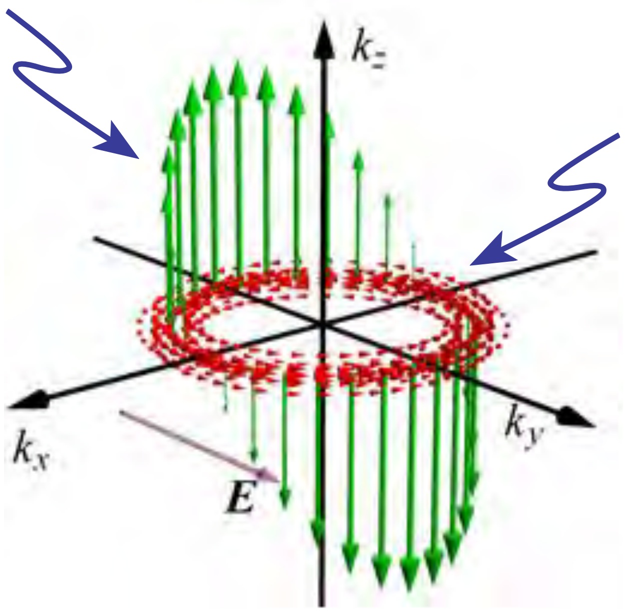
- anomalous velocity: $\mathbf{v}(\mathbf{k}) = \frac{\partial \varepsilon}{\partial \mathbf{k}} - \frac{e}{\hbar} \mathbf{E} \times \mathbf{\Omega}(\mathbf{k})$ **Karplus, Kohn, Luttinger**

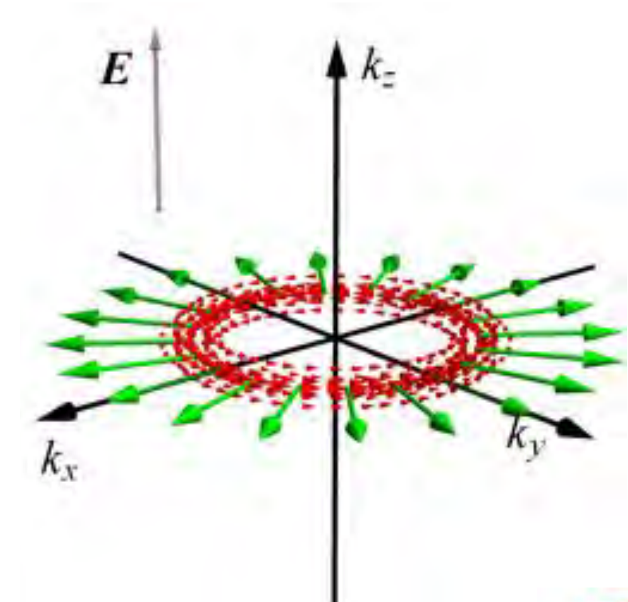
- transverse current: $\mathbf{j}_t = \frac{e^2}{\hbar} \int \frac{d^3k}{(2\pi)^3} f(\mathbf{k})\, \mathbf{E} \times \mathbf{\Omega}(\mathbf{k})$ ← Berry curvature

- differential current: $\mathbf{j}_{t,\phi} = \frac{e^2}{\hbar} \frac{R}{8\pi^2} \left(1 - \frac{m}{\mu}\right) \mathbf{E} \times \hat{\mathbf{e}}_\phi$ ← universal part

transverse current

Berry curvature



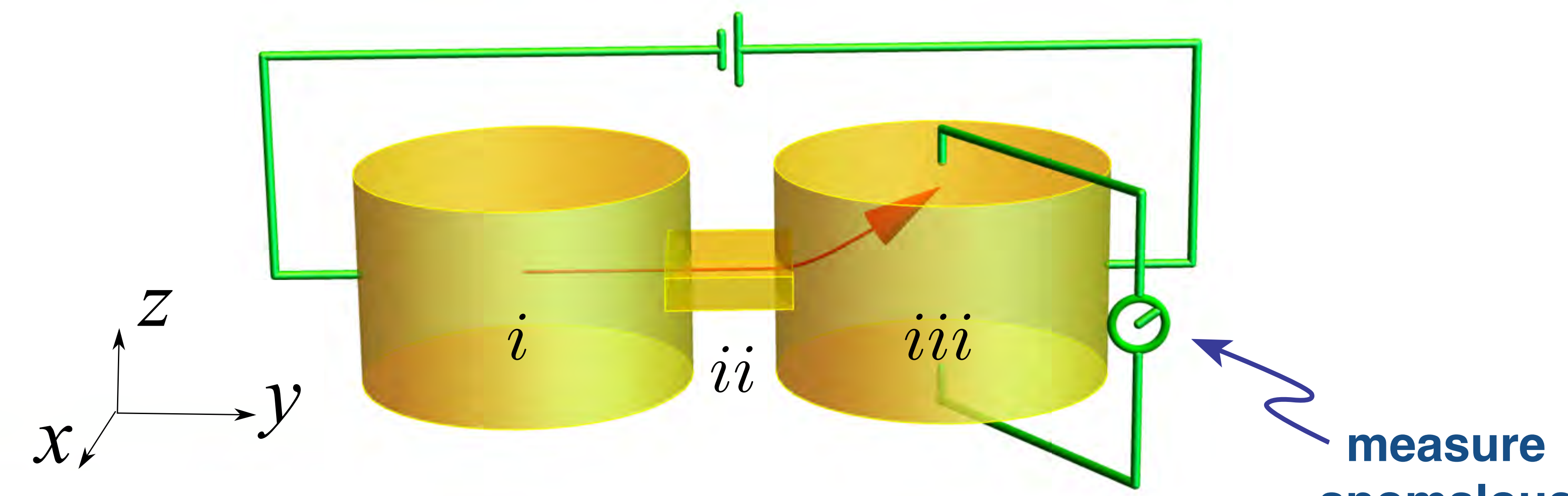


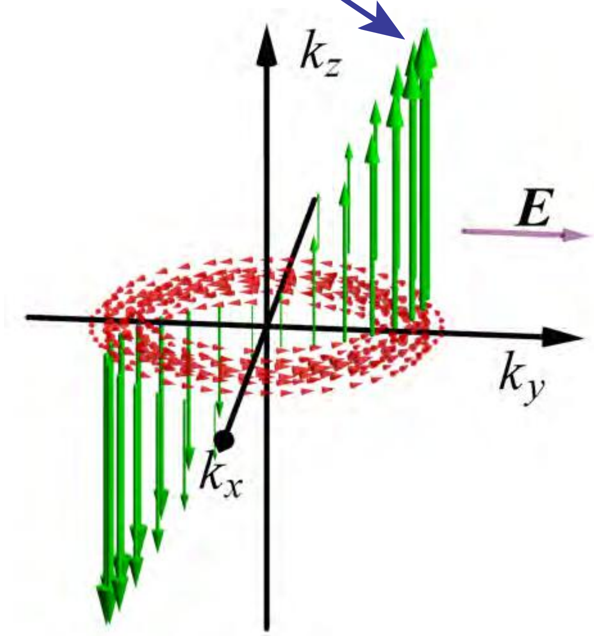
⚠ Anomalous current vanishes after integrating over ϕ 😞

Dirac nodal-line semimetal

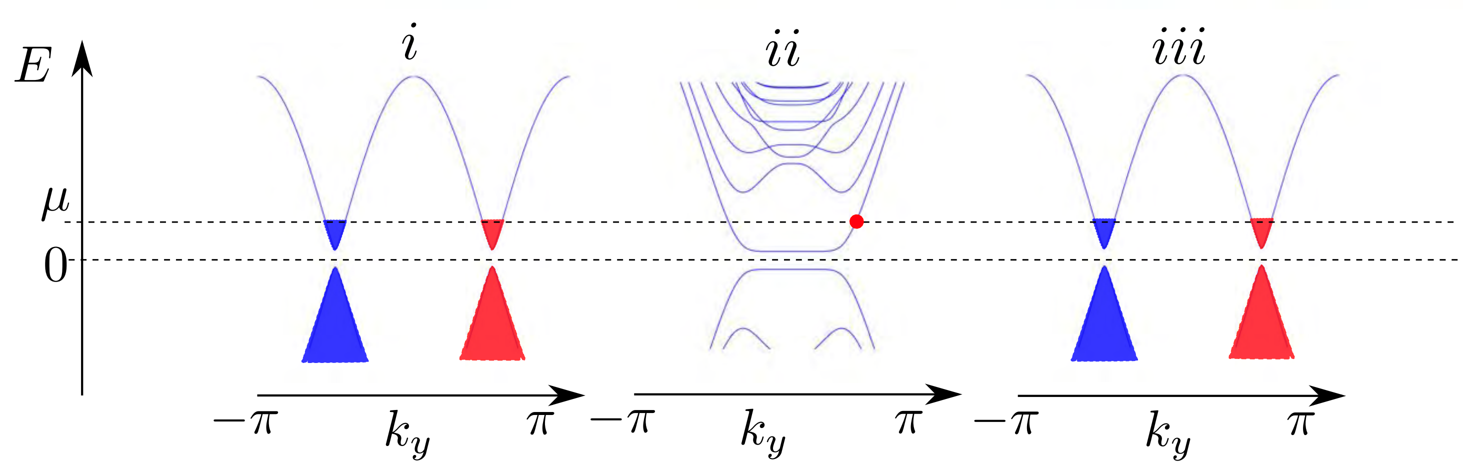
Drumhead surface states as a momentum filter:

- Consider dumbbell geometry:





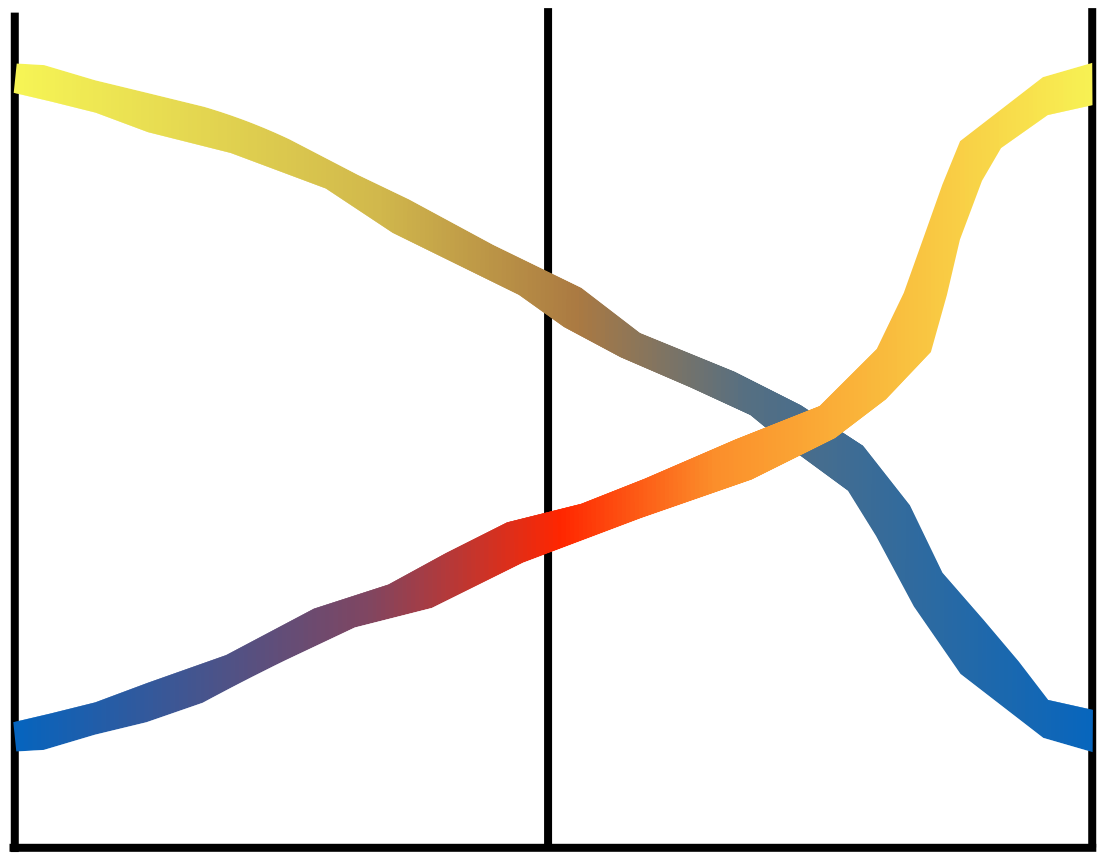
— band structures for $k_x = 0$:



