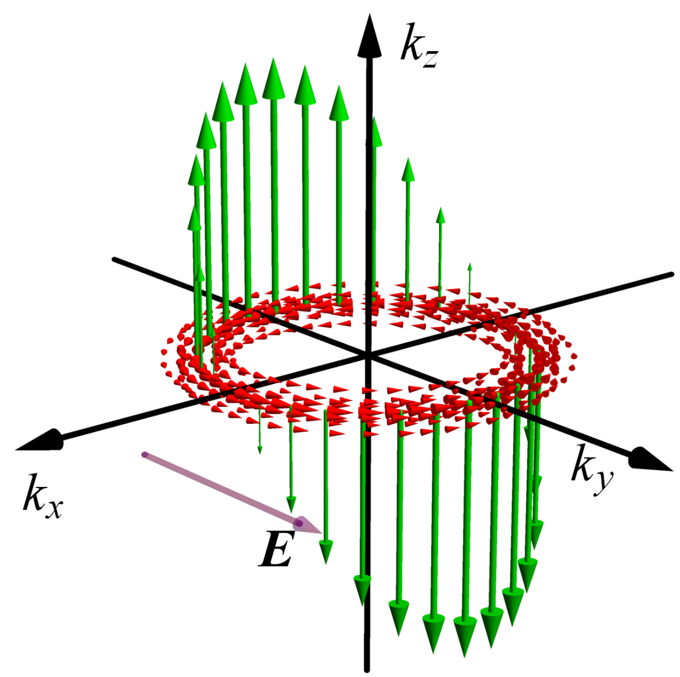
Crystalline topological semi-metals

Andreas P. Schnyder

Max Planck Institute for Solid State Research, Stuttgart



Review article: Rev. Mod. Phys. 88, 035005 (2016)

May 31st, 2017

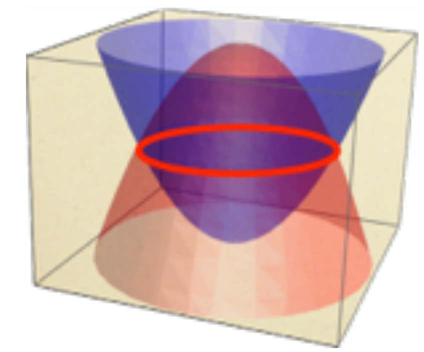
IFIMAC Conference Series, Universidad Autonoma de Madrid, Spain

Outline

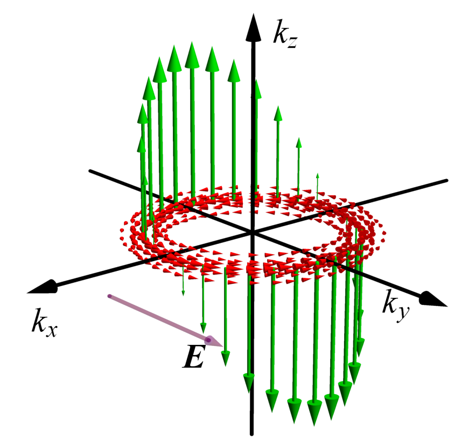
1. Introduction: Topological band theory
   - Classification of crystalline topological materials

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	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	$M\mathbb{Z}_2$	$M\mathbb{Z}$	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

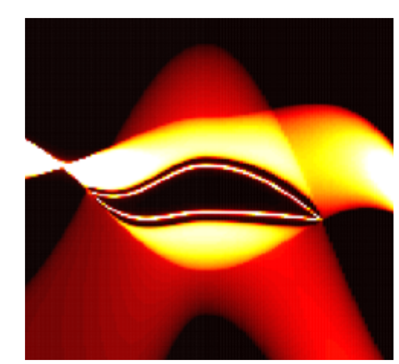
2. Topological nodal-line semimetals
   - Ca_3P_2, Zr_5Si_3



3. Quantum anomalies in nodal-line semimetals
   - Parity anomaly & anomalous transport



4. Dirac line nodes w/ non-symmorphic symmetries
   - $CuBi_2O_4$



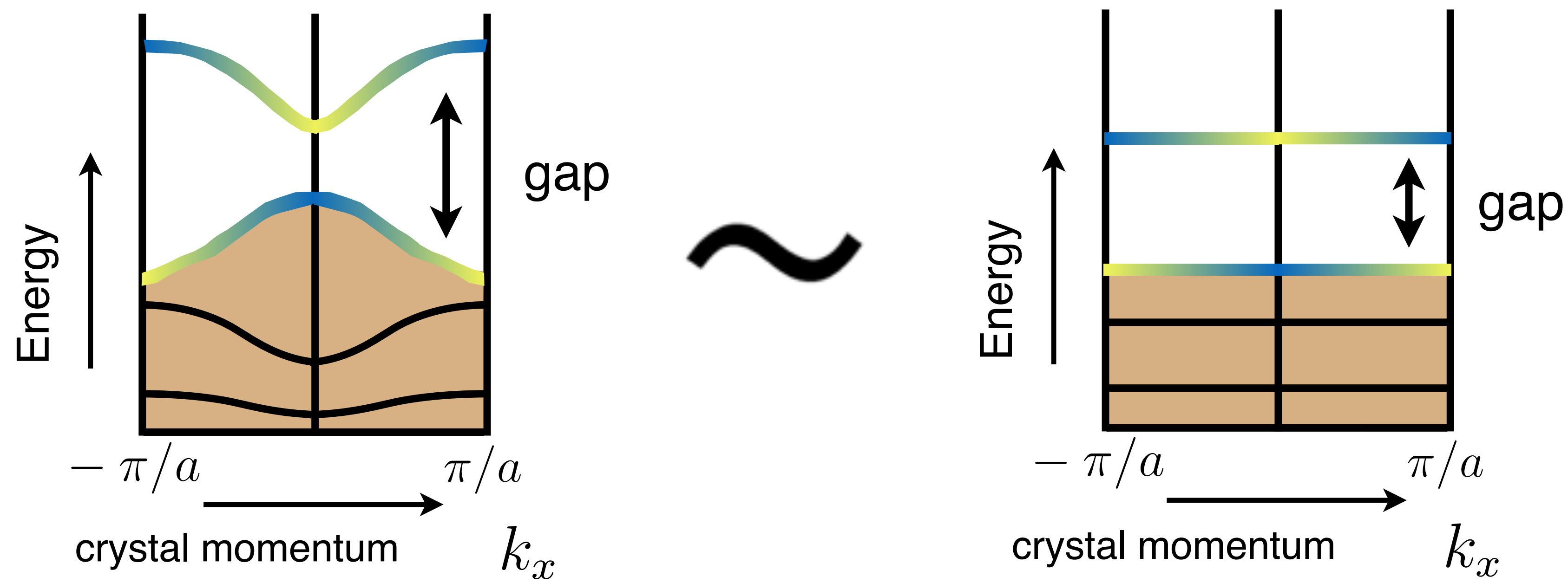
4. Conclusions & Outlook

Review article: Rev. Mod. Phys. 88, 035005 (2016)

Topological band theory

- Consider band structure: $H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

- **(i) Topological equivalence for insulators:**



▷ symmetries to consider: *time-reversal symmetry, particle-hole,*
reflection, inversion (parity)

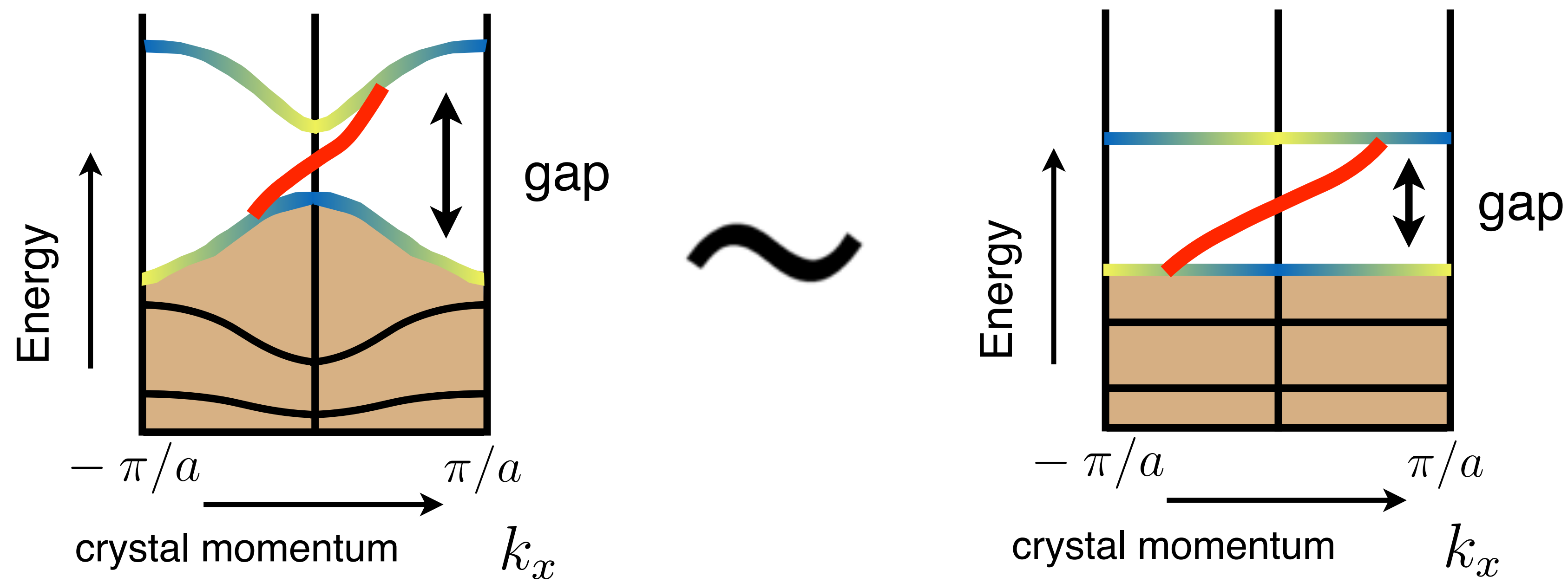
▷ top. equivalence classes distinguished by: $$n_{\mathbb{Z}} = \frac{i}{2\pi} \int_{\substack{\text{filled} \\ \text{states}}} \mathcal{F}\, d\mathbf{k} \;\in\; \mathbb{Z}$$

topological invariant

Topological band theory

- Consider band structure: $H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

- **(i) Topological equivalence for insulators:**



▷ symmetries to consider: *time-reversal symmetry, particle-hole,*
reflection, inversion (parity)

▷ top. equivalence classes distinguished by: $$n_{\mathbb{Z}} = \frac{i}{2\pi}\int_{\text{filled states}} \mathcal{F}\, d\mathbf{k} \;\in\; \mathbb{Z}$$

topological invariant

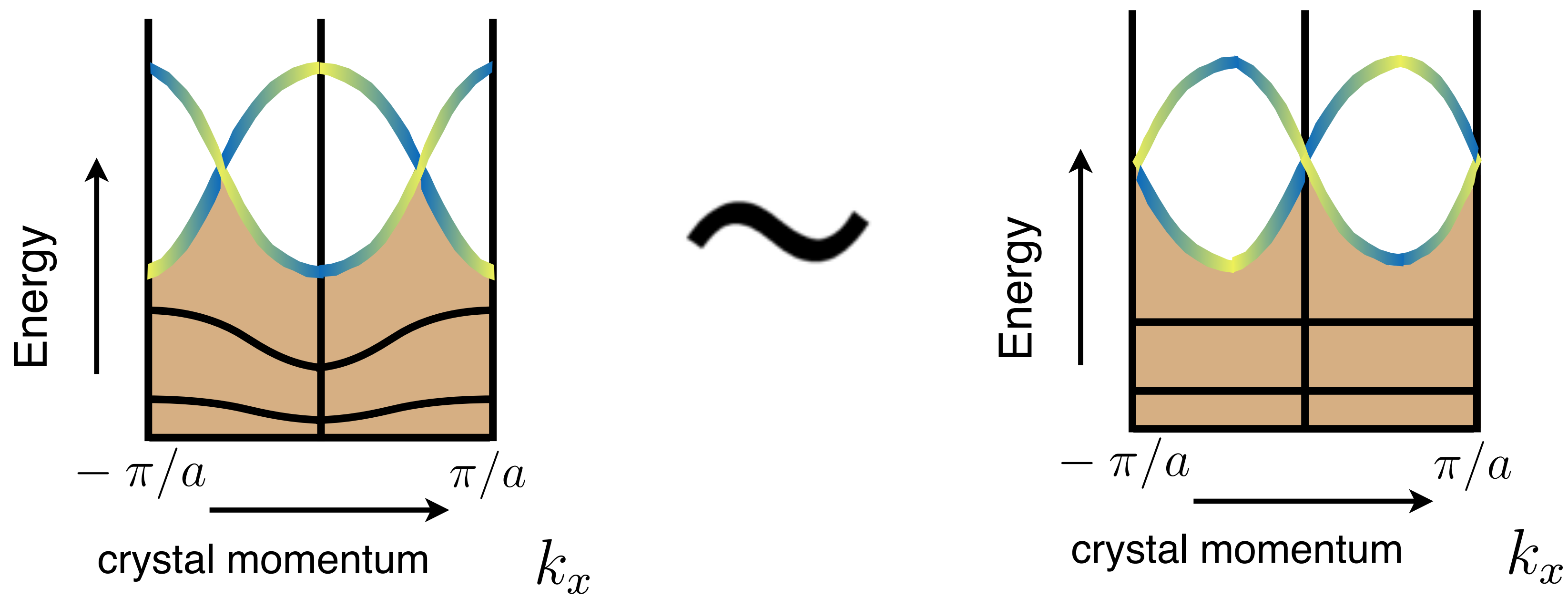
- **Bulk-boundary correspondence:**

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

Topological band theory

- Consider band structure: $H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

- **(ii) Topological equivalence for band crossings:**



▷ symmetries to consider: *time-reversal symmetry, particle-hole, reflection, inversion (parity)*

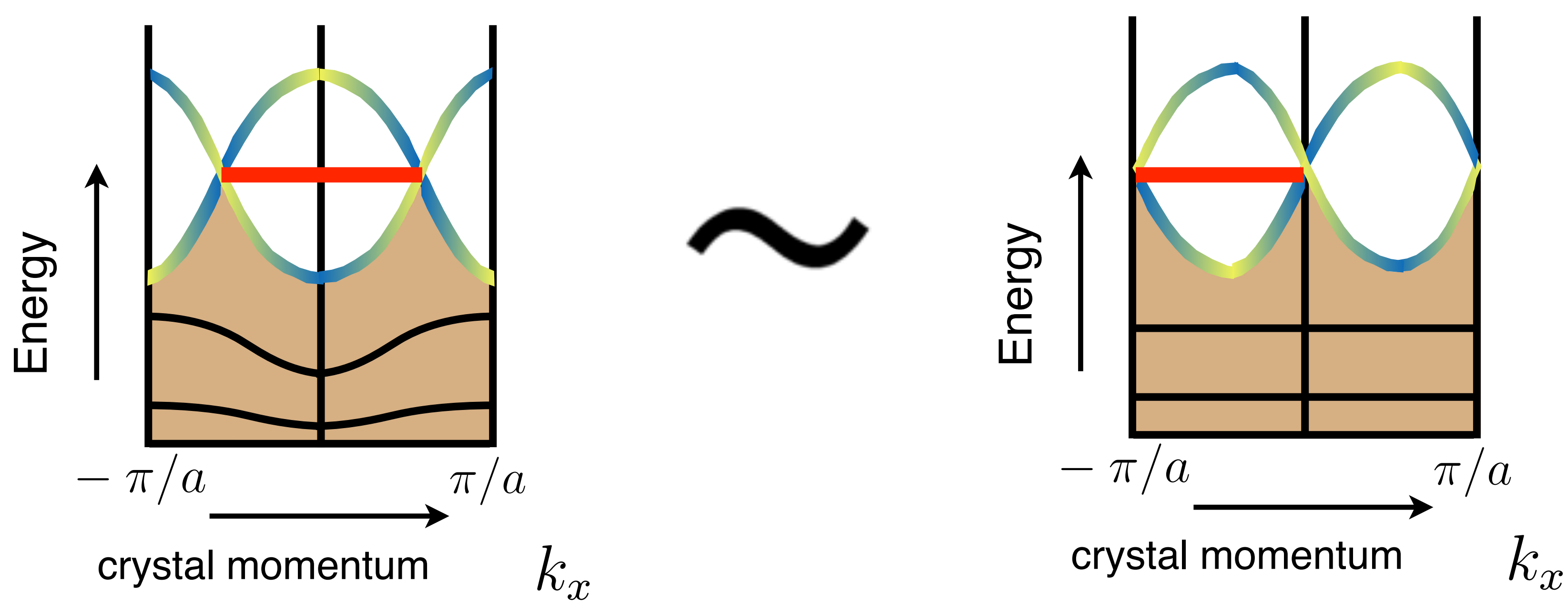
▷ top. equivalence classes distinguished by: $$n_{\mathbb{Z}} = \frac{i}{2\pi} \int_{\text{filled states}} \mathcal{F}\, d\mathbf{k} \in \mathbb{Z}$$

topological invariant

Topological band theory

- Consider band structure: $H(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n(\boldsymbol{k})\rangle$

