Topological materials with reflection symmetry

Andreas P. Schnyder

Max Planck Institute for Solid State Research, Stuttgart

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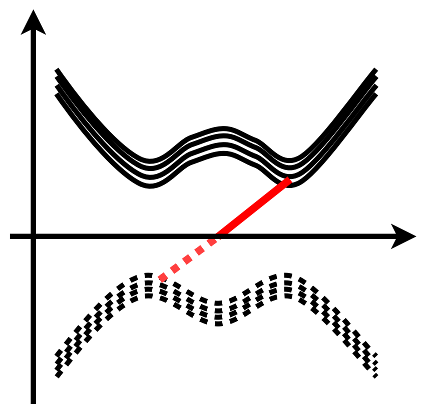
in collaboration with:

C.-K. Chiu, Y.-H. Chan, M. Y. Chou, Y. Nohara, A. Yaresko

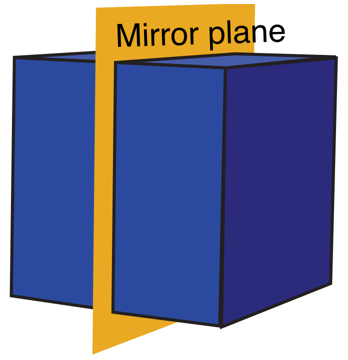
KITP Workshop Ismatter 2015

Outline

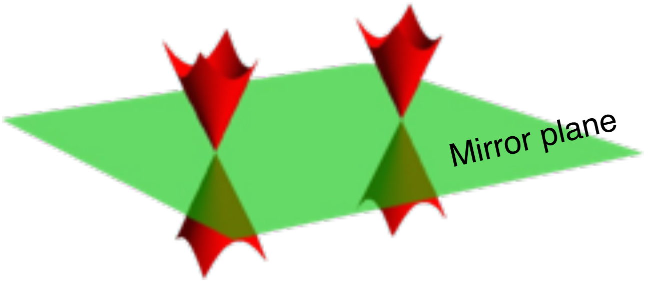
1. Introduction
   - Topological equivalence
   - Mirror reflection symmetry



2. Reflection symmetry protected TIs and SCs
   - Classification of reflection symmetric TIs and SCs
   - Examples: SnTe, Ca_3PbO, Sr_3PbO



3. Reflection symmetry protected semimetals and nodal superconductors
   - Classification schemes
   - Examples: Ca_3P_2, $PbTaSe_2$



4. Conclusions & Outlook

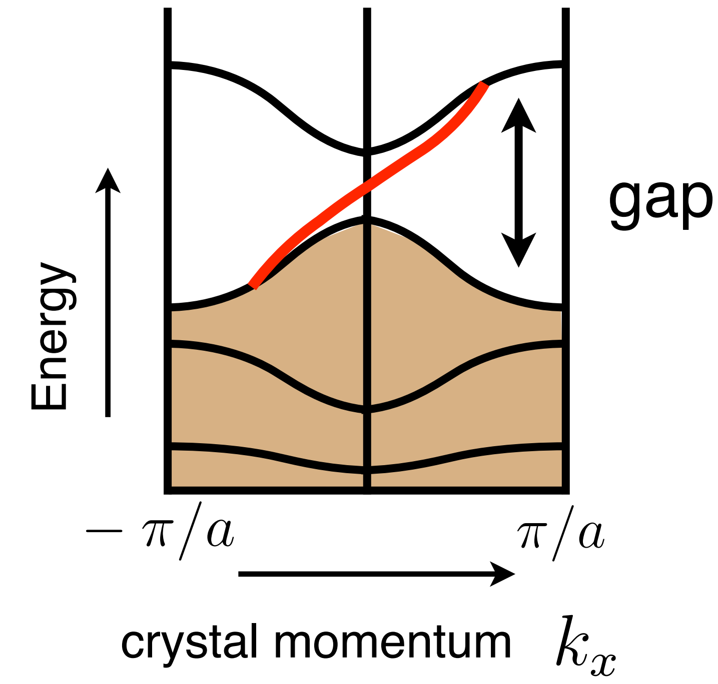
Topological band theory

- Consider band structure with a gap:

$$H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$$

— *band insulator*: E_F between conduction and valence bands

— *superconductor*: band structure of Bogoliubov quasiparticles



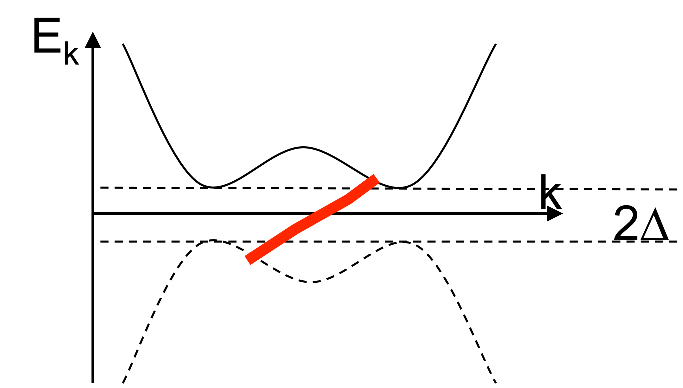
- **Topological equivalence:**

> Two band structures are equivalent if they can be continuously deformed into one another without closing the energy gap and without breaking the **symmetries** of the band structure.

▹ symmetries to consider:

— particle-hole symmetry, time-reversal symmetry

— reflection symmetry, rotation symmetry, etc.



▹ top. equivalence classes distinguished by:

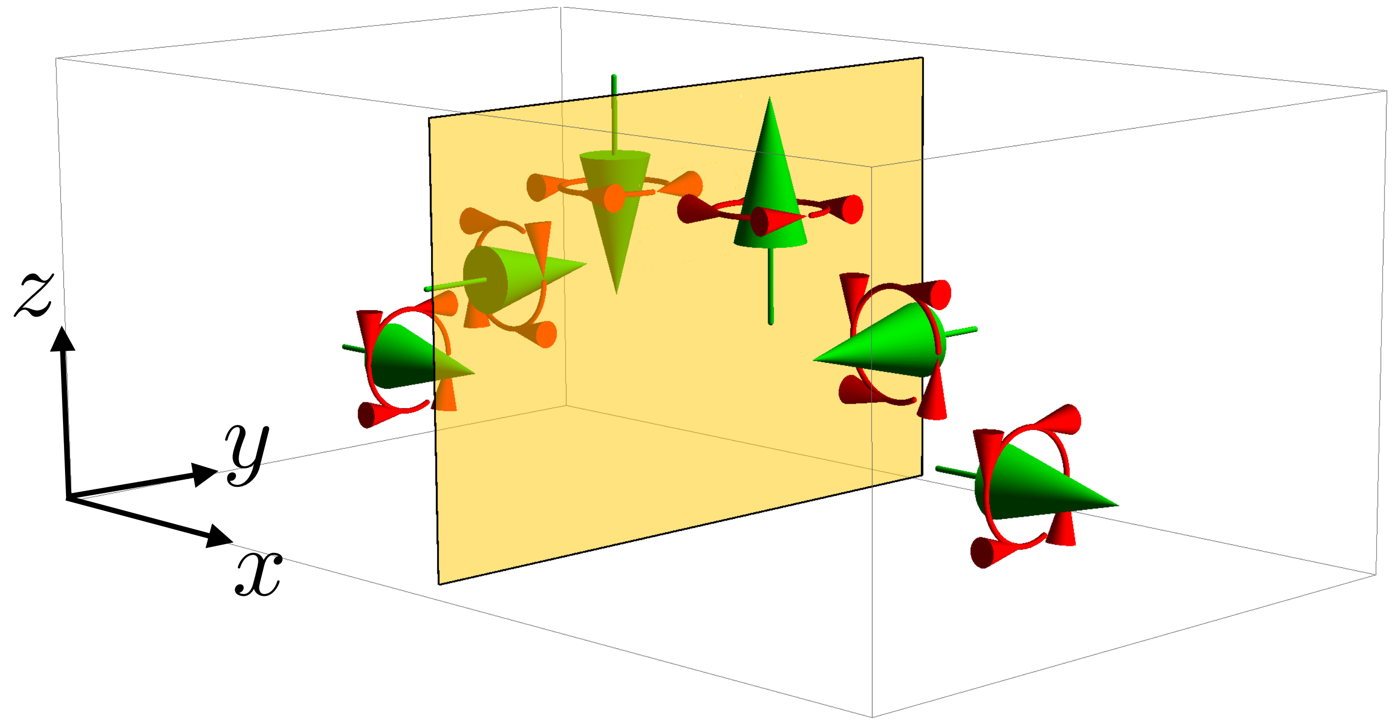
Berry curvature

topological invariant (e.g. Chern no): $n_{\mathbb{Z}} = \dfrac{i}{2\pi}\displaystyle\int_{\substack{\text{filled}\\\text{states}}} \mathcal{F}\, d\mathbf{k} \in \mathbb{Z}$

- **Bulk-boundary correspondence:**

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

Reflection symmetry



- Consider reflection R: $x \to -x$

$$\boxed{\begin{array}{l} R^{-1}\mathcal{H}(-k_x,k_y,k_z)R = \mathcal{H}(k_x,k_y,k_z) \\ \text{with} \quad R = s_x \end{array}}$$

— w.l.o.g.: eigenvalues of $R \in \{-1,+1\}$

Teo, Fu, Kane PRB '08

- **mirror Chern number:**

$$k_x = 0 \implies \mathcal{H}(0,k_y,k_z)R - R\mathcal{H}(0,k_y,k_z) = 0$$

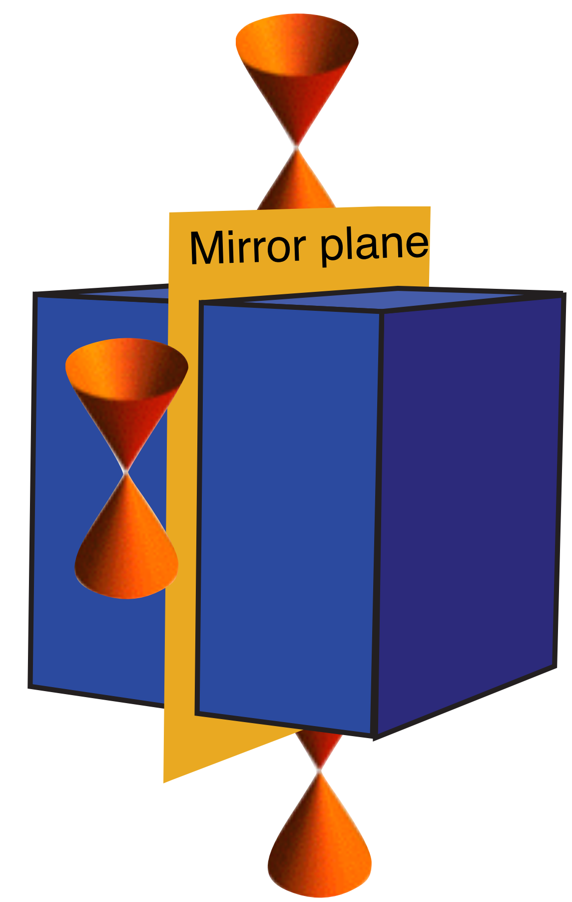
— project $\mathcal{H}(0,k_y,k_z)$ onto eigenspaces of R: $\boxed{\mathcal{H}_\pm(k_y,k_z)}$

$$n^\pm_{\mathcal{M}} = \frac{1}{4\pi}\int_{\text{2D BZ}} \mathcal{F}_\pm \, d^2\mathbf{k}$$

Berry curvature in $\pm$ eigenspace

— total Chern number: $n_{\mathcal{M}} = n^+_{\mathcal{M}} + n^-_{\mathcal{M}}$

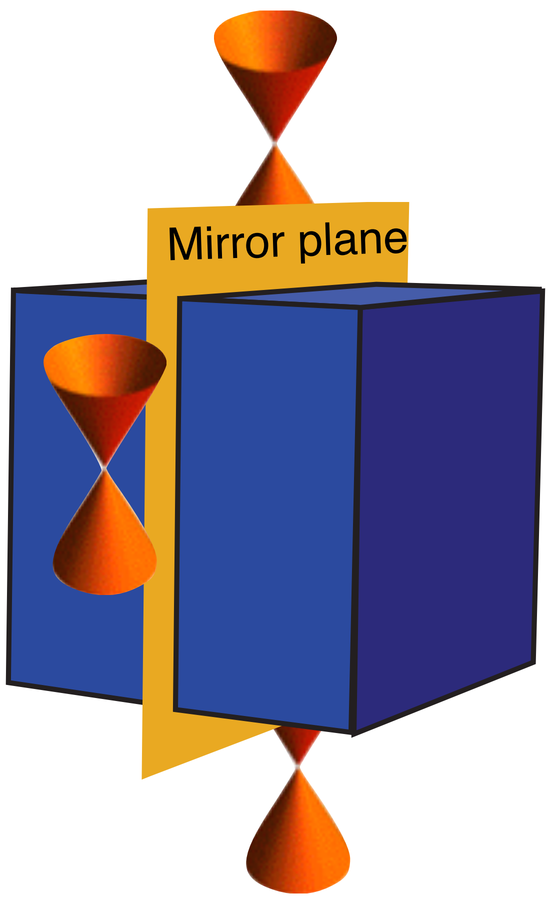
— mirror Chern number: $n_{\mathcal{M}} = n^+_{\mathcal{M}} - n^-_{\mathcal{M}}$



- Bulk-boundary correspondence:

— zero-energy states on surfaces that are left invariant under the mirror symmetry

2. Classification of topological insulators and superconductors with reflection symmetry



Global symmetries: Ten symmetry classes

— Non-spatial symmetries: symmetries that act *locally* in real space

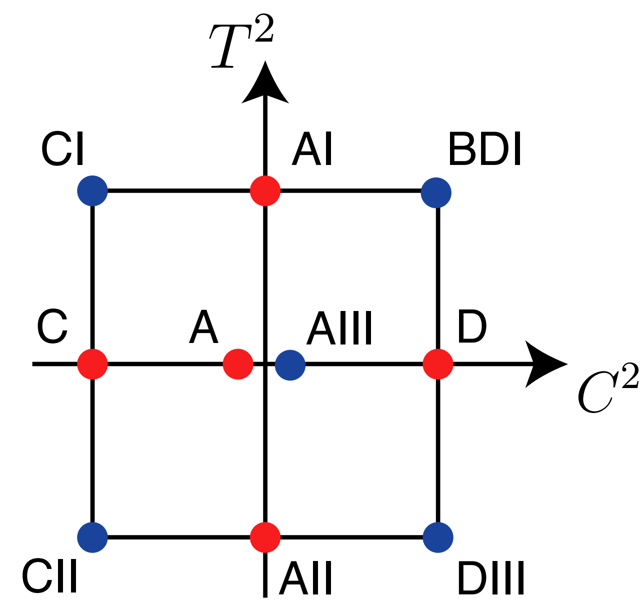
- time-reversal: $T\mathcal{H}(\mathbf{k})T^{-1} = +\mathcal{H}(-\mathbf{k});$ $\quad T^2 = \pm 1$
- particle-hole: $C\mathcal{H}(\mathbf{k})C^{-1} = -\mathcal{H}(-\mathbf{k});$ $\quad C^2 = \pm 1$
- sublattice: $S\mathcal{H}(\mathbf{k})S^{-1} = -\mathcal{H}(\mathbf{k});$ $\quad S \propto TP$

ten symmetry classes

Altland-Zirnbauer Random Matrix Classes

Class	Symmetry T	C	S
A	0	0	0
AIII	0	0	1
AI	1	0	0
BDI	1	1	1
D	0	1	0
DIII	-1	1	1
AII	-1	0	0
CII	-1	-1	1
C	0	-1	0
CI	1	-1	1

"Bott clock"



Classification of reflection symmetry protected topological materials

Reflection symmetry **+** non-spatial symmetries (TRS, PHS, SLS)