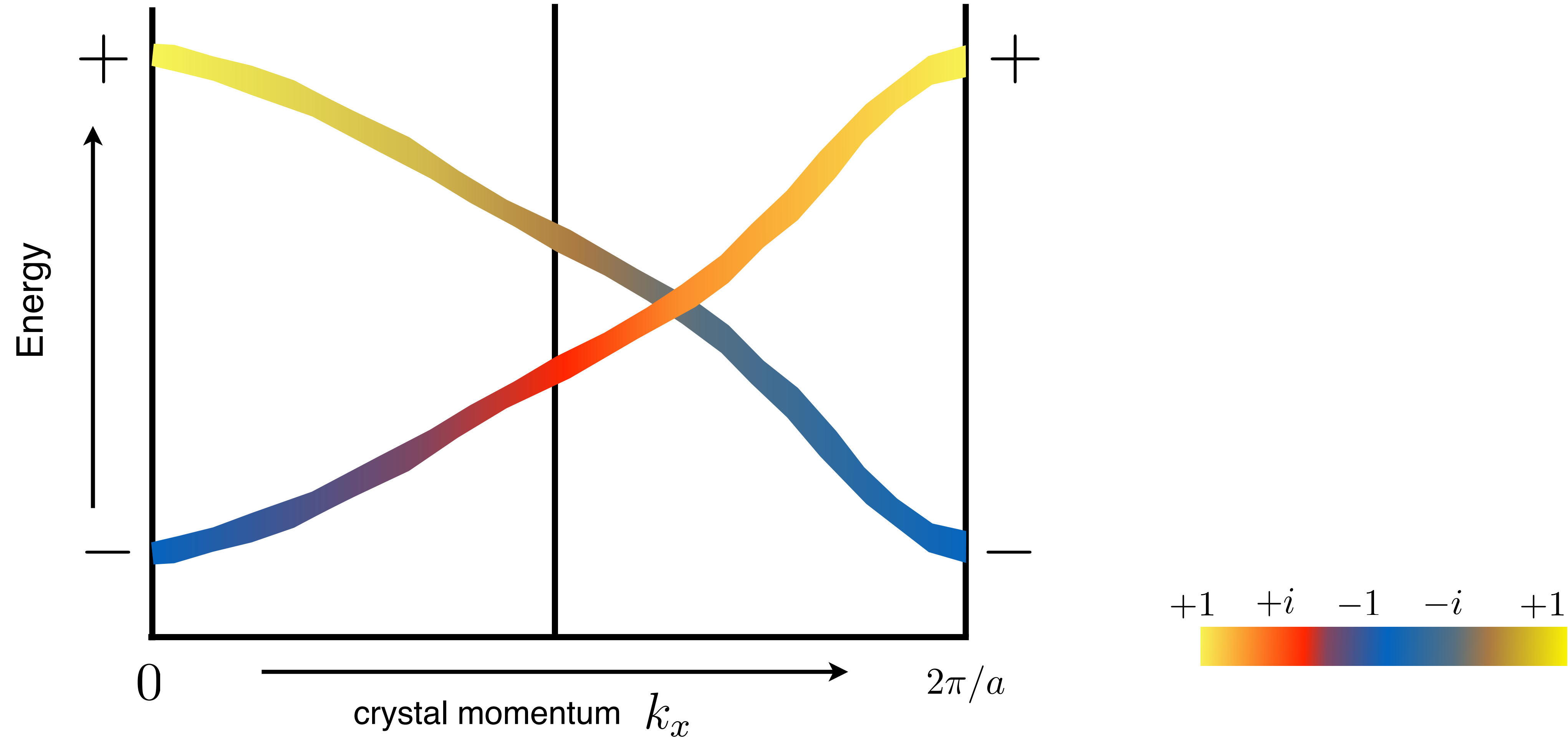
$\Longrightarrow$ Drumhead surface states act as a filter

$\Longrightarrow$ Transverse current can be measured!

3. Symmetry-enforced band crossings



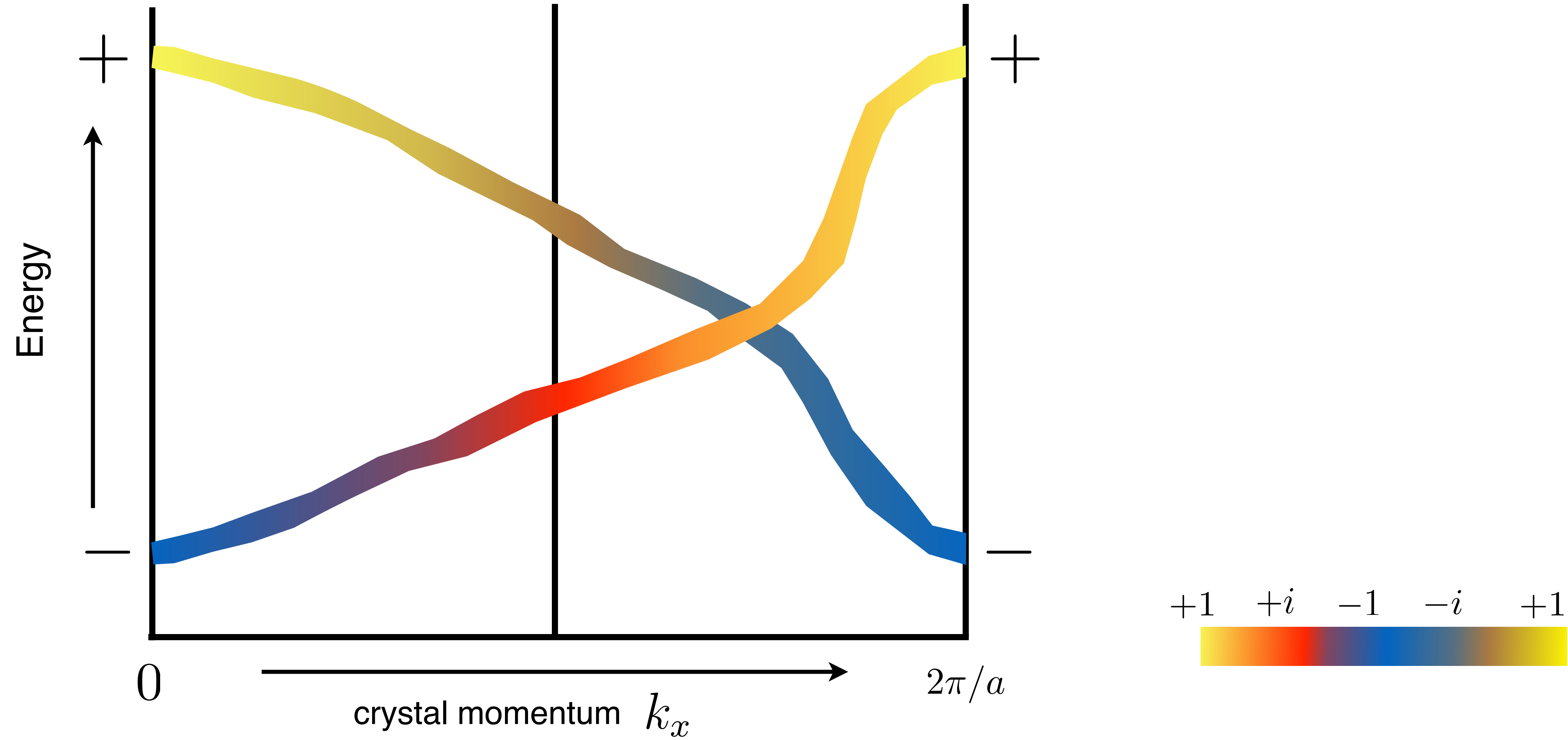
Symmetry-enforced band crossings



- protected by *non-symmorphic* crystal symmetry (possibly together with non-spatial sym)
- exhibits local topological charge $n_{\mathbb{Z}}$ and *global* topological charge $m_{\mathbb{Z}_2}$
- globally stable, movable but *not removable*

$\Longrightarrow$ classification tells you that band crossing is *symmetry required!*

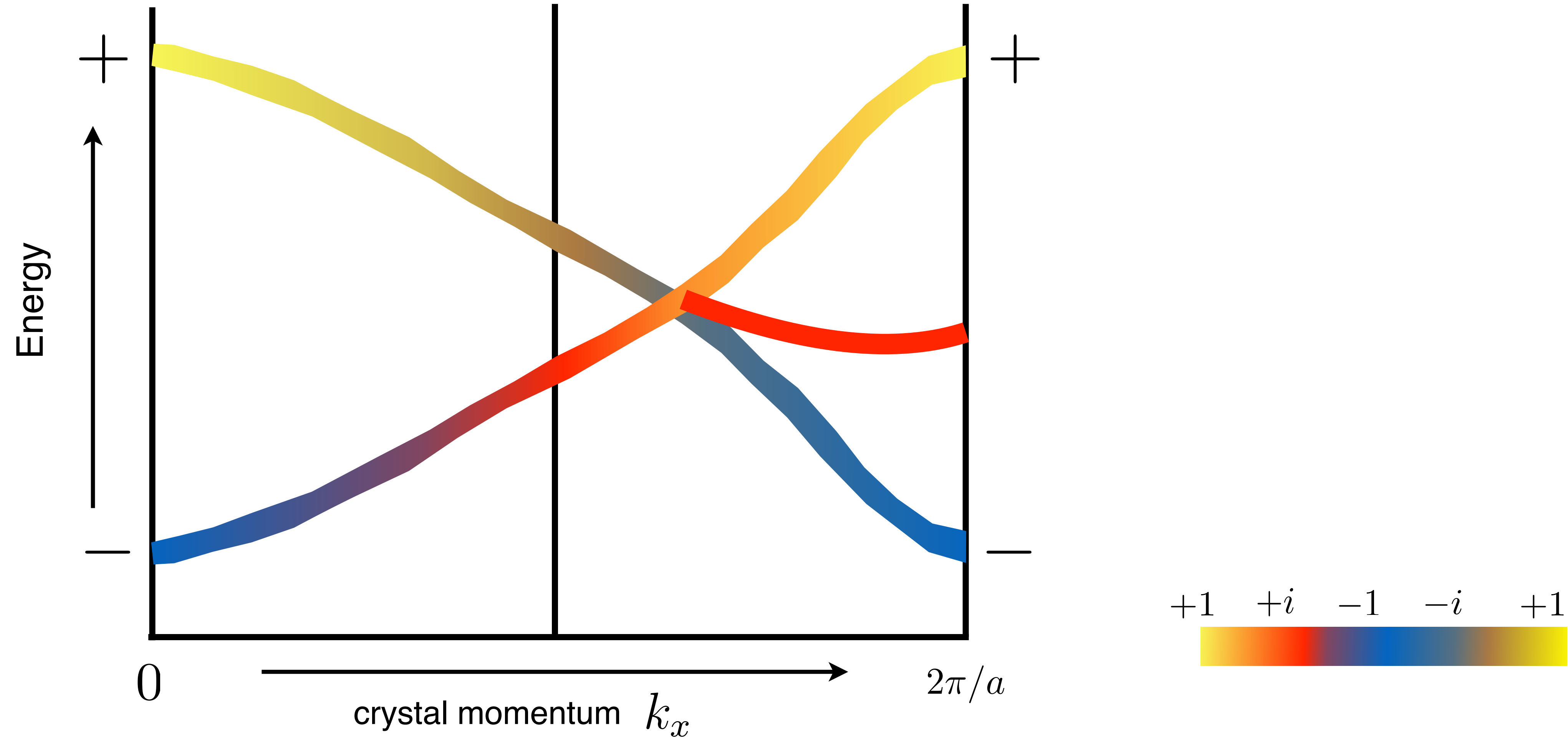
Symmetry-enforced band crossings



- protected by *non-symmorphic* crystal symmetry (possibly together with non-spatial sym)
- exhibits local topological charge $n_{\mathbb{Z}}$ and *global* topological charge $m_{\mathbb{Z}_2}$
- globally stable, movable but *not removable*