- **(ii) Topological equivalence for band crossings:**



▷ symmetries to consider: *time-reversal symmetry, particle-hole, reflection, inversion (parity)*

▷ top. equivalence classes distinguished by: $$n_{\mathbb{Z}} = \frac{i}{2\pi}\int_{\substack{\text{filled}\\ \text{states}}} \mathcal{F}\, d\mathbf{k} \ \in\ \mathbb{Z}$$

topological invariant

- **Bulk-boundary correspondence:**

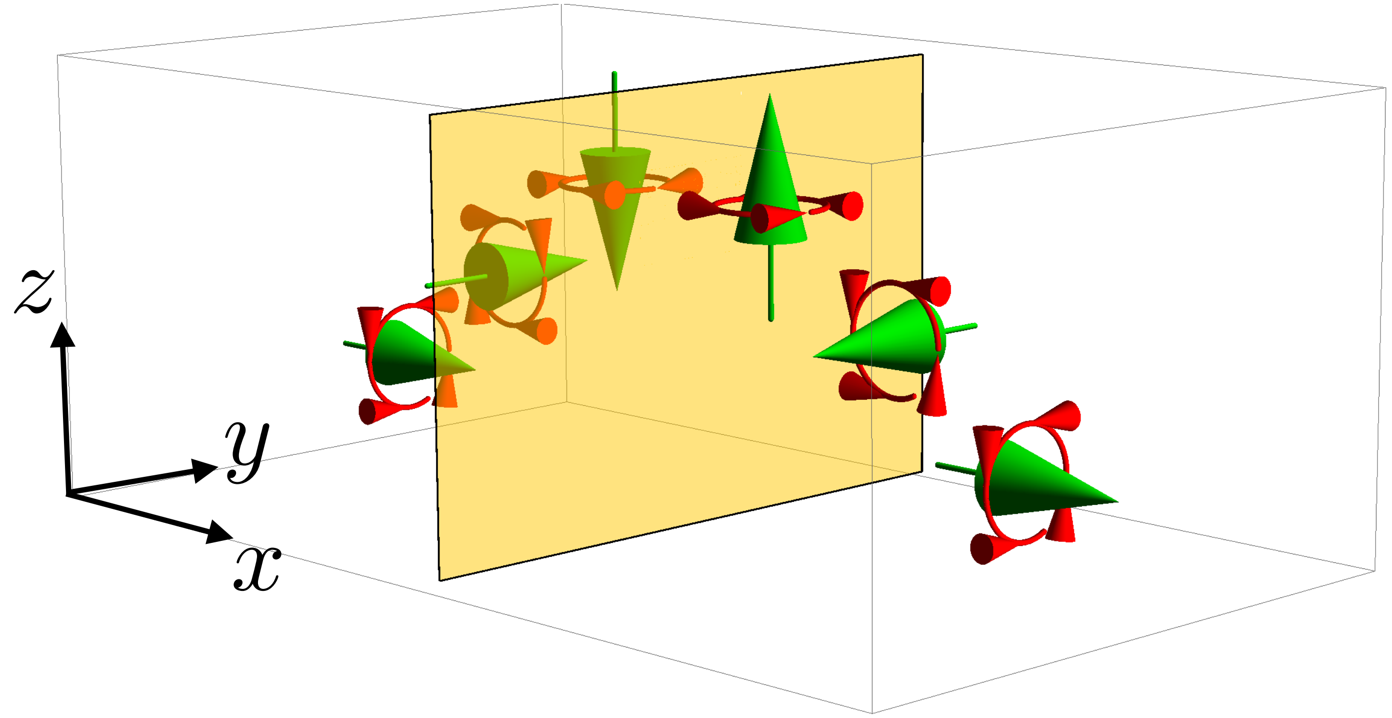
$$|n_{\mathbb{Z}}| = \#\,\text{gapless edge states (or surface states)}$$

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: $n_{\mathcal{M}} = n^{+}_{\mathcal{M}} + n^{-}_{\mathcal{M}}$

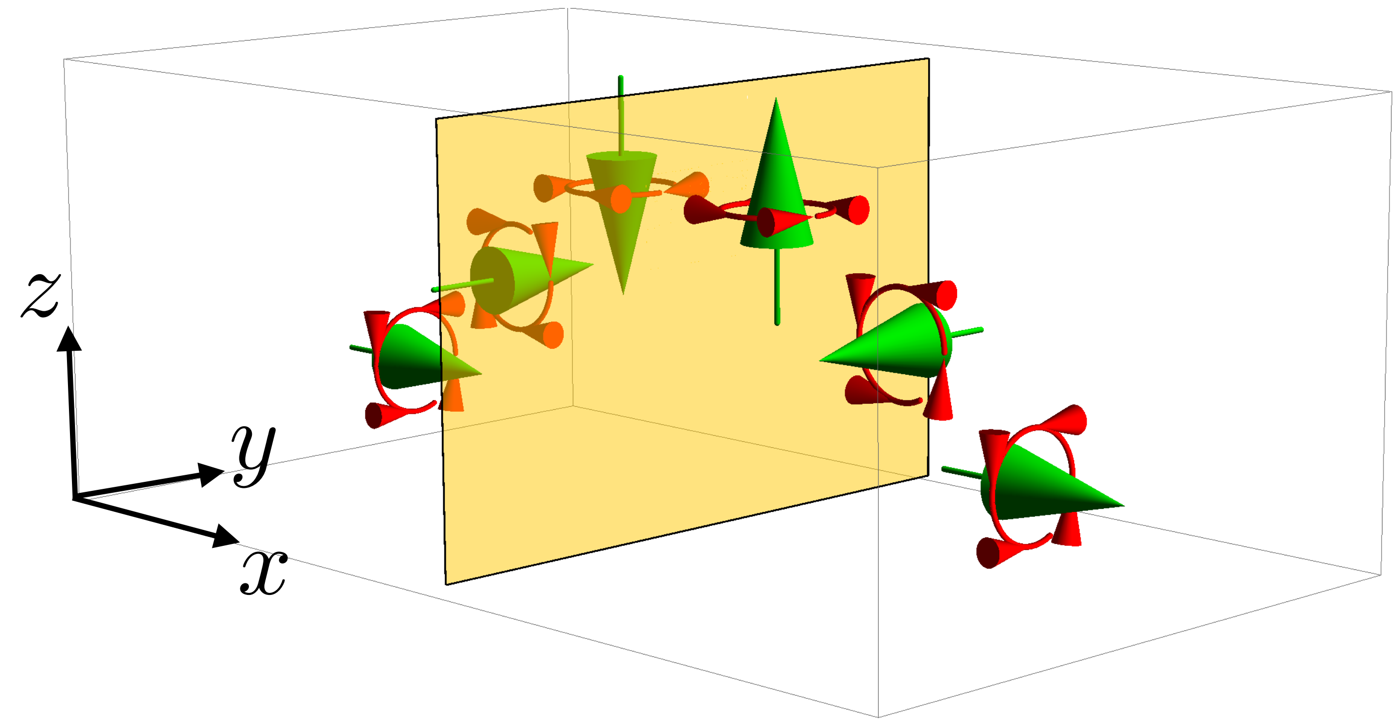
— mirror Chern number: $n_{\mathcal{M}} = n^{+}_{\mathcal{M}} - n^{-}_{\mathcal{M}}$

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

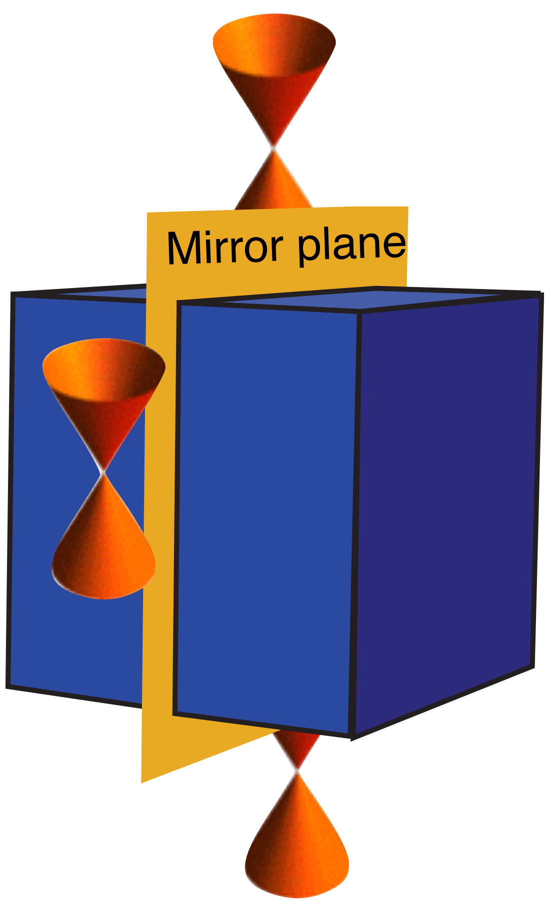
- **mirror Chern number:**

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

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

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

Berry curvature in $\pm$ eigenspace



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

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

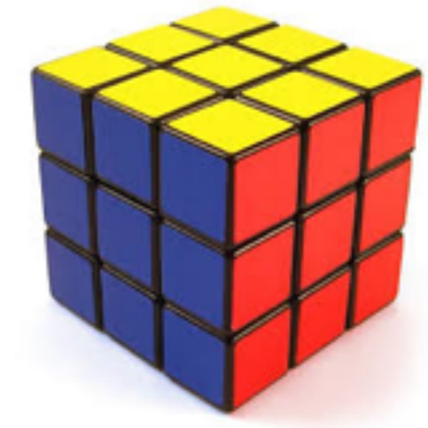
- Bulk-boundary correspondence:

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

Classification of *free-fermion* systems with reflection symmetry

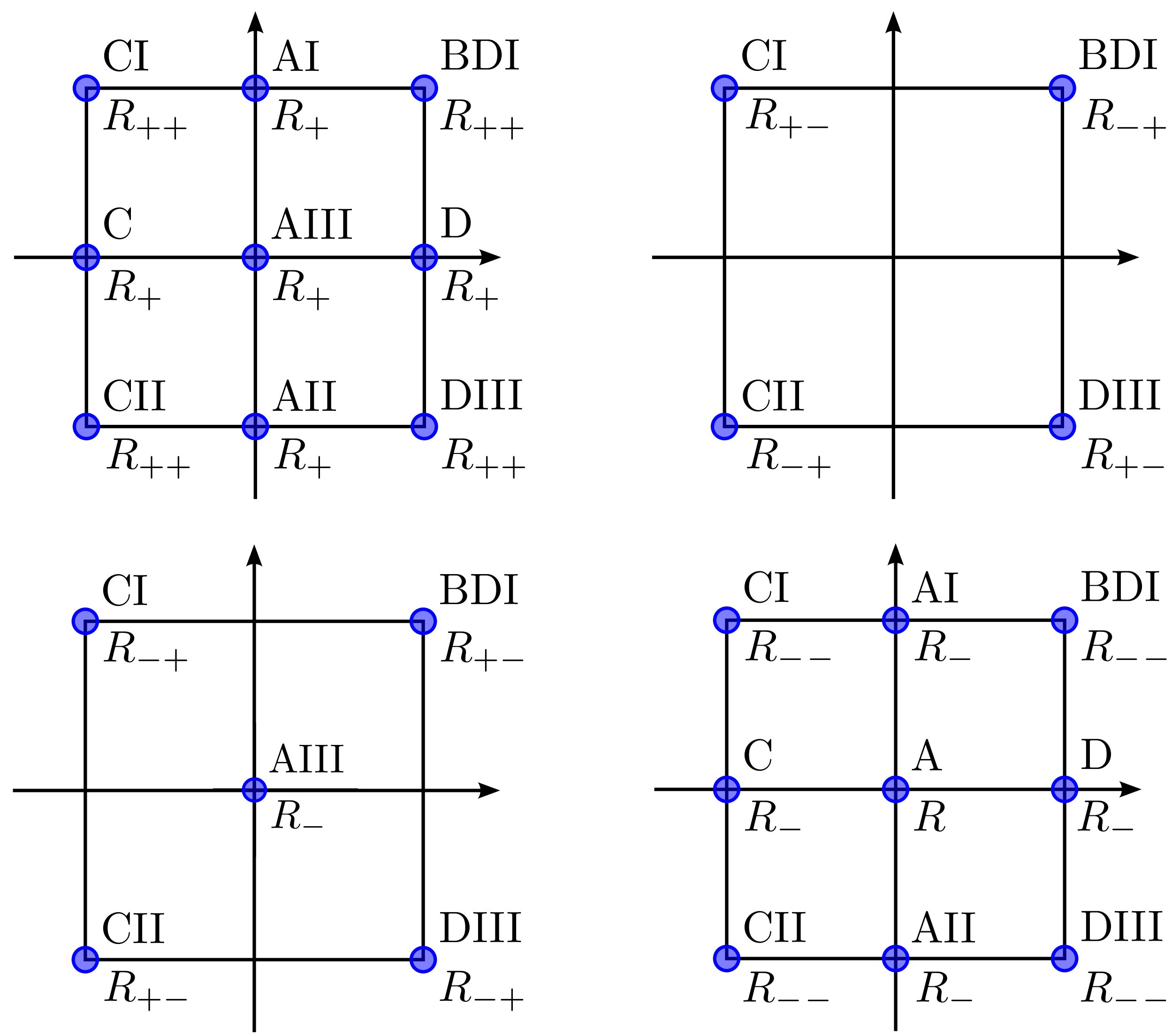
R_+ : R commutes with T (C or S)

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"



PRB 90, 205136 (2014); PRL 116, 156402 (2016)

Classification of *free-fermion* systems with reflection symmetry

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

Reflection	TI/TSC FS1 FS2
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 or topological semi-metal protected by reflection symmetry?

