Z. Song, Z. Fang and CF, PRL 119, 246402 (2017)
CF and L. Fu, arXiv:1709.01929
Z. Song, T. Zhang, Z. Fang and CF arXiv:1711.11049
Z. Song, T. Zhang and CF arXiv:1711.11050

Quantitative Mappings from Symmetry to Topology

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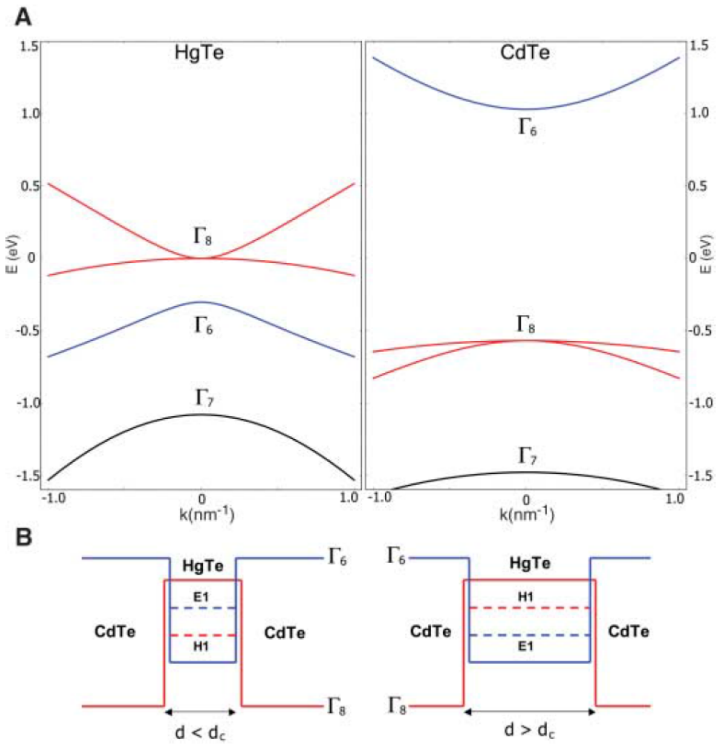
May. 5th, 2018

Symmetries in band structures

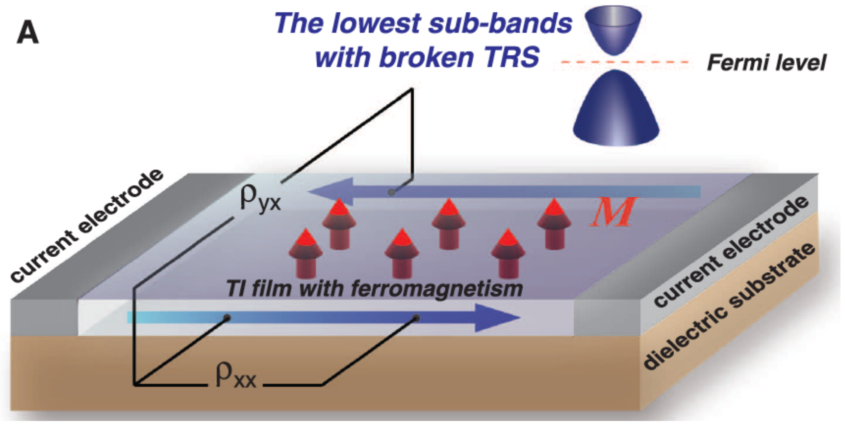
- Theory of crystallographic space groups: 32 point groups, 230 space groups and 1651 magnetic groups in 3D.
- Representation theory in band structures: each band is an irreducible representation of the little group at a given momentum.
- Symmetry data can be routinely extracted ab intio, i. e., a SOLVED problem.



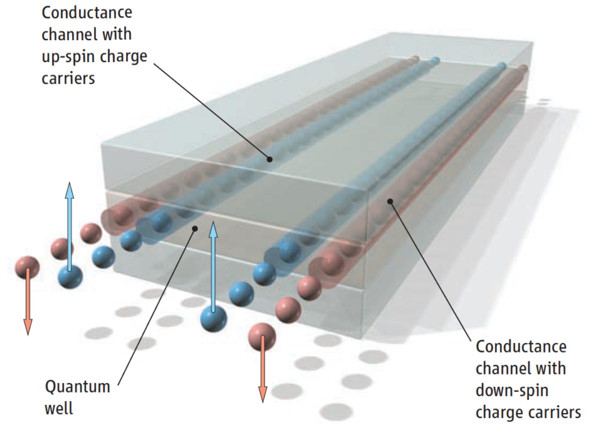
Bernevig et al, Science 2006

Topology in band structures

- Chern insulators
- Topological insulators protected by time-reversal symmetry
- Topological crystalline insulators