$\Longrightarrow$ classification tells you that band crossing is *symmetry required!*

Symmetry-enforced band crossings



- protected by *non-symmorphic* crystal symmetry (possibly together with non-spatial sym)
- exhibits local topological charge $n_{\mathbb{Z}}$ and *global* topological charge $m_{\mathbb{Z}_2}$
- **Bulk-boundary correspondence:**

$$|n_{\mathbb{Z}}| = \#\,\text{gapless edge states (or surface states)}$$

Strategy for discovery of topological semi-metals

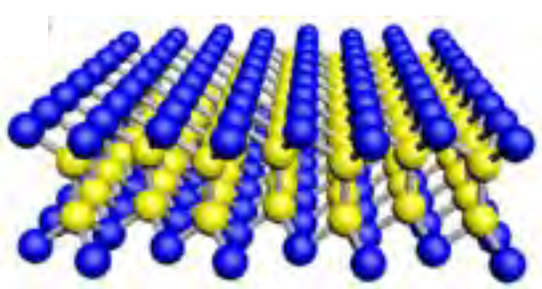
(i) Consider 157 non-symmorphic space groups

$\Rightarrow$ identify those space groups with symmetry-enforced band crossings using symmetry eigenvalues and compatibility between irreps

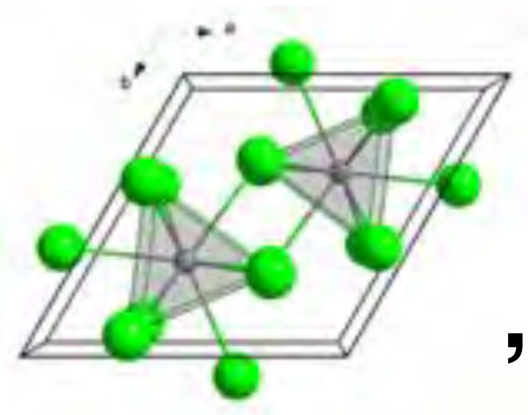
$P6_1$ (#169) , $P6_3/m$ (#176) , $P6_122$ (#178) , ...

FIZ Karlsruhe ICSD

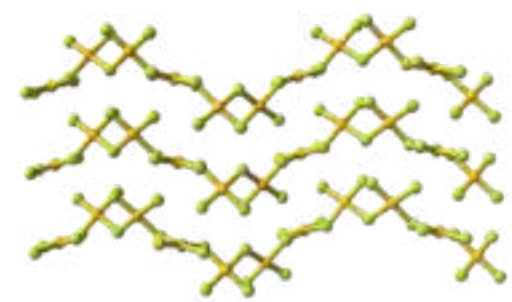
(ii) Perform a database search for materials in these space groups



In_2Se_3 ,



$LaBr_3$,



AuF_3 , ...

(iii) Compute DFT band structures, topological invariants, surface states, etc.

— to check whether band crossings and surface states are near E_F

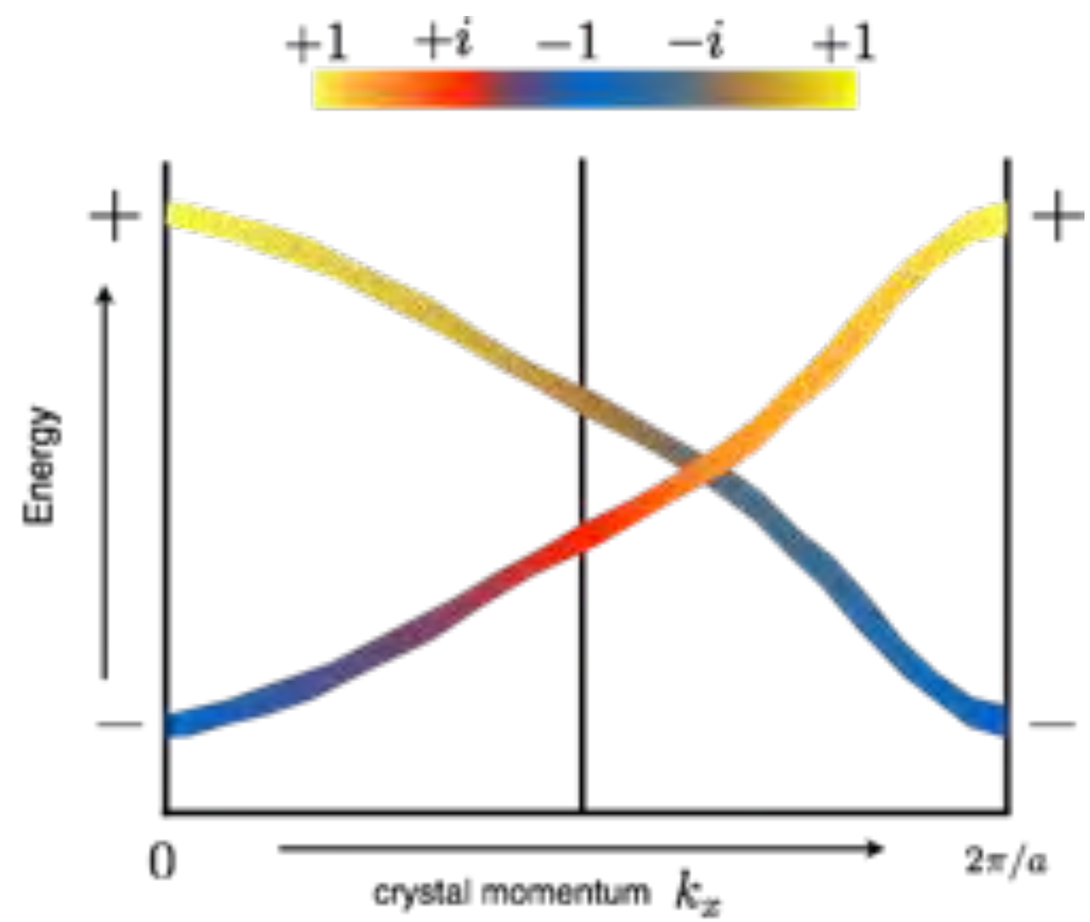
3.2 How non-symmorphic symmetries lead to enforced band crossings

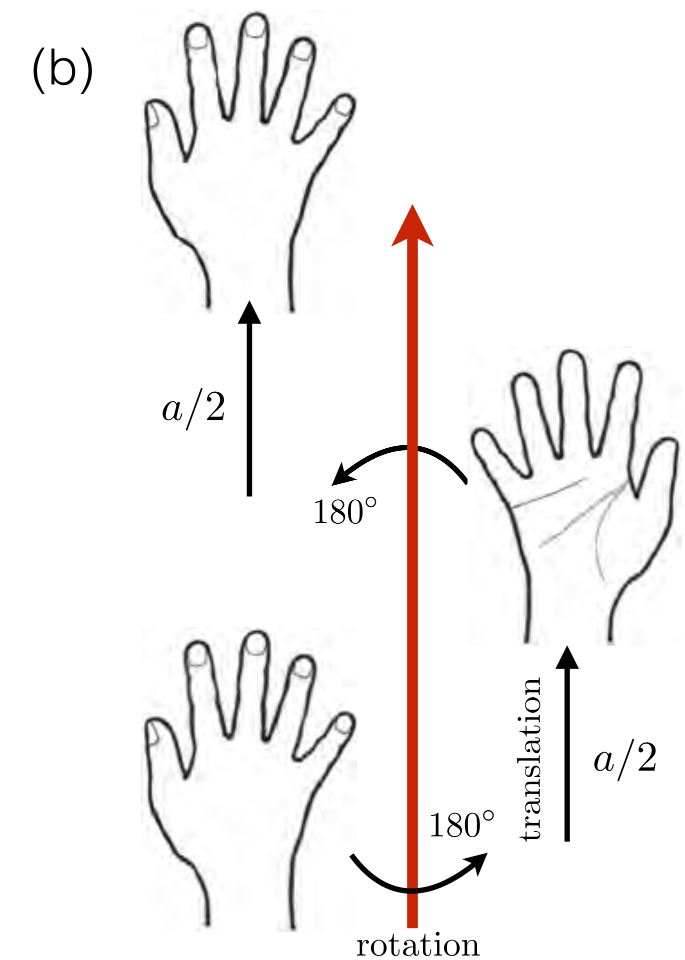
- screw rotation symmetry:

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

$$G(k) = \begin{pmatrix} 0 & e^{-ik} \\ 1 & 0 \end{pmatrix} \qquad G^2(k) = \sigma_0 e^{-ik}$$

- eigenvalues: $G\,|\psi_\pm(\mathbf{k})\rangle = \pm e^{-ik/2}\,|\psi_\pm(\mathbf{k})\rangle$





Nonsymmorphic symmetries lead to enforced band crossings

- $G(k)$ does not commute with σ_3

$$\Rightarrow \; H(k) = \begin{pmatrix} 0 & q(k) \\ q^*(k) & 0 \end{pmatrix} \qquad\qquad E = \pm |q(k)|$$

- symmetry constraint: $q(k) e^{ik} = q^*(k)$
- show that $q(k)$ must have zero, using contradiction

$$z := e^{ik} \qquad\qquad f(z) := q(k)$$

$$\Rightarrow \quad z = f^*(z)/f(z) \; = e^{2i\mathrm{Arc}[f(z)]}$$

winds once

winds twice

$\Longrightarrow f(z)$, $q(k)$ must vanish at some k by contradiction

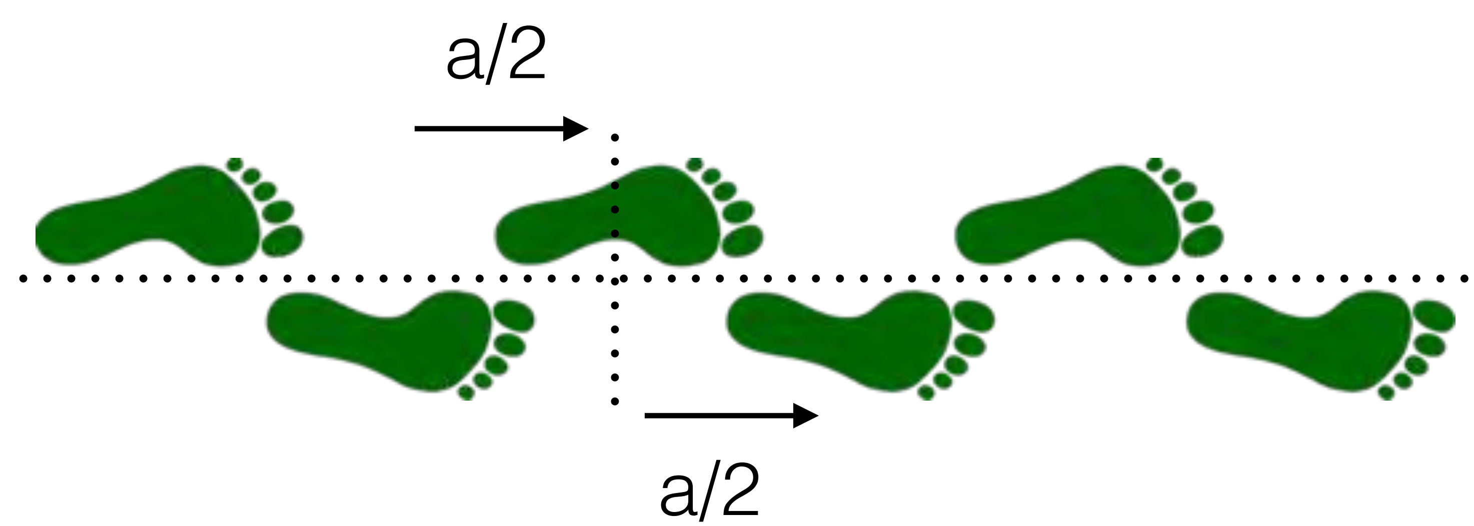
3.2 Weyl nodal-line semimetal

ZrIrSn in SG #190

- Glide reflection (rank two):