Classification of *free-fermion* systems with reflection symmetry

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

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	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	$M\mathbb{Z}_2$	$M\mathbb{Z}$	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

PRB 90, 205136 (2014)

PRL 116, 156402 (2016)

Classification of *free-fermion* systems with reflection symmetry

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

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	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	[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	$M\mathbb{Z}_2$	$M\mathbb{Z}_2$	[illegible]	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]	$T\mathbb{Z}_2$	$\mathbb{Z}_2$
	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

graphene

Ca_3PbO, Sr_3PbO

PRB 90, 205136 (2014)

PRL 116, 156402 (2016)

Reduction of classification with *interactions*

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

			$D = 8n + d, n = 0, 1, 2 \cdots$							
Ref.	Class	Clifford Algebra	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
R	A	Cl_{d+2}/Cl_{d+2}	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_{2^{4n+5}}$	0
R_+	AIII	Cl_{d+3}/Cl_{d+3}	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_{2^{4n+5}}$
R_-	AIII	Cl_{d+2}/Cl_{d+2}	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_{2^{4n+5}}$	0
$R_{+(+)}$	AI	$Cl_{2,d+2}/Cl_{2,d+2}$	$\mathbb{Z}_{2^{4n+2}}$	0	0	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	BDI	$Cl_{d+1,4}/Cl_{2,d+1}$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_2$
	D	$Cl_{d,4}/Cl_{2,d}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0	$\mathbb{Z}_{2^{4n+5}}$	0
	DIII	$Cl_{d,5}/Cl_{3,d}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0	$\mathbb{Z}_{2^{4n+5}}$
	AII	$Cl_{4,d}/Cl_{4,d}$	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0
	CII	$Cl_{d+3,2}/Cl_{5,d}$	0	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0
	C	$Cl_{2+d,2}/Cl_{d+3,1}$	0	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+5}}$	0
	CI	$Cl_{2+d,3}/Cl_{2,d+3}$	0	0	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+5}}$
$R_{-(-)}$	AI	$Cl_{1,d+3}/Cl_{1,d+3}$	0	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+5}}$	0
	BDI	$Cl_{2+d,3}/Cl_{1,d+2}$	0	0	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+6}}$
	D	$Cl_{d+1,3}/Cl_{1,d+1}$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	DIII	$Cl_{d+1,4}/Cl_{2,d+1}$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_2$
	AII	$Cl_{3,d+1}/Cl_{3,d+1}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	0
	CII	$Cl_{d+4,1}/Cl_{4,d+1}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$
	C	$Cl_{3+d,1}/Cl_{d+2,2}$	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0
	CI	$Cl_{d+3,2}/Cl_{1,d+4}$	0	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0
R_{-+}	BDI	Cl_{d+4}/Cl_{d+2}	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_{2^{4n+5}}$	0
R_{-+}	CII	Cl_{d+4}/Cl_{d+4}	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0
R_{+-}	DIII	Cl_{d+4}/Cl_{d+2}	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_{2^{4n+5}}$	0
R_{+-}	CI	Cl_{d+4}/Cl_{d+4}	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_{2^{4n+4}}$	0
R_{+-}	BDI	$Cl_{d+1,3}/Cl_{1,d+1}$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
R_{+-}	CII	$Cl_{d+3,1}/Cl_{4,d}$	$\mathbb{Z}_{2^{4n+1}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0
R_{-+}	DIII	$Cl_{d,4}/Cl_{2,d}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0	0	0	$\mathbb{Z}_{2^{4n+5}}$	0
R_{-+}	CI	$Cl_{2+d,2}/Cl_{1,d+3}$	0	0	$\mathbb{Z}_{2^{4n+2}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+5}}$	0

PRB 95, 195108 (2017)

Reduction of classification with *interactions*

U_+ : U commutes with T (C or S) U_- : U anti-commutes with T (C or S)

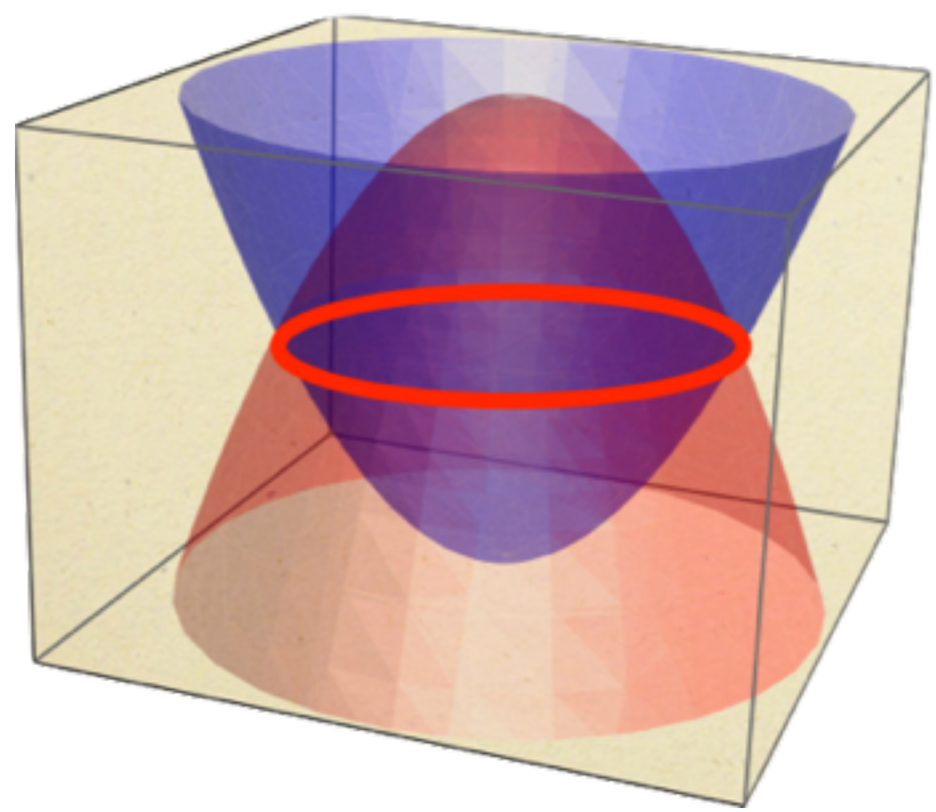
		$D = 8n + d, n = 0, 1, 2 \cdots$							
Rot.	Class	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
U	A	0	0	0	0	0	0	0	0
U_+	AIII	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+5}}$	$\mathbb{Z}_{2^{4n+5}}$
U_-	AIII	0	0	0	0	0	0	0	0
$U_{+(+)}$	AI	$\mathbb{Z}_{2^{4n+2}}$	0	0	0	$\mathbb{Z}_{2^{4n+3}}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	BDI	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+5}}$	$\mathbb{Z}_{2^{4n+6}}$
	D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	0	0	$\mathbb{Z}_2$
	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0	$\mathbb{Z}_{2^{4n+5}}$	$\mathbb{Z}_2$
	AII	0	0	0	0				
	CII	$\mathbb{Z}_{2^{4n+1}}$	$\mathbb{Z}_{2^{4n+1}}$	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$
	C	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0
	CI	0	0	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+4}}$	0
$U_{-(-)}$	AI	0	0	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	BDI	$\mathbb{Z}_{2^{4n+2}}$	0	0	0	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	D	0	0	0	0	0	0	0	0
	DIII	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+5}}$	$\mathbb{Z}_{2^{4n+5}}$
	AII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	0
	CII	$\mathbb{Z}_{2^{4n+1}}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_{2^{4n+3}}$	0	0	0
	C	0	0	0	0	0	0	0	0
	CI	$\mathbb{Z}_{2^{4n+1}}$	$\mathbb{Z}_{2^{4n+1}}$	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+2}}$	$\mathbb{Z}_{2^{4n+3}}$	$\mathbb{Z}_{2^{4n+4}}$	$\mathbb{Z}_{2^{4n+5}}$	$\mathbb{Z}_{2^{4n+5}}$
U_{-+}	BDI	$\mathbb{Z}_2$	0	0	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
U_{-+}	CII	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0
U_{+-}	DIII	0	0	0	0	0	0	0	0
U_{+-}	CI	0	0	0	0	0	0	0	0
U_{+-}	BDI	0	0	0	0	0	0	0	0
U_{+-}	CII	0	0	0	0	0	0	0	0
U_{-+}	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	0	0
U_{-+}	CI	0	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0

SSH model / Kitaev chain

PRB 95, 195108 (2017)

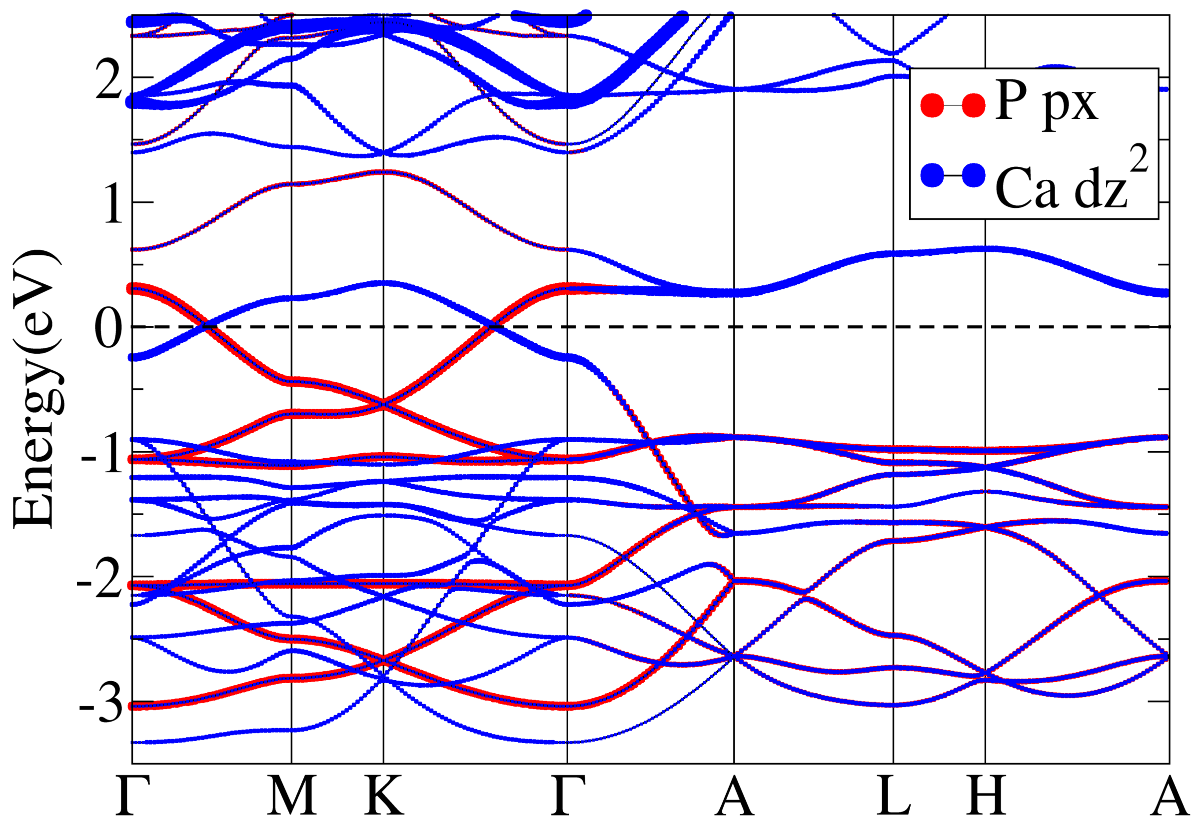
2. Topological nodal line semi-metals

Ca_3P_2 , Zr_5Si_3



Topological nodal lines in Ca_3P_2

▶ Band structure:



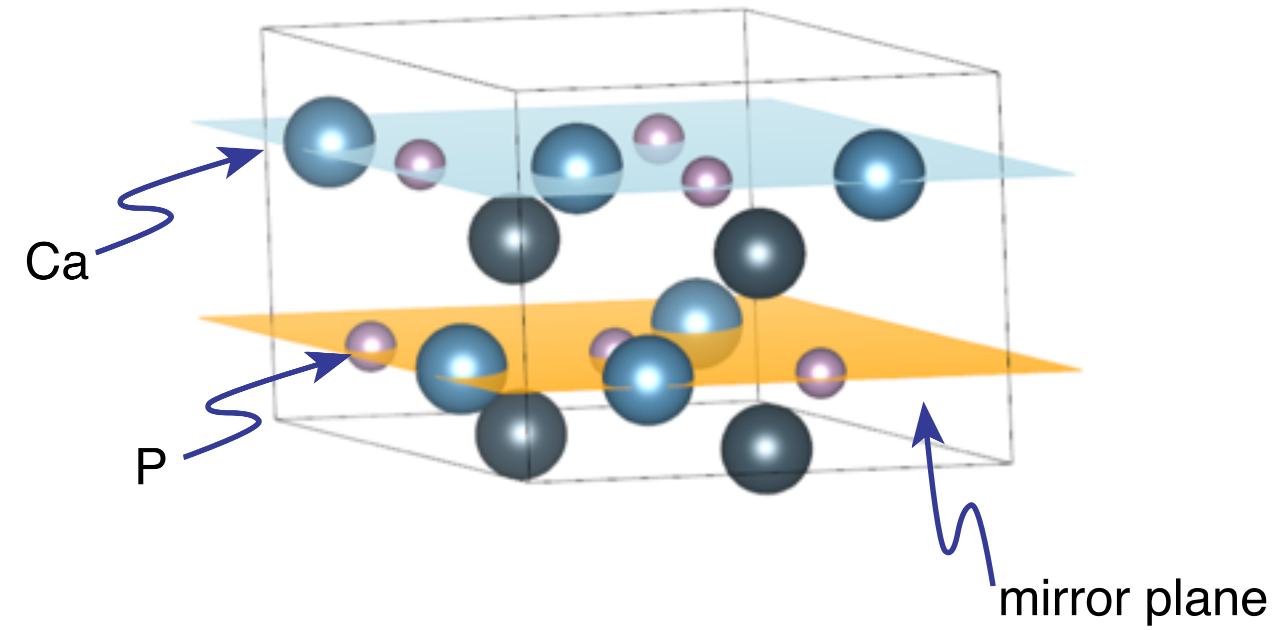
charge balanced: Ca^{2+} — P^{3-}

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

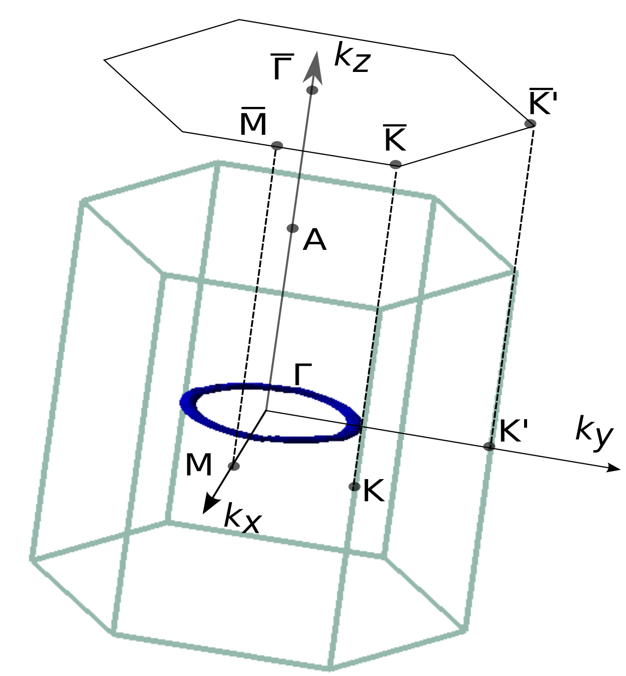
Ca: d_{z^2} orbitals from 6 Ca atoms

P: p_x orbitals from 6 P atoms

▶ Crystal structure $P6_3/mcm$



▶ Dirac ring within reflection plane



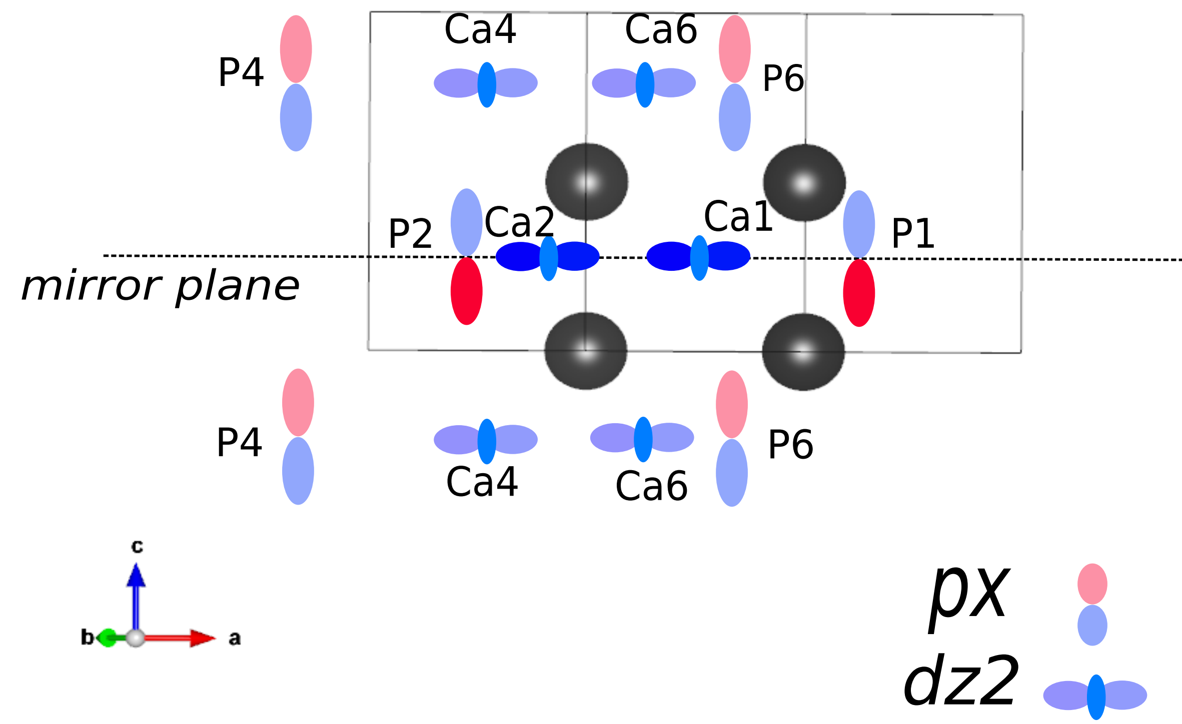
Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Topological nodal line: Mirror invariant

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

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

$$R(\mathbf{k}) = \begin{pmatrix} 1_{3\times3} & 0 & 0 & 0 \\ 0 & 1_{3\times3}e^{-ik_z} & 0 & 0 \\ 0 & 0 & -1_{3\times3} & 0 \\ 0 & 0 & 0 & -1_{3\times3}e^{-ik_z} \end{pmatrix}$$

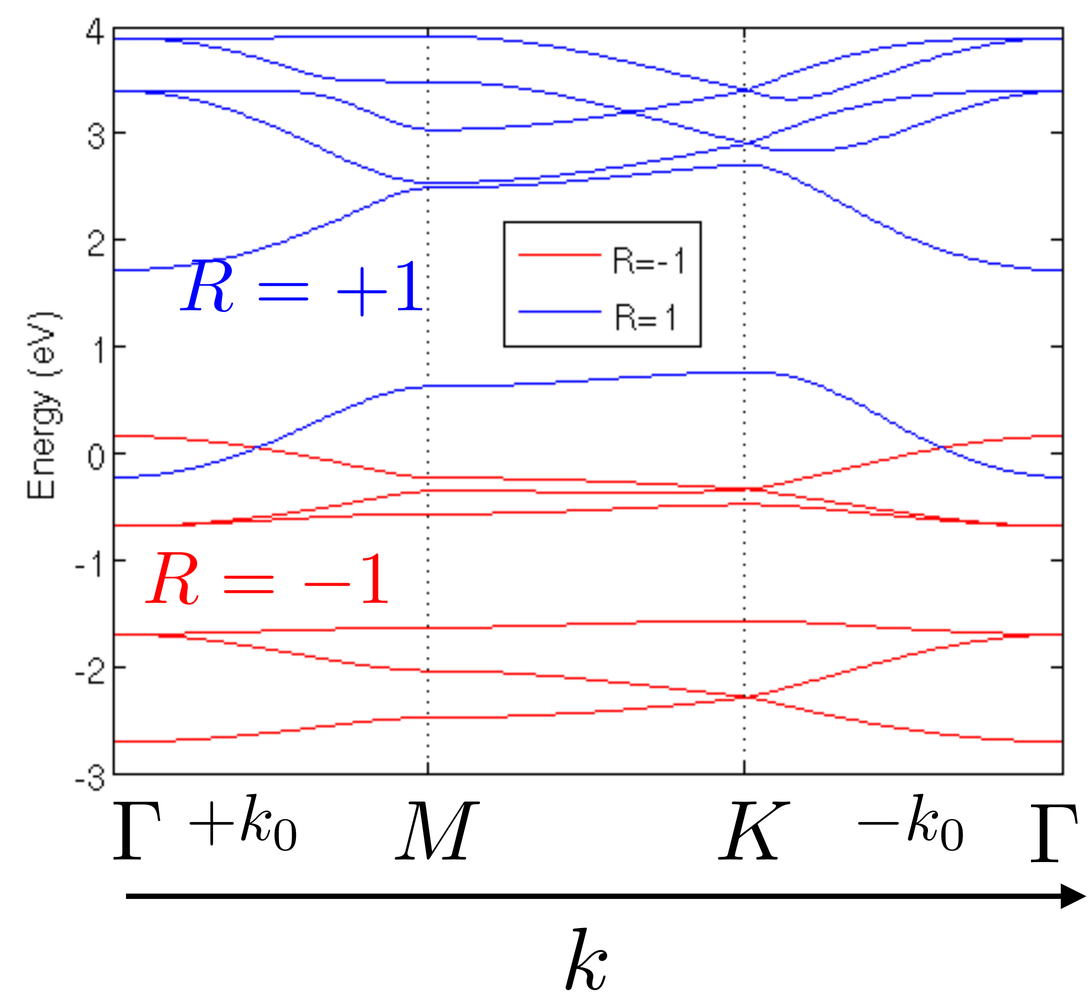


- **Mirror invariant:**

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

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

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



Chan, Chiu, Chou, Schnyder, Phys. Rev. B 93, 205132 (2016)

Topological nodal line: Berry phase invariant

▶ **Berry phase:**

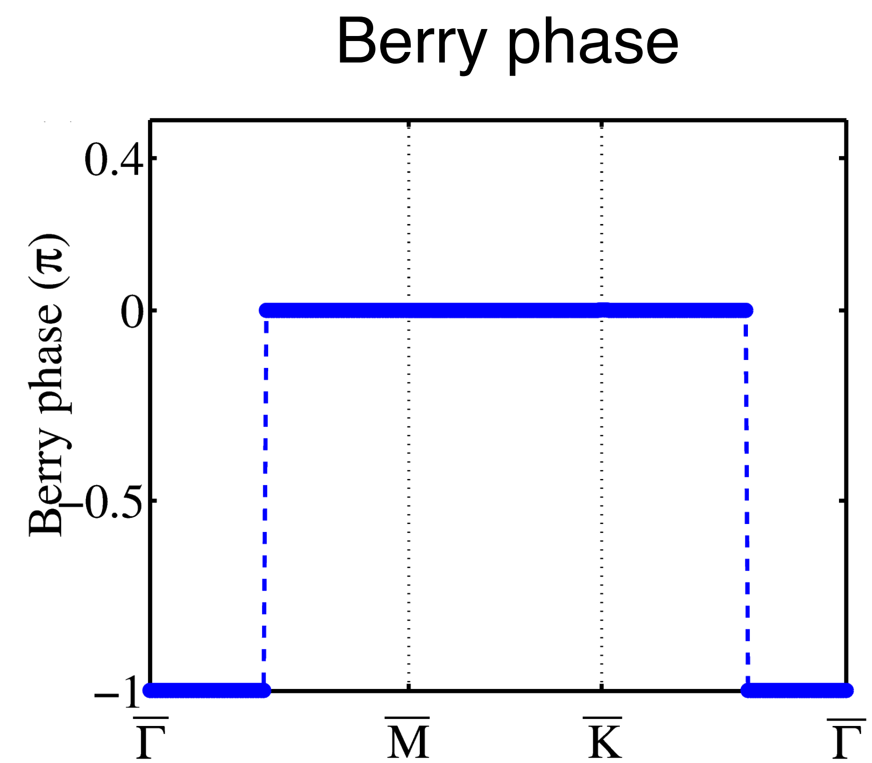
$$\mathcal{P}(k_{\parallel}) = -i \sum_{j \in \text{filled}} \int_{-\pi}^{\pi} \left\langle u_{k_\perp}^{(j)} \middle| \partial k_\perp \middle| u_{k_\perp}^{(j)} \right\rangle dk_\perp$$

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

– In Ca_3P_2 Berry phase is quantized due to:

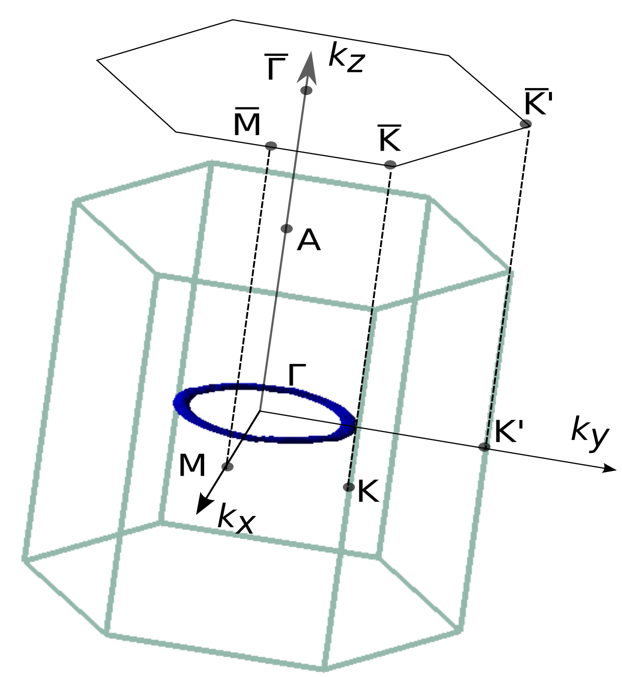
(i) reflection symmetry $z \to -z$

(ii) inversion + time-reversal symmetry



▶ **Relation btw Berry phase & mirror invariant:**

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



PRL 116, 156402 (2016)

Phys. Rev. B 93, 205132 (2016)

Drumhead surface state and Berry phase

▶ **Berry phase & charge polarization:**

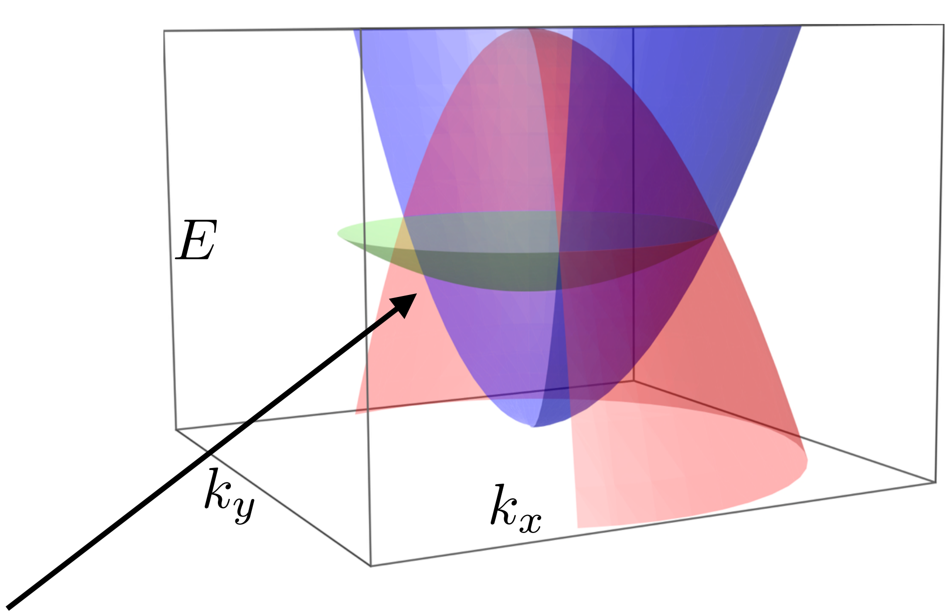
$$\mathcal{P}(k_{\|}) = -i \sum_{j \in \text{filled}} \int_{-\pi}^{\pi} \left\langle u_{k_\perp}^{(j)} \middle| \partial k_\perp \middle| u_{k_\perp}^{(j)} \right\rangle dk_\perp$$

Bulk-boundary correspondence:

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

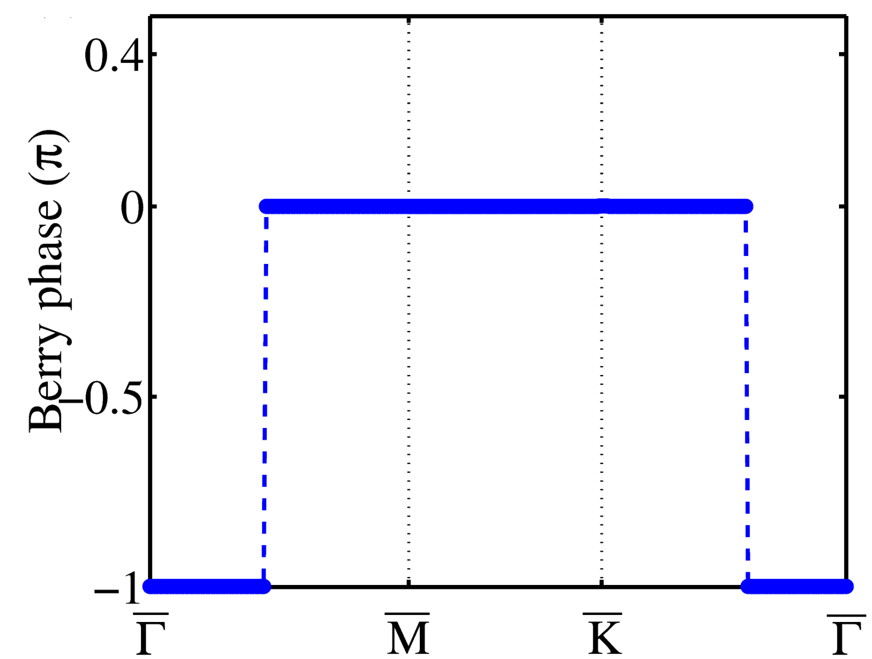
King-Smith and Vanderbilt PRB '93

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

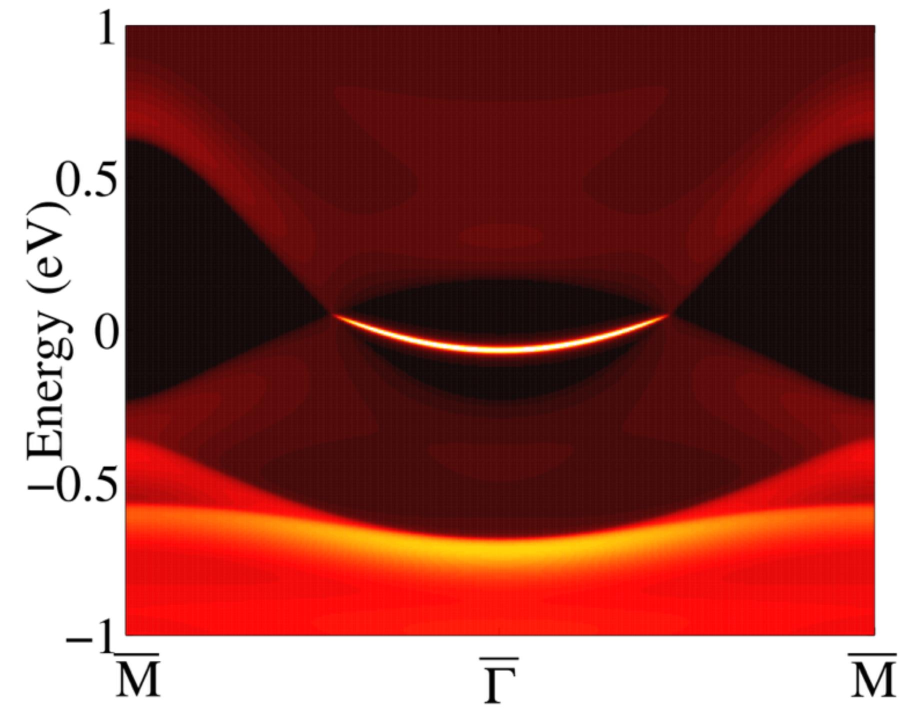


Drumhead surface state

Berry phase

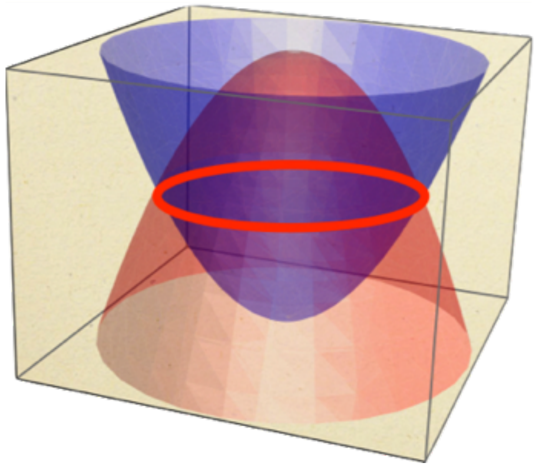


Surface spectrum



Phys. Rev. B 93, 205132 (2016)