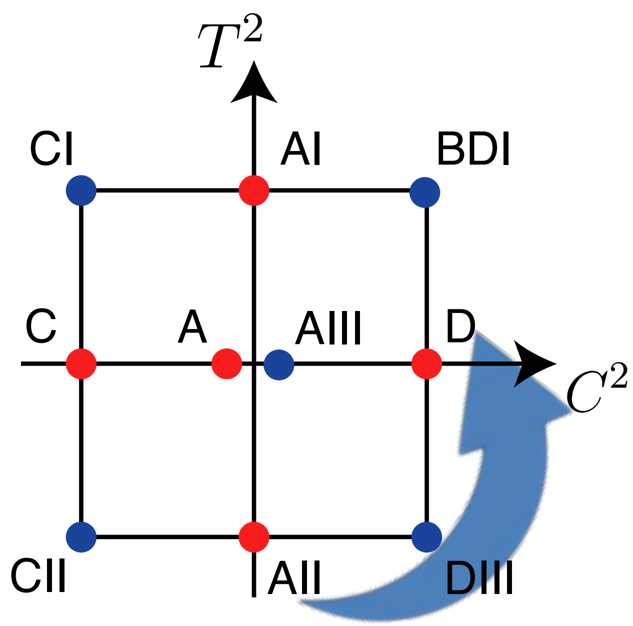
▶ Symmetries of $\mathcal{H}_{\pm}(k_y, k_z)$:

(i) $R_+ \ : \ R$ commutes with T $(C$ or $S)$

➡ same symmetries as full Hamiltonian $\mathcal{H}(\mathbf{k})$

(ii) $R_- \ : \ R$ anti-commutes with T $(C$ or $S)$

➡ effective symmetry class shifts by two on "Bott clock"



▶ Classification of reflection symmetric topological materials depends on:

- whether R commutes or anti-commutes with TRS, PHS, SLS

$\Rightarrow$ **27 symmetry classes**

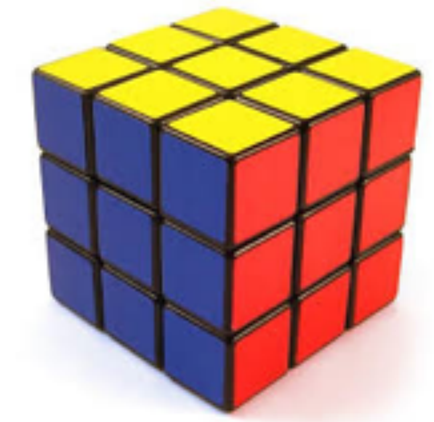
27 classes

R	A
R_+	AIII
R_-	AIII
R_+,R_{++}	AI BDI D DIII AII CII C CI
R_-,R_{--}	AI BDI D DIII AII CII C CI
R_{-+}	BDI, CII
R_{+-}	DIII, CI
R_{+-}	BDI
R_{-+}	DIII
R_{+-}	CII
R_{-+}	CI

Classification of reflection symmetry protected topological insulators and superconductors

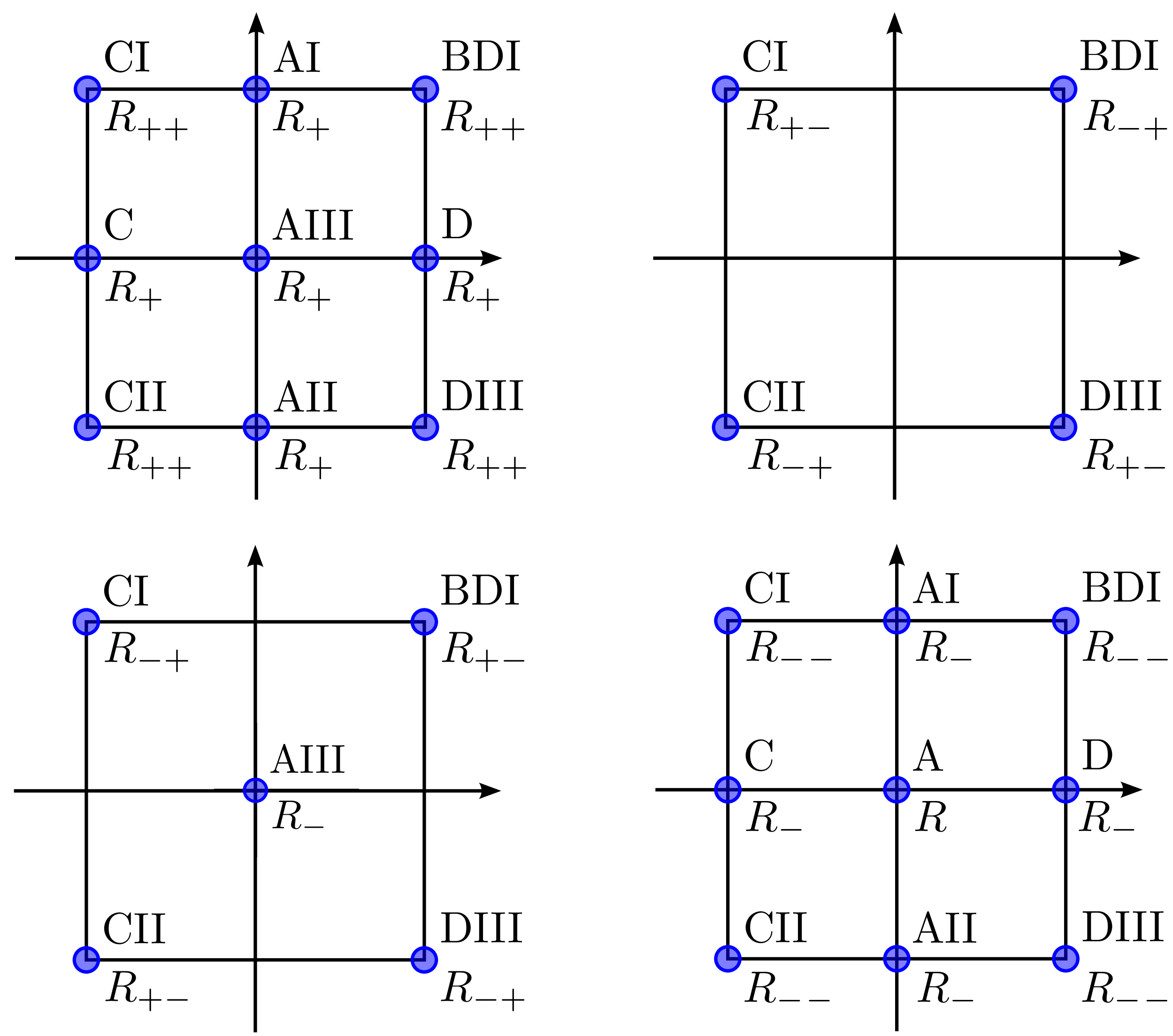
R_+ : R commutes with T (C or S)

R_- : R anti-commutes with T (C or S)



Reflection	sym. class
R	A
R_+	AIII
R_-	AIII
R_+,R_{++}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_-,R_{--}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_{-+}	BDI, CII
R_{+-}	DIII, CI
R_{+-}	BDI
R_{-+}	DIII
R_{+-}	CII
R_{-+}	CI

"Bott cube"



Chiu, Yao, Ryu, PRB 2013; Morimoto, Furusaki PRB 2013; Chiu, Schnyder PRB 2014;

Classification of reflection symmetry protected topological insulators and superconductors

R_+ : R commutes with T (C or S)
R_- : R anti-commutes with T (C or S)

Reflection	sym. class
R	A
R_+	AIII
R_-	AIII
R_+,R_{++}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_-,R_{--}	AI
	BDI
	D
	DIII
	AII
	CII
	C
	CI
R_{-+}	BDI, CII
R_{+-}	DIII, CI
R_{+-}	BDI
R_{-+}	DIII
R_{+-}	CII
R_{-+}	CI

For which symmetry class and dimension is there a topological insulator/superconductor protected by reflection symmetry?

Chiu, Yao, Ryu, PRB 2013; Morimoto, Furusaki PRB 2013; Chiu, Schnyder PRB 2014;

Symmetries and Dirac Hamiltonians

Dirac Hamiltonian in spatial dimension d : $\mathcal{H}(k) = \sum_{i=1}^{d} k_i \gamma_i + m\gamma_0$ $\quad E_{\pm} = \pm\sqrt{m^2 + \sum_{i=1}^{d} k_i^d}$

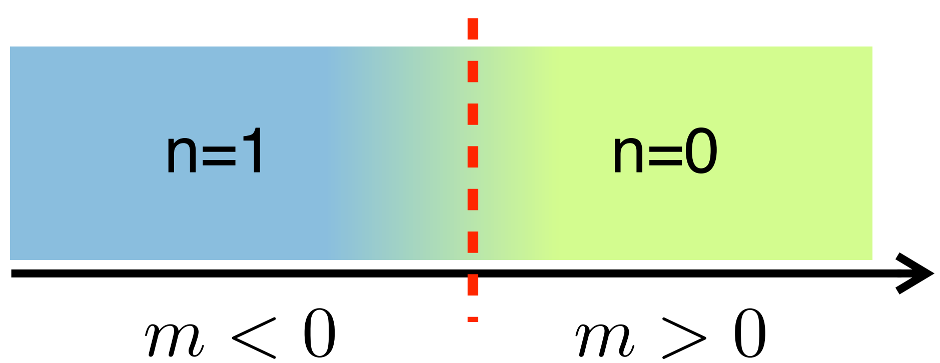
- Gamma matrices γ_i obey: $\{\gamma_i, \gamma_j\} = 2\delta_{ij} \qquad i = 0, 1, \dots, d$

- TRS, PHS, chiral symmetry and reflection ($k_1 \rightarrow -k_1$) lead to the conditions:

$$[\gamma_0, T] = 0 \qquad \{\gamma_{i\neq 0}, T\} = 0 \qquad \{\gamma_i, S\} = 0 \qquad \{\gamma_1, R\} = 0$$

$$\{\gamma_0, C\} = 0 \qquad [\gamma_{i\neq 0}, C] = 0 \qquad [\gamma_{i\neq 1}, R] = 0$$

- Topological phase transition as a function of mass term $m\gamma_0$



? are there *extra symmetry preserving* mass terms $M\gamma_{d+1}$ that connect the two phases without gap closing?

$$\{\gamma_{d+1}, \gamma_i\} = 0 \quad i = 0, 1, \cdots 2 \qquad E_{\pm} = \pm\sqrt{m^2 + M^2 + \sum_{i=1}^{d} k_i^d}$$

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

Classification of reflection symmetry protected topological insulators and superconductors

R_+ : R commutes with T (C or S)

R_- : R anti-commutes with T (C or S)

Reflection	sym. class	d=1	d=2	$\boxed{d=3}$	d=4	d=5	d=6	d=7	d=8
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	[illegible]	[illegible]	[illegible]	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	[illegible]	[illegible]	[illegible]	$T\mathbb{Z}_2$
	$\boxed{\text{AII}}$	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$\boxed{M\mathbb{Z}}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0

SnTe, Ca_3PbO, Sr_3PbO

Chiu, Yao, Ryu, PRB 2013; Morimoto, Furusaki PRB 2013

SnTe is a reflection symmetry protected TI

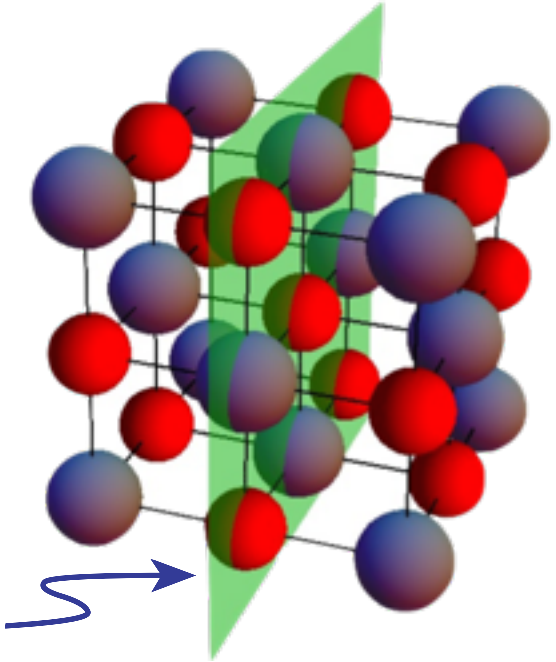
- Effective low-energy Hamiltonian:

Hsieh, Fu, et al. 2012

Tanaka, Ando, et al., 2012, 2013

$$\mathcal{H} = \varepsilon(\mathbf{k})\sigma_z + v(\sin k_x s_y - \sin k_y s_x) \otimes \sigma_x + v_z \sin k_z \sigma_y$$

$(s_i : \text{ spin}; \quad \sigma_i : \text{ orbitals})$



Reflection plane

- Symmetries:

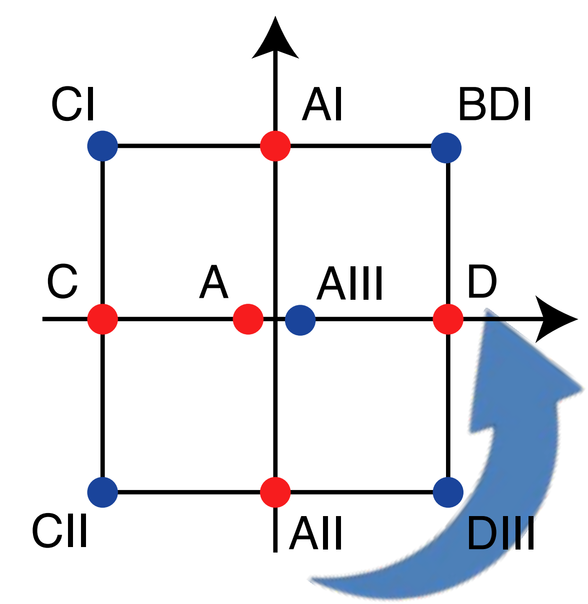
– Time-reversal: $T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k}) \qquad T = i s_y \mathcal{K} \qquad T^2 = -1$ (class AII)

– Reflection ($x \to -x$): $R^{-1}\mathcal{H}(-k_x, k_y, k_z)R = \mathcal{H}(k_x, k_y, k_z) \qquad \text{with } R = s_x$

– project $\mathcal{H}(\mathbf{k})$ onto *eigenspaces of* R: (i.e., $s_x = \pm 1$)

$$\mathcal{H}_\pm(k_y, k_z) = \varepsilon_{\mathbf{k}}\sigma_z \mp v \sin k_y \sigma_x + v_z \sin k_z \sigma_y = \mathbf{m}_\pm(\mathbf{k}) \cdot \vec{\sigma}$$

R anti-commutes with T: $TRT^{-1} = -R \qquad R_-$



class AII → class D

Particle-hole symmetry: $C^{-1}\mathcal{H}_\pm(-\mathbf{k})C = -\mathcal{H}_\pm(-\mathbf{k}) \qquad \text{with } C = \sigma_x \mathcal{K}$

SnTe is a reflection symmetry protected TI

Tanaka, Ando, et al., Nat. Phys. 2012, 2013

- Effective Hamiltonian within mirror plane:

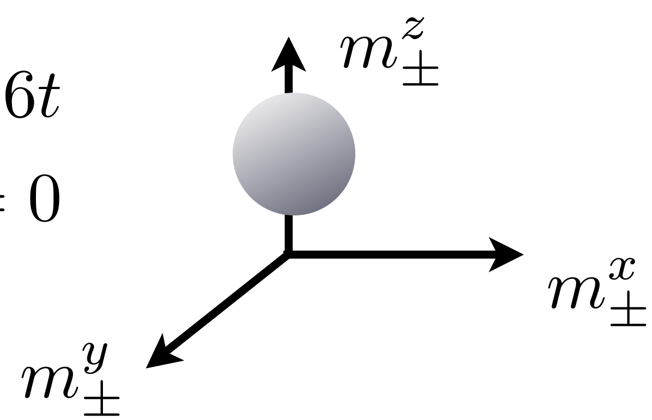
$$\mathcal{H}_{\pm}(k_y, k_z) = \varepsilon_{\mathbf{k}} \sigma_z \mp v \sin k_y \sigma_x + v_z \sin k_z \sigma_y = \mathbf{m}_{\pm}(\mathbf{k}) \cdot \vec{\sigma}$$

$$E = \pm |\mathbf{m}_{\pm}(\mathbf{k})| \qquad \hat{\mathbf{m}}_{\pm} = \frac{\mathbf{m}_{\pm}(\mathbf{k})}{|\mathbf{m}_{\pm}(\mathbf{k})|}$$

trivial phase

$|\mu| > 6t$

$n_{\pm} = 0$

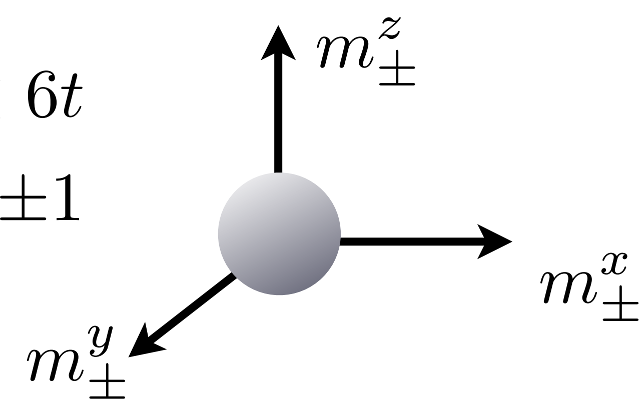


no surface states

non-trivial phase

$|\mu| < 6t$

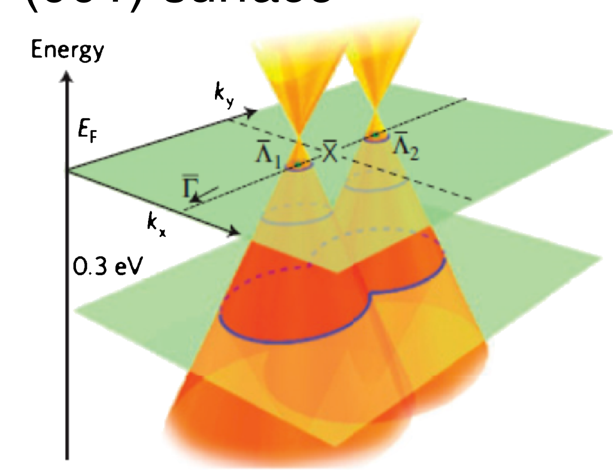
$n_{\pm} = \pm 1$



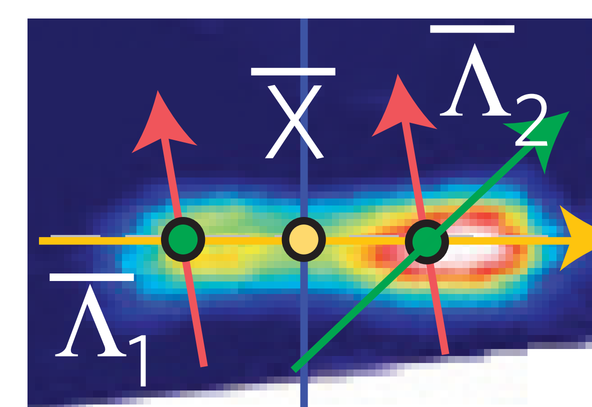
two pairs of surface states

$$\Longrightarrow \quad n_{\pm} = \frac{1}{8\pi} \int_{\text{2D BZ}} d^2\mathbf{k}\, \epsilon^{\mu\nu} \underbrace{\hat{\mathbf{m}}_{\pm} \cdot \left[\partial_{k_\mu} \hat{\mathbf{m}}_{\pm} \times \partial_{k_\nu} \hat{\mathbf{m}}_{\pm} \right]}_{\text{Berry curvature}}$$

(001) surface



ARPES on SnTe



- **Mirror Chern number:** $n_{\mathcal{M}} = (n_+ - n_-)$
- **Bulk-boundary correspondence:**

  $|n_{\mathcal{M}}| = \#$ Dirac cone surface states

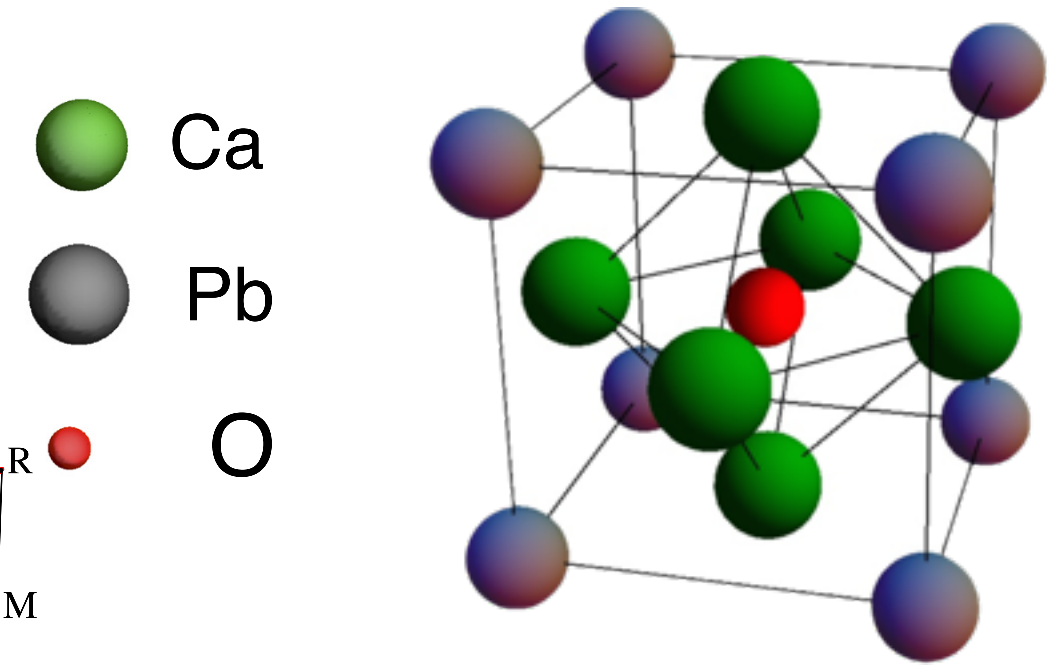
  for SnTe: $n_{\mathcal{M}} = 2$

Ca_3PbO is a reflection symmetry protected TI

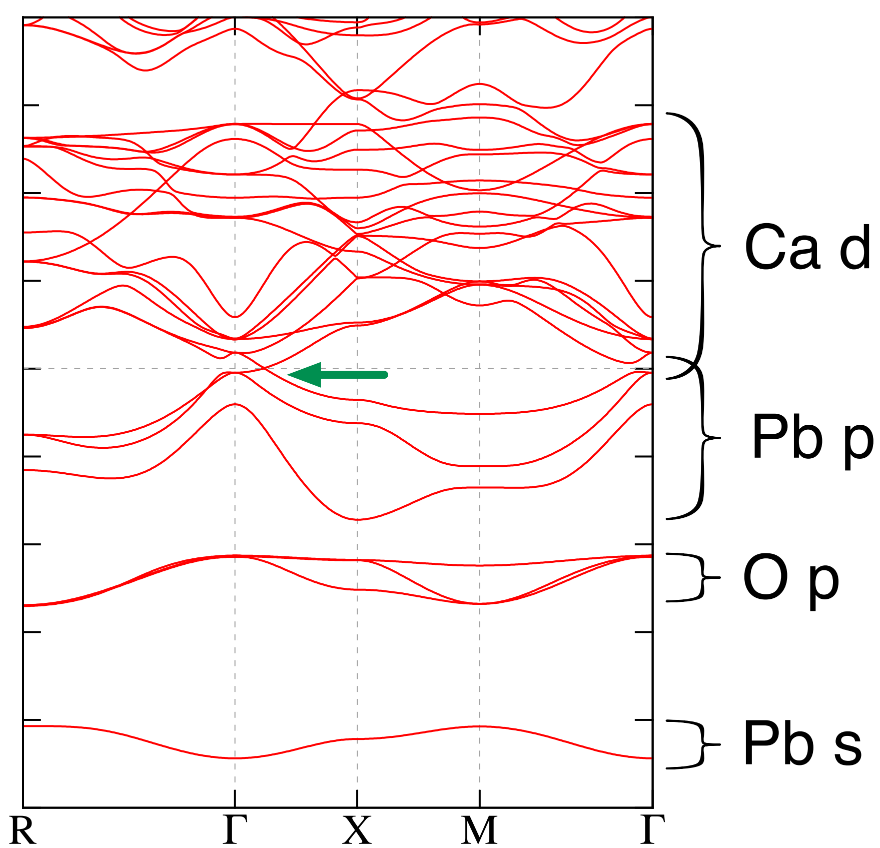
- Anti-perovskites: Ca_3PbO, Sr_3PbO

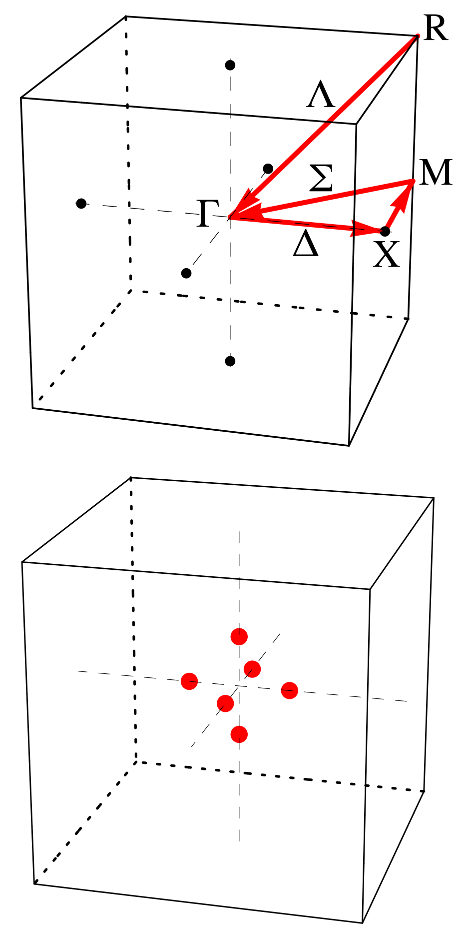
  Kariyado & Ogata JPSJ '12

  Hsieh, Fu et al., PRB '14



- Band structure (without SOC):





- Orbital character of bands:

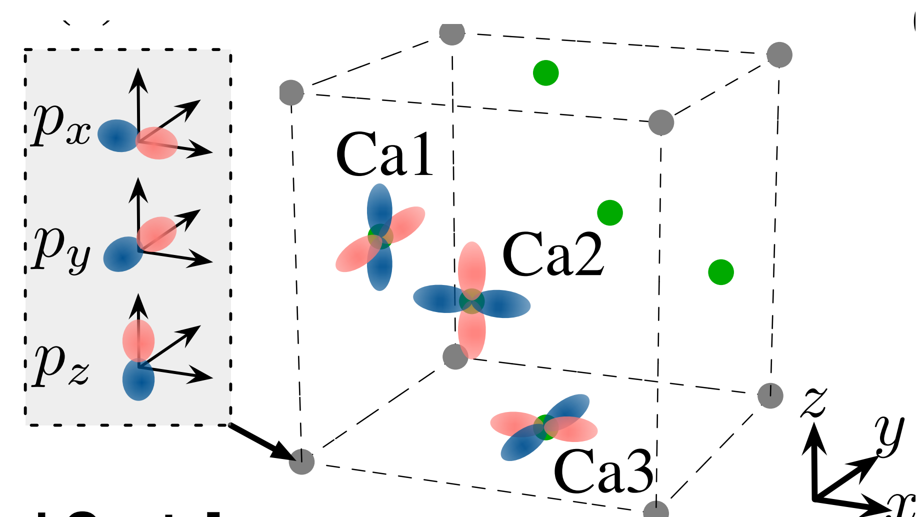
  Pb: $|p_x\rangle\,,|p_y\rangle\,,|p_z\rangle$

  Ca: $|d_{x^2-y^2}\rangle\,,|d_{x^2-z^2}\rangle\,,|d_{y^2-z^2}\rangle$

- Opening of bulk gap:

  hybridisation w/ Ca $|d_{xy}\rangle\,,|d_{xz}\rangle\,,|d_{yz}\rangle$

  + SOC opens up bulk gap of ~10 meV



[after Kariyado and Ogata]

Ca_3PbO is a reflection symmetry protected TI

- Anti-perovskites: Ca_3PbO, Sr_3PbO

  Kariyado & Ogata JPSJ '12

  Hsieh, Fu et al., PRB '14

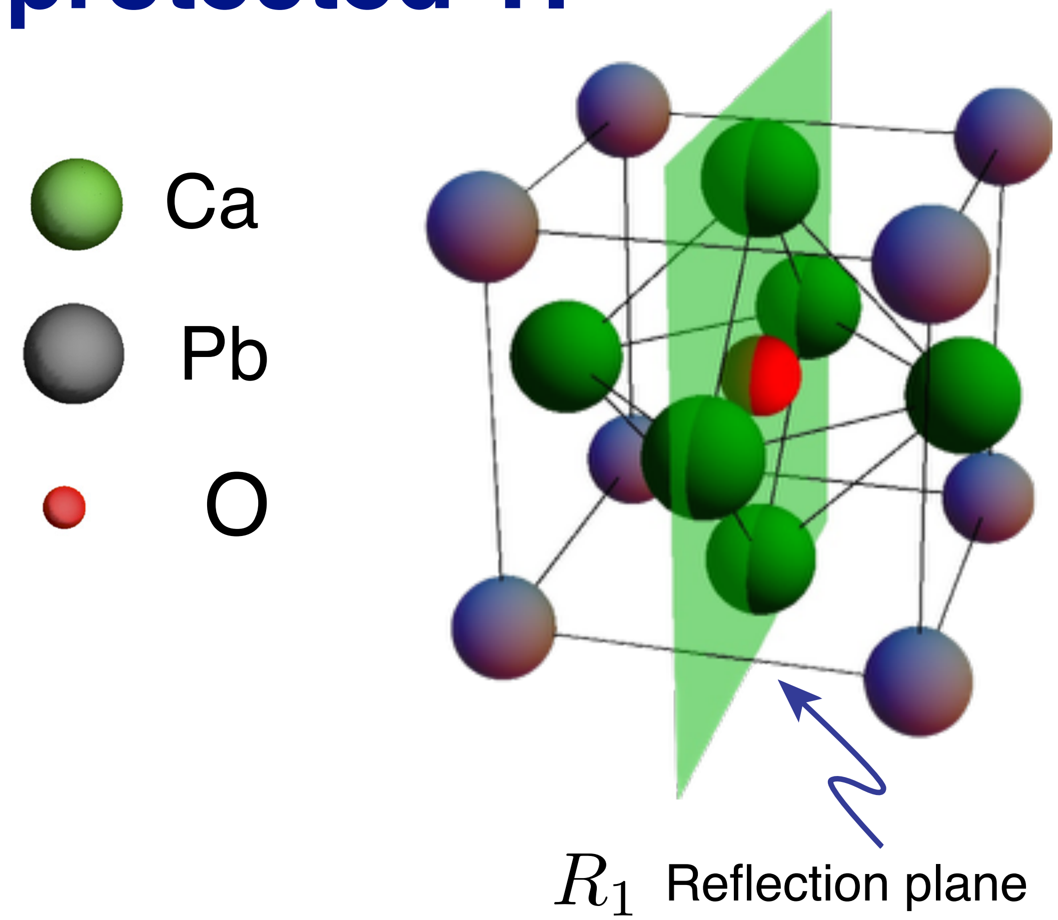
- Symmetries:

  – Time-reversal: $T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k})$

  $$T = is_y\mathcal{K} \qquad T^2 = -1$$

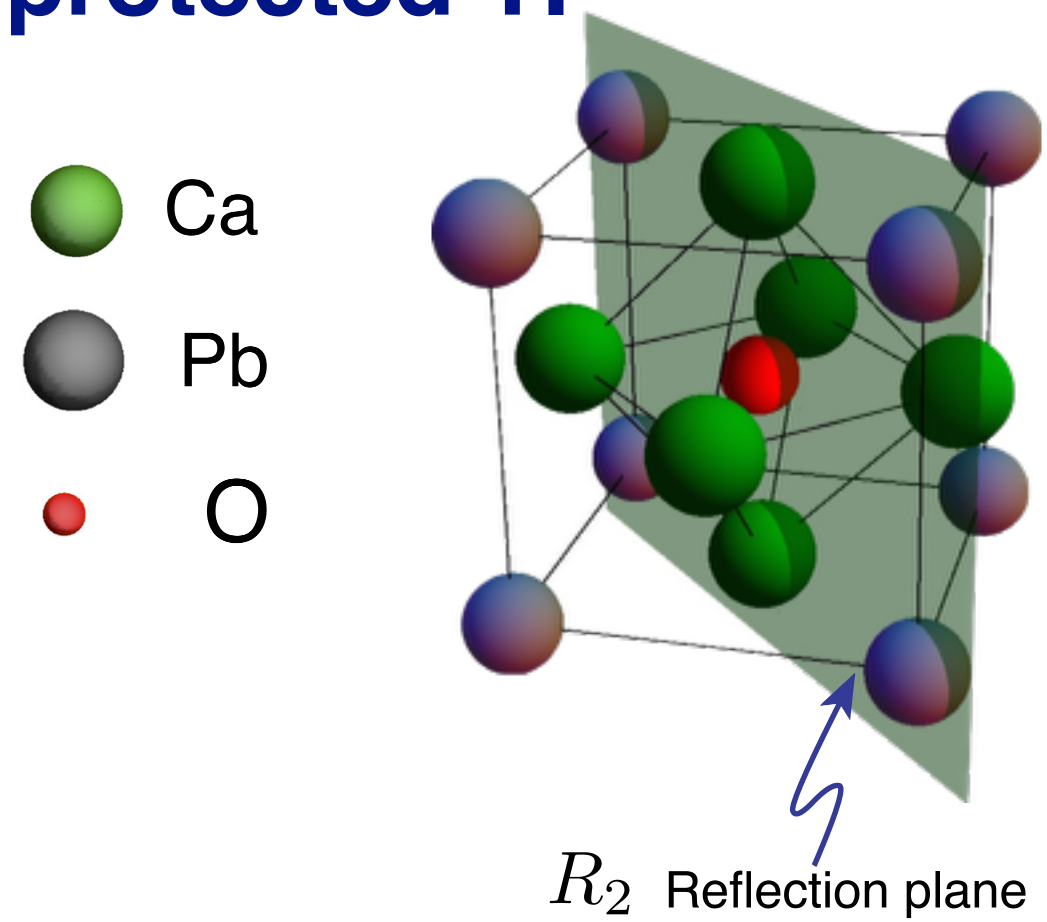
  – two reflection symmetries : R_1 and R_2

  $$R_1^{-1}\mathcal{H}(-k_x, k_y, k_z)R_1 = \mathcal{H}(k_x, k_y, k_z)$$



Chiu, Nohara, Chan, Schnyder, in preparation

Ca_3PbO is a reflection symmetry protected TI



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- Symmetries:

  – Time-reversal: $T^{-1}\mathcal{H}(-\mathbf{k})T = +\mathcal{H}(\mathbf{k})$

  $$T = i s_y \mathcal{K} \qquad T^2 = -1$$

  – two reflection symmetries : R_1 and R_2

  $$R_1^{-1}\mathcal{H}(-k_x, k_y, k_z)R_1 = \mathcal{H}(k_x, k_y, k_z)$$

  $$R_2^{-1}\mathcal{H}(-k_y, -k_x, k_z)R_2 = \mathcal{H}(k_x, k_y, k_z)$$

  R_j anti-commutes with T: $TR_jT^{-1} = -R_j$ $\quad R_-$

- Topological invariants:

  – two mirror Chern numbers: $n_{\mathcal{M}_1}, n_{\mathcal{M}_2}$

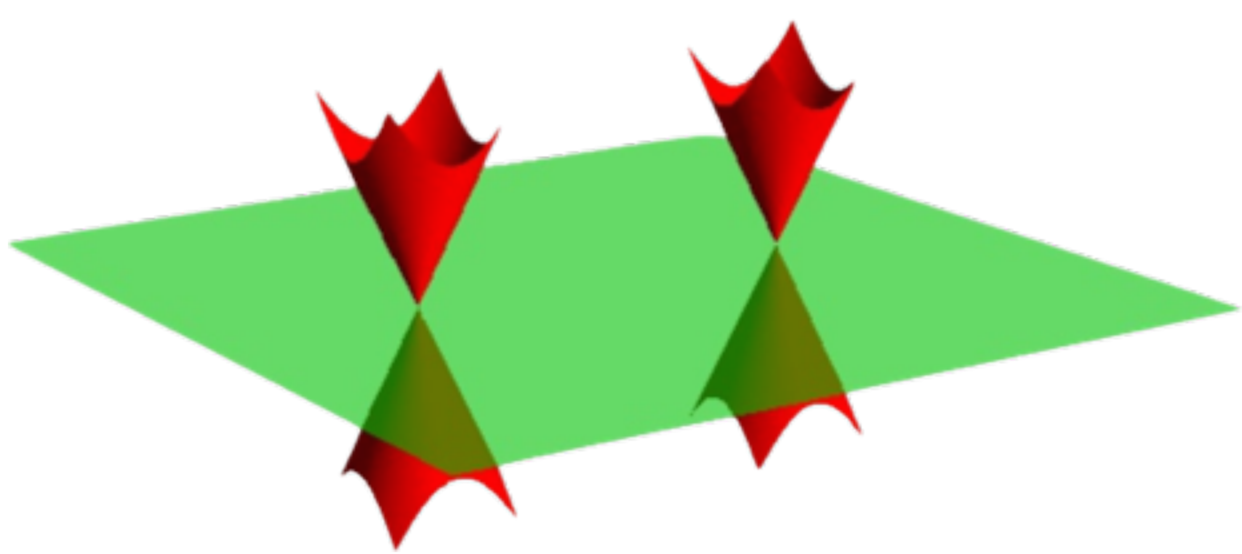
  – for Ca_3PbO, Sr_3PbO: $n_{\mathcal{M}_1} = -2, \; n_{\mathcal{M}_2} = +2$

  $\Longrightarrow 2 \times 2$ Dirac cone surface states

Chiu, Nohara, Chan, Schnyder, in preparation

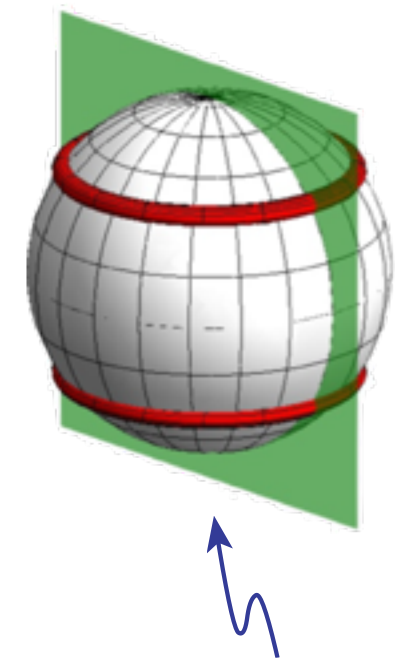
3. Reflection symmetry protected topological semimetals and nodal superconductors

A Fermi surface in a semimetal (or a nodal line in a superconductor) is topologically stable if there does not exist any **symmetry** preserving mass term that opens up a full gap in the spectrum.



Reflection symmetry protected topological semimetals and nodal SCs

? How about topology of reflection symmetric semimetals and nodal superconductors?

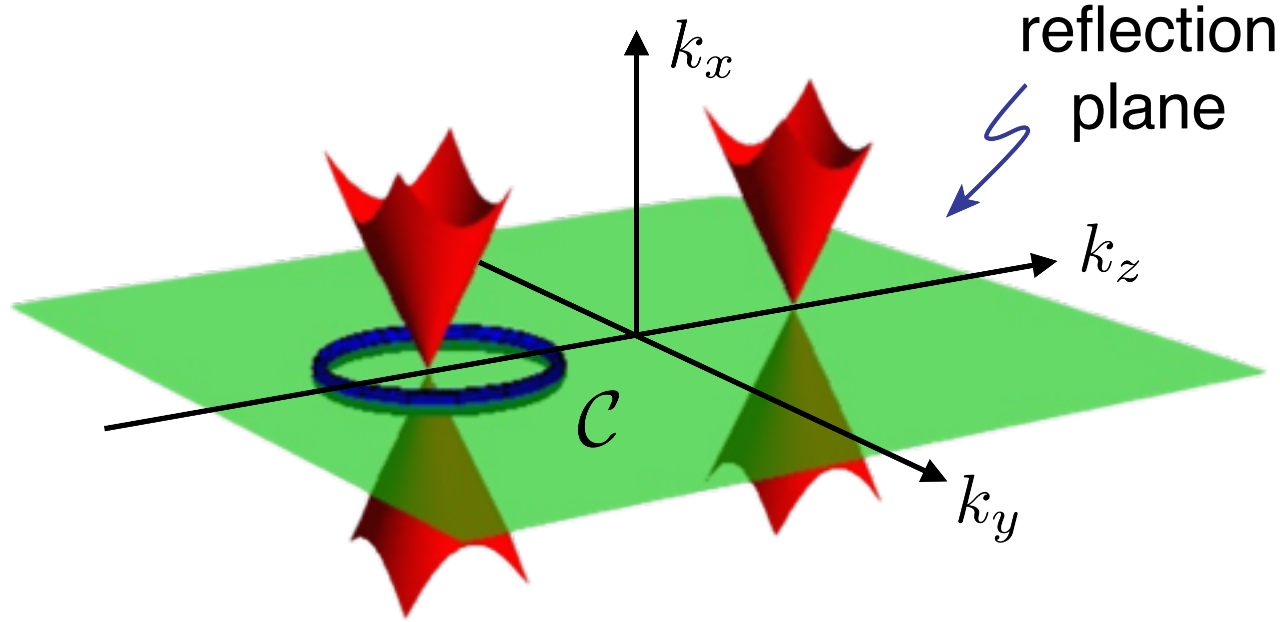


▶ Problem: Global topological number ill-defined (no gap!)

Solution: (assume translational symmetry)

⟹ Define **momentum-dependent topological number**

$$\boxed{W^{\pm}_{\mathcal{C}} = \frac{1}{2\pi} \oint_{\mathcal{C}} \omega_{\pm}(\mathbf{k}) dk_l}$$



$\mathcal{C}$ *does* enclose Fermi point

$$W^{\pm}_{\mathcal{C}} = \pm 1 \quad \Rightarrow \text{topologically stable}$$

Classification of reflection symmetric semimetals and nodal SCs

Reflection symmetry **+** global symmetries (TRS, PHS, SLS)

Chiu, Schnyder, PRB 2014

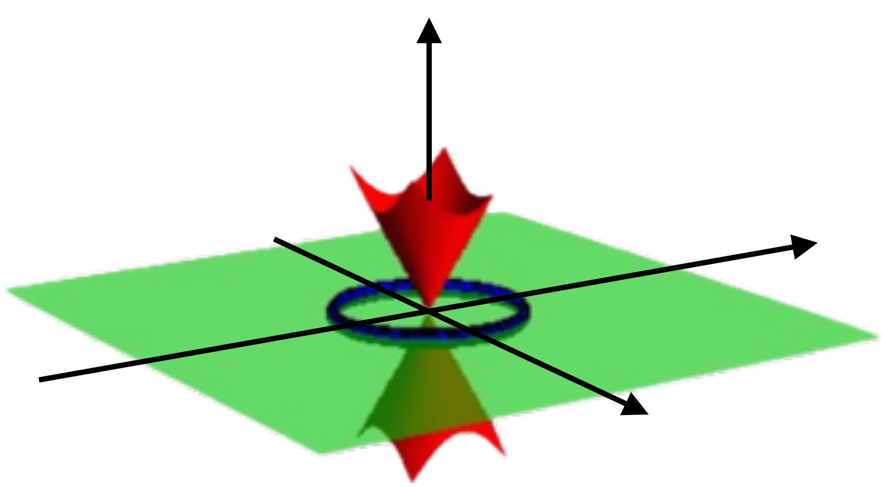
▶ Classification of reflection symmetric topological semimetals and superconductors depends on:

- whether R commutes or anti-commutes with TRS, PHS, SLS

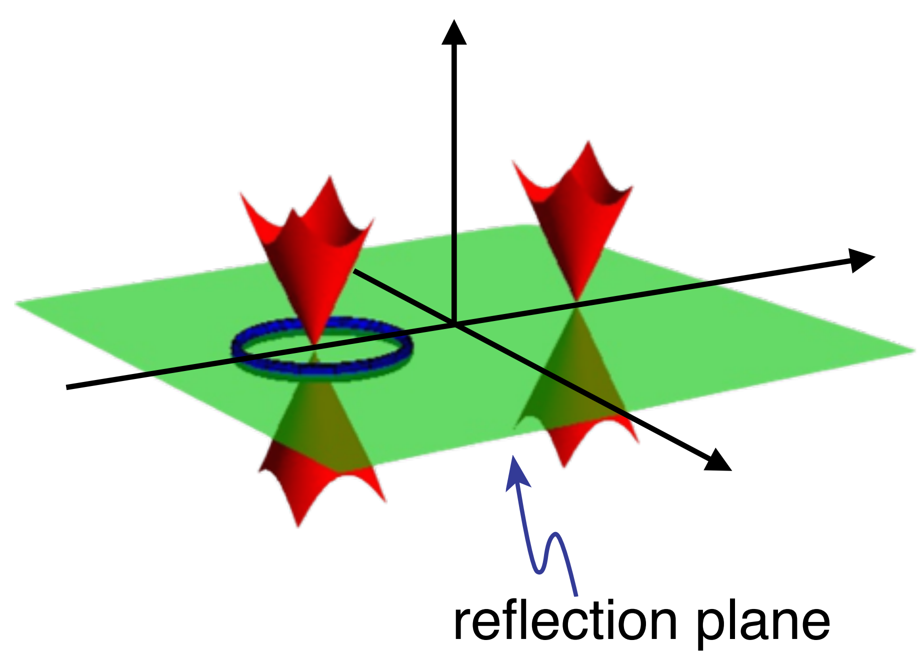
  $\Rightarrow$ **27 symmetry classes**

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

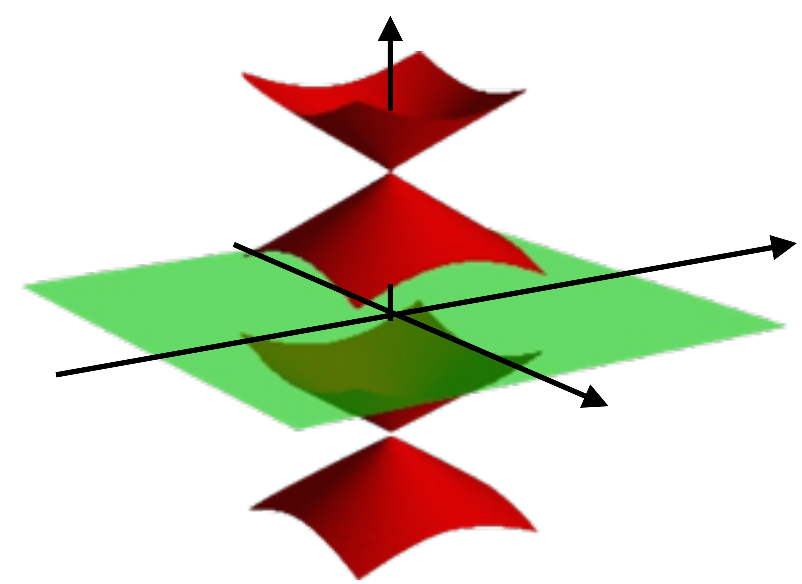
(i) Fermi surface is invariant under reflection and global symmetries



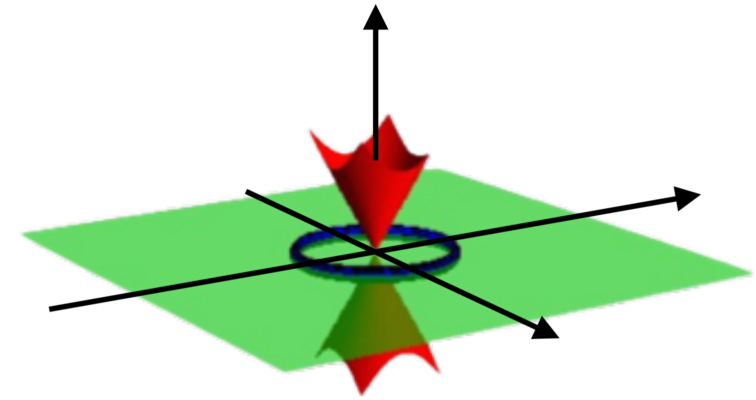
(ii) Fermi surface is only invariant under reflection



(iii) Fermi surface is not invariant under reflection & global sym.