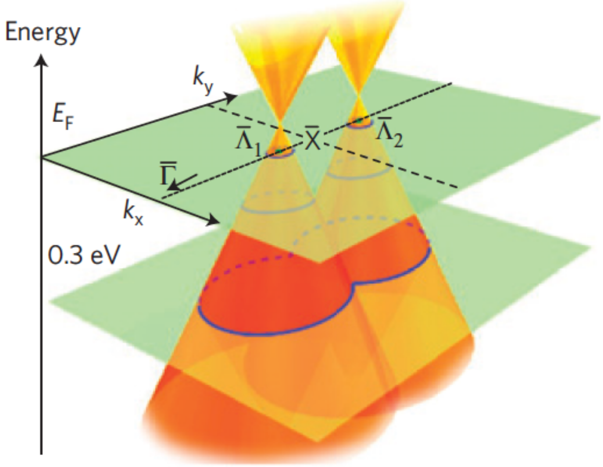


Chang et al, Science 2013



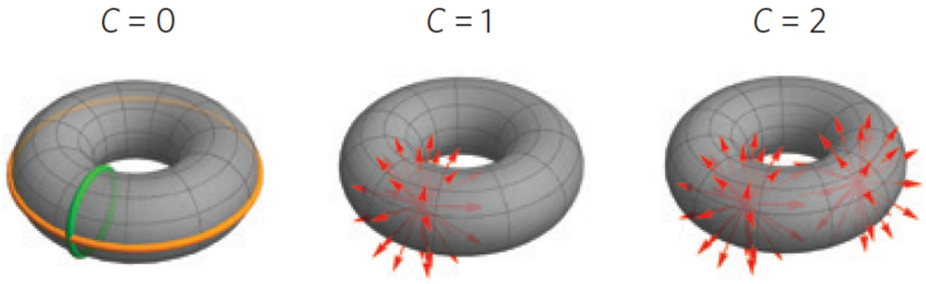
Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

Konig et al, Science 2007



Tanaka et al, Nat Phys 2012
Dziawa et al, Nat Mat 2012
Xu et al, Nat Comm 2012

Quantified topology: topological invariants



- Chern number (TKNN number)

$$i\int dk^2(\partial_x u^*\partial_y u - \partial_y u^*\partial_x u)$$

- Z_2-index in TI: $(-1)^{\xi} = \Pi_{K\in TRIM} Pf[W(K)]$
- Various invariants in TCI
  - Mirror Chern number: $i\int dk^2(\partial_x u_M^*\partial_y u_M - \partial_y u_M^*\partial_x u_M)$
  - Glide-plane Z_2-index Fang and Fu 2015, Shiozaki et al 2015

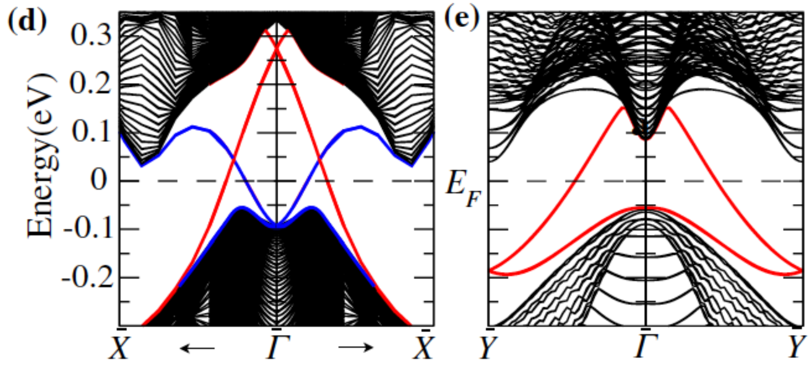
$$\sum_{j=1,\dots,N_{occ}/2}\log(\lambda^I_{j+}) + B^I_+ = \sum_{j=1,\dots,N_{occ}/2}\log(\lambda^I_{j-}) + 2n_I\pi \qquad \sum_{j=1,\dots,N_{occ}/2}\log(\lambda^{II}_{j+}) + B^{II}_+ = \sum_{j=1,\dots,N_{occ}/2}\log(\lambda^{II}_{j-}) + 2n_{II}\pi$$

$$\sum_{j=1,\dots,N_{occ}/2}[\log(\lambda^I_{j+}) + \log(\lambda^I_{j-})] + B_0 = \sum_{j=1,\dots,N_{occ}/2}[\log(\lambda^{II}_{j+}) + \log(\lambda^{II}_{j-})] + 2n_0\pi \qquad z_2 = (n_I + n_{II} + n_0) \bmod 2$$

  - Rotation Z_2, inversion Z_2, screw axis Z_2, S_4 Z_2···

Introducing topological invariants of TCI

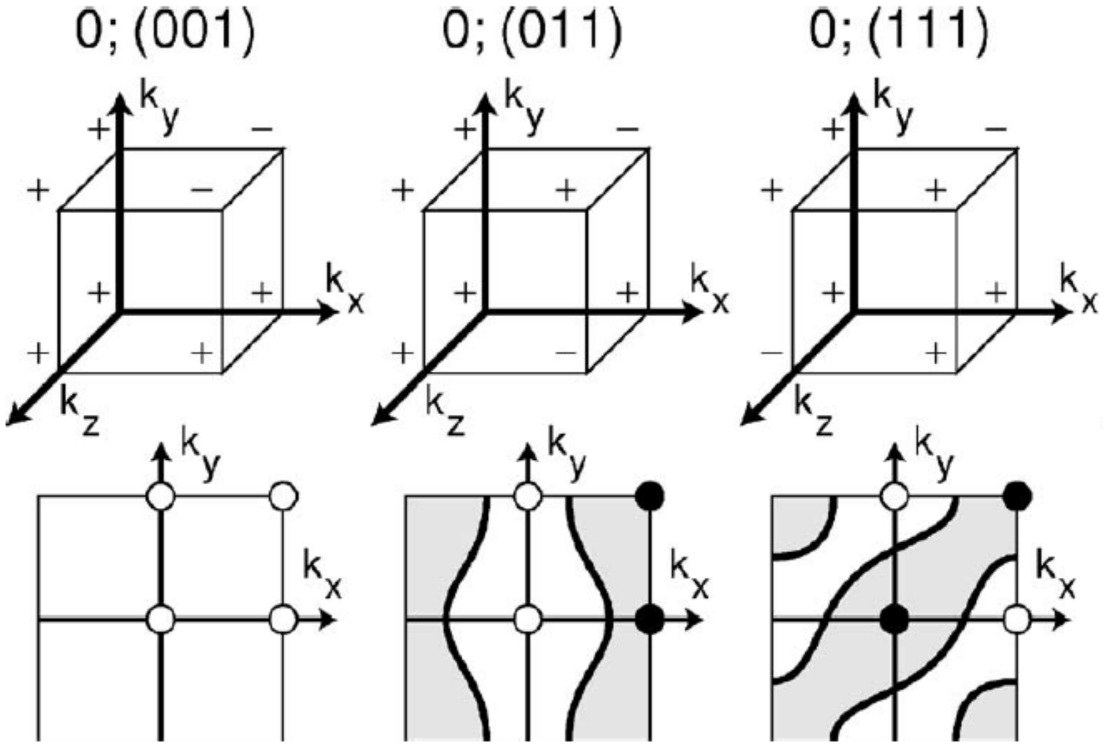
- Weak Z_2-indices (weak TI)
  - Symmetry: translation and time-reversal
  - Up to three indices
  - Surface: two Dirac cones