Low-energy effective theory for Ca_3P_2



- low-energy effective Hamiltonian:

even in k

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

- symmetry operators:

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

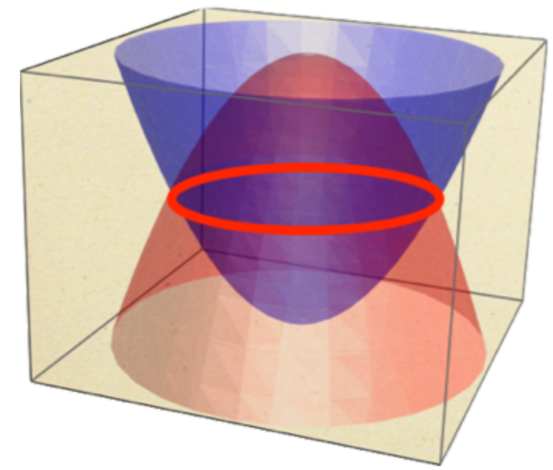
- Gap-opening term τ_x is symmetry forbidden:

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

  — breaks PT symmetry: $(PT)^{-1}\tau_x(PT) = -\tau_x$

$\Rightarrow$ nodal line is stable

Low-energy effective theory for Ca_3P_2



- low-energy effective Hamiltonian:

even in k

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

- 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 PT symmetry: $(PT)^{-1}\tau_x(PT) = -\tau_x$

$\Rightarrow$ nodal line is stable

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

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

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

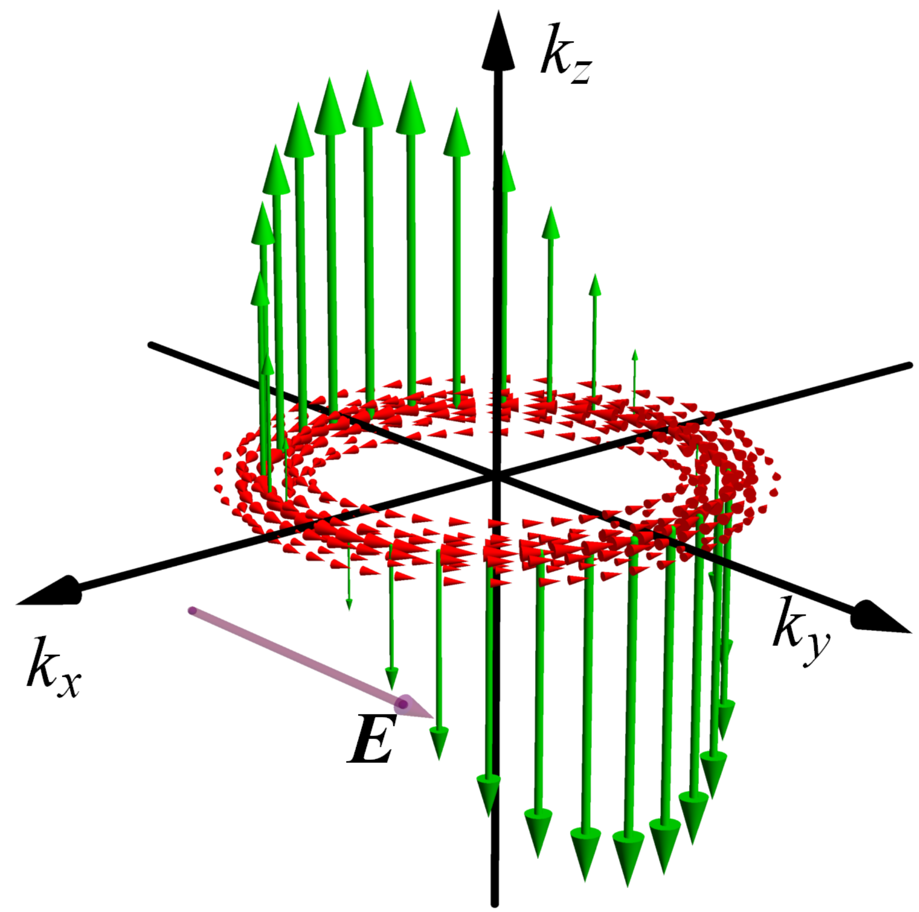
- (PT)-symmetric:

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

- but breaks R:

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

3. Anomaly in nodal line semi-metals



Parity anomaly in nodal-line semi-metals

Quantum Anomaly:

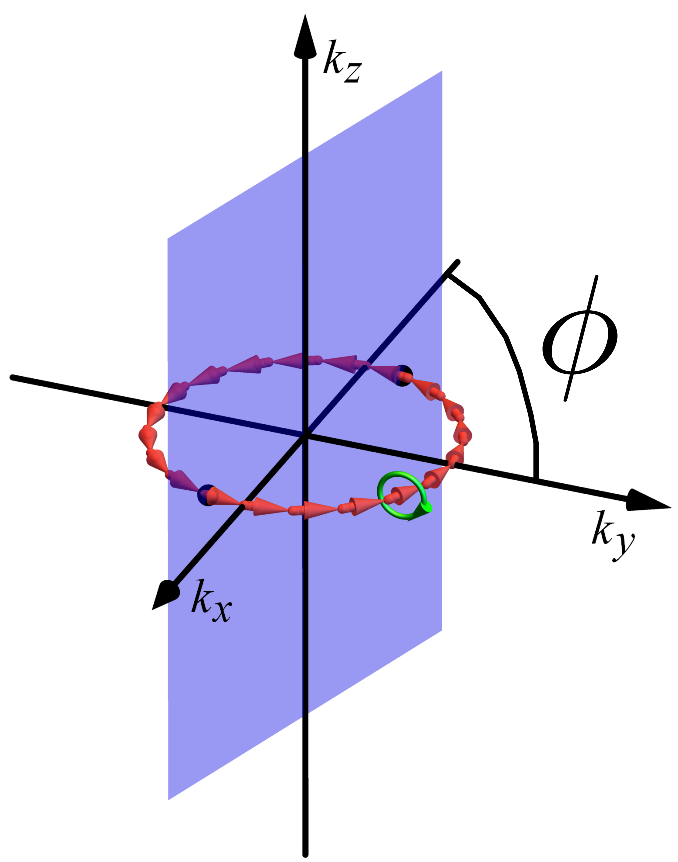
Symmetry of classical action broken by regularization of quantum theory

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 semi-metal?



$\Longrightarrow$ consider family of 2D subsystems

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

Parity anomaly in nodal-line semi-metals

Parity anomaly for a 2D subsystem:

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

breaks PT symmetry

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

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

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

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

Berry phase

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

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

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

$\Rightarrow$ transverse charge response to applied EM field

Parity anomaly in nodal-line semi-metals

R: radius of nodal ring m: small PT breaking term $\mathbf{E}$: electric field

Anomalous transport within semi-classical response theory:

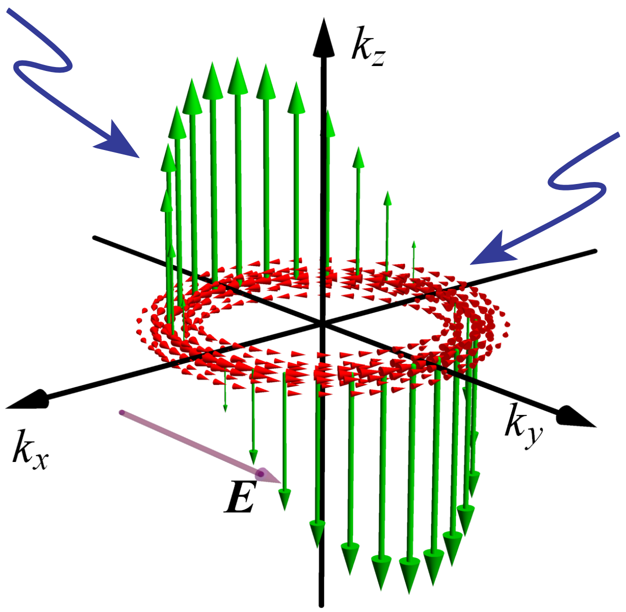
- anomalous velocity: $$\mathbf{v}(\mathbf{k}) = \frac{\partial \varepsilon}{\partial \mathbf{k}} - \frac{e}{\hbar}\mathbf{E} \times \mathbf{\Omega}(\mathbf{k})$$ **Xia, Chiung, Niu RMP 10**

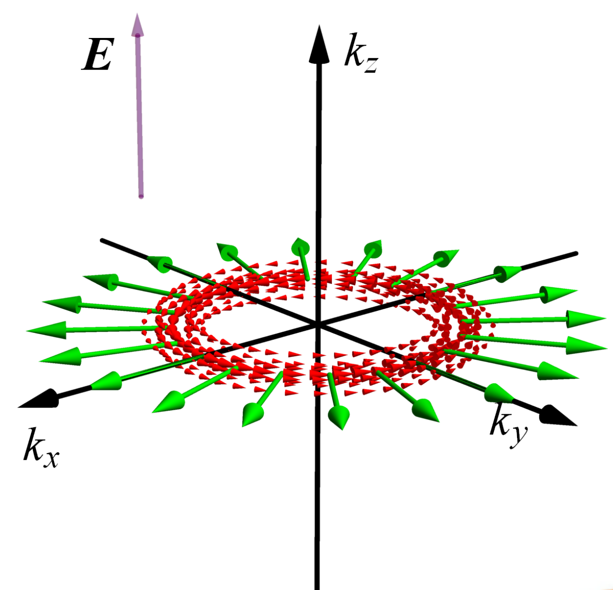
- transverse current: $$\mathbf{j}_t = \frac{e^2}{\hbar}\int \frac{d^3k}{(2\pi)^3} f(\mathbf{k})\, \mathbf{E} \times \mathbf{\Omega}(\mathbf{k})$$ Berry curvature

- 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





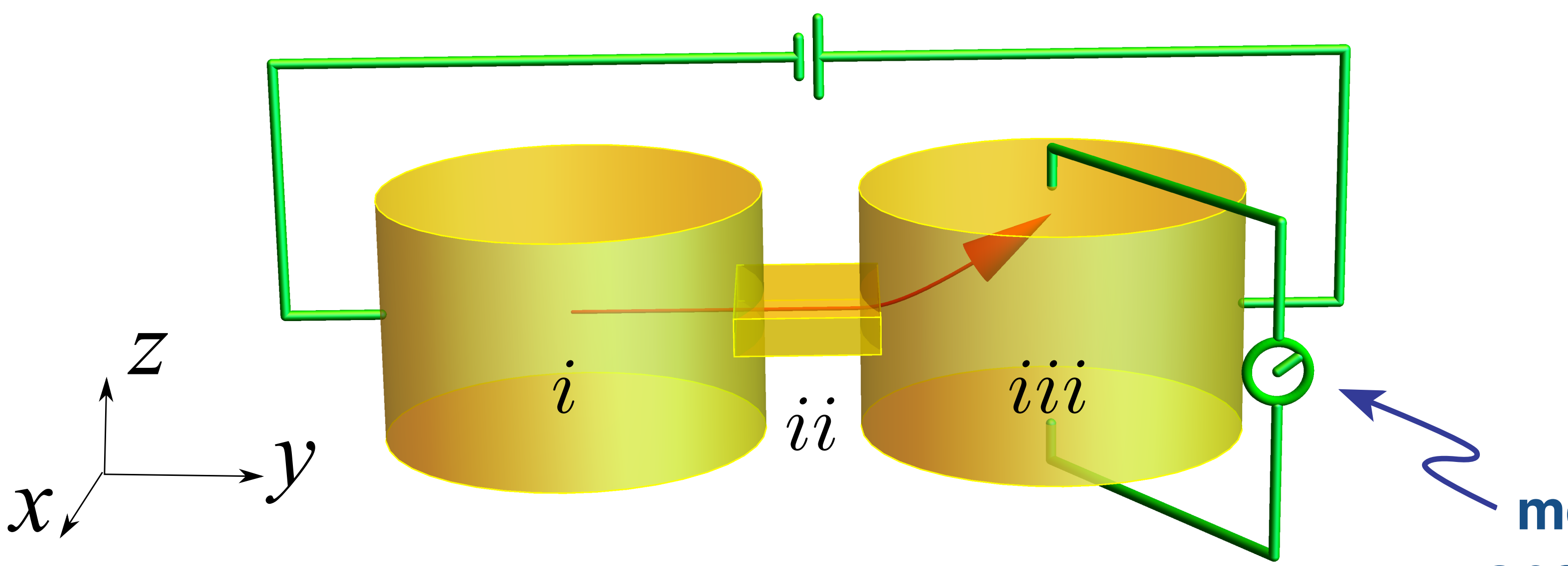
Anomalous current vanishes after integrating over ϕ

