PREDICTION AND DISCOVERY OF TOPOLOGICAL MATERIALS: WANNIER CHARGE CENTERS AND Z2PACK PACKAGE

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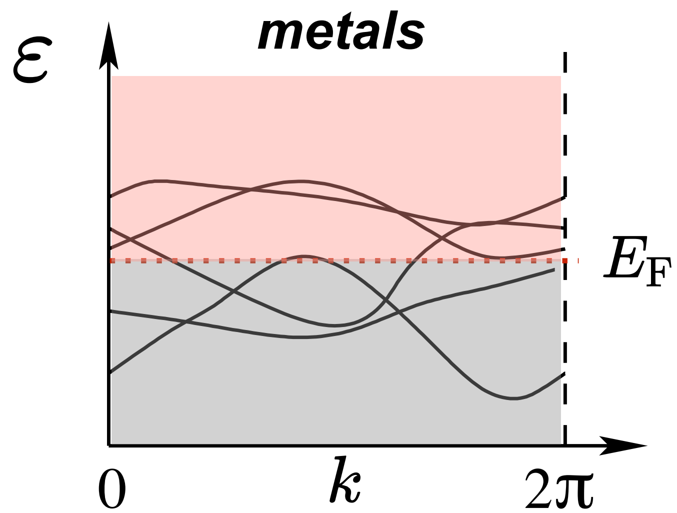
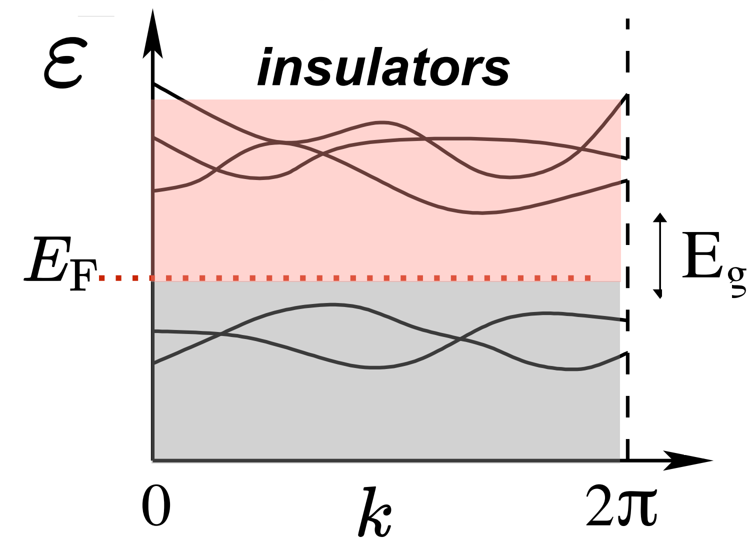
Introduction to Topological Materials

Band theory: $H(\mathbf{k})|u_{n\mathbf{k}}\rangle = \varepsilon_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle$ **DFT** → **Energy bands** ε_{nk}

Eigenvalue classification:

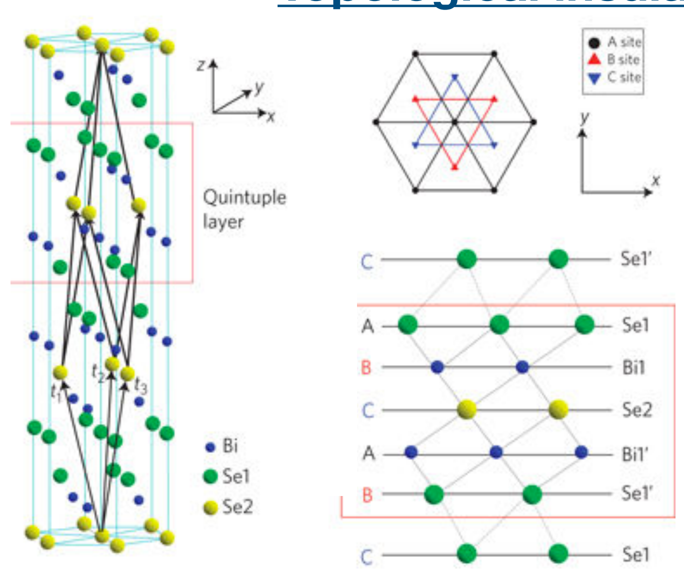


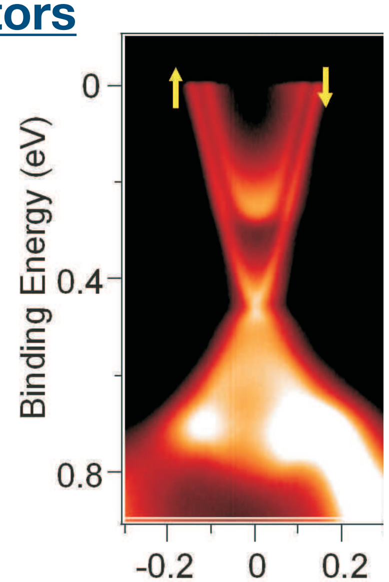


Topological band theory: $H(\mathbf{k})|u_{n\mathbf{k}}\rangle = \varepsilon_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle$ **DFT** → **Bloch bands** $|u_{n\mathbf{k}}\rangle$

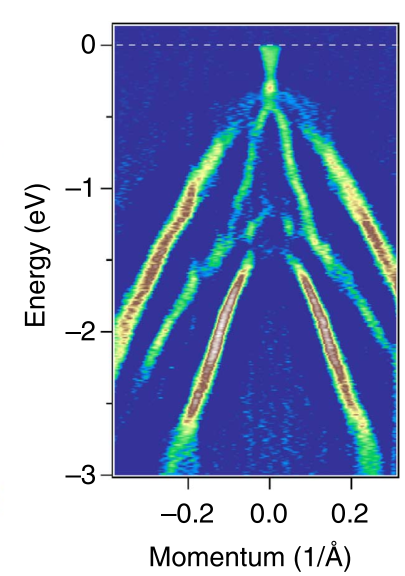
Eigenstate classification: Topological invariants provide richer classification