$$M = (m|\vec{\tau})$$

$$M^2 = \hat{T}$$



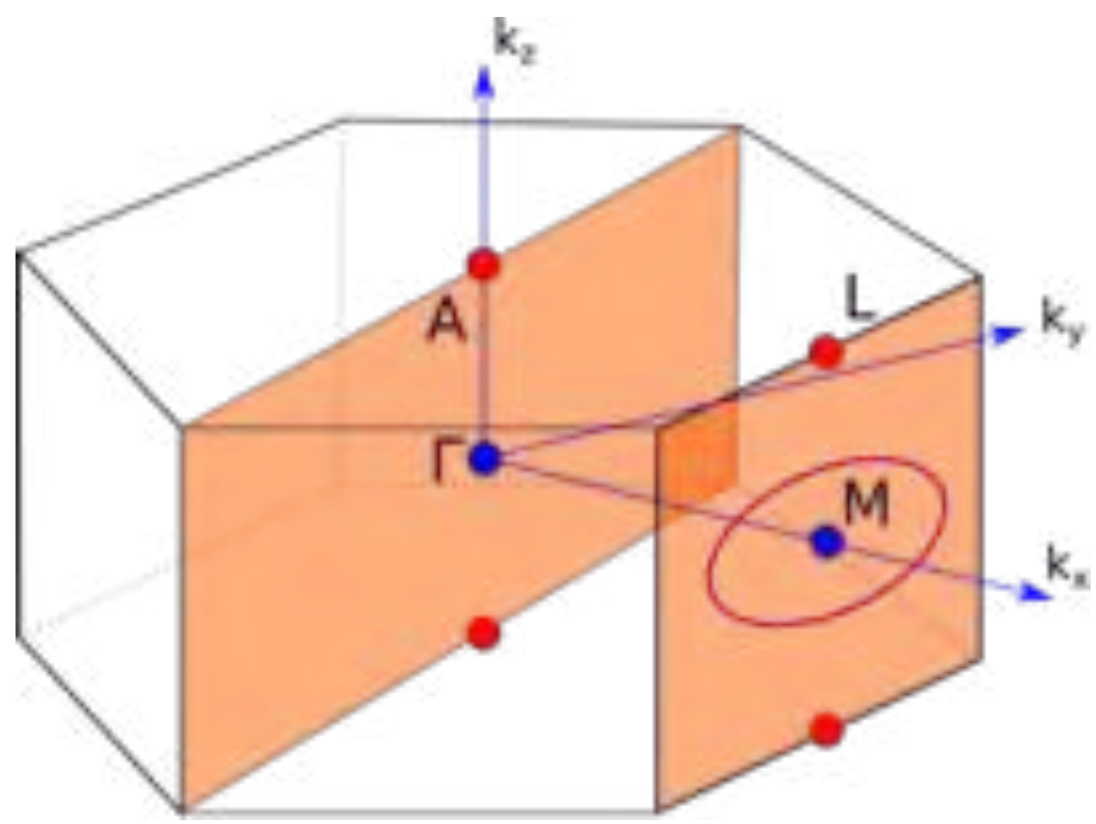
Weyl nodal-line semimetal

- glide reflection symmetry: $M_x \;:\; (x, y, z) \to (-x, y, z + \frac{1}{2})$
- invariant planes: $k_x = 0 \quad \& \quad k_x = \pi$
- symmetry eigenvalues: $M_x^2 = -\hat{T}_z = -e^{-ik_z} \;\Rightarrow\; \text{EVs: } \pm\, ie^{-ik_z/2}$

due to spin part

- $|\psi(\mathbf{k})\rangle$ in invariant planes are simultaneous eigenstates of M_x

$$\Longrightarrow \quad \boxed{M_x \, |\psi_\pm(\mathbf{k})\rangle = \pm i e^{-ik_z/2} \, |\psi_\pm(\mathbf{k})\rangle}$$

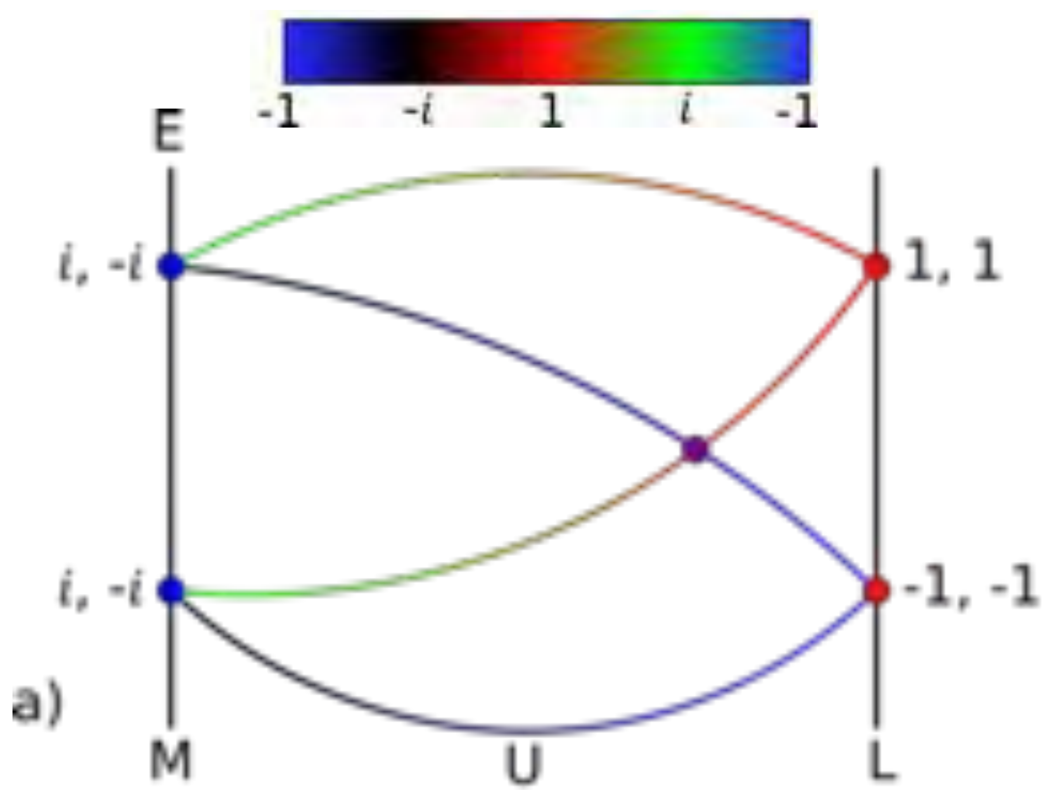


Weyl nodal-line semimetal

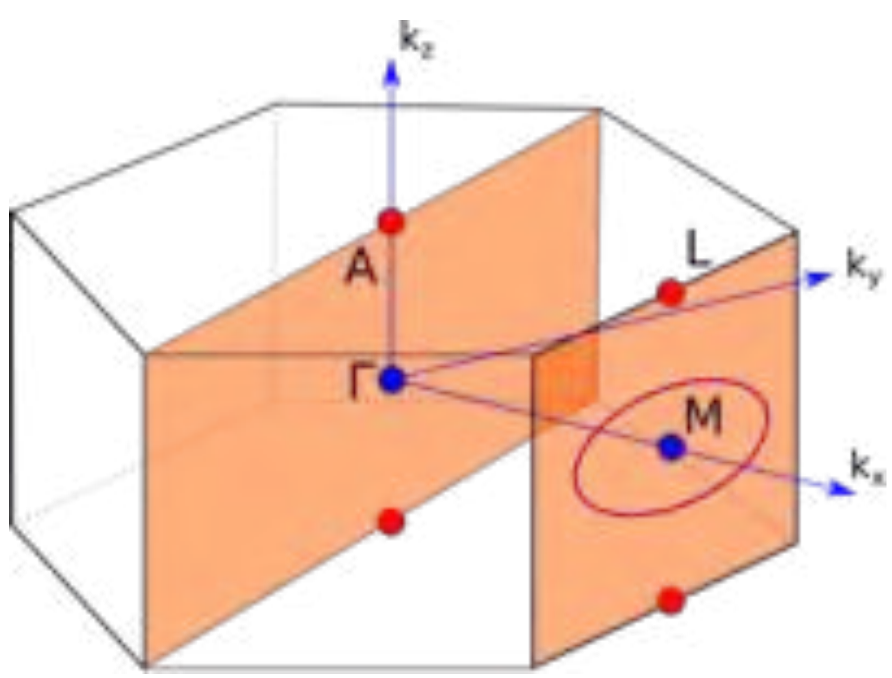
$$M_x \left|\psi_\pm(\mathbf{k})\right\rangle = \pm i e^{-ik_z/2} \left|\psi_\pm(\mathbf{k})\right\rangle$$