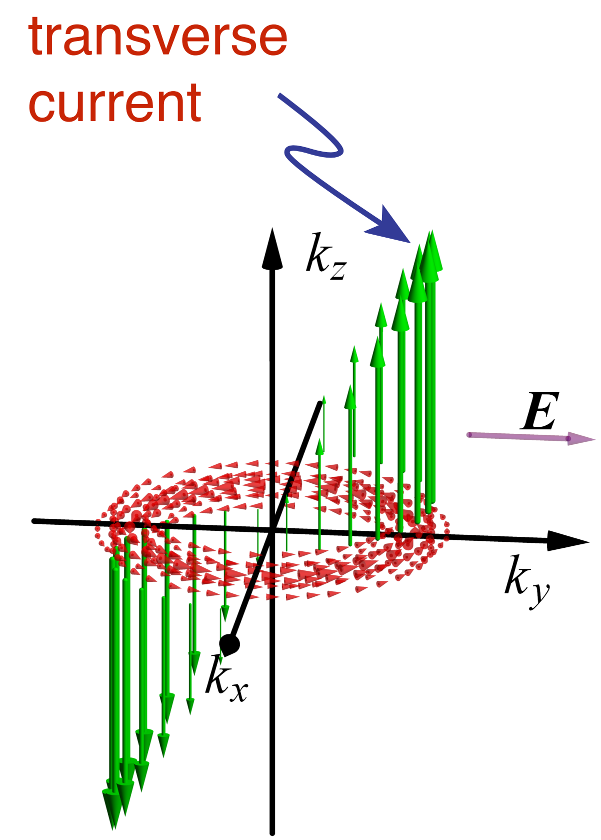
arXiv:1703.05958

Parity anomaly in nodal-line semi-metals

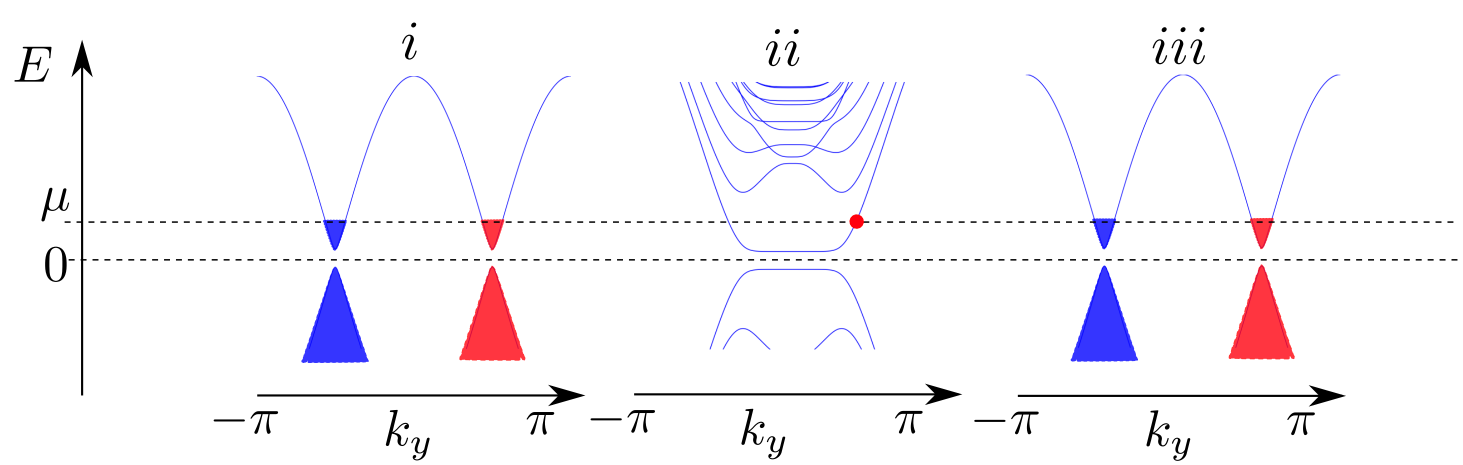
Drumhead surface states as a momentum filter:

- Consider dumbbell geometry:





— band structures for $k_x = 0$:

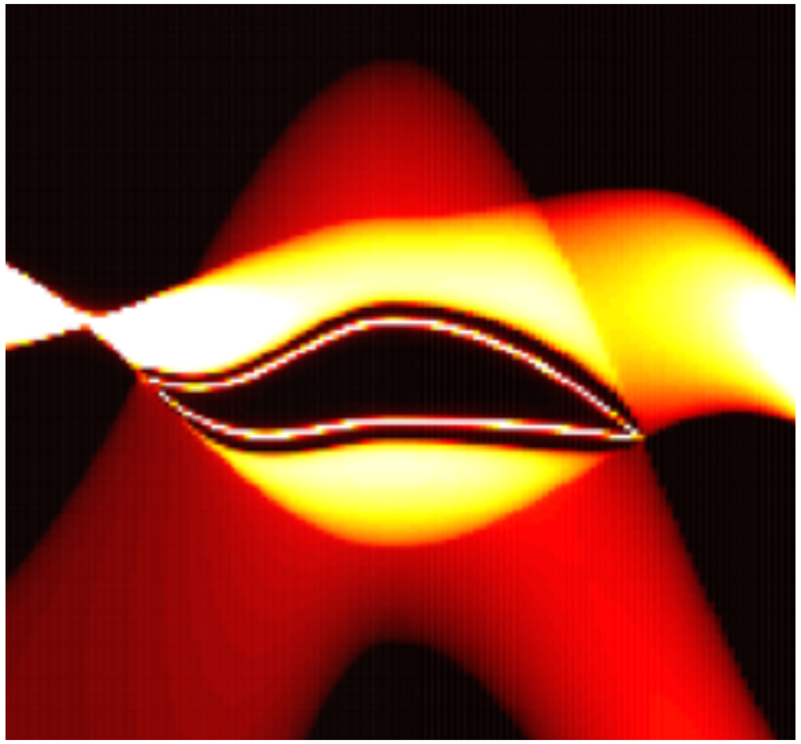


$\Longrightarrow$ Drumhead surface states act as a filter

$\Longrightarrow$ Transverse current can be measured!

arXiv:1703.05958

4. Dirac line nodes protected by non-symmorphic symmetries

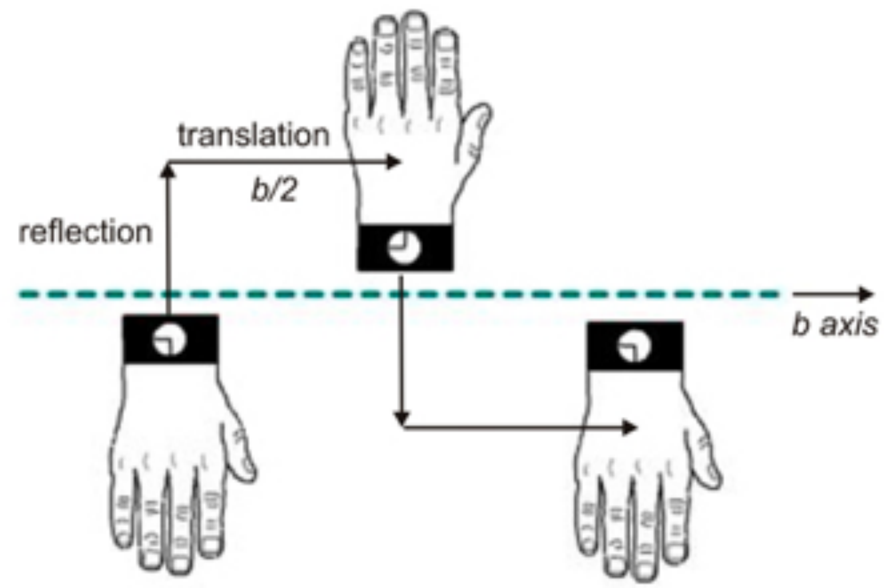


Non-symmorphic symmetries

- Glide reflection
  (rank two):

$$\mathbf{g} = (m|\vec{\tau})$$

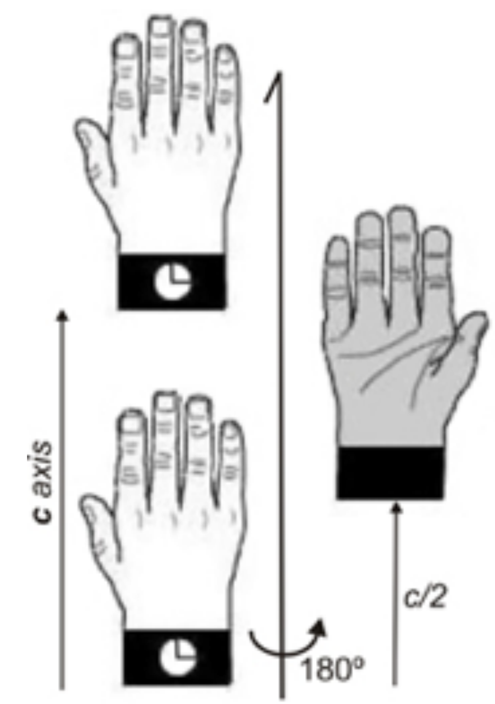
$$\mathbf{g}^2 = T$$



- n-fold screw rotation
  (rank n=2,3,4,6):

$$\mathbf{s}_n = (C_n|\vec{\tau})$$

$$(\mathbf{s}_n)^n = T$$

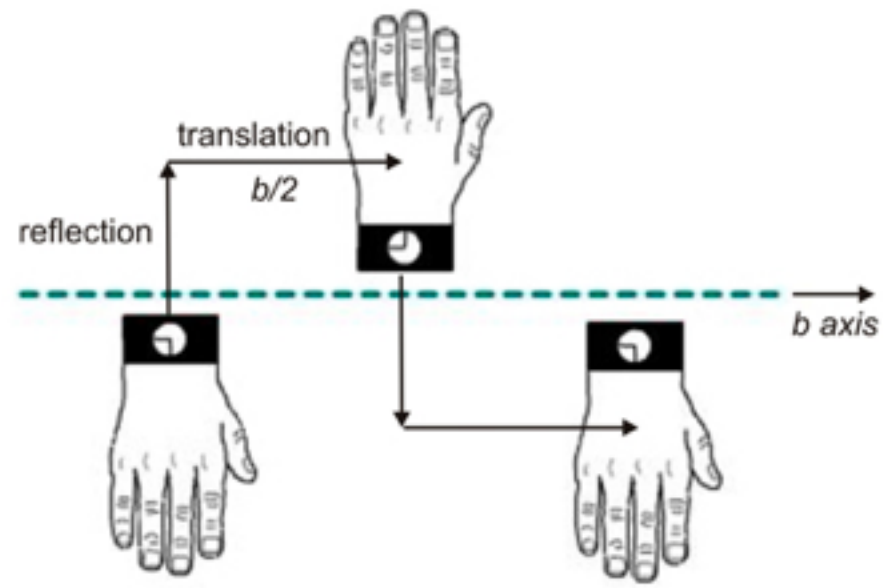


Non-symmorphic symmetries

- Glide reflection (rank two):

$$\mathbf{g} = (m|\vec{\tau})$$

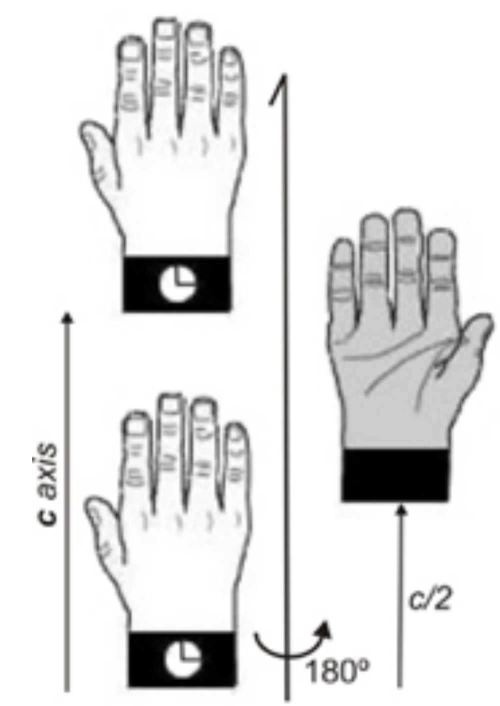
$$\mathbf{g}^2 = T$$



- n-fold screw rotation (rank n=2,3,4,6):

$$\mathbf{s}_n = (C_n|\vec{\tau})$$

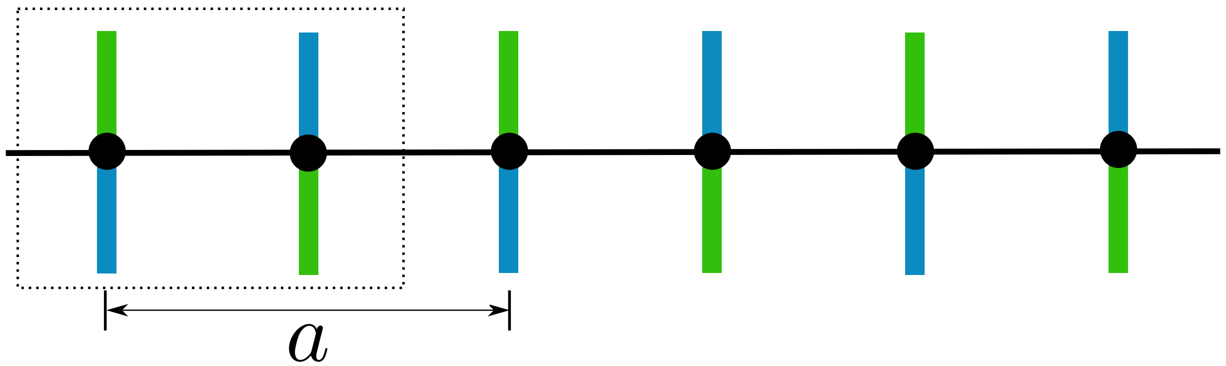
$$(\mathbf{s}_n)^n = T$$



? Can non-symmorphic symmetries impose new constraints on band topology?

Constraints of non-symmorphic symmetry on band structure

- Consider 2-fold screw rotation in 1D:



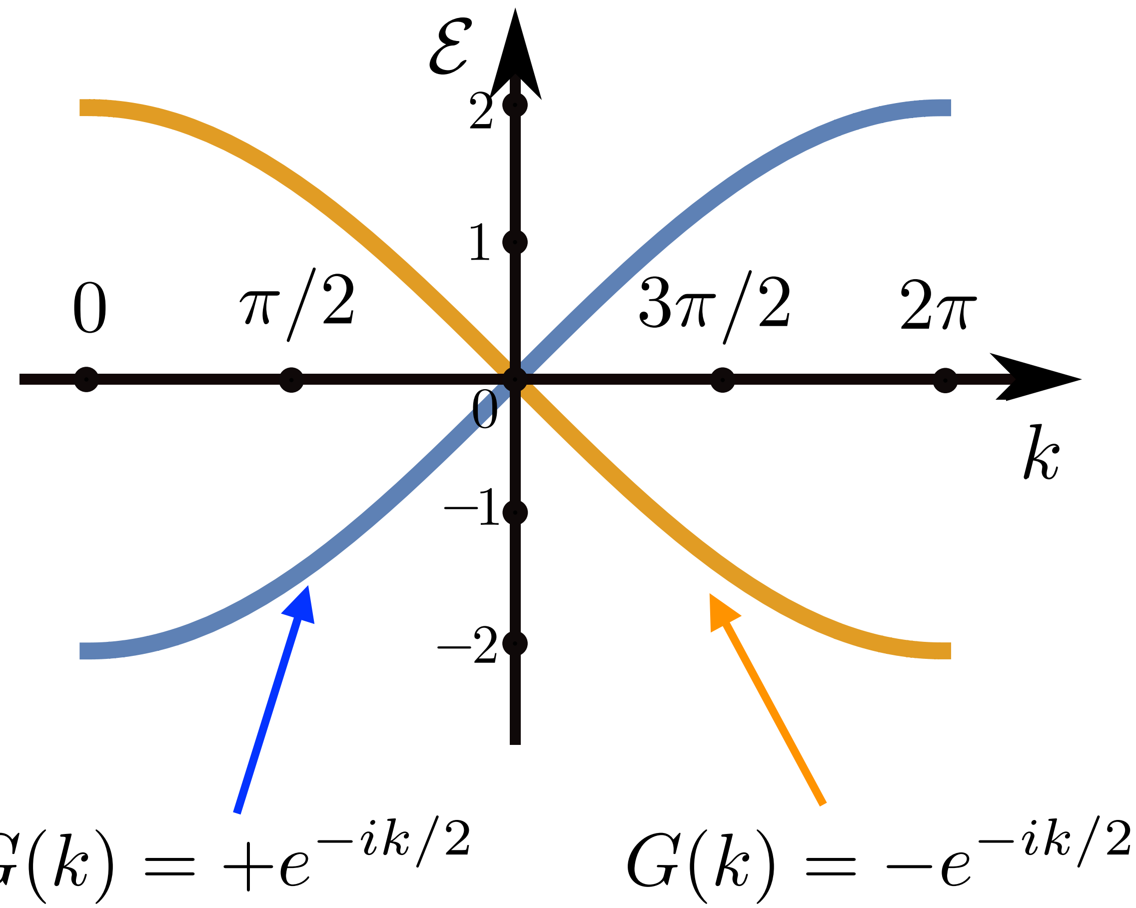
$$G(k) = \begin{pmatrix} 0 & e^{-ik} \\ 1 & 0 \end{pmatrix} \qquad G(k)\mathcal{H}(k)G^{-1}(k) = \mathcal{H}(k)$$