Gapless Dirac Hamiltonians



(i) Nodal point is *invariant* under non-spatial symmetries

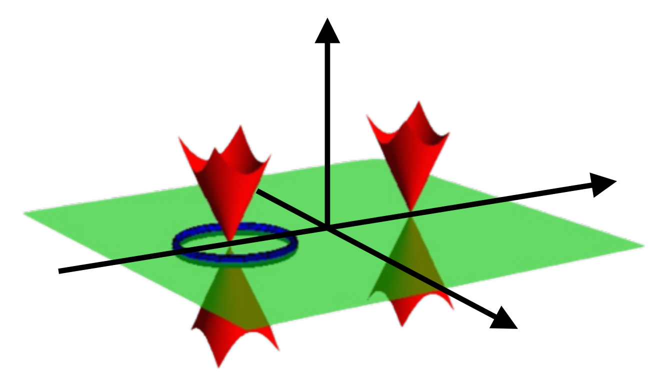
$$\mathcal{H}(k) = \sum_{i=1}^{d} k_i \gamma_i \qquad E_{\pm} = \pm\sqrt{\sum_{i=1}^{d} k_i^2}$$

? are there *symmetry preserving* mass terms $M\gamma_{d+1}$ that open up a gap in the spectrum?

$$\{\gamma_{d+1}, \gamma_i\} = 0 \quad i = 0, 1, \cdots 2 \qquad E_{\pm} = \pm\sqrt{M^2 + \sum_{i=1}^{d} k_i^2}$$

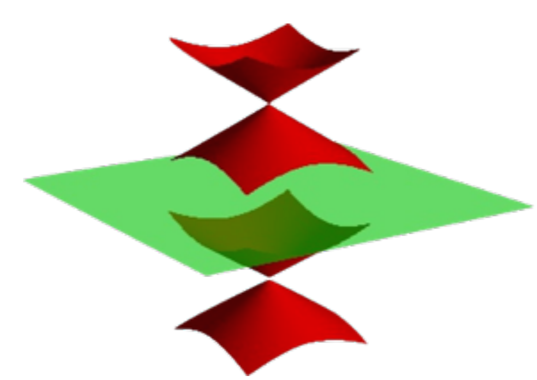
NO: topologically non-trivial **YES:** topologically trivial

– to distinguish between $\mathbb{Z}_2$ and $\mathbb{Z}$ classification consider doubled version of Hamiltonian



(ii) & **(iii)** Nodal points *pairwise related* by non-spatial symmetries

$$\mathcal{H}(k) = \sum_{i=1}^{p-1} \sin k_i \gamma_i + \left(1 - p + \sum_{i=1}^{p} \cos k_i\right)\gamma_0$$



– nodal superconductor with $(d-p)$-dimensional node

Classification of reflection symmetric semimetals and nodal SCs

Reflection symmetry **+** global symmetries (TRS, PHS, SLS)

Chiu, Schnyder, PRB 2014

▶ Classification of reflection symmetric topological semimetals and superconductors depends on:

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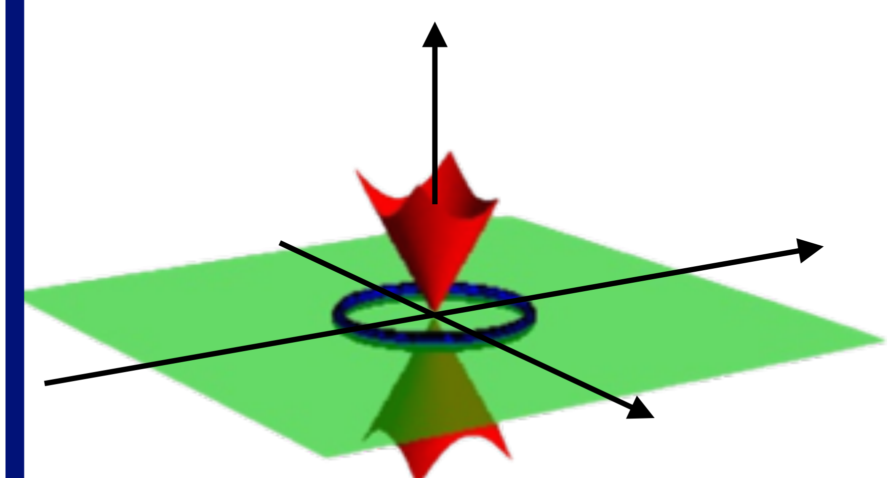
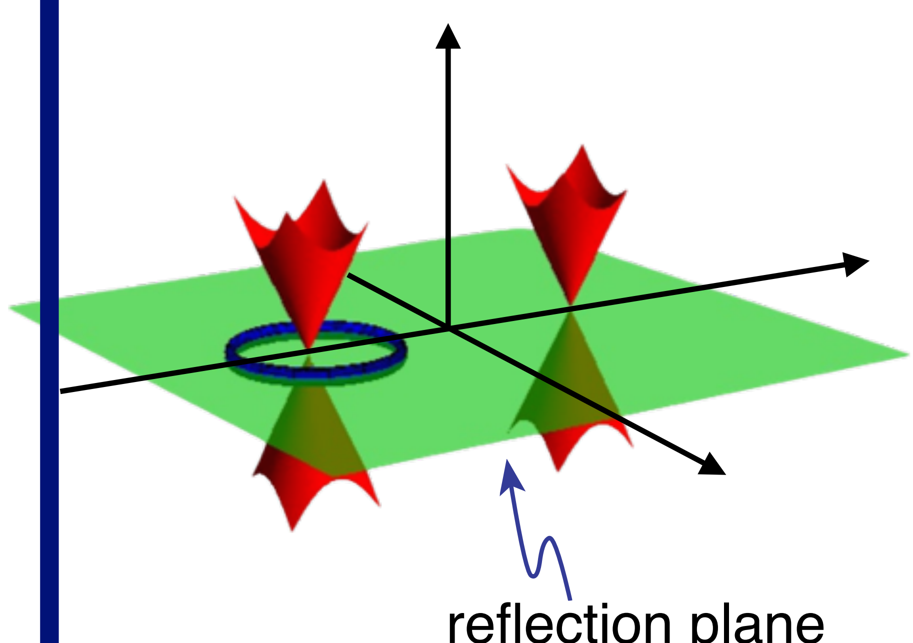
  $\Rightarrow$ **27 symmetry classes**

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

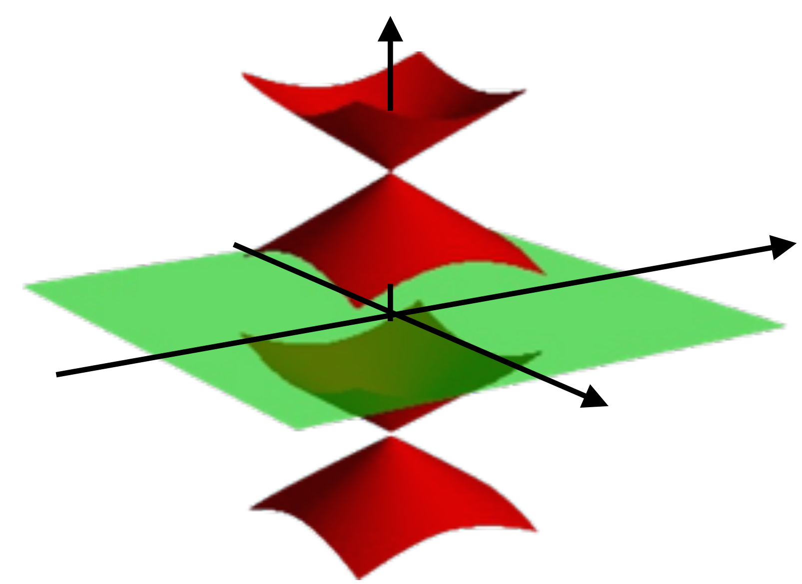
(i) Fermi surface is invariant under reflection and global symmetries



(ii) Fermi surface is only invariant under reflection



(iii) Fermi surface is not invariant under reflection & global sym.



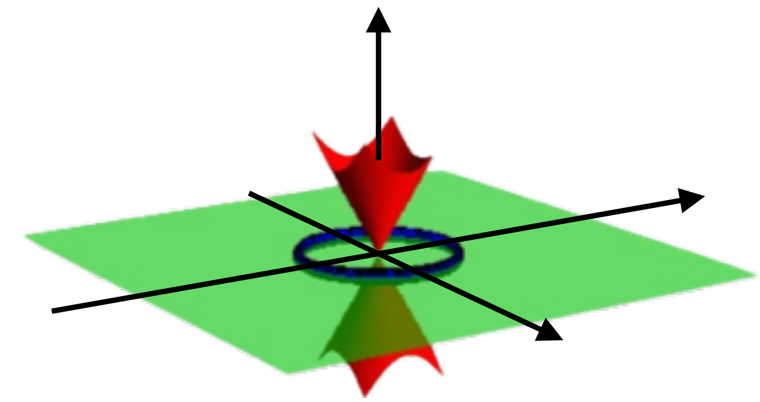
Classification of reflection symmetric semimetals and nodal SCs

(i) Fermi surface invariant under reflection and global symmetries

$$p = d - d_{\mathrm{FS}}$$

classification of *Fermi points* with $d_{\mathrm{FS}} = 0$ in **d** dimensions

classification of *fully gapped* topological materials in **d+1** dimensions



Reflection	sym. class	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	[illegible]	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0	[illegible]	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$
	AII	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z}\oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}_2\oplus\mathbb{Z}_2$	$M\mathbb{Z}\oplus\mathbb{Z}$	0

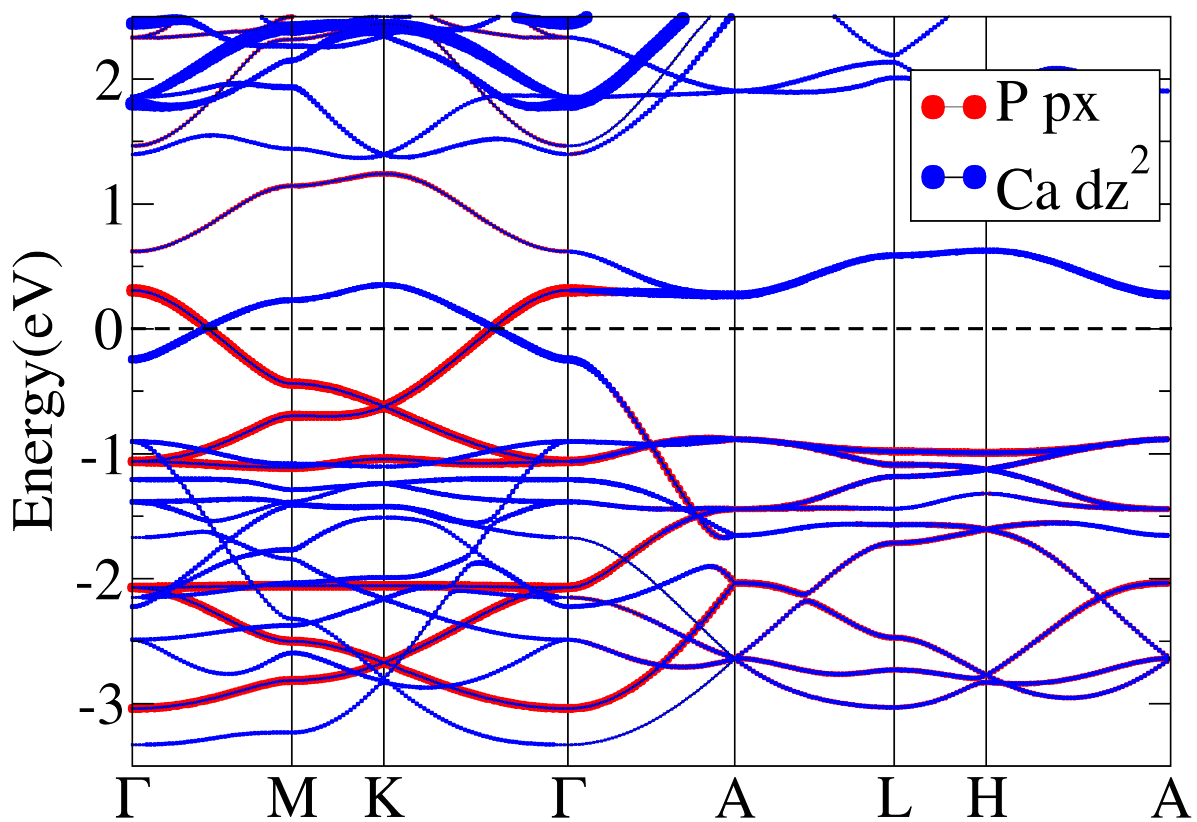
Ca_3P_2

Chiu, Schnyder PRB 90, 205136 (2014)

Topological nodal lines in Ca_3P_2

L. Xie, L. Schoop, R. Cava, *et. al.* , APL Mat. 3, 083602 (2015)

▶ Band structure:



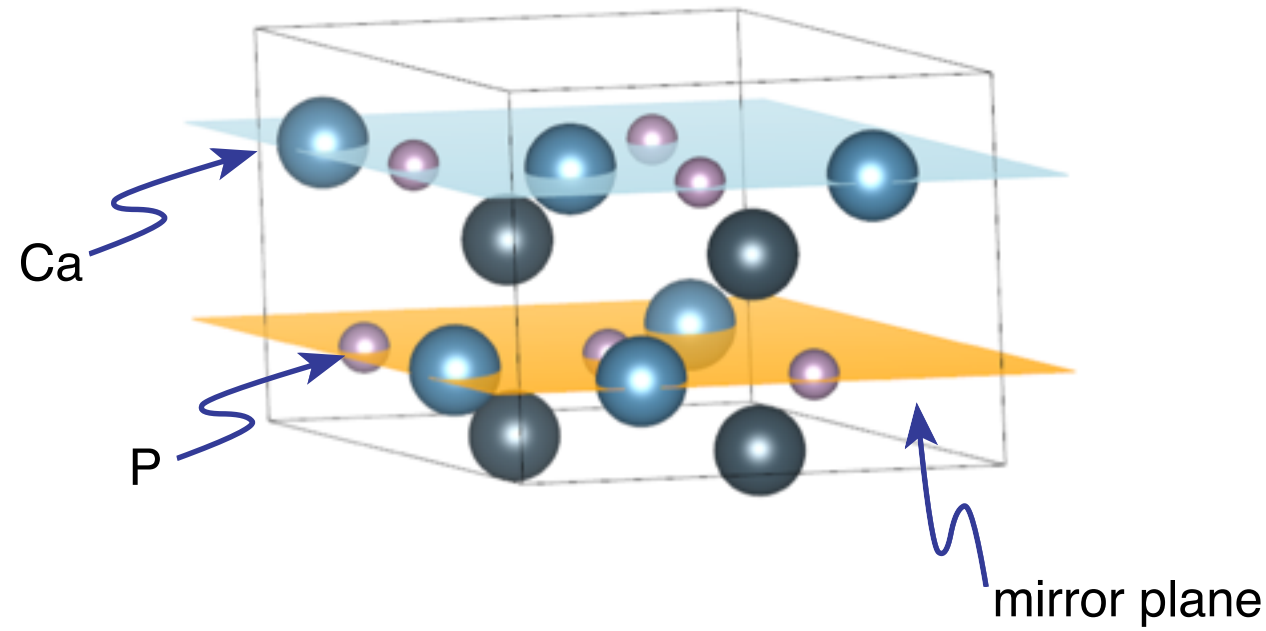
charge balanced: Ca^{2+} — P^{3-}

▶ Orbital character of bands near E_F:
(6 Ca atoms, 6 P atoms)