- add time-reversal symmetry: $T = i\sigma_y \mathcal{K}$

$\Longrightarrow$ pairs up states with complex conjugate EVs at the TRIMs



$k_z = 0$ $k_z = \pi$



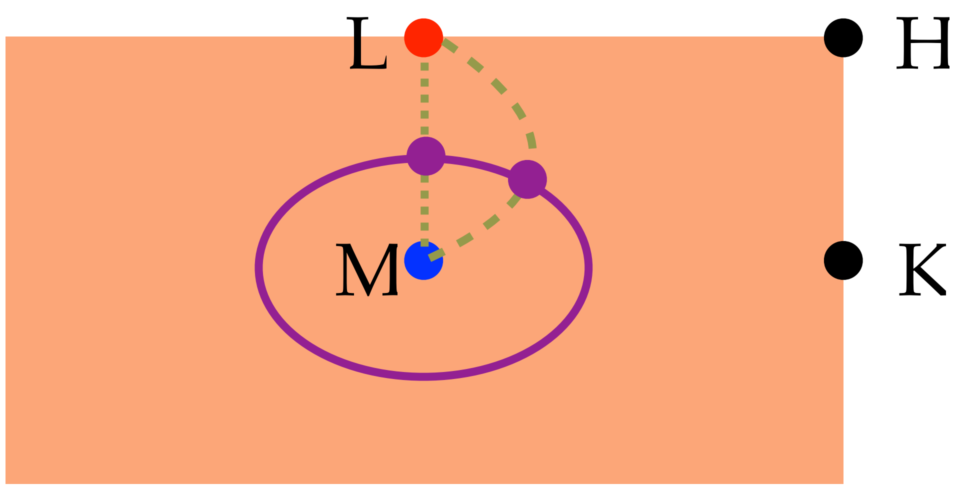
$\Longrightarrow$ hourglass dispersion

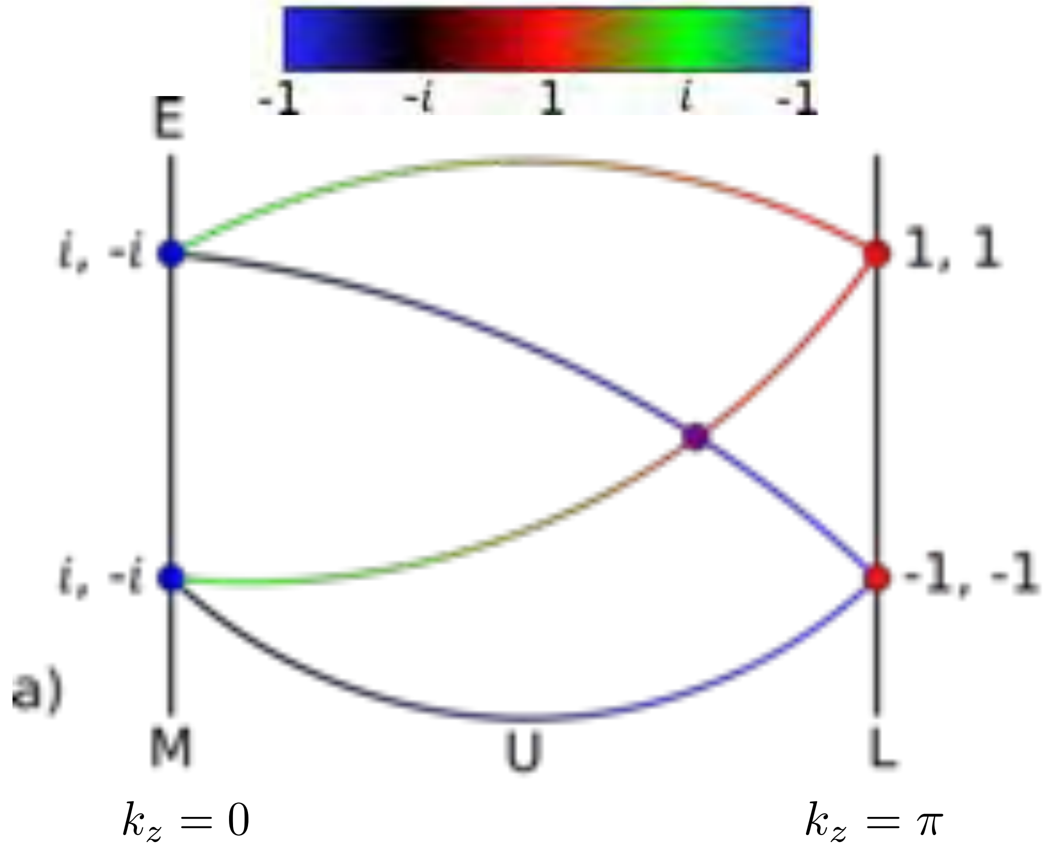
Weyl nodal-line semimetal

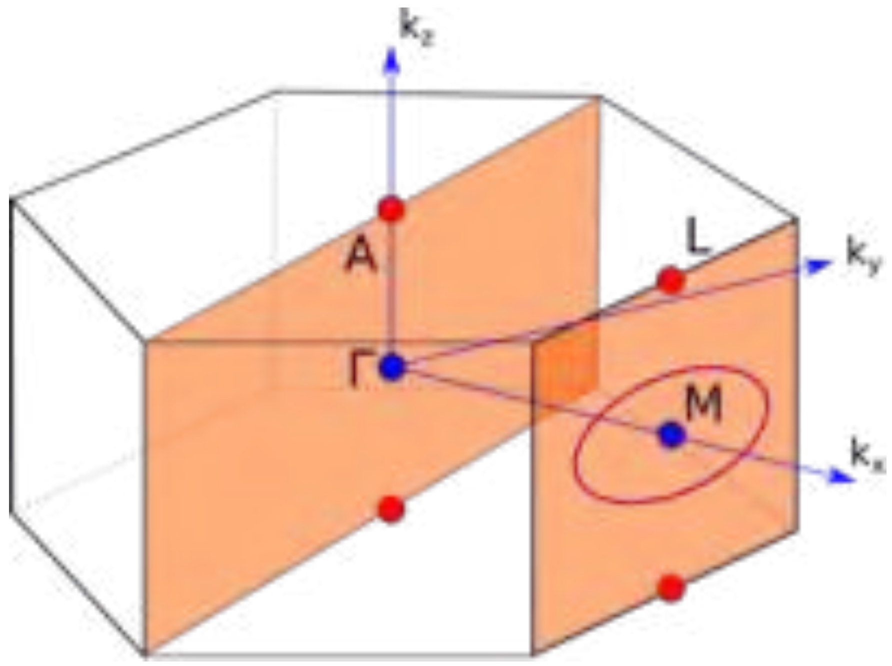
$$M_x \left|\psi_\pm(\mathbf{k})\right\rangle = \pm i e^{-ik_z/2} \left|\psi_\pm(\mathbf{k})\right\rangle$$

- add time-reversal symmetry: $T = i\sigma_y \mathcal{K}$

$\Longrightarrow$ pairs up states with complex conjugate EVs at the TRIMs







$\Longrightarrow$ Weyl nodal line within mirror plane

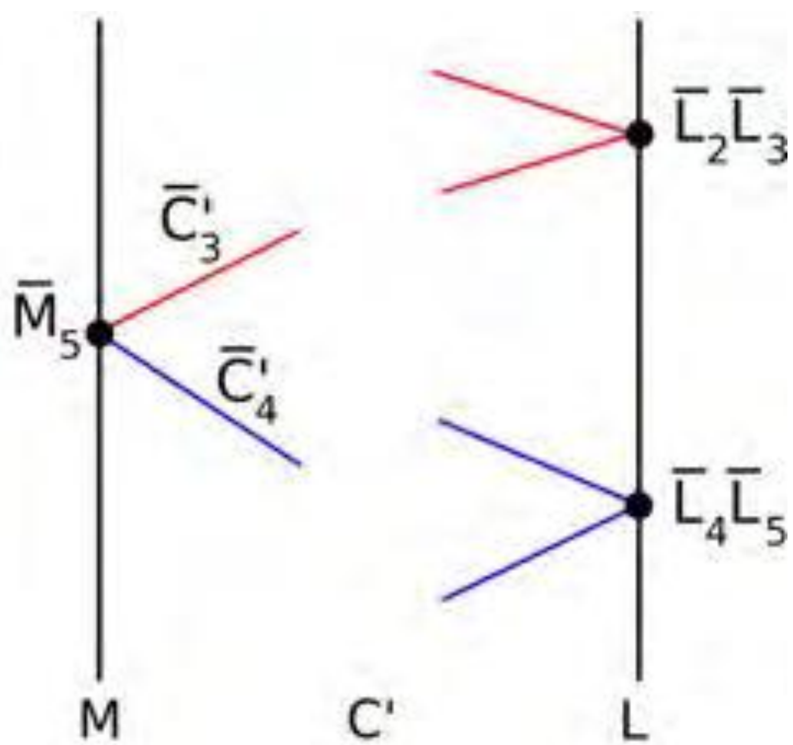
Weyl nodal-line semimetal

- consider *time-reversal* invariant little-group irreps at TRIMs and within mirror plane C':

$$\text{M:}\ \bar{M}_5 \quad \text{L:}\ \bar{L}_2\bar{L}_3,\ \bar{L}_4\bar{L}_5 \quad \text{C':}\ \bar{C}'_3,\ \bar{C}'_4$$

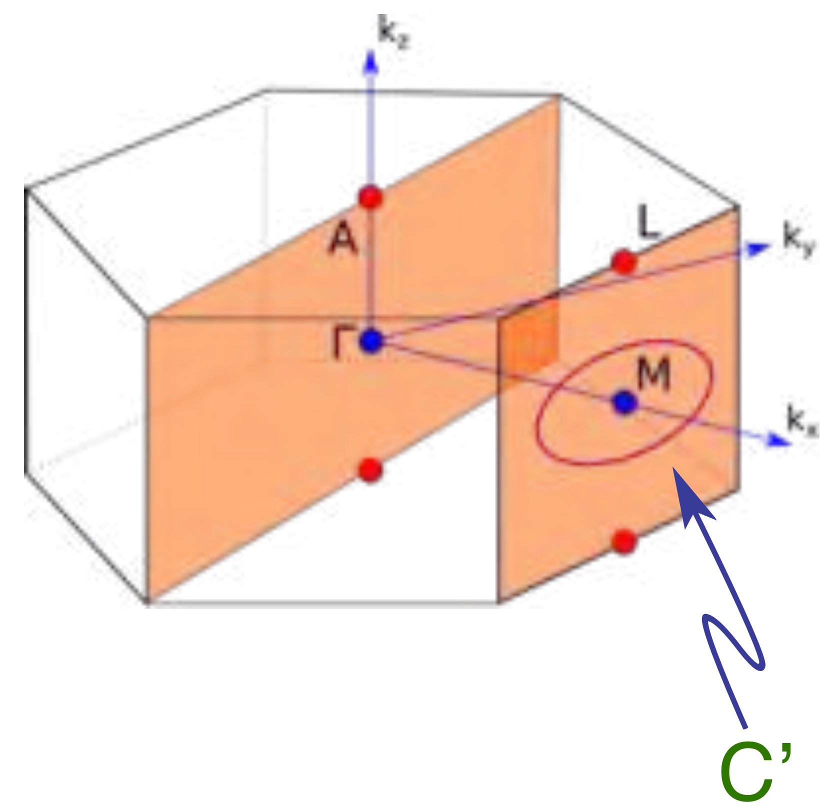
- compatibility relation between irreps tell us how irreps split as we move from M,L $\longrightarrow$ C'

$$\mathbf{D}_M \downarrow \mathcal{G}_{C'} = \mathbf{D}_{C'} \qquad \text{(subduction)}$$



Miller, Love, *Pruett* 1967

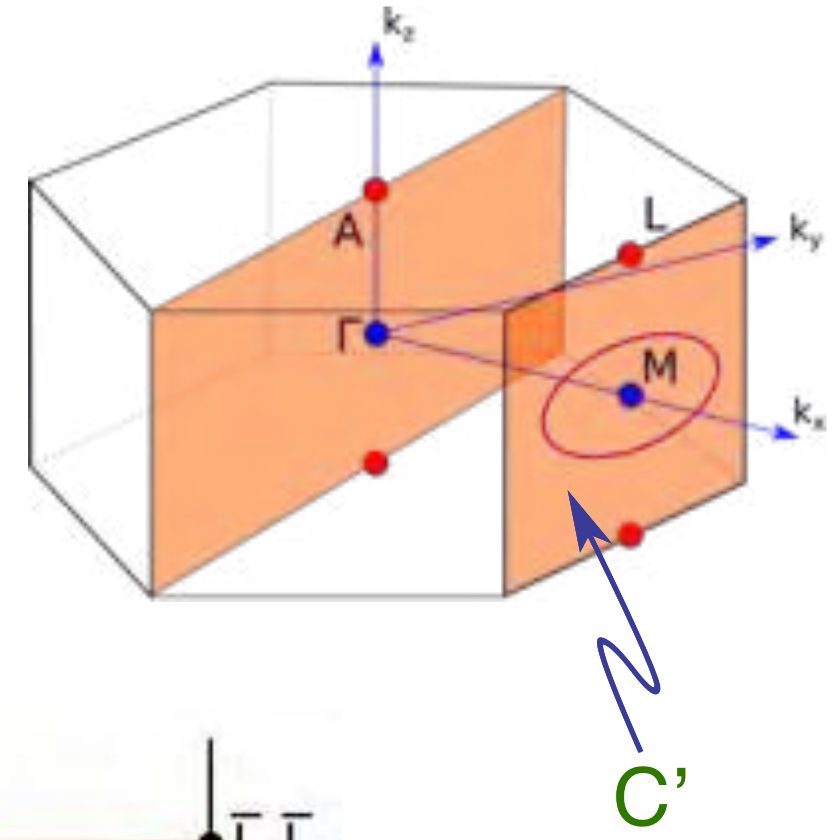
Irrep\Element	E	M_x
$\bar{M}_5$	$\begin{pmatrix} +1 & 0 \\ 0 & +1 \end{pmatrix}$	$\begin{pmatrix} +i & 0 \\ 0 & -i \end{pmatrix}$
$\bar{L}_2$	$+1$	-1
$\bar{L}_3$	$+1$	-1
$\bar{L}_4$	$+1$	$+1$
$\bar{L}_5$	$+1$	$+1$
$\bar{C}'_3$	$+1$	$e^{\frac{i}{2}(\pi+k_z)}$
$\bar{C}'_4$	$+1$	$e^{-\frac{i}{2}(\pi-k_z)}$