- Since $G^2(k) = e^{-ik}\sigma_0$

$\Longrightarrow$ EVs are $\pm e^{-ik/2}$

$\Longrightarrow$ states switch positions

$\Longrightarrow$ band crossing required by non-symmorphic symmetry



2-fold screw rotation in 1D

PRB 94, 195109 (2016)

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

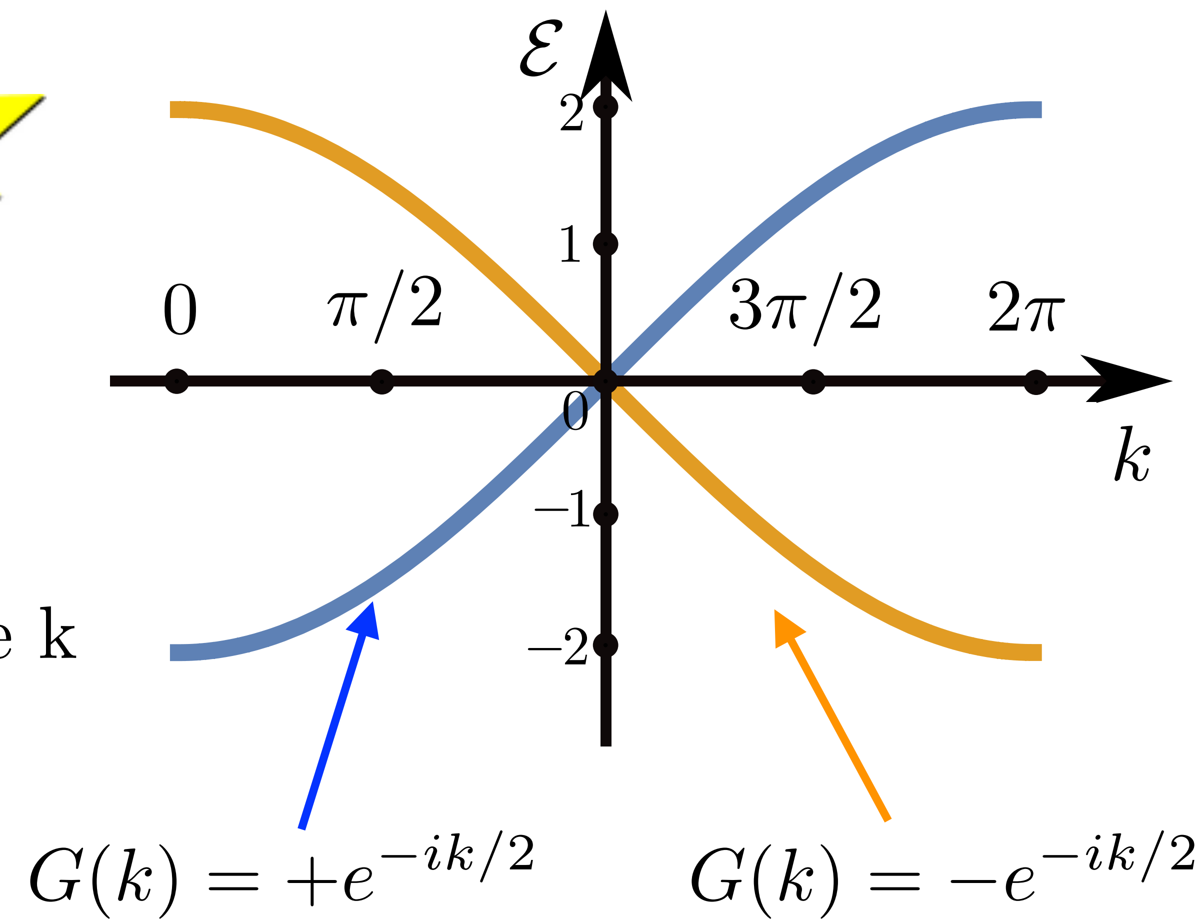
$$G(k) \text{ anti-commutes with } \sigma_3 \quad \Rightarrow \quad H(k) = \begin{pmatrix} o & q(k) \\ q^*(k) & 0 \end{pmatrix}$$

- symmetry constraint: $\quad q(k)e^{ik} = q^*(k) \qquad (\star)$

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

$$(\star) \quad \Rightarrow \quad z = \frac{f^*(z)}{f(z)}$$

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



$\Longrightarrow \qquad$ By contradiction $q(k) = 0$ at some k

$\Longrightarrow \qquad$ band crossing btw 0 and 2π

2-fold screw rotation in 1D

PRB 94, 195109 (2016)

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

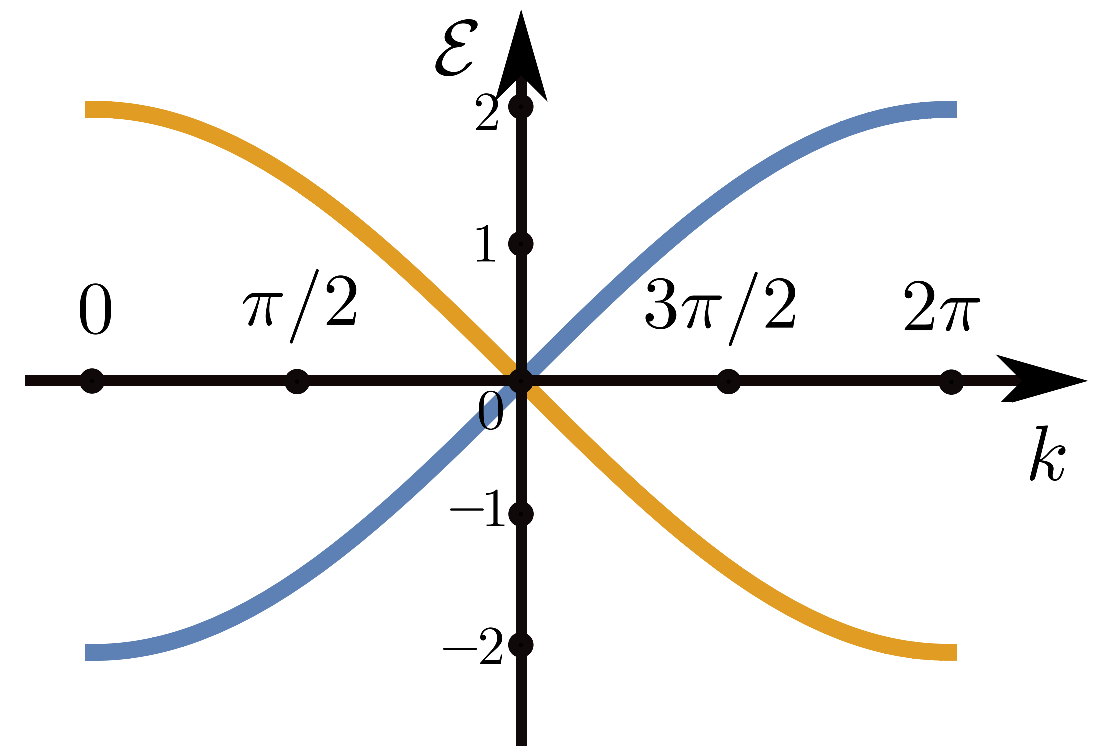
$$G(k) \text{ anti-commutes with } \sigma_3 \quad \Rightarrow \quad H(k) = \begin{pmatrix} o & q(k) \\ q^*(k) & 0 \end{pmatrix}$$

- symmetry constraint: $\quad q(k)e^{ik} = q^*(k) \qquad (\star)$

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

$$(\star) \quad \Rightarrow \quad z = \frac{f^*(z)}{f(z)}$$

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



$\Longrightarrow$ By contradiction $q(k) = 0$ at some k

$\Longrightarrow$ band crossing btw 0 and 2π

NOTE 1: Holds also for multi-band systems with chiral sym. $(q(k) = \mathrm{Det}[\Delta(k)])$

2-fold screw rotation in 1D

PRB 94, 195109 (2016)

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

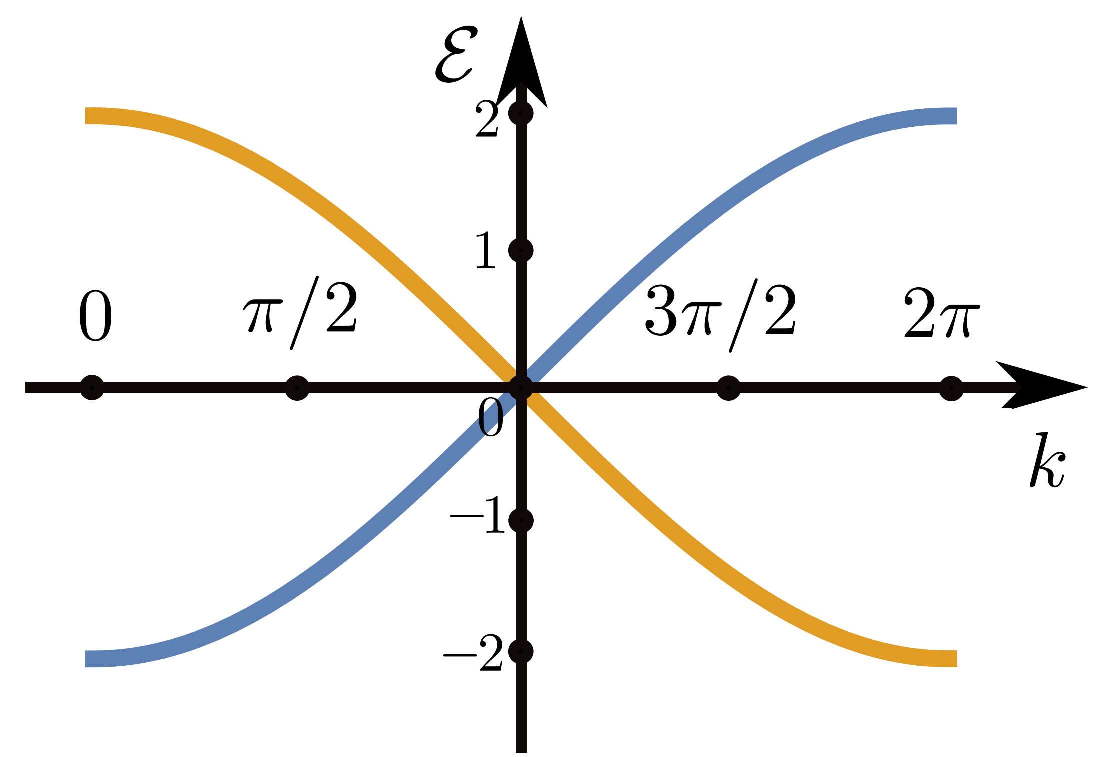
$$G(k) \text{ anti-commutes with } \sigma_3 \quad \Rightarrow \quad H(k) = \begin{pmatrix} o & q(k) \\ q^*(k) & 0 \end{pmatrix}$$

- symmetry constraint: $\quad q(k)e^{ik} = q^*(k) \qquad (\star)$

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

$$(\star) \quad \Rightarrow \quad z = \frac{f^*(z)}{f(z)}$$

$$f^*(z)/f(z) = e^{2i\text{Arc}[f(z)]}$$



$\Longrightarrow$ By contradiction $q(k) = 0$ at some k

$\Longrightarrow$ band crossing btw 0 and 2π

NOTE 1: Holds also for multi-band systems with chiral sym. $(q(k) = \text{Det}[\Delta(k)])$

NOTE 2: Position of band crossing point can be anywhere in BZ

2-fold screw rotation & inversion in 1D

PRB 94, 195109 (2016)

- Consider 2-fold screw rotation *G* and inversion $\hat{P}$

(i) $\hat{P}$ and G anti-commute, $\hat{P}G(k)\hat{P}^{-1} = -G(-k)$:

$$\Longrightarrow q(k) = -q^*(-k), \qquad q(k) = \sum_{n=0}^{\infty} \frac{\lambda_n}{i} \left(e^{ink} - e^{-i(n+1)k} \right)$$

$\Longrightarrow$ band crossing at $k = 0$

(ii) $\hat{P}$ and G commute, $\hat{P}G(k)\hat{P}^{-1} = +G(-k)$:

$$\Longrightarrow q(k) = +q^*(-k), \qquad q(k) = \sum_{n=0}^{\infty} \lambda_n \left(e^{ink} + e^{-i(n+1)k} \right)$$

$\Longrightarrow$ band crossing at $k = \pi$

Position	$G, \hat{P}$
$k = 0$	$\hat{P}G = -G^\dagger \hat{P}$
$k = \pi$	$\hat{P}G = G^\dagger \hat{P}$

$CuBi_2O_4$: Dirac ring protected by glide reflection

- anti-ferromagnetic insulator w/ space group #56.367 (Pc'cn)
- Important symmetries:
  - time-reversal ∗ inversion: $(PT)^2 = -1$

    $\Rightarrow$ all bands doubly degenerate $|\psi(k)\rangle, PT|\psi(k)\rangle$
  - glide reflection: $\{R_x, \tau = (1/2, 0, 1/2)\}$

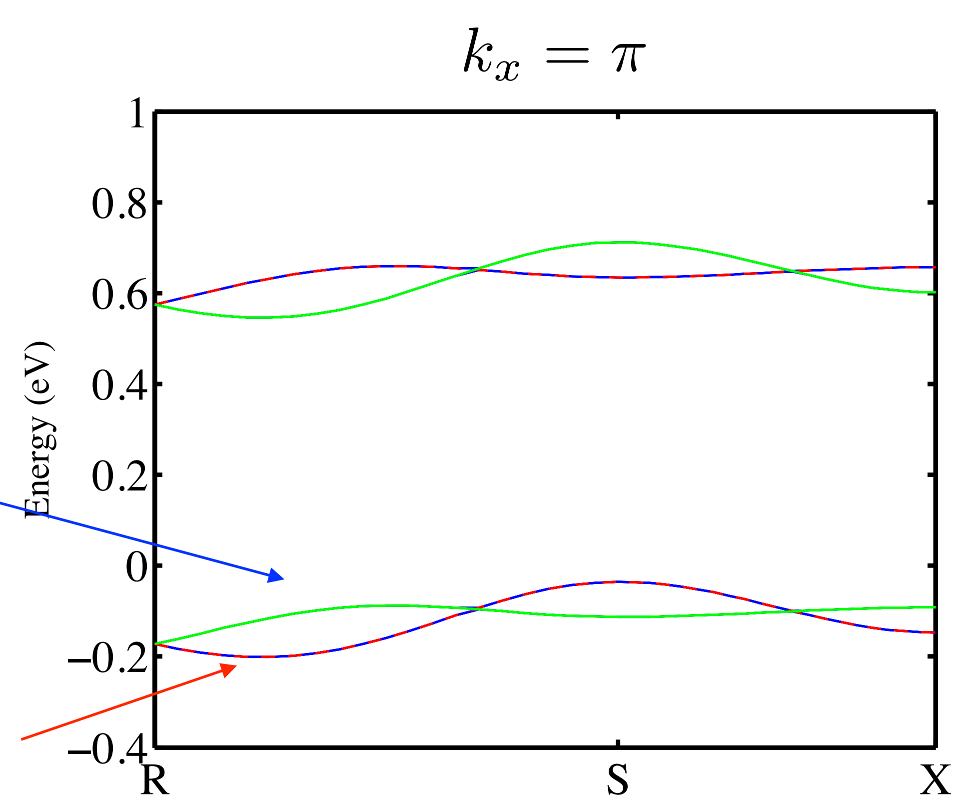
    $\Rightarrow$ 4-fold degenerate Dirac ring at $k_x = \pi$