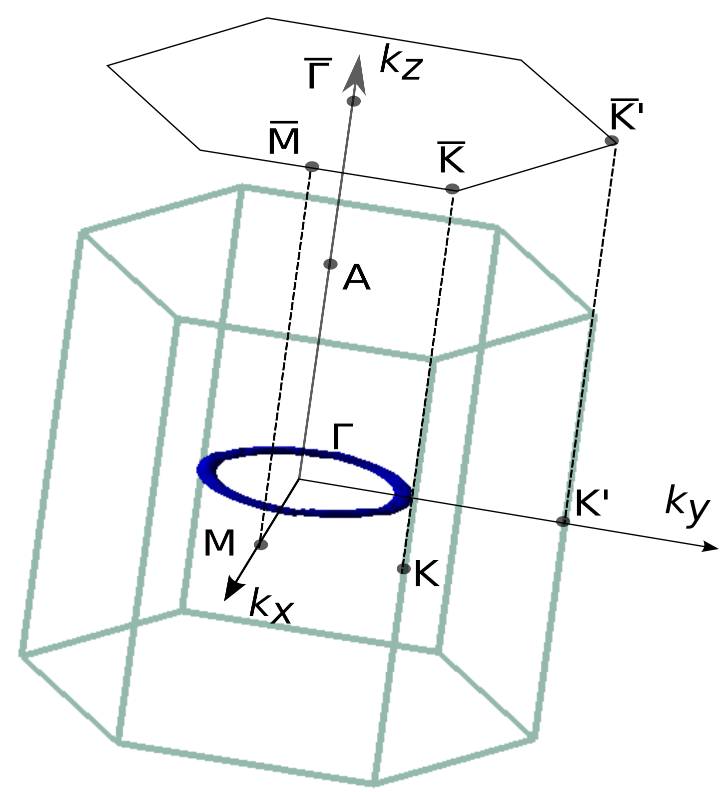
Ca: d_{z^2} orbitals from 6 Ca atoms

P: p_x orbitals from 6 P atoms

▶ Crystal structure $P6_3/mcm$



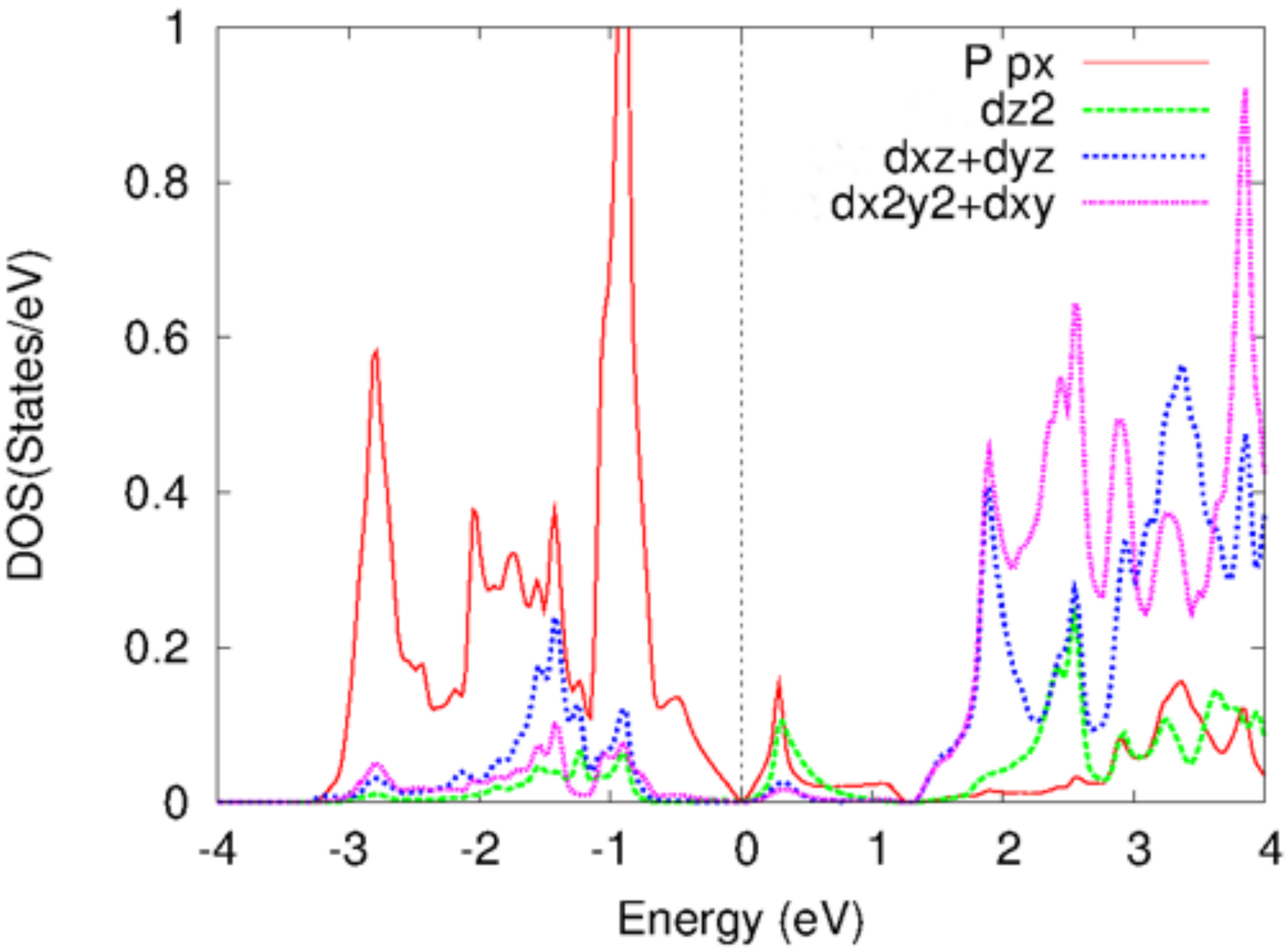
▶ Dirac ring within reflection plane

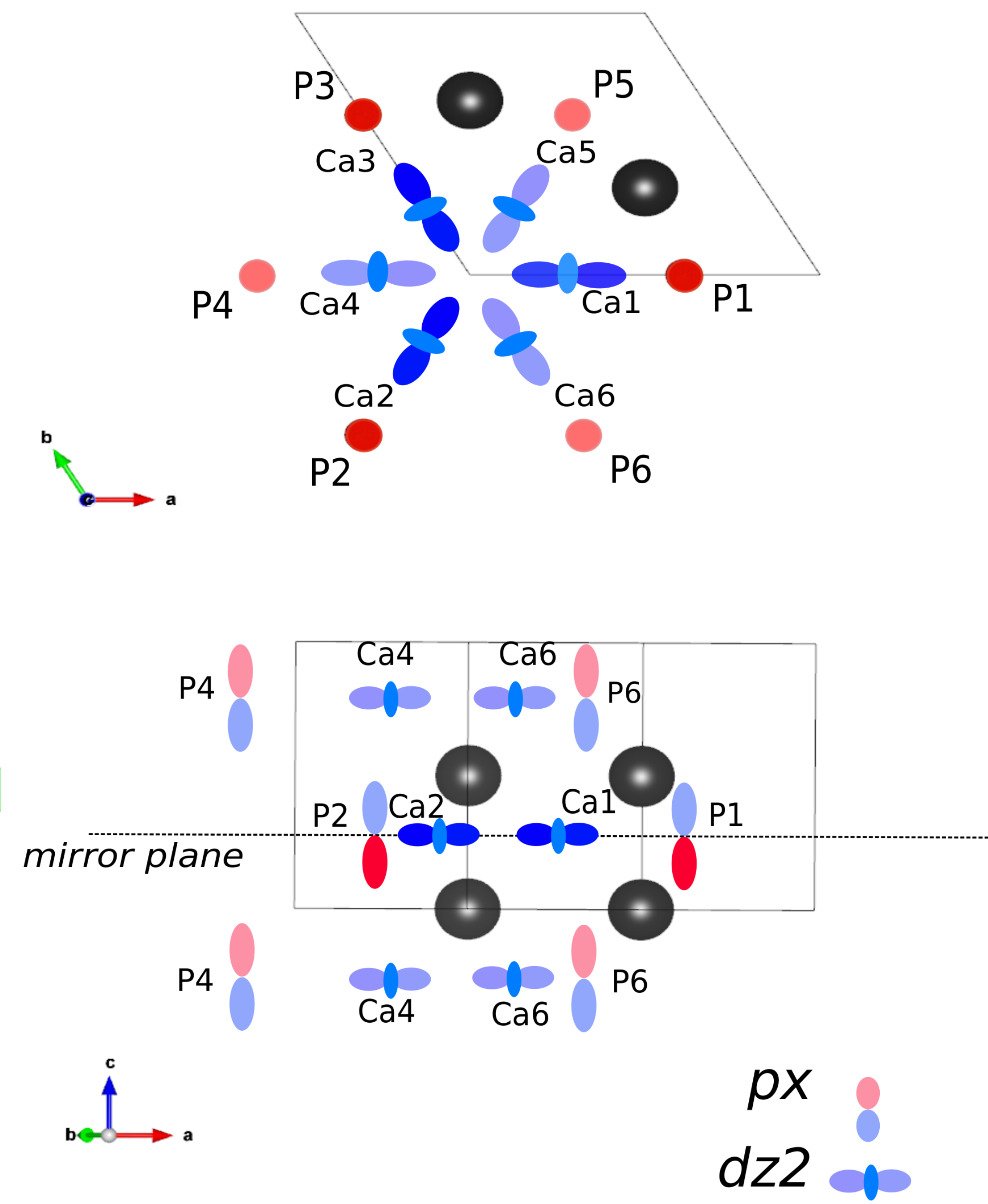


Topological nodal lines in Ca_3P_2

L. Xie, L. Schoop, R. Cava, *et. al.* , APL Mat. 3, 083602 (2015)

- Band structure:





- Orbital character of bands near E_F:
  (6 Ca atoms, 6 P atoms)

  Ca: d_{z^2} orbitals from 6 Ca atoms

  P: p_x orbitals from 6 P atoms

Tight-binding Hamiltonian for Ca_3P_2

- Tight-binding Hamiltonian

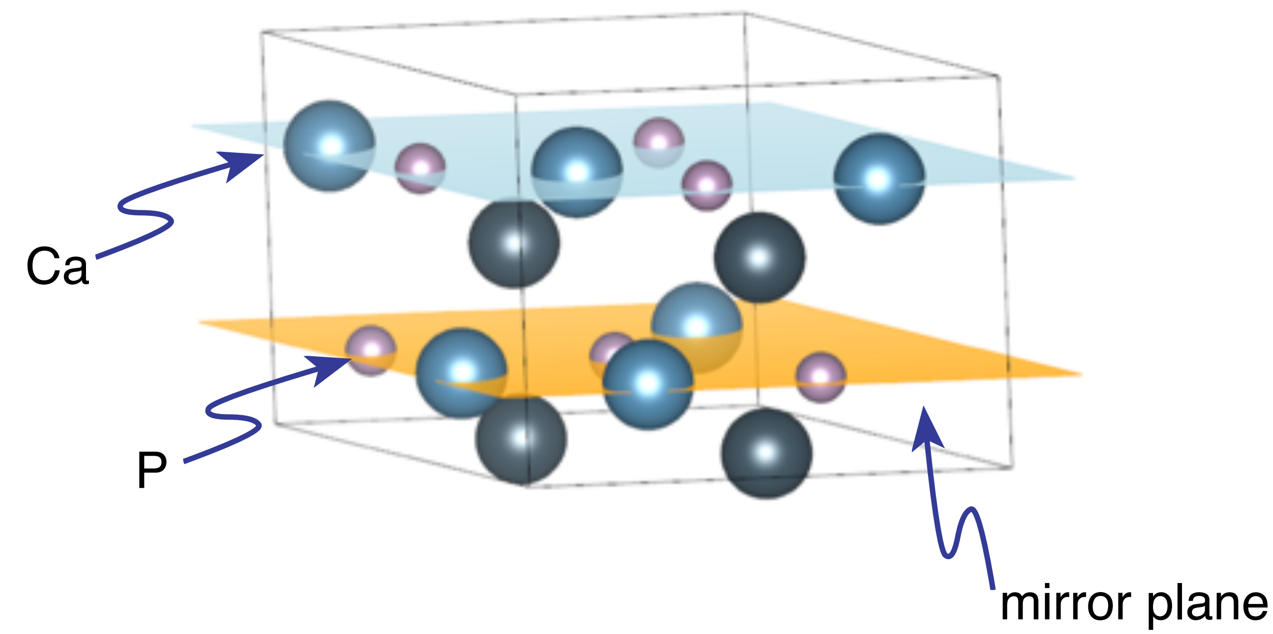
(SOC small, spin degree can be neglected)

Ca: d_{z^2} orbitals from 6 Ca atoms

P: p_x orbitals from 6 P atoms

$$H(\mathbf{k}) = \begin{pmatrix} \mathrm{H}_{\mathrm{CaCa}} & \mathrm{H}_{\mathrm{CaP}} \\ \mathrm{H}_{\mathrm{PCa}} & \mathrm{H}_{\mathrm{PP}} \end{pmatrix} \qquad H_{ij} = \begin{pmatrix} h_{ij}^{\mathrm{ll}} & h_{ij}^{\mathrm{lu}} \\ h_{ij}^{\mathrm{ul}} & h_{ij}^{\mathrm{uu}} \end{pmatrix}$$

- Crystal structure $P6_3/mcm$



- Symmetries:

– Time-reversal: $T = \mathbb{1}\mathcal{K} \qquad T^2 = +1 \qquad \Longrightarrow \text{class AI}$

– Reflection ($z \to -z$):

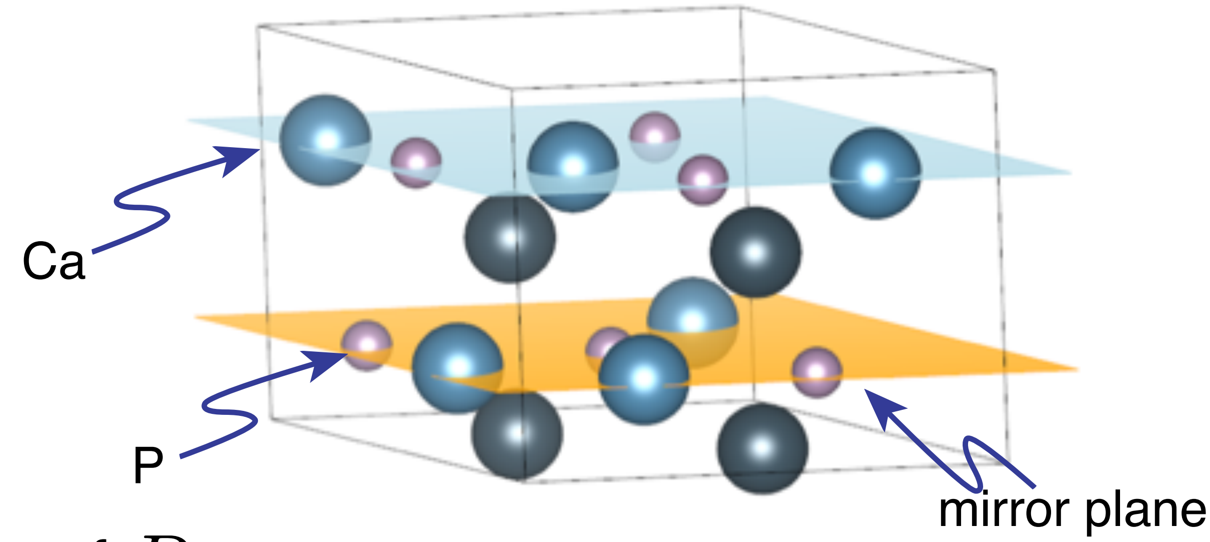
$$R^{-1}\mathcal{H}(k_x, k_y, -k_z)R = \mathcal{H}(k_x, k_y, k_z) \qquad R(\mathbf{k}) = \begin{pmatrix} 1_{3\times3} & 0 & 0 & 0 \\ 0 & 1_{3\times3}e^{-ik_z} & 0 & 0 \\ 0 & 0 & -1_{3\times3} & 0 \\ 0 & 0 & 0 & -1_{3\times3}e^{-ik_z} \end{pmatrix}$$