Topological insulators

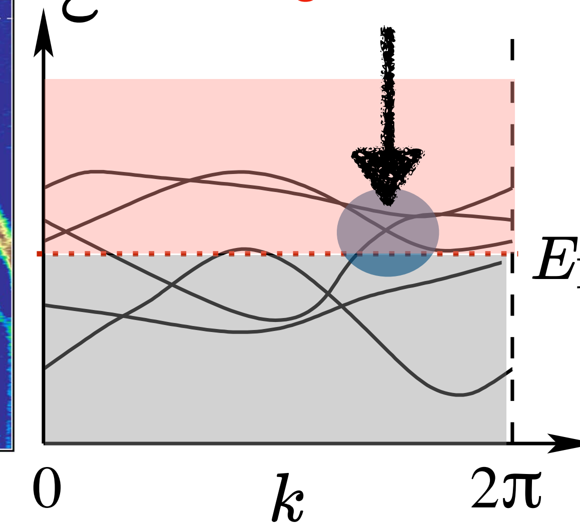




Topological metals



Band degeneracies



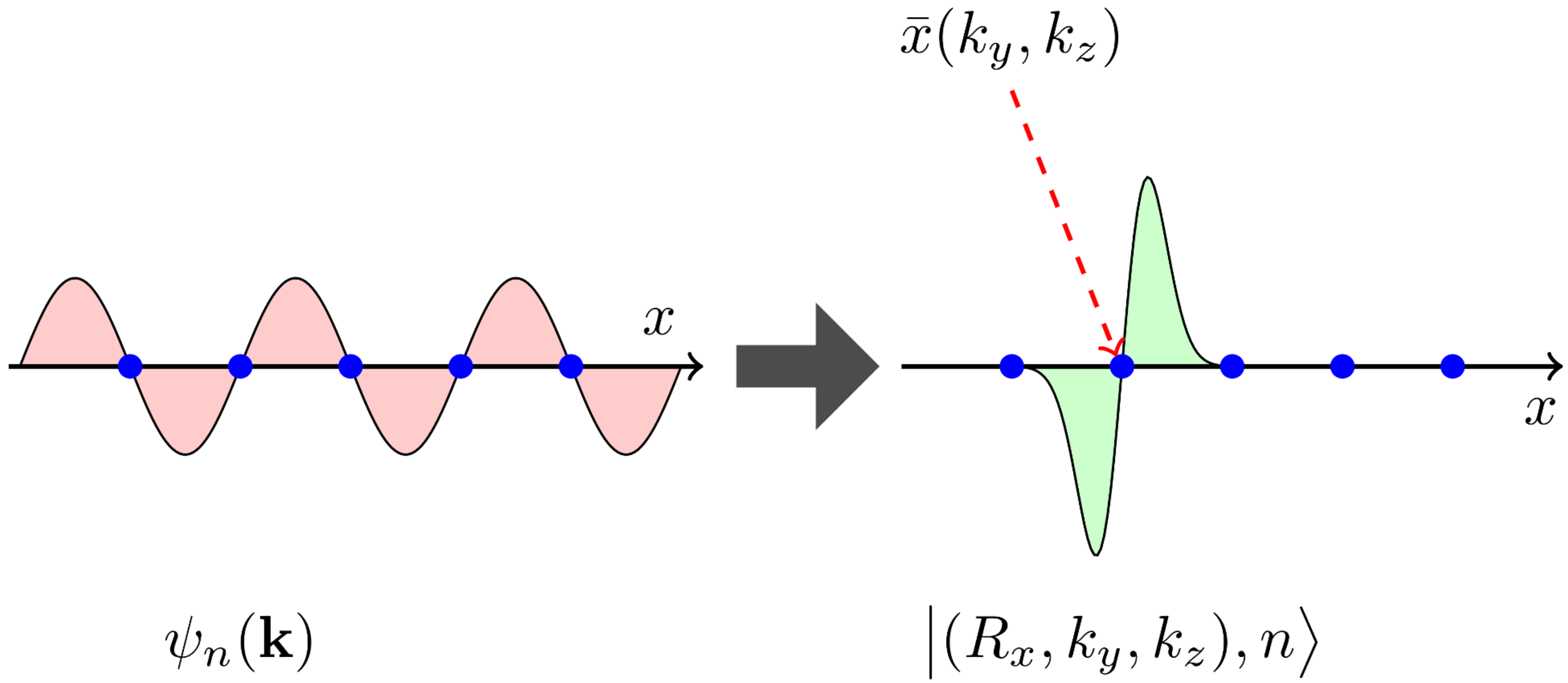
2D Dirac Fermions Bi_2Se_3

Method: hybrid Wannier functions

Hybrid Wannier function: $$|(R_x, k_y, k_z), n\rangle = \frac{1}{2\pi}\int e^{ik_xR_x}|\Psi_{n,\mathbf{k}}\rangle dk_x$$

Localized in *x*, delocalized in *y* and *z*

Hybrid Wannier centers: $$\bar{x}_n(k_y, k_z) = \langle (R_x, k_y, k_z), n|\hat{X}|(R_x, k_y, k_z), n\rangle$$



Sgiarovello, Peressi, Resta, PRB'03
Soluyanov, Vanderbilt PRB'11
Yu, Qi, Bernevig, Fang, Dai PRB'11

Track the centers as a function of *k* to understand the charge motion!

Physics with Hybrid Wannier Functions: Electronic Polarization and Chern Numbers

Electronic polarization of a 1D insulator:

$$P_x = \sum_{n}^{\mathrm{N_{occ}}} \bar{x}_n \mod 1$$

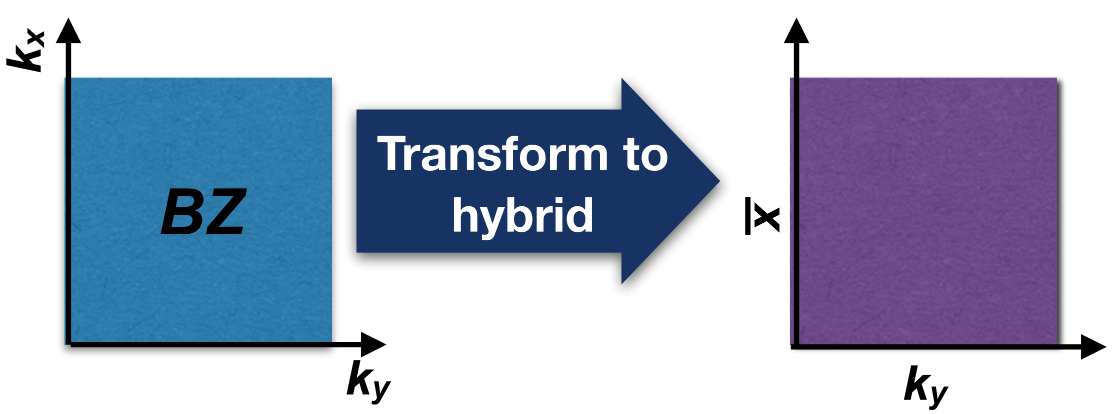
in 1D Wannier functions are always exponentially localized

Parallel transport $|u_{nk}\rangle$ across BZ to get $\bar{x}_n$

Chern numbers of a 2D insulator:

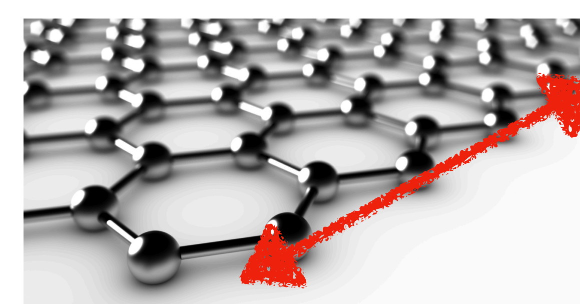
$$C = \frac{1}{2\pi}\int_{BZ} dk_x dk_y \left[\partial_{k_x}\langle u_{n\mathbf{k}}|\partial_{k_y}|u_{n\mathbf{k}}\rangle - \partial_{k_y}\langle u_{n\mathbf{k}}|\partial_{k_x}|u_{n\mathbf{k}}\rangle\right]$$

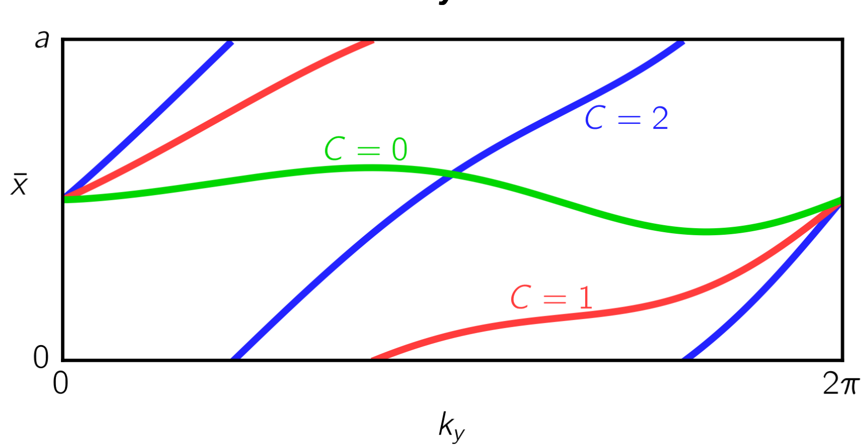
$$C \in \mathbb{Z}$$

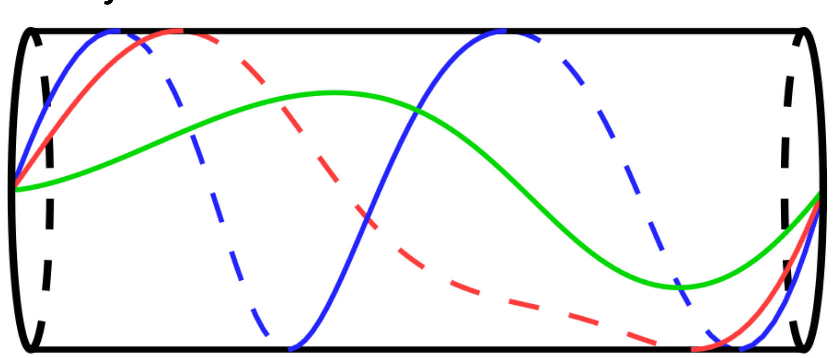


$$\sigma_{xy} = C\frac{2e}{h}$$

IQHE without magnetic field







$$C = [P_x(k_y = 2\pi) - P_x(k_y = 0)]$$

Individual Chern Numbers

Not isolated bands or degeneracies are present in the spectrum

$$\mathcal{H} = \bigoplus_i \mathcal{H}_i$$

Split the Hilbert space into subspaces related by symmetry

$$P_{\mathbf{k}} = \sum_i P_{\mathbf{k}}^{(i)}; \qquad UP_{\mathbf{k}}^{(i)}U^{-1} = P_{U^{-1}\mathbf{k}}$$

Obtain the individual Chern numbers

$$c_i = \frac{i}{2\pi} \int_M \mathrm{Tr}\left\{ P_{\mathbf{k}}^{(i)} \left[\partial_{k_1} P_{\mathbf{k}}^{(i)}, \partial_{k_2} P_{\mathbf{k}}^{(i)} \right] \right\} \mathrm{d}k_1 \wedge \mathrm{d}k_2$$

Relation to the total Chern number

$$C = \sum_i c_i$$

Vanishing *<u>total</u>* Chern number does not exclude a topological phase!

Time-Reversal Symmetric Z_2 Insulators

Anti-unitary time-reversal operator for spinful fermions:

$$\theta^2 = -1$$

Kramers pairs of occupied bands:

$$\theta|u_I(\mathbf{k})\rangle = |u_{II}(-\mathbf{k})\rangle$$