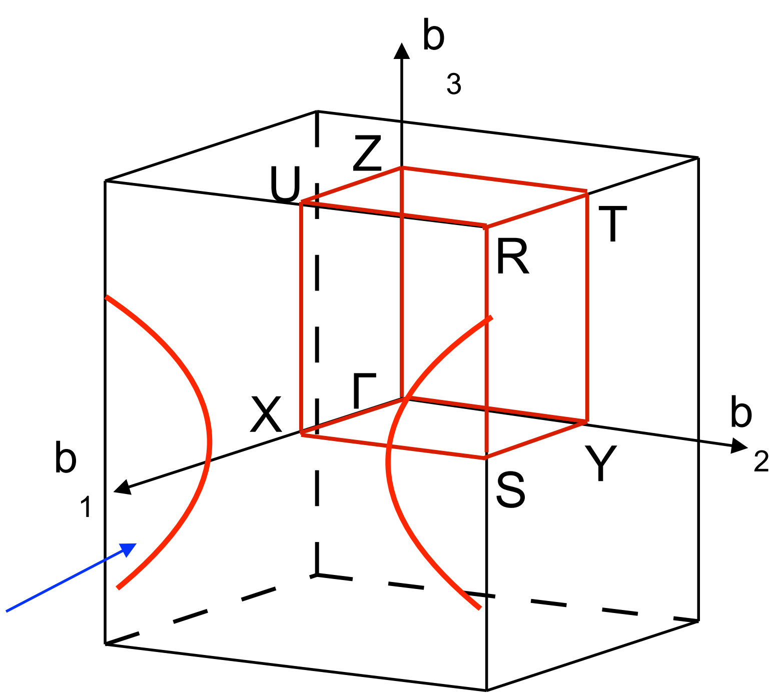
$[R_x, PT]=0$ $\Rightarrow$ band crossing at $k_x = \pi$

$R_x = \pm i e^{ik_z/2}$

$R_x = i e^{ik_z/2}$

$R_x = -i e^{ik_z/2}$

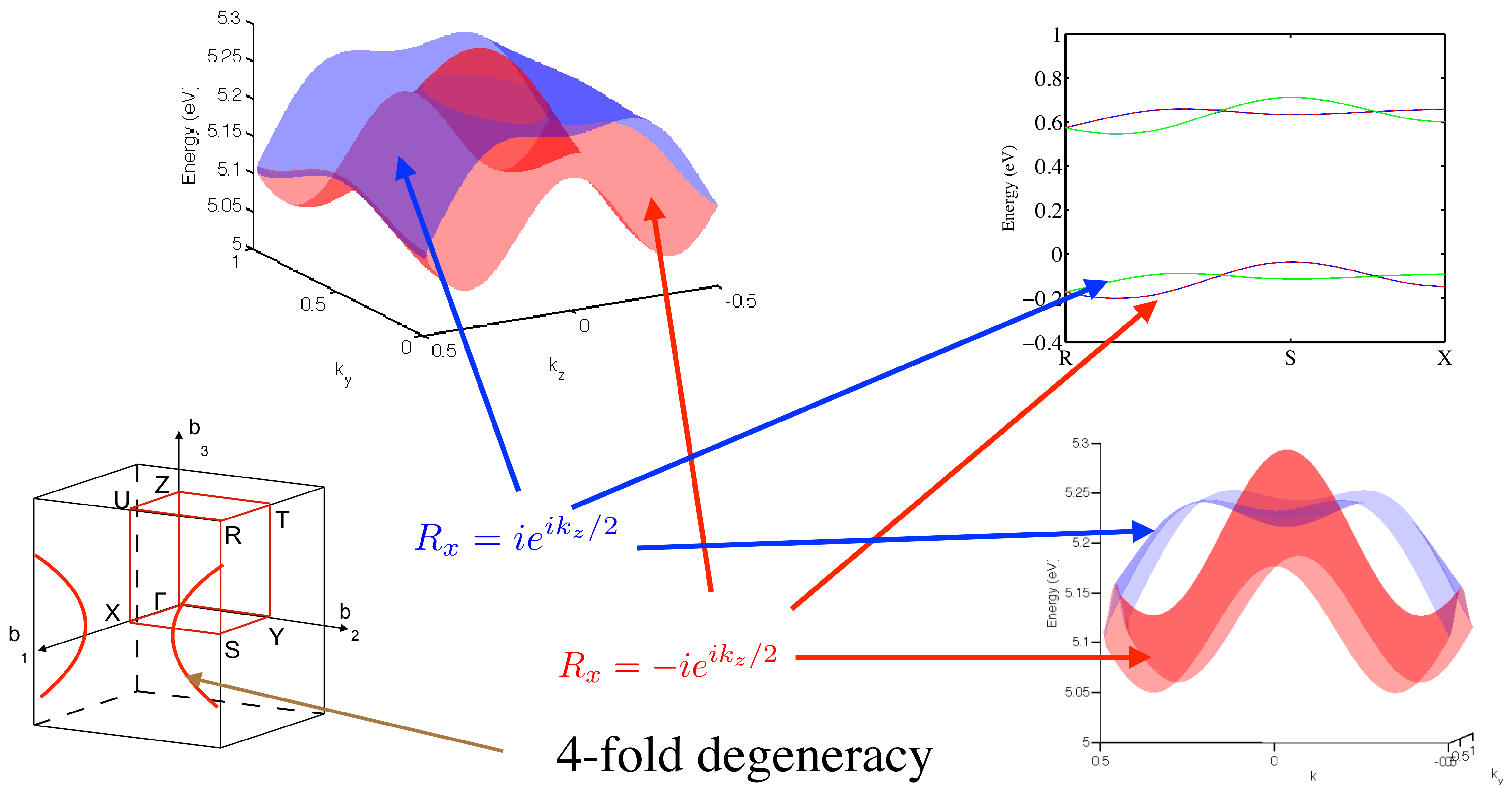




Dirac ring

$CuBi_2O_4$: Dirac ring protected by glide reflection

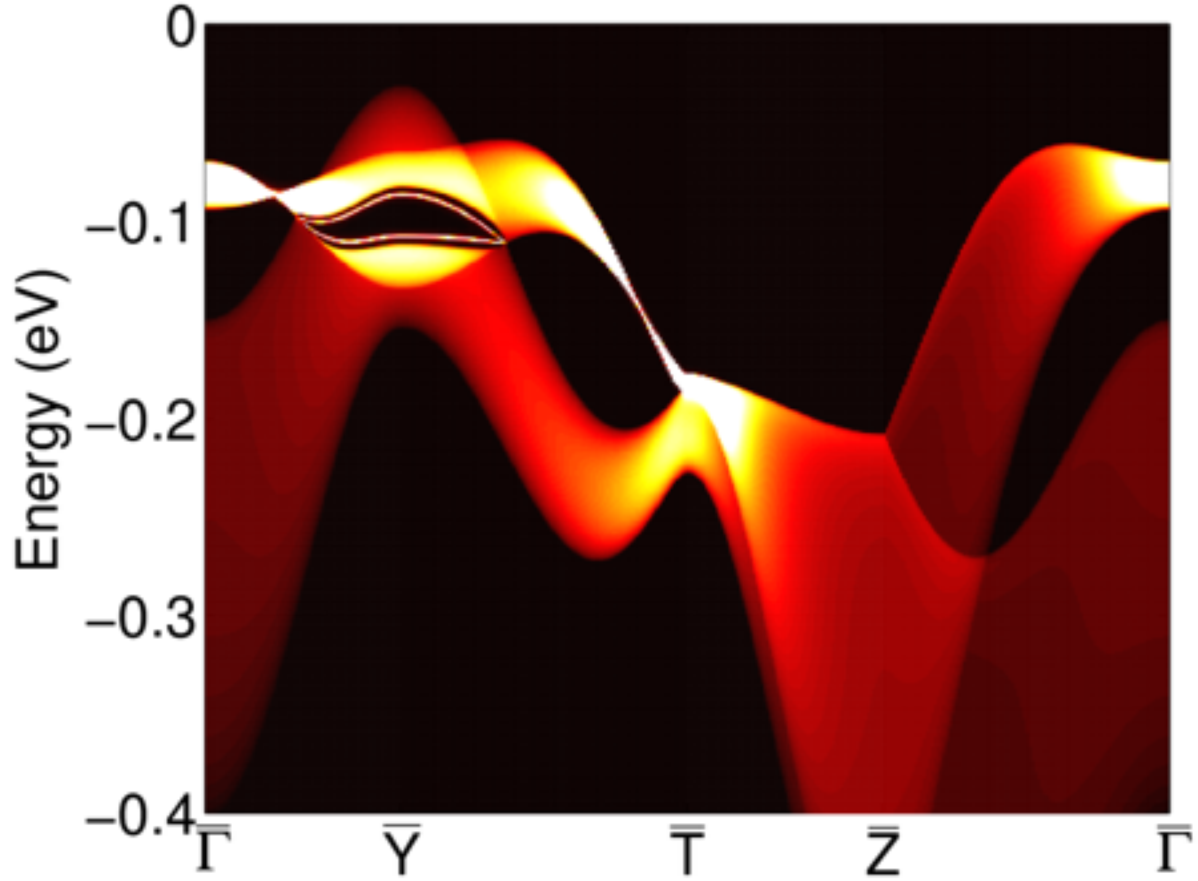
- 4-fold degenerate ring protected by PT and glide reflection

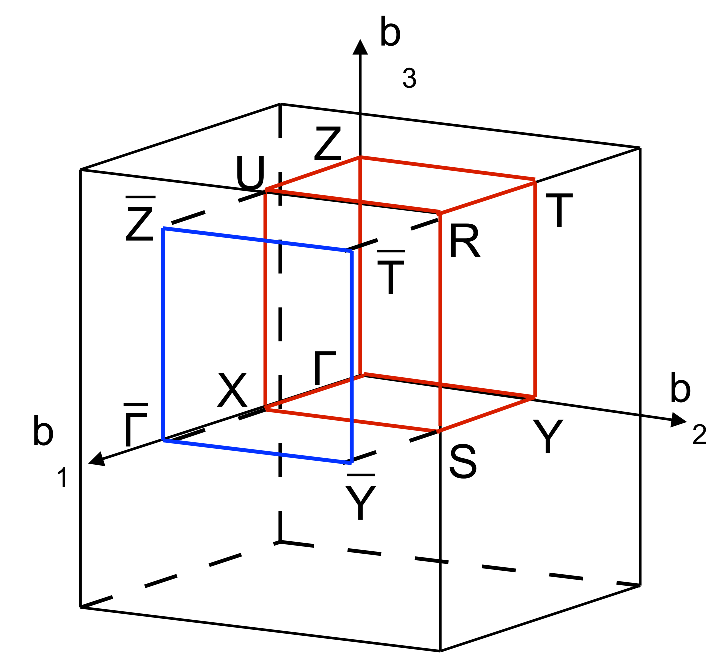


$CuBi_2O_4$: Double drumhead surface states

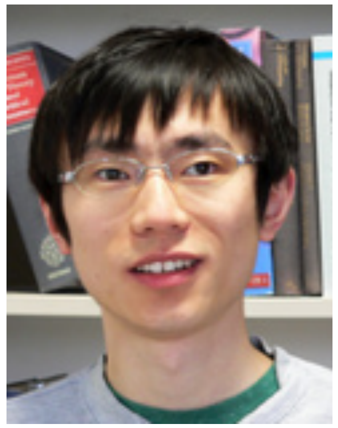
- *Double drumhead surface states* bound by Dirac ring

(100) surface

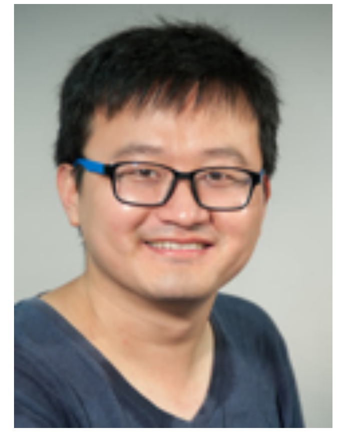




Acknowledgments



Yuxin Zhao
(MPI-FKF/Nanjing)



Wenbin Rui
(MPI-FKF)

M. Hirschmann
(MPI-FKF)

Xue-Yang Song
(U Peking)

Yang-Hao Chan
(A. Sinica, Taiwan)

Ching-Kai Chiu
(Uni Maryland)

Conclusions and Outlook

- Classification of crystalline topological materials
  - w/ reflection symmetry
  - w/ PT and CP symmetry

PRB 90, 205136 (2014)

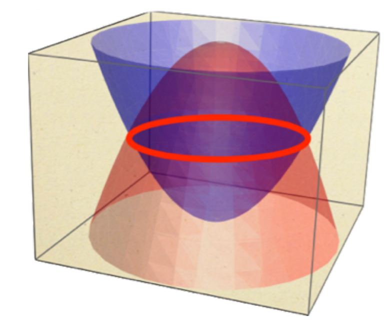
PRL 116, 156402 (2016)

PRB 95, 195108 (2017)

Reflection	TI/TSC	d=1	d=2	d=3	d=4	d=5	d=6	d=7	d=8
	FS1	p=8	p=1	p=2	p=3	p=4	p=5	p=6	p=7
	FS2	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	$M\mathbb{Z}_2$	$M\mathbb{Z}$	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

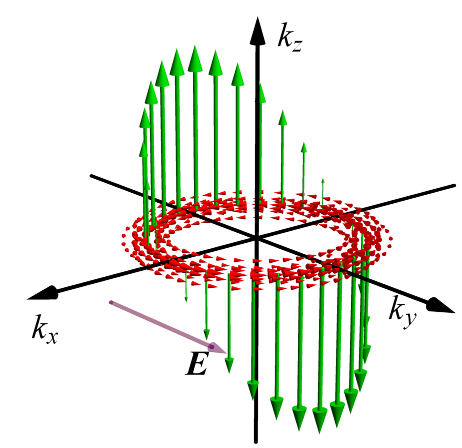
- Topological nodal line semimetals
  - Drumhead surface states Ca_3P_2, Zr_5Si_3

PRB 93, 205132 (2016) **PRL 116, 156402 (2016)**



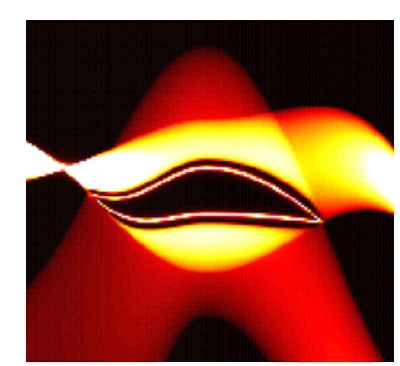
- Quantum anomalies in nodal-line semimetals
  - Parity anomaly & anomalous transport

arXiv:1703.05958



- Dirac line nodes with non-symmorphic symmetries
  - $CuBi_2O_4$

to be published



Review article:
Rev. Mod. Phys 88, 035005 (2016)