$ZrTe_5$

Theory: Weng et al PRX 2014

Experiment: Wu et al PRX 2016

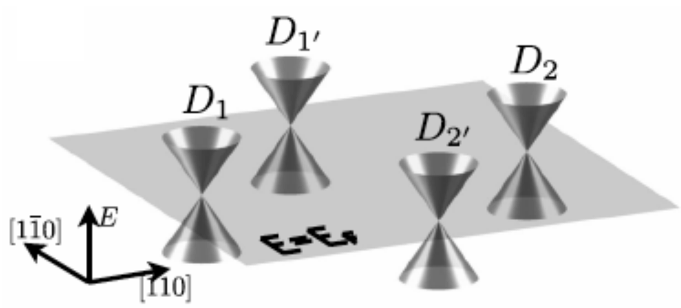


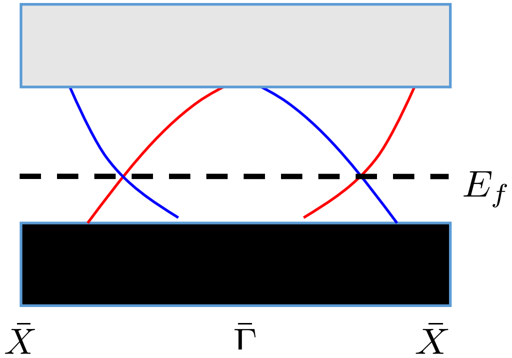
Fu and Kane, PRB 2007

Introducing topological invariants of TCI

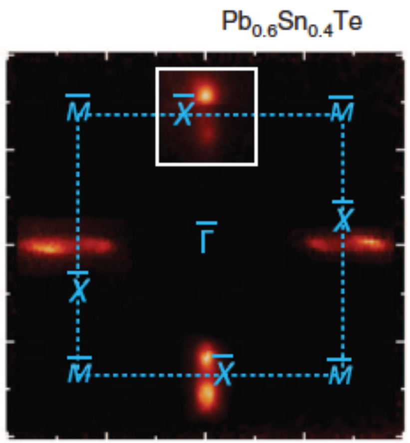
- Mirror Chern number protected by mirror plane and time-reversal

$$[H(k_x, 0, k_z), M_{xz}] = 0 \Rightarrow H(k_x, 0, k_z) = \left[\begin{array}{c:c} H_{+i} & 0 \\ \hdashline 0 & H_{-i} \end{array}\right] \Rightarrow \begin{array}{l} C_{+i} : \text{Chern number of } H_{+i} \\ C_{-i} : \text{Chern number of } H_{-i} \end{array}$$