– Inversion ($\mathbf{r} \to -\mathbf{r}$):

$$I^{-1}H(-\mathbf{k})I = H(\mathbf{k}) \qquad I = \tau_0 \otimes \rho_x \otimes \mathbb{1}_{3\times3}$$

Chan, Chiu, Chou, Schnyder, arXiv:1510.02759

Topological nodal line: Mirror invariant



- **Reflection** $(z \to -z)$:

$$R^{-1}\mathcal{H}(k_x, k_y, -k_z)R = \mathcal{H}(k_x, k_y, k_z)$$

- within mirror planes $k_z = 0, \pi$: $[H, R] = 0$

— eigenstates of $\mathcal{H}$ are simultaneous eigenstates of R

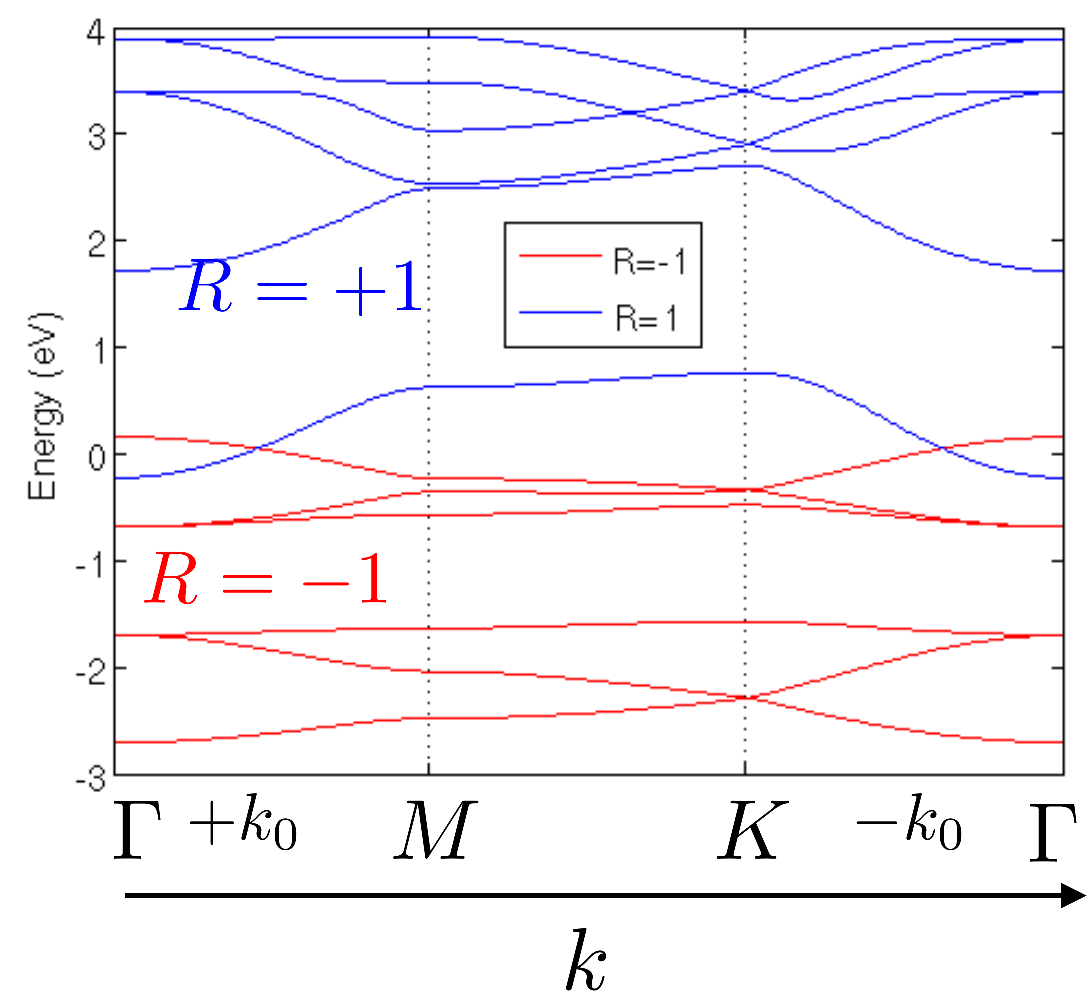
— eigenstates of $\mathcal{H}$ are in the eigenspace of either $R = +1$ or $R = -1$

- **Mirror invariant:**

— number of occupied states with $R = +1$

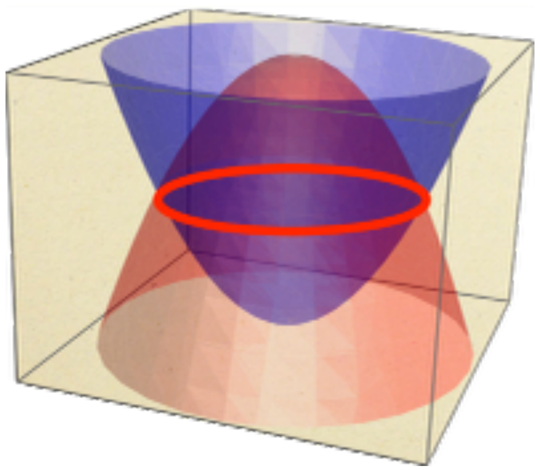
$$N^0_{M\mathbb{Z}} = n^{+,0}_{\text{occ}}(|k| > k_0) - n^{+,0}_{\text{occ}}(|k| < k_0)$$

$$n^{+,0}_{\text{occ}}(k) = \begin{cases} 1 & |k| < k_0 \\ 0 & |k| > k_0 \end{cases}$$



see also: Burkov, Hook, Balents PRB 11

Low-energy effective theory for Ca_3P_2



- low-energy effective Hamiltonian:

even in k

$$H_{\rm eff}(\mathbf{k}) = (k_{\parallel}^2 - k_0^2)\tau_z + k_z \tau_y + f(\mathbf{k})\tau_0$$

- symmetry operators:

— reflection: $R = \tau_z$ — time-reversal: $T = \tau_0 \mathcal{K}$ — inversion: $I = \tau_z$

- Gap-opening term τ_x is symmetry forbidden:

— breaks reflection symmetry: $R^{-1}\tau_x R = -\tau_x$

— breaks inversion + TRS: $(IT)^{-1}\tau_x IT = -\tau_x$

$\Rightarrow$ nodal line is stable

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

$$H_{\rm eff}(\mathbf{k}) \otimes \sigma_0 = (k_{\parallel}^2 - k_0^2)\tau_z \otimes \sigma_0 + k_z \tau_y \otimes \sigma_0 + f(\mathbf{k})\tau_0 \otimes \sigma_0$$

— consider gap opening term $\hat{m} = \tau_x \otimes \sigma_y$:

- (IT)-symmetric:

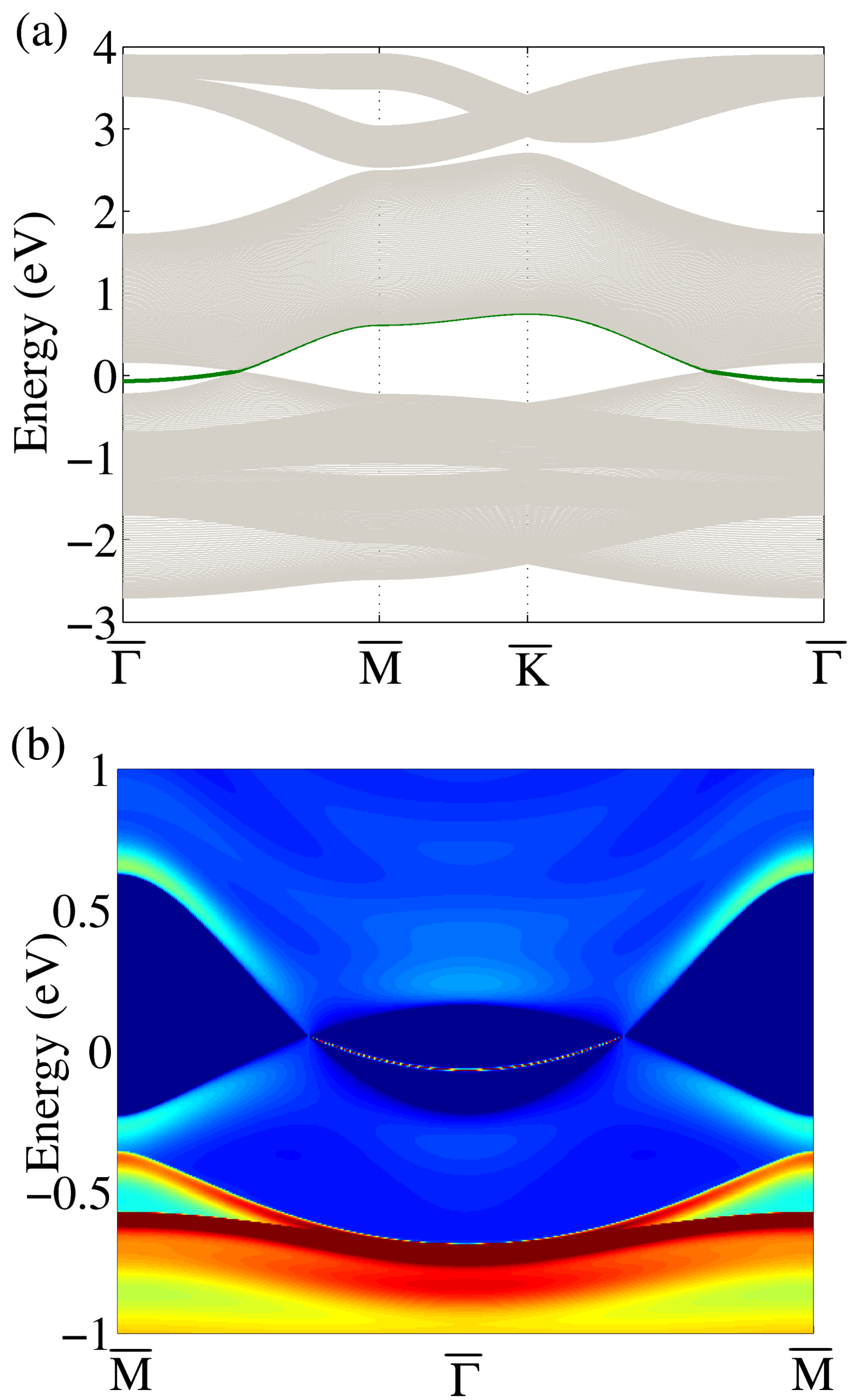
$$(\tau_z \otimes \sigma_0 \mathcal{K})^{-1} \hat{m} (\tau_z \otimes \sigma_0 \mathcal{K}) = \hat{m} \qquad \Rightarrow \mathbb{Z}_2 \text{ classification}$$

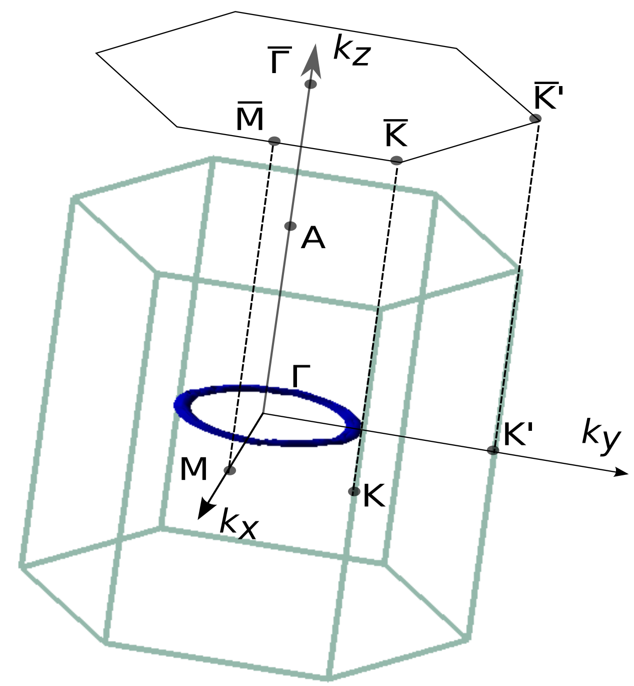
- but breaks R:

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

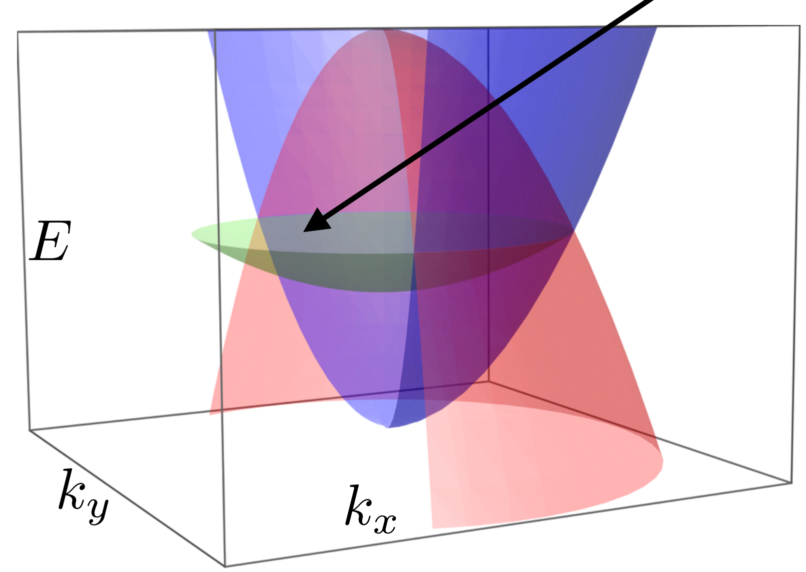
Drumhead surface state and Berry phase

- ▶ **Nearly flat surface states connecting Dirac ring**





Drumhead surface state



Chan, Chiu, Chou, Schnyder, arXiv:1510.02759

Drumhead surface state and Berry phase

▶ **Berry phase & charge polarization:**

$$\mathcal{P}(k_{\|}) = -i \sum_{j\in\text{filled}} \int_{-\pi}^{\pi} \left\langle u_{k_\perp}^{(j)} \middle| \partial k_\perp \middle| u_{k_\perp}^{(j)} \right\rangle dk_\perp$$

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

King-Smith and Vanderbilt PRB 93

— $\mathcal{P}(k_{\|}) \neq 0 \Rightarrow$ surface state

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

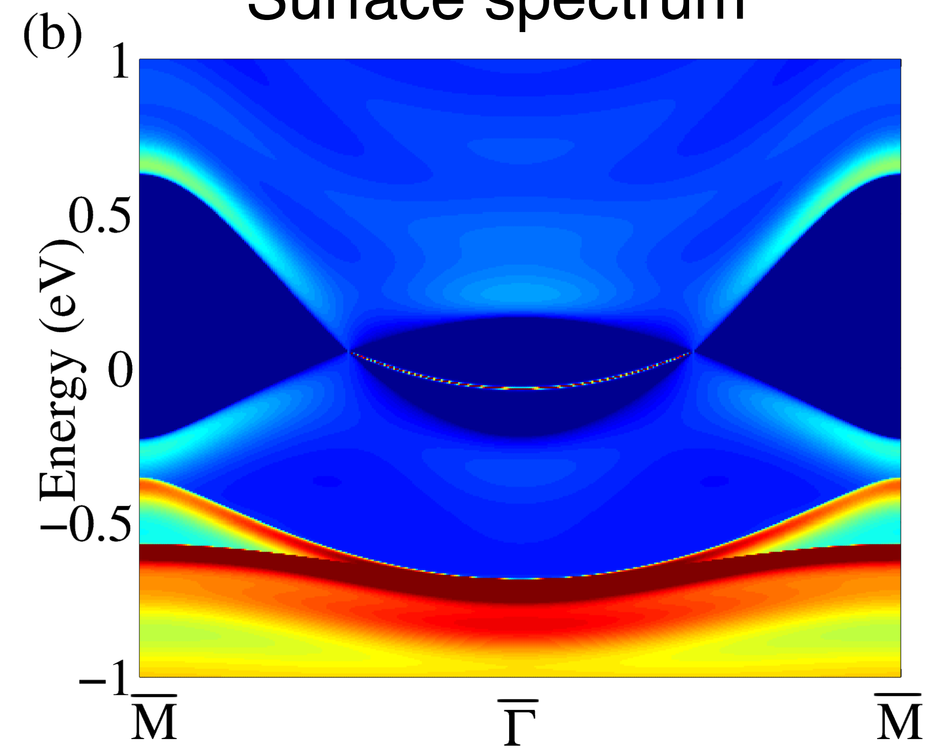
— In Ca_3P_2 Berry phase is quantized due to:

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

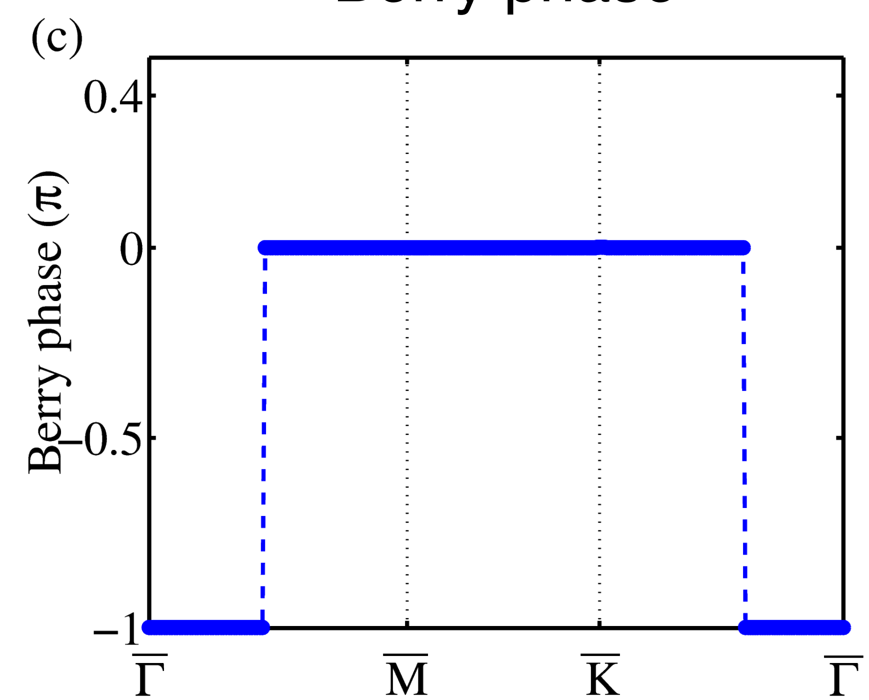
(ii) inversion + time-reversal symmetry

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

Surface spectrum



Berry phase



Relation between Berry phase and mirror invariant

$$\boxed{(-1)^{n_{\mathrm{occ}}^{+,0}(k)+n_{\mathrm{occ}}^{+,\pi}(k)} e^{i\partial R} = e^{i\mathcal{P}(k)}}$$

with $\partial R = i \sum_{j \in \mathrm{filled}} \int_0^{\pi} \left\langle u_{k_z}^{(j)} \middle| R_{k_z}^{\dagger} \left(\partial_{k_z} R_{k_z}\right) \middle| u_{k_z}^{(j)} \right\rangle dk_z$

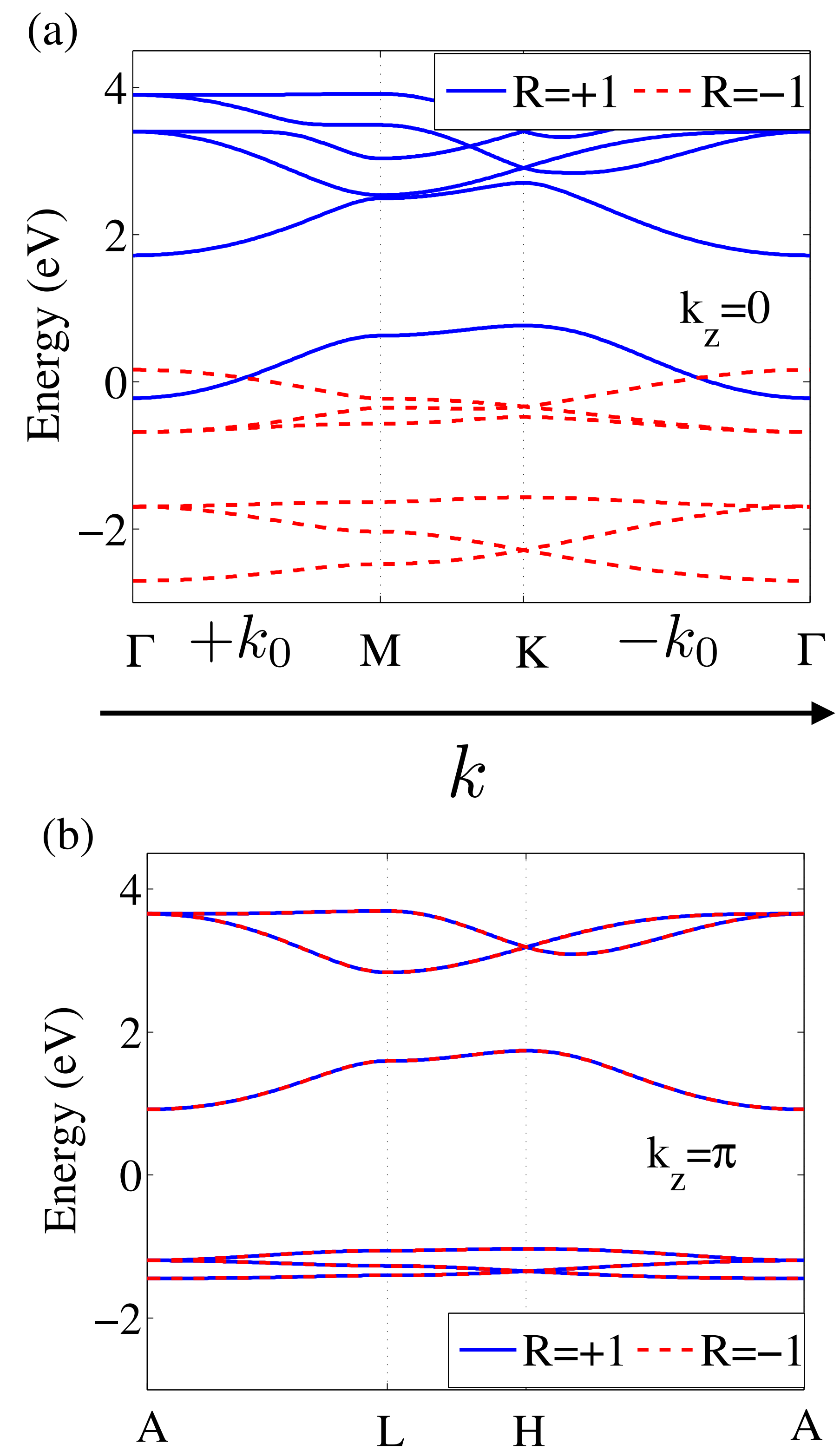
— mirror invariants are easier to compute than Berry phase

— for Ca_3P_2:

$$n_{\mathrm{occ}}^{+,0}(k) = \begin{cases} 1 & |k| < k_0 \\ 0 & |k| > k_0 \end{cases}$$

$$n_{\mathrm{occ}}^{+,\pi}(k) = 3 \;\; \forall k \qquad \partial R = 3$$

$\Rightarrow$ relation holds ✓

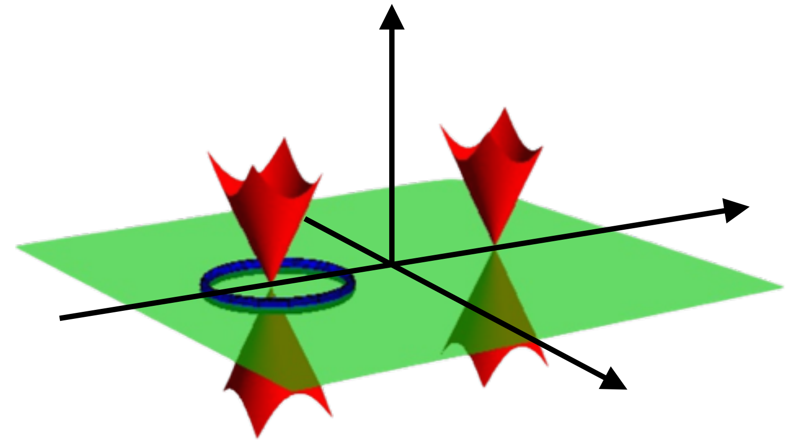


Chan, Chiu, Chou, Schnyder, arXiv:1510.02759

Classification of reflection symmetric semimetals and nodal SCs

(ii) Fermi surface only invariant under reflection

$$p = d - d_{\mathrm{FS}}$$



classification of *Fermi points* with $d_{\mathrm{FS}} = 0$ in **d** dimensions ⟷ classification of *fully gapped* topological materials in **d-1** dimensions

Reflection	sym. class	p=2	p=3	p=4	p=5	p=6	p=7	p=8	p=1
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z} \oplus \mathbb{Z}$	0	$M\mathbb{Z} \oplus \mathbb{Z}$	0	$M\mathbb{Z} \oplus \mathbb{Z}$	0	$M\mathbb{Z} \oplus \mathbb{Z}$	0
R_+,R_{++}	AI	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	[illegible]	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$
	D	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	AII	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CII	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
	C	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CI	0	0	0	$2M\mathbb{Z}$	0	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
R_-,R_{--}	AI	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	BDI	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	D	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$
	AII	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0	$2M\mathbb{Z}$
	C	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0	0
	CI	0	$2M\mathbb{Z}$	0	$T\mathbb{Z}_2$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0
R_{-+}	BDI, CII	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0
R_{+-}	DIII, CI	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0	$2M\mathbb{Z}$	0	$2\mathbb{Z}$	0
R_{+-}	BDI	$M\mathbb{Z} \oplus \mathbb{Z}$	0	0	0	$2M\mathbb{Z} \oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$
R_{-+}	DIII	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z} \oplus \mathbb{Z}$	0	0	0	$2M\mathbb{Z} \oplus 2\mathbb{Z}$	0
R_{+-}	CII	$2M\mathbb{Z} \oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z} \oplus \mathbb{Z}$	0	0	0
R_{-+}	CI	0	0	$2M\mathbb{Z} \oplus 2\mathbb{Z}$	0	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$M\mathbb{Z} \oplus \mathbb{Z}$	0

graphene

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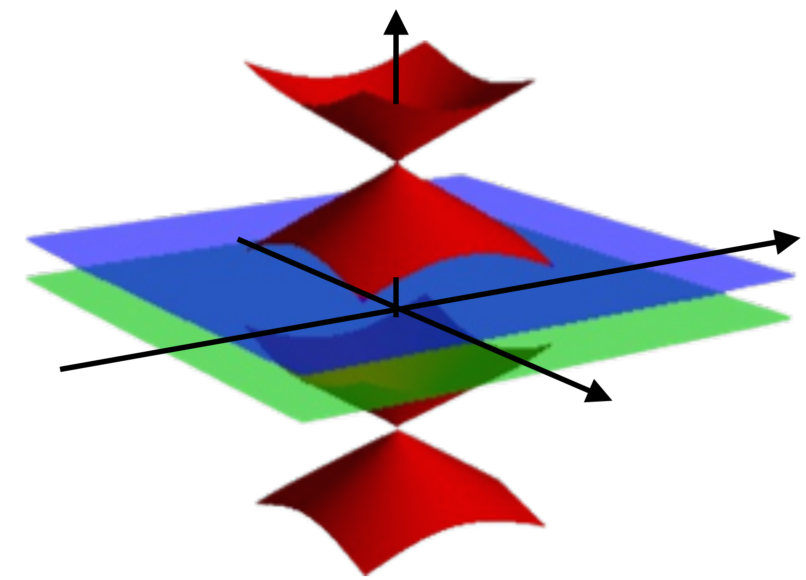
Classification of reflection symmetric semimetals and nodal SCs

(iii) Fermi surface not invariant under reflection & global symmetries



- consider combined symmetries, e.g.: $\widetilde{T} = RT$

$$\widetilde{T}^{-1} H(k_x, -\tilde{\mathbf{k}}) \widetilde{T} = +H(k_x, \tilde{\mathbf{k}})$$

$\Longrightarrow$ Fermi surface is invariant under combined symmetry

Reflection	sym. class	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
R	A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
R_+	AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
R_+,R_{++}	AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$
	BDI	$C\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$
	D	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	DIII	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
	AII	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	CII	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	C	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$	0
	CI	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	$\mathbb{Z}$
R_-,R_{--}	AI	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$	0	0	0
	BDI	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$	0	0
	D	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$	0
	DIII	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$
	AII	$2\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$	0
	CII	0	$2\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$C\mathbb{Z}_2$
	C	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	CI	0	$C\mathbb{Z}_2$	0	$2\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
R_{+-}	CI	$C\mathbb{Z}_2$	0	0	0	0	0	0	$C\mathbb{Z}_2$
R_{-+}	BDI	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	0	0	0	0	0
R_{+-}	DIII	0	0	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	0	0	0
R_{-+}	CII	0	0	0	0	0	$C\mathbb{Z}_2$	$C\mathbb{Z}_2$	0

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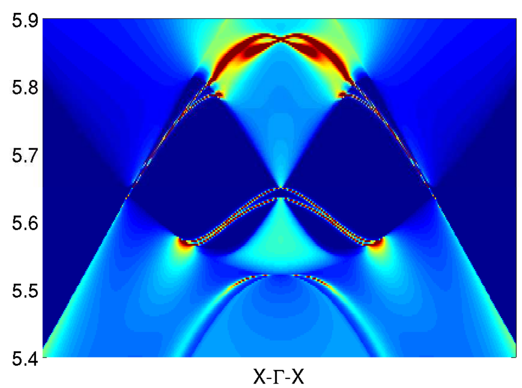
Conclusions and Outlook

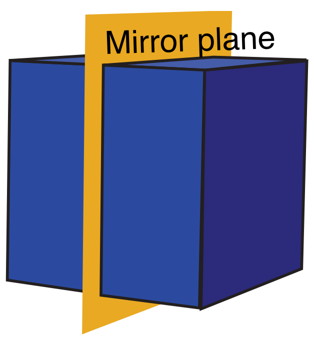
- Topological classification schemes:

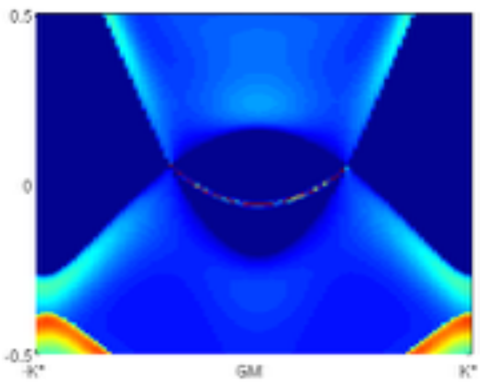
  (i) bring order to the growing zoo of topological materials

  (ii) give guidance for the search and design of new topological states

  (iii) link the properties of the surface states to the bulk wave function topology







Review articles: arXiv:1505.03535; J. Phys.: Condens. Matter 27, 243201 (2015)

- Candidate materials for topological matter:
  - Anti-perovskites: Ca_3PbO, Sr_3PbO, Ba_3PbO (class AII with R_-)
  - Dirac semi-metals with *rotation symmetry*: Cd_3As_2, Na_3Bi (class DIII with R_{--})
  - Nodal ring protected by reflections symmetry: Ca_3P_2, $PbTaSe_2$ (class A with R)
  - Non-centrosymmetric SCs: $CePt_3Si$, $CeIrSi_3$, $CeRhSi_3$ (class DIII)
  - Chiral d-wave SC: SrPtAs (class C)
  - etc.