Weyl nodal-line semimetal

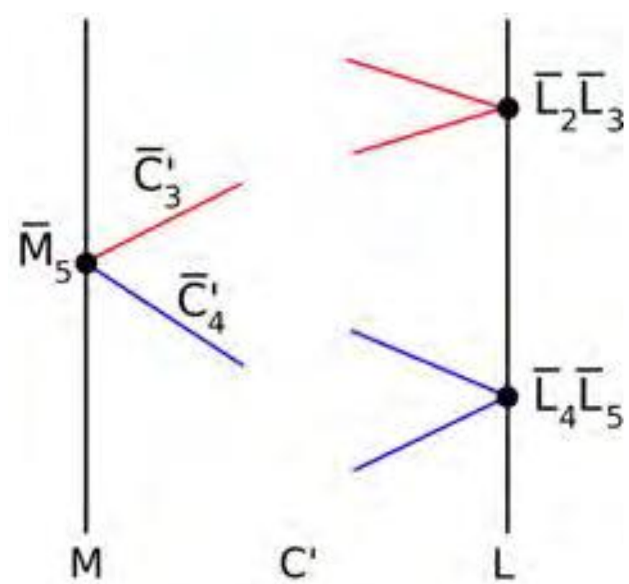
- consider *time-reversal* invariant little-group irreps at TRIMs and within mirror plane C':

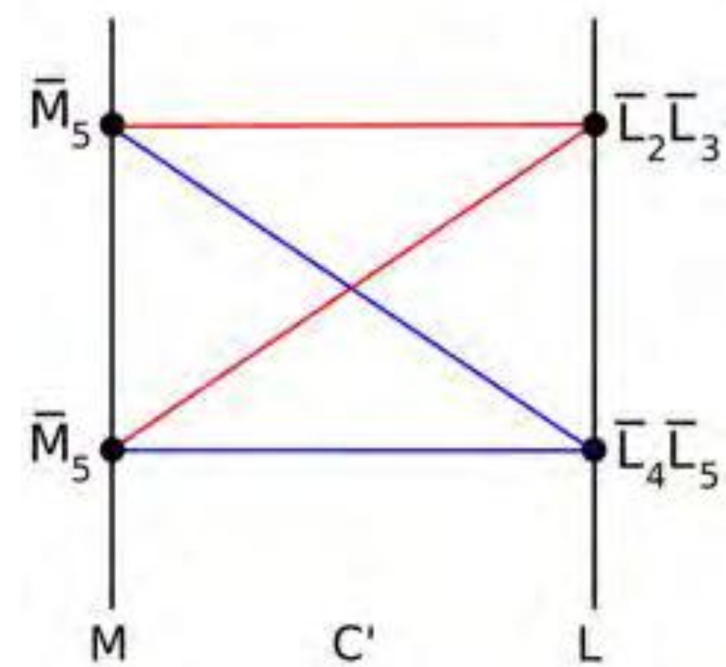
$$\mathrm{M:}\ \bar{M}_5 \qquad \mathrm{L:}\ \bar{L}_2\bar{L}_3,\ \ \bar{L}_4\bar{L}_5 \qquad \mathrm{C':}\ {\color{red}\bar{C}'_3},\ \ {\color{blue}\bar{C}'_4}$$



- compatibility relation between irreps tell us how irreps split as we move from $\mathrm{M,L} \longrightarrow \mathrm{C'}$

$$\mathbf{D}_M \downarrow \mathcal{G}_{C'} = \mathbf{D}_{C'} \qquad \text{(subduction)}$$





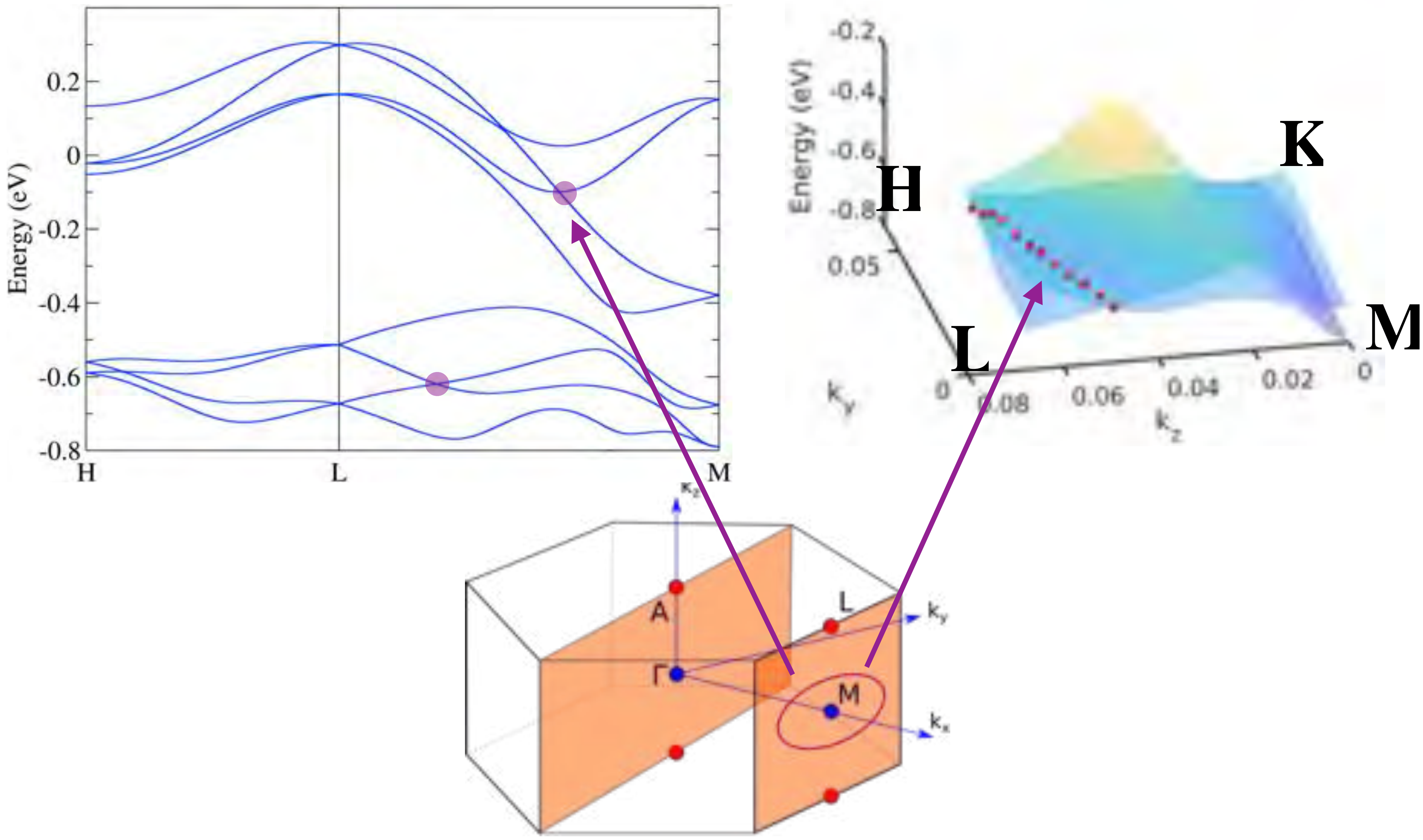
- bands need to connect, such that compatibility relations are satisfied

$$\Longrightarrow \text{Weyl nodal line within mirror plane C'}$$

Miller, Love, *Pruett* 1967

Weyl nodal-line semimetal

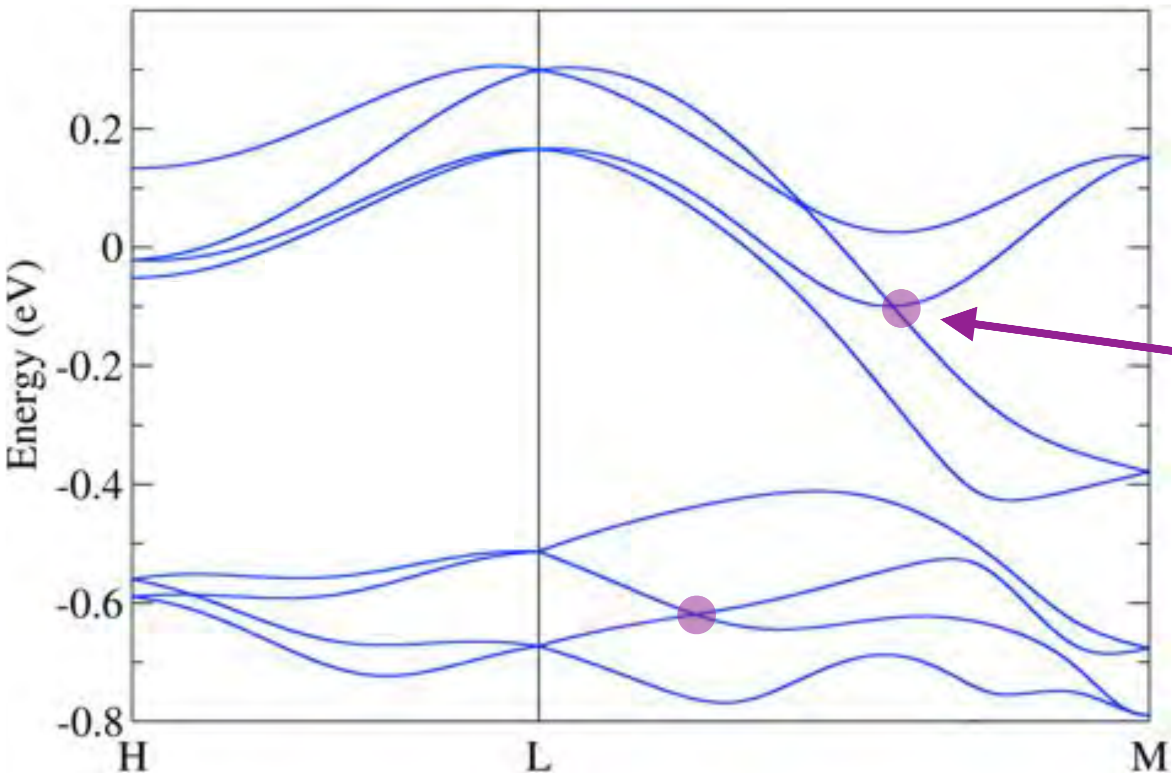
- DFT band structure of ZrIrSn:

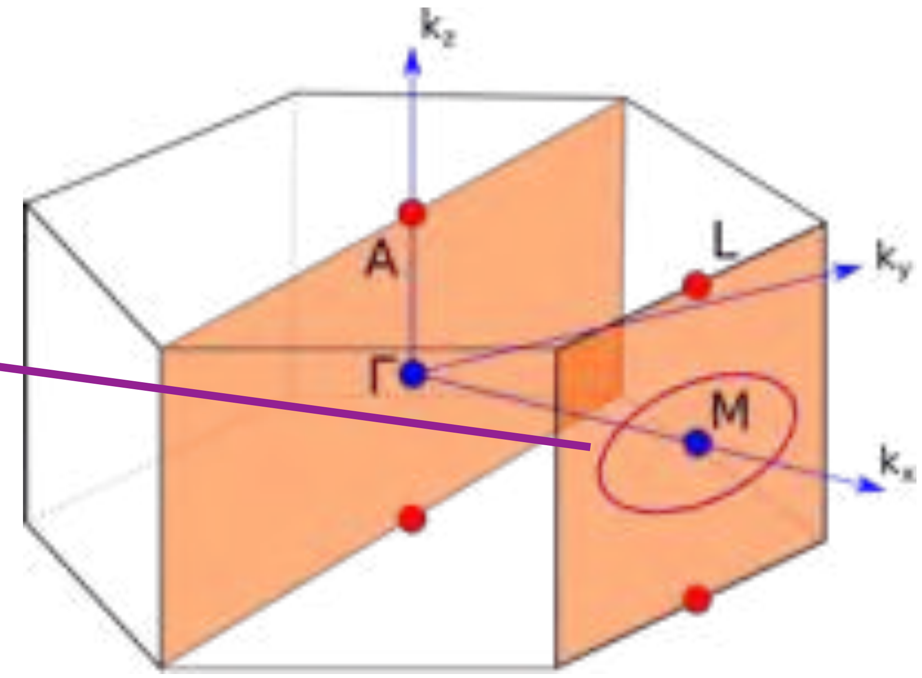


— Weyl nodal line characterized by quantized π-Berry phase

Weyl nodal-line semimetal

- DFT band structure of ZrIrSn:





- Experimental consequences:

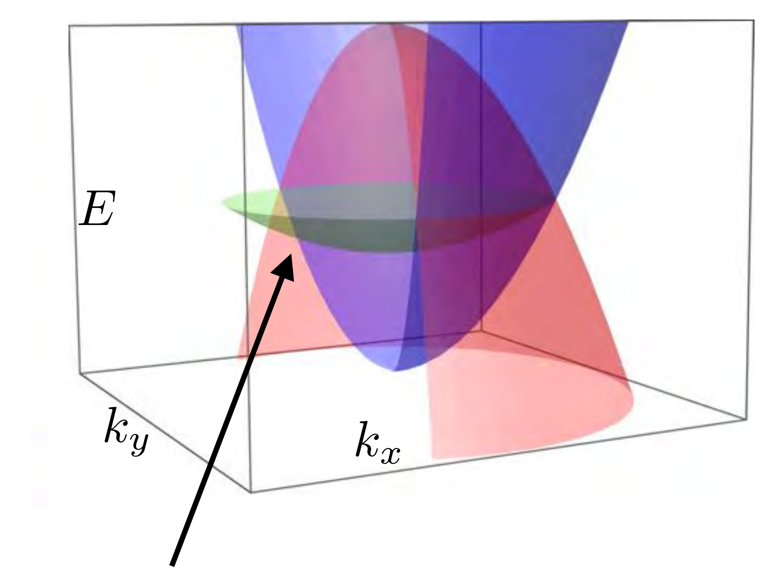
— Bulk-boundary correspondence:

$\Longrightarrow$ drumhead surface state

— Large Berry curvature:

$\Longrightarrow$ large anomalous Hall effect

$\Longrightarrow$ anomalous magnetoelectric responses



3.2 Dirac nodal-line semimetal

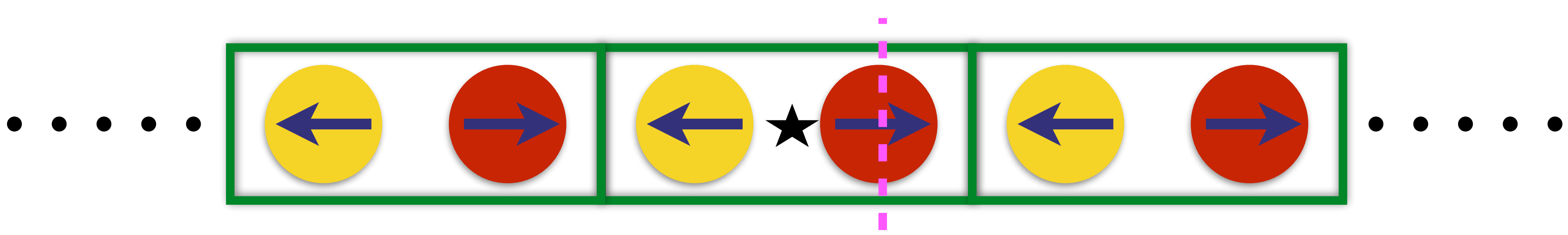
$LaBr_3$

Off-center symmetries:

- Pair of non-symmorphic symmetries

$$G = (g|\vec{\tau}_\perp), \;\; G' = (g'|\vec{\tau}'_\perp)$$

with *different* reference points



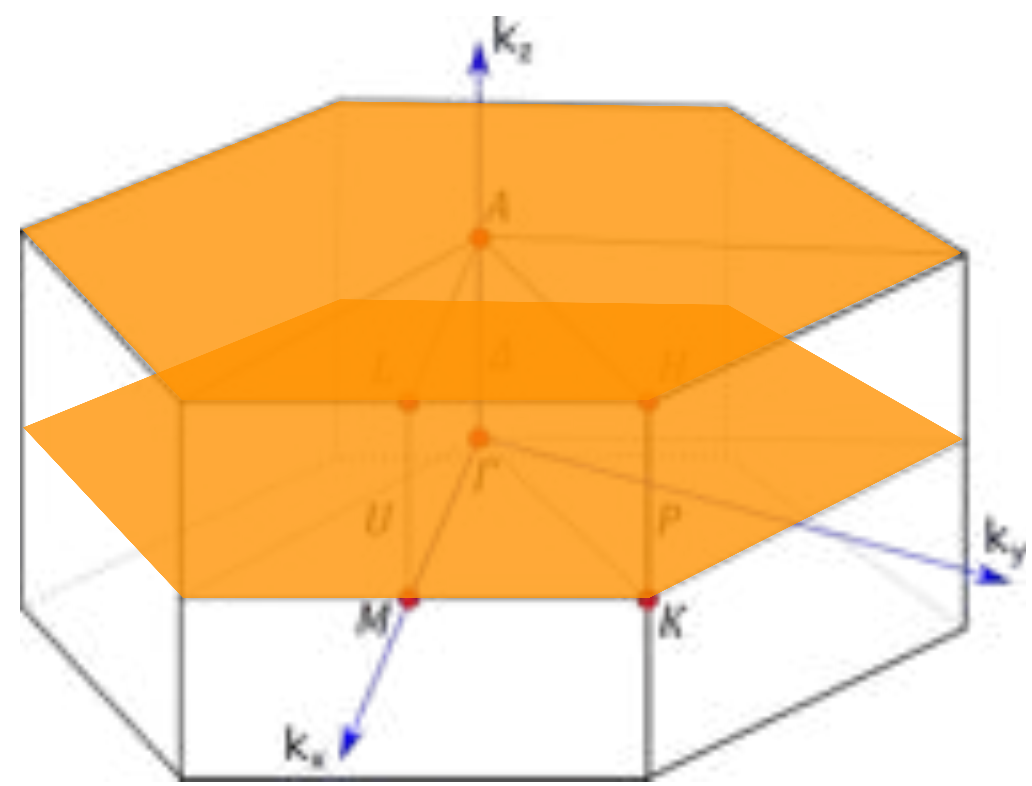
Dirac nodal-line semimetal

- off-centered symmetries: $(\widetilde{M}_z, P)$

$$\widetilde{M}_z \; : \; (x,y,z) \rightarrow (x,y,-z+\tfrac{1}{2}) \qquad P \; : \; (x,y,z) \rightarrow (-x,-y,-z)$$

- invariant planes: $k_z = 0 \quad \& \quad k_z = \pi$
- symmetry eigenvalues: $(\widetilde{M}_z)^2 = -1 \;\Rightarrow\; \widetilde{M}_z \,|\psi_\pm(\mathbf{k})\rangle = \pm i \,|\psi_\pm(\mathbf{k})\rangle$

$$\boxed{\widetilde{M}_z P \,|\psi_\pm(\mathbf{k})\rangle = e^{ik_z} P \widetilde{M}_z \,|\psi_\pm(\mathbf{k})\rangle}$$



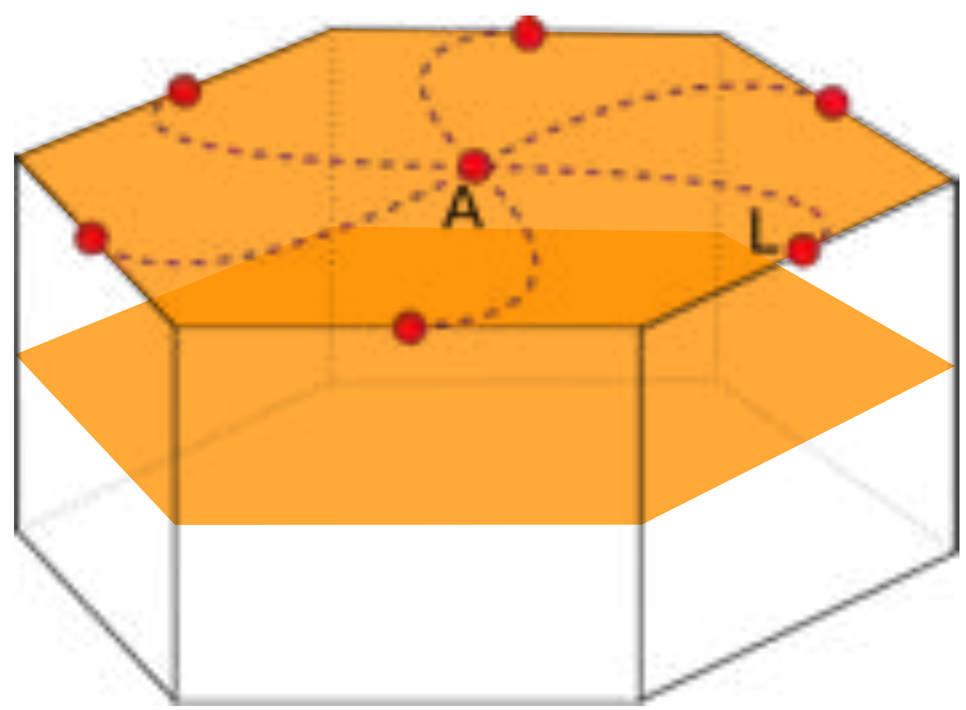
Dirac nodal-line semimetal

$$\widetilde{M}_z P \left|\psi_\pm(\mathbf{k})\right\rangle = e^{ik_z} P \widetilde{M}_z \left|\psi_\pm(\mathbf{k})\right\rangle$$

- add time-reversal symmetry: $T = i\sigma_y \mathcal{K}$

$$\widetilde{M}_z \left[PT \left|\psi_\pm(\mathbf{k})\right\rangle\right] = \mp i e^{ik_z} PT \left|\psi_\pm(\mathbf{k})\right\rangle \qquad k_z \in \{0, \pi\}$$

$\Rightarrow$ the crossing of two Kramers degenerate bands within the $k_z = \pi$ plane is protected by $\widetilde{M}_z$



Dirac nodal-line semimetal

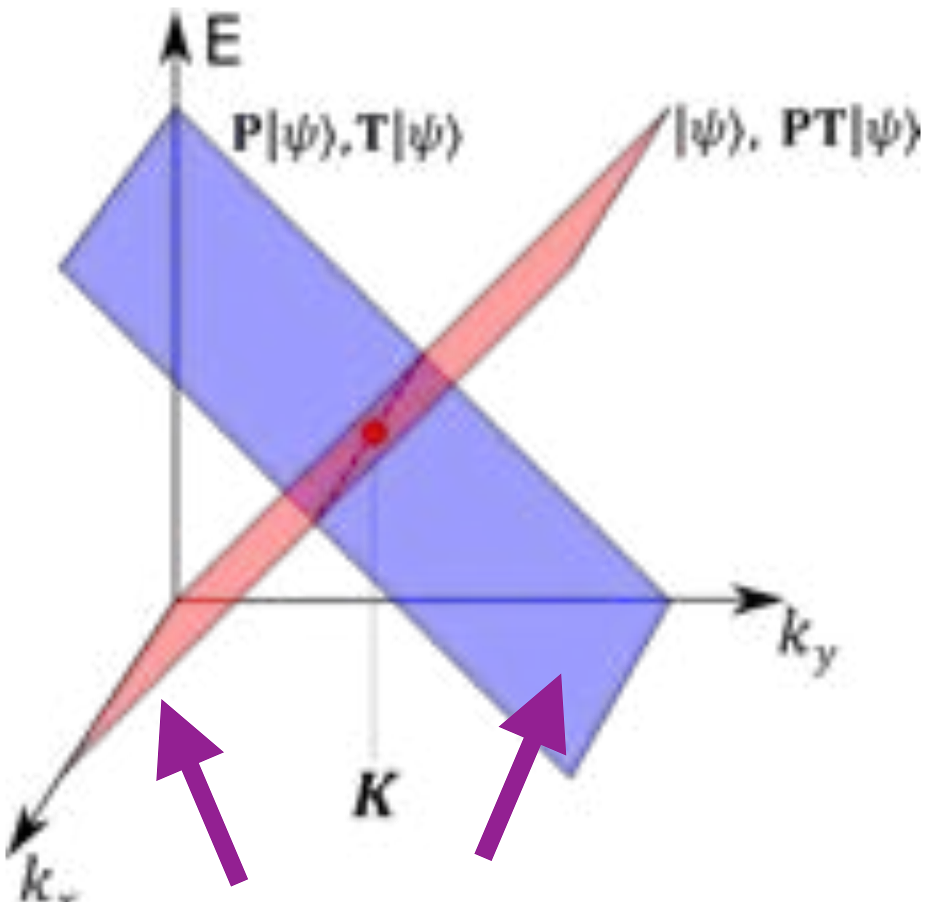
— Dirac nodal line is in fact *symmetry enforced*