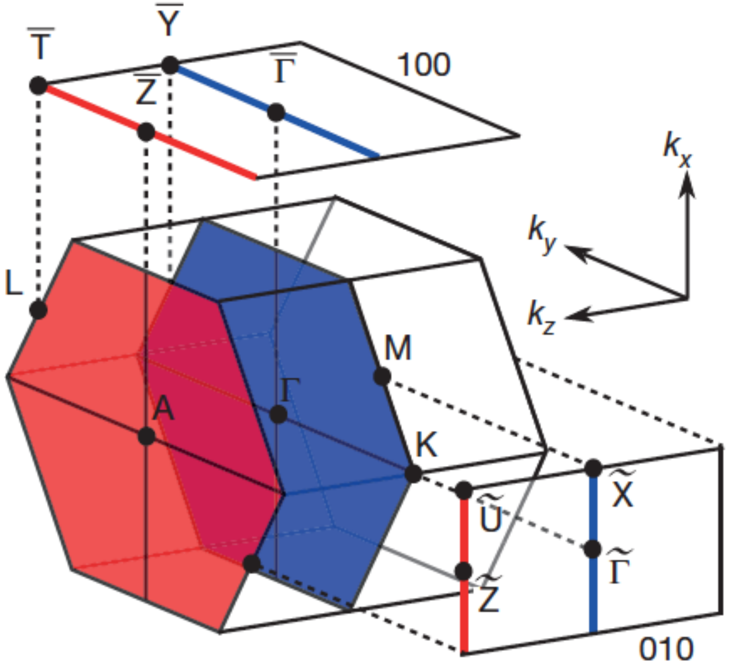
$$C_{+i} = +2,$$
$$C_{-i} = -2.$$

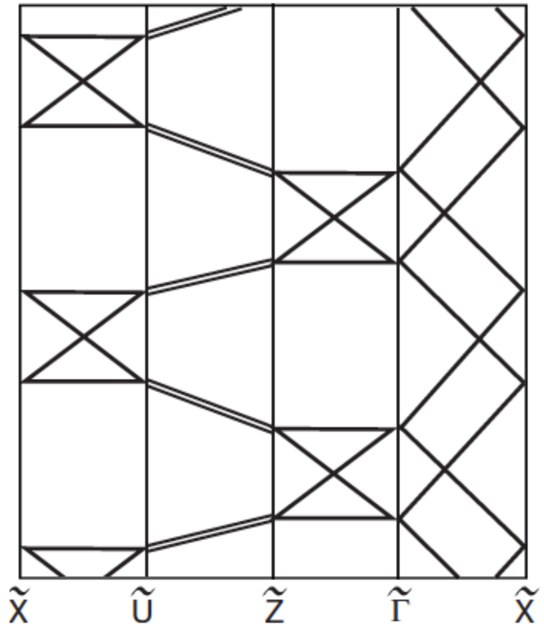


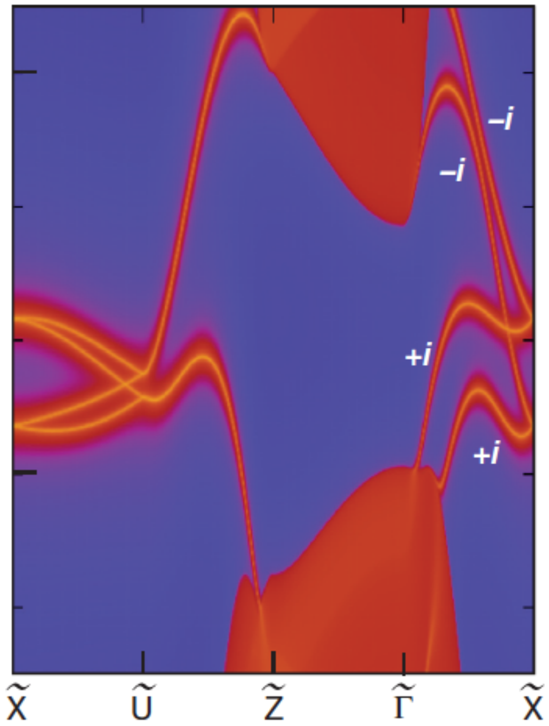
Hsieh et al, Nat Comm 2012
Dziawa et al, Nat Mat 2012
Tanaka et al, Nat Phys 2012
Xu et al, Nat Comm 2012

Introducing topological invariants of TCI

- Glide plane Z_2 protected by glide plane and time-reversal





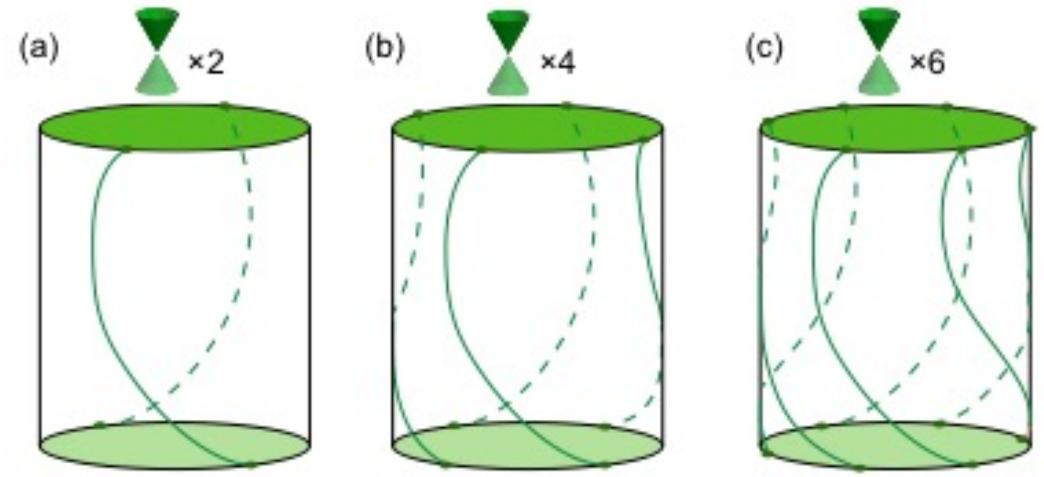


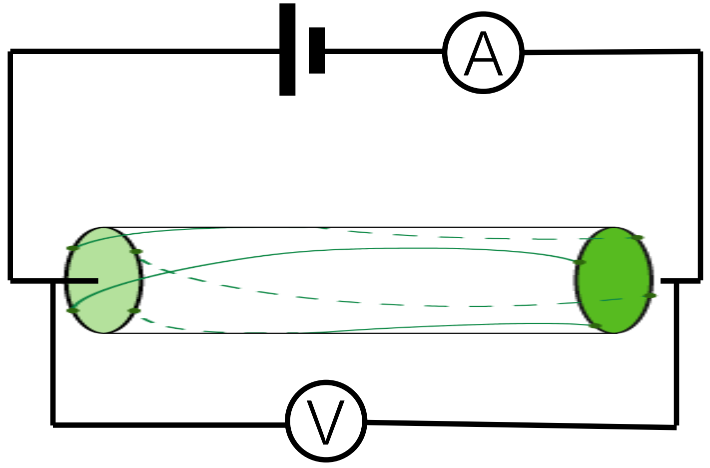
Theory: Wang et al, Nature 2016
Experiment: Ma et al, Sci Adv 2017

Song, Fang and CF, PRL 2017
CF and Fu, arXiv:1709.01929

Introducing topological invariants of TCI

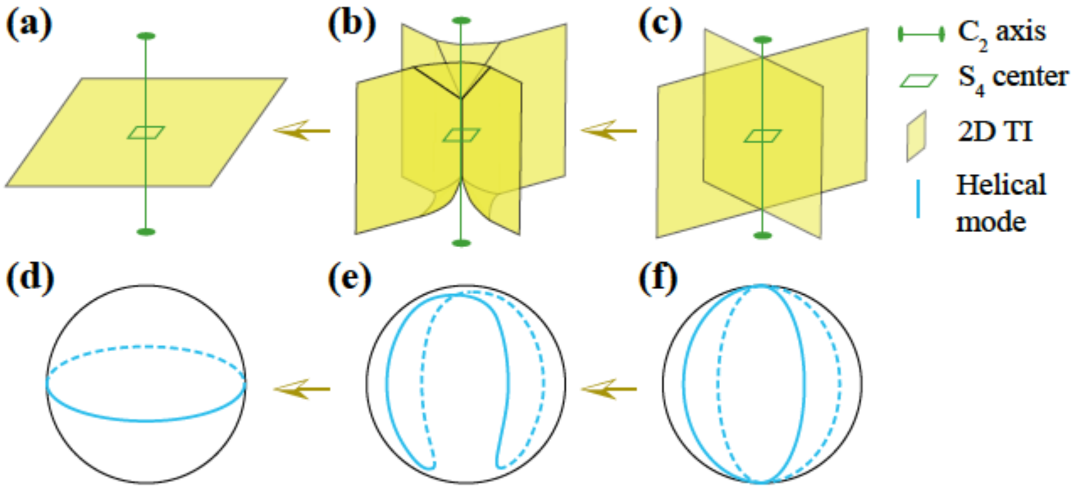
- Z_2-invariants protected by $C_{2,4,6}$-fold rotation plus time-reversal
  - Bulk invariants do not have close form
  - 2D Dirac cones on the top and bottom
  - 1D helical states on the side
- Z_2-invariants protected by 2-, 4-, 6-fold screw axes plus time-reversal
  - No Dirac cones, just helical states on the side

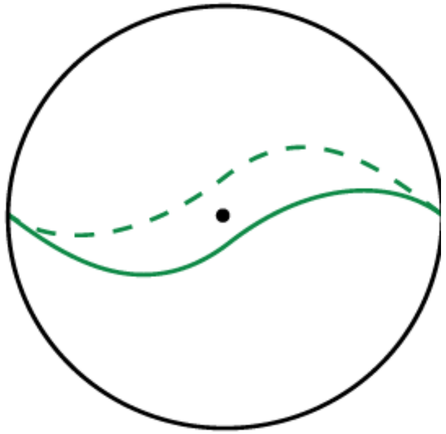




Introducing topological invariants of TCI

- Z_2-invariant protected by $S_4: (x, y, z) \to (-y, x, -z)$ and time-reversal   Song et al, arXiv:1711.11049, Khalaf et al, arXiv 2017
- Z_2-invariant protected by inversion $S_2: (x, y, z) \to (-x, -y, -z)$ and time-reversal   Turner et al 2010, Hughes et al 2011, CF and Fu, arXiv:1709.01929
- These are examples of "high order TI"





Fu-Kane formula and alike

- Fu-Kane formula maps inversion eigenvalues to invariants in TI

$$z_2 = \sum_{K \in \mathrm{TRIM}} \frac{[N^+(K) - N^-(K)]}{2} \ \mathbf{mod}\ 2$$

Fu and Kane PRL 2007

- There are also formulas mapping rotation eigenvalues to Chern numbers

$$(-1)^C = \prod_{i \in \mathrm{occ.}} \zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M)$$

$$i^C = \prod_{i \in \mathrm{occ.}} (-1)^F \xi_i(\Gamma)\xi_i(M)\zeta_i(Y)$$

$$e^{i2\pi C/3} = \prod_{i \in \mathrm{occ.}} (-1)^F \theta_i(\Gamma)\theta_i(K)\theta_i(K'),$$

$$e^{i\pi C/3} = \prod_{i \in \mathrm{occ.}} (-1)^F \eta_i(\Gamma)\theta_i(K)\zeta_i(M),$$

Fang et al PRB 2012

Generalized Fu-Kane formula?

- An invariant protected by group S cannot be represented by the eigenvalues of S, but may be represented by the eigenvalues of G, where $S \subset G$.
- A general mapping from symmetry eigenvalues of G to the topological invariants or topological nodes protected by S may greatly enhance the efficiency of the search of new topological materials.

Symmetry data of G $\Rightarrow$ Topological invariants of S

Two theoretical tools:

1. Symmetry-based indicators (lossless compression of symmetry data)
2. Layer construction (fixed point wave functions of 3D TCI)

Lossless compression of symmetry data

Symmetry data of space group 225: 11 integers Z^{11}

k point	irreducible representations
Γ	$2E_{\frac{1}{2}g} + E_{\frac{1}{2}u} + F_{\frac{3}{2}u}$
L	$E_{\frac{3}{2}g} + 2E_{\frac{1}{2}g} + 2E_{\frac{1}{2}u}$
W	$2E_{\frac{3}{2}} + 3E_{\frac{1}{2}}$
X	$2E_{\frac{1}{2}g} + 2E_{\frac{1}{2}u} + E_{\frac{3}{2}u}$

Symmetry data from VASP for SnTe

Symmetry indicator of 225: Z_8

$$Z_8 = 4$$

Po et al, Nat Comm 2017
Bradlyn et al, Nature 2017

Symmetry-based indicators $X_{BS} = \{BS\}/\{AI\}$

Without SOC (spinless)

Table 4 Symmetry-based indicators of band topology for systems with time-reversal symmetry and negligible spin-orbit coupling

X_{BS}	Space groups
$\mathbb{Z}_2$	3, 11, 14, 27, 37, 48, 49, 50, 52, 53, 54, 56, 58, 60, 66, 68, 70, 75, 77, 82, 85, 86, 88, 103, 124, 128, 130, 162, 163, 164, 165, 166, 167, 168, 171, 172, 176, 184, 192, 201, 203
$\mathbb{Z}_2 \times \mathbb{Z}_2$	12, 13, 15, 81, 84, 87
$\mathbb{Z}_2 \times \mathbb{Z}_4$	147, 148
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	10, 83, 175
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	2

X_{BS} the quotient group between the group of band structures and that of atomic insulators

Lossless compression of symmetry data as far as topology is concerned:
1. Nonzero indicator -> Not an AI
2. Different indicators -> different topologies
3. Same indicators -> cannot distinguish their topologies using symmetry eigenvalues

With SOC (spinful)

Table 3 Symmetry-based indicators of band topology for systems with time-reversal symmetry and significant spin-orbit coupling

X_{BS}	Space groups
$\mathbb{Z}_2$	81, 82, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 215, 216, 217, 218, 219, 220
$\mathbb{Z}_3$	188, 190
$\mathbb{Z}_4$	52, 56, 58, 60, 61, 62, 70, 88, 126, 130, 133, 135, 136, 137, 138, 141, 142, 163, 165, 167, 202, 203, 205, 222, 223, 227, 228, 230
$\mathbb{Z}_8$	128, 225, 226
$\mathbb{Z}_{12}$	176, 192, 193, 194
$\mathbb{Z}_2 \times \mathbb{Z}_4$	14, 15, 48, 50, 53, 54, 55, 57, 59, 63, 64, 66, 68, 71, 72, 73, 74, 84, 85, 86, 125, 129, 131, 132, 134, 147, 148, 162, 164, 166, 200, 201, 204, 206, 224
$\mathbb{Z}_2 \times \mathbb{Z}_8$	87, 124, 139, 140, 229
$\mathbb{Z}_3 \times \mathbb{Z}_3$	174, 187, 189
$\mathbb{Z}_4 \times \mathbb{Z}_8$	127, 221
$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	175, 191
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	11, 12, 13, 49, 51, 65, 67, 69
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	83, 123
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$	2, 10, 47

X_{BS} the quotient group between the group of band structures and that of atomic insulators

Remaining questions

- Explicit formulas for the indicators?
- Given a band structure having nonzero indicator, is it a topological (crystalline) insulator or topological semimetal?
- If a TCI, what are the topological invariants?
- If a TSM, what and where are the nodes?

Insulator or semimetal?

- Spinful: in any space group for any nonzero set of indicators, there always exists one corresponding TCI.

- Spinless: in any space group for any nonzero set of indicators, the band structure must be gapless, having nodes at generic momenta.

Mapping indicators to invariants

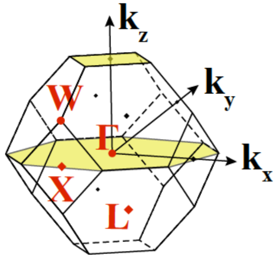
- For each nonzero set of indicators, we list all possible combinations of topological invariants protected by the space group. It is usually a one-to-many mapping.
- Example of SnTe:

k point	irreducible representations
Γ	$2E_{\frac{1}{2}g} + E_{\frac{1}{2}u} + F_{\frac{3}{2}u}$
L	$E_{\frac{3}{2}g} + 2E_{\frac{1}{2}g} + 2E_{\frac{1}{2}u}$
W	$2E_{\frac{3}{2}} + 3E_{\frac{1}{2}}$
X	$2E_{\frac{1}{2}g} + 2E_{\frac{1}{2}u} + E_{\frac{3}{2}u}$

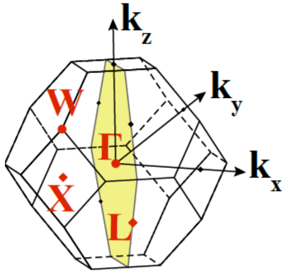
Symmetry data

$Z_8 = 4$

Symmetry indicators



$\delta_{m(001)}=4$
$\delta_{2r(110)}=0$
$\delta_{2r(001)}=0$
$\delta_{2s}=0$
$\delta_{2i}=0$



$\delta_{m(110)}=2$
$\delta_{2r(110)}=1$
$\delta_{2r(001)}=1$
$\delta_{2s}=1$
$\delta_{2i}=0$

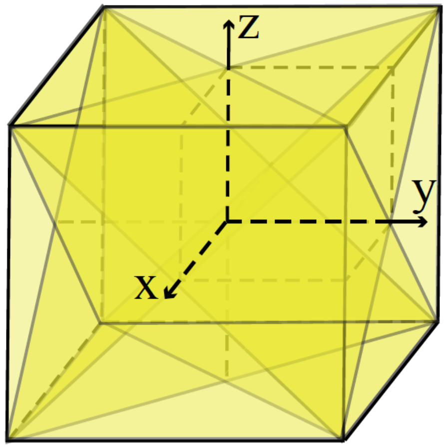
Topological invariants

Spinful: mapping indicators to invariants

- Using the method of layer construction to obtain all TCIs.
- For each LC, calculate the invariants in real space.
- For each LC, calculate the indicators in momentum space.
- Match!

$Z_8 = 4$

k-space



Layer construction

Real space

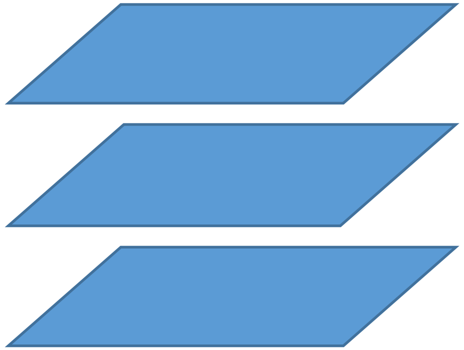
$C_{m(110)}=2$ $\delta_{h(110)}=1$ $\delta_{r(110)}=1$ $\delta_{r(001)}=1$

$\delta_{s(110)}=1$ $\delta_{s(001)}=1$ $\delta_{S4}=1$

Layer construction

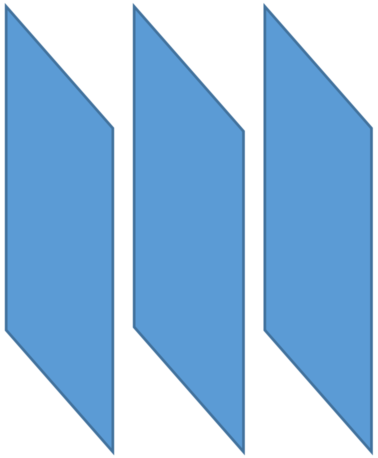
- Atomic insulators: decoupled atoms symmetrically arranged
- Layer construction of TCI: decoupled 2D TIs symmetrically arranged.
- All known TCIs can be layer-constructed.

Song et al, PRX 2017



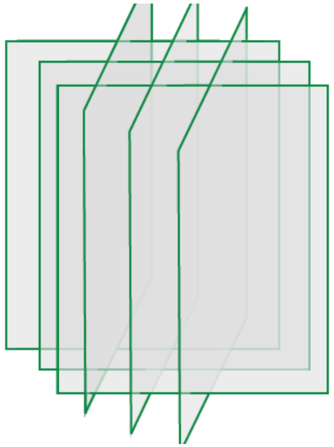
Mirror TCI

Ezawa, PRB 2016



Hourglass TCI

Fang and Fu, 2017



C_4 TCI

Spinless: mapping indicators to topological nodes

- Relate indicators to topological invariants for sub-manifolds of Brillouin zone.
- All indicators correspond to topological nodes at generic momenta, including nodal lines and Weyl points.
  - Centrosymmetric: types, numbers and configurations of all nodal lines
  - Noncentrosymmetric: numbers, charge and configurations of all Weyl points

Z. Song, T. Zhang and CF arXiv:1711.11050

Example (spinless)

- CaP_3

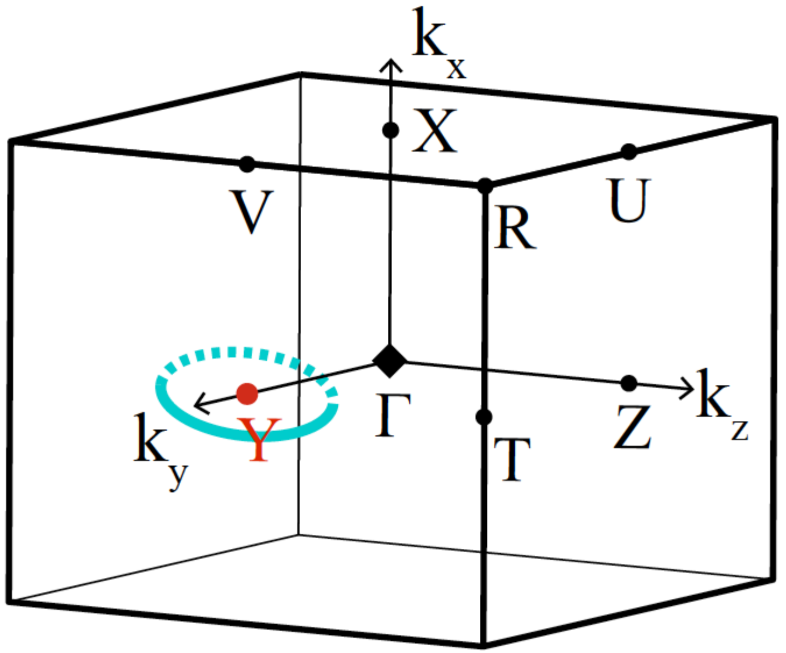
Symmetry data: Z^{16}

k point	irreducible representations
Γ	$14E_g + 11E_u$
R	$12E_g + 13E_u$
T	$13E_g + 12E_u$
U	$12E_g + 13E_u$
V	$13E_g + 12E_u$
X	$13E_g + 12E_u$
Y	$13E_g + 12E_u$
Z	$13E_g + 12E_u$

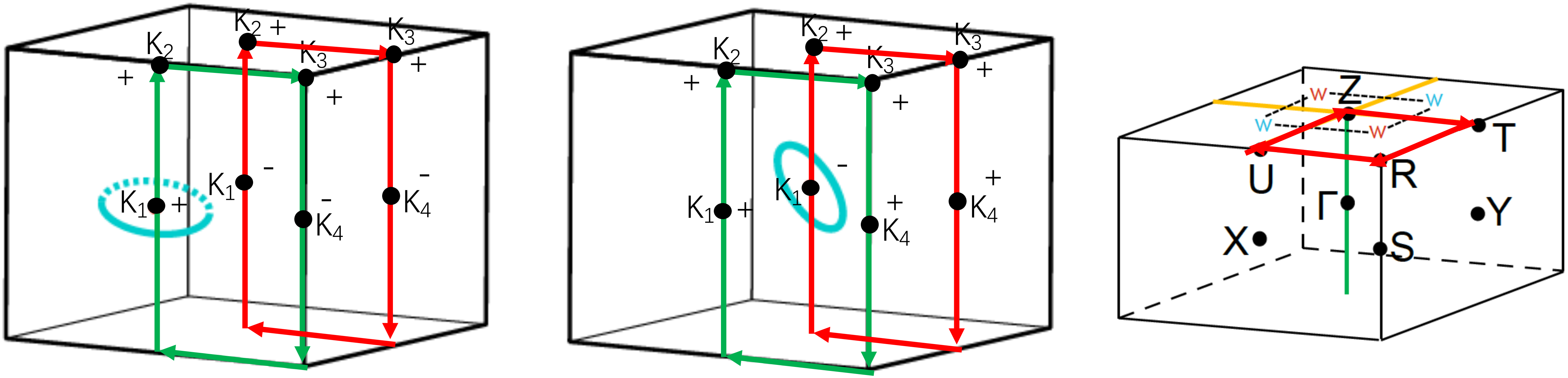
Indicator: $Z_2^3 \times Z_4$

(010;1)

Confirmed in Xu et al PRB 2017



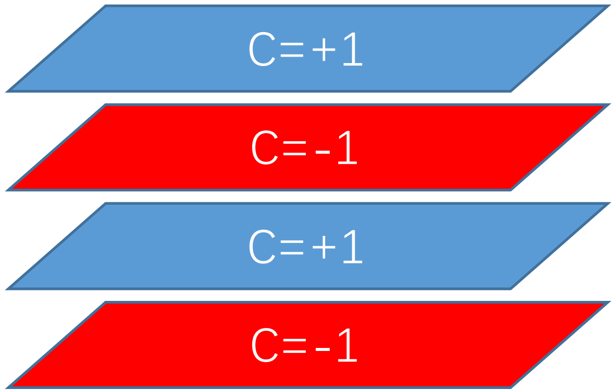
Indicators as Berry phases of submanifolds



Extension to other symmetry classes

- Superconductors (BdG classes): layer construction + wire construction
- Magnetic group insulators are generally constructed by layers of Chern insulators

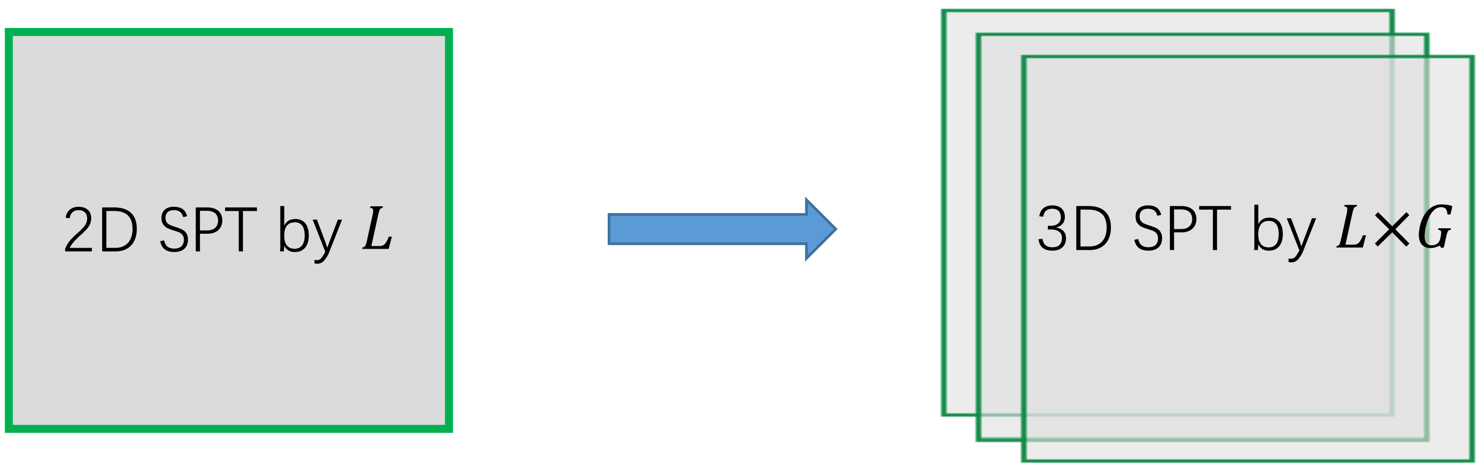
3D TSC protected by C_4 and T



AFM TI protected by $T*T_z$

Extension to strongly interacting SPT

2D TI protected by T + Arranged in a set of G-symmetric planes = 3D TCI protected by $T\times G$



2D SPT protected by local symmetry group L + Arranged in a set of G-symmetric planes = 3D SPT protected by $L\times G$

See Huang et al arXiv 2017 for the case without local symmetry

Summary

- We find the explicit formulas for all symmetry-based indicators in the presence of time reversal symmetry.
- We establish a mapping from the symmetry eigenvalues of a band structure at high-symmetry points to its topological data.
  - In the presence of SOC, we give all possible combinations of invariants
  - In the absence of SOC, we give all possible configurations of nodes
- Byproducts
  - The classification of TCI
  - An exhaustive enumeration of all layer constructions that can be extended to strongly interacting systems