- at the TRIMs $\mathbf{K}$, Bloch states form quartet of mutually orthogonal, degenerate states

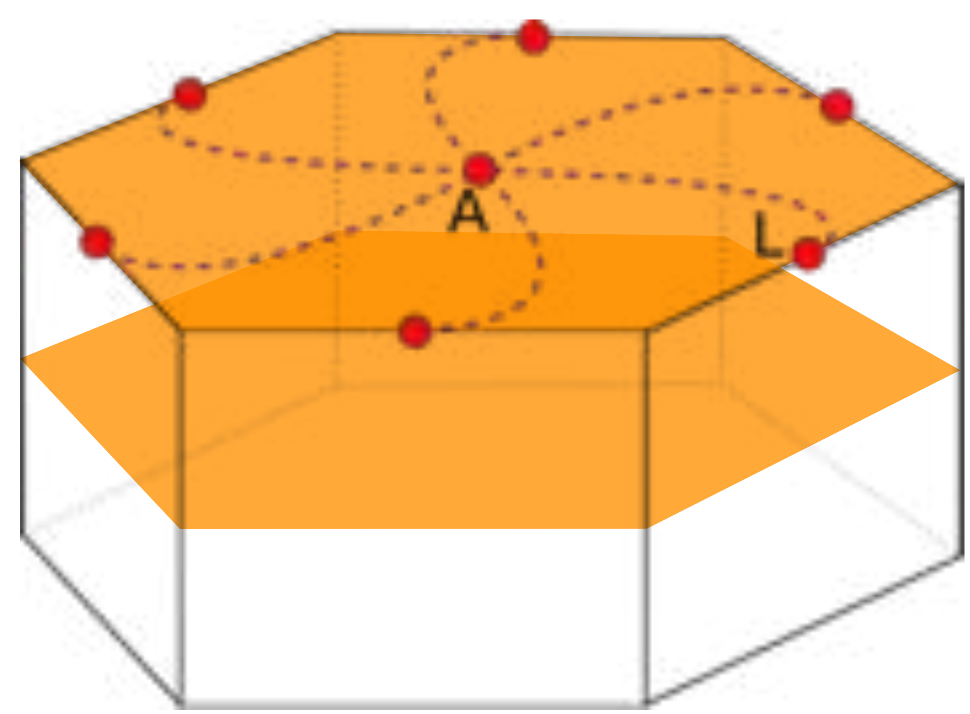
$$|\psi_\pm(\mathbf{K})\rangle \ , \ P\,|\psi_\pm(\mathbf{K})\rangle \ , \ T\,|\psi_\pm(\mathbf{K})\rangle \ , \ PT\,|\psi_\pm(\mathbf{K})\rangle$$

- consider pair of degenerate states:

$$|\psi_\pm(\mathbf{K}+\mathbf{k})\rangle \quad \overset{P,T}{\longleftrightarrow} \quad |\psi_\pm(\mathbf{K}-\mathbf{k})\rangle$$

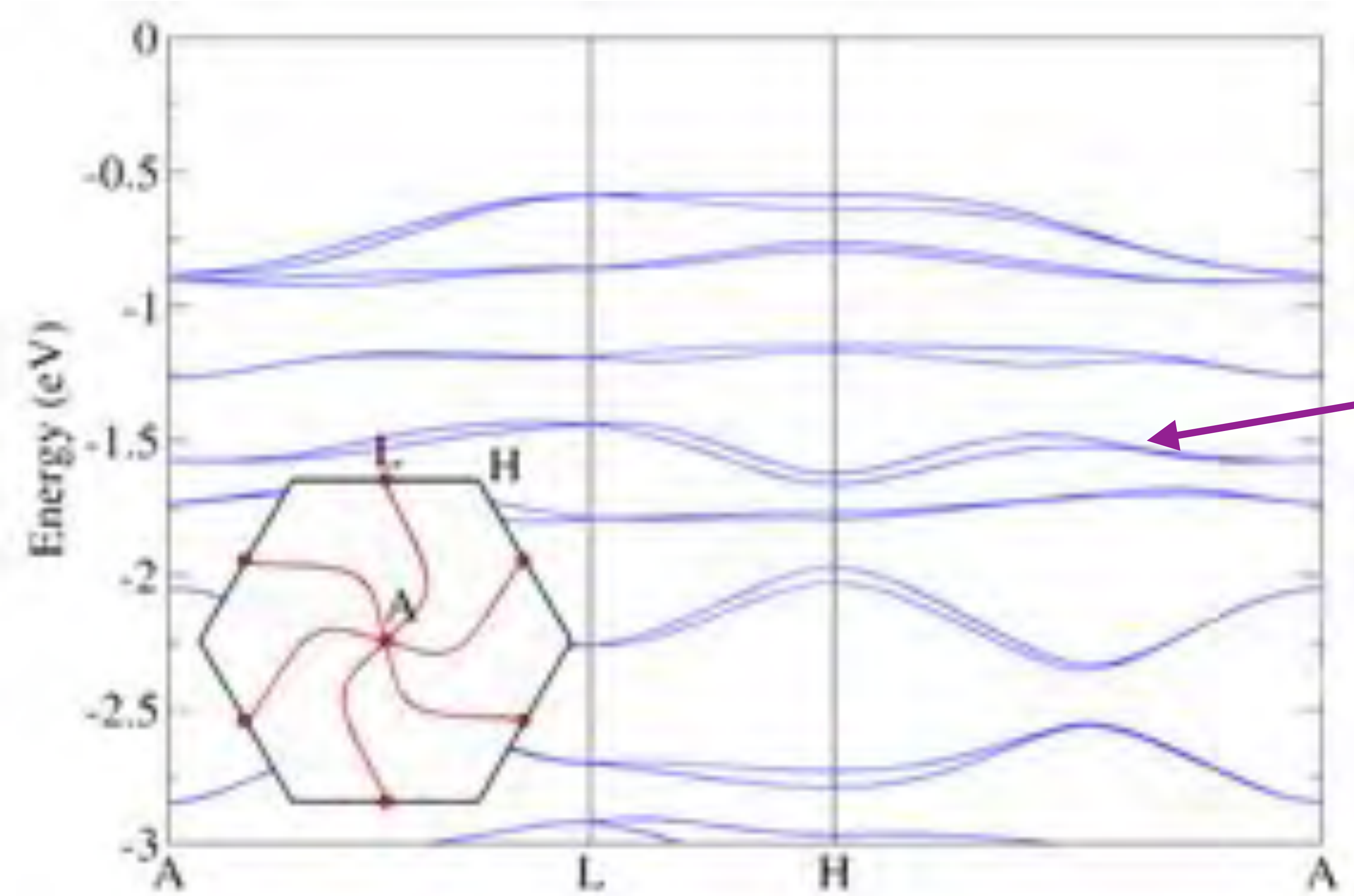


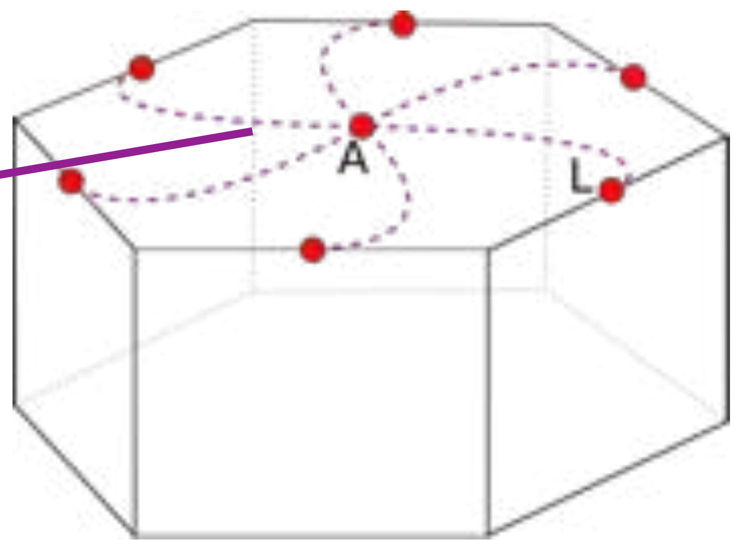
opposite $\widetilde{M}_z$ eigenvalue



Dirac nodal-line semimetal

- DFT calculation of $LaBr_3$:



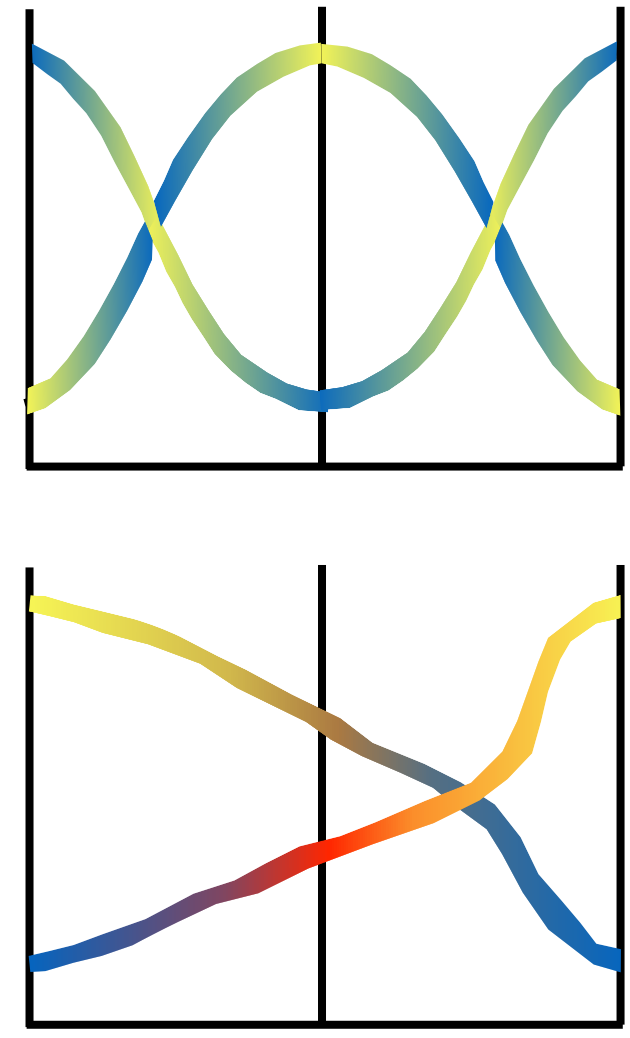


— star-shaped nodal line characterized by Wilson loop

— Bulk-boundary correspondence:

$$\Longrightarrow \text{double drumhead surface state}$$

4. Conclusion and outlook



— studied accidental band crossings

— symmetry enforced band crossings

— strategy for materials discovery

— several examples

- Open questions for future research

  — topology of magnets

  — effects of electron-electron correlation

  — need for better topological materials

    $\Rightarrow$ use, e.g., discussed strategy for materials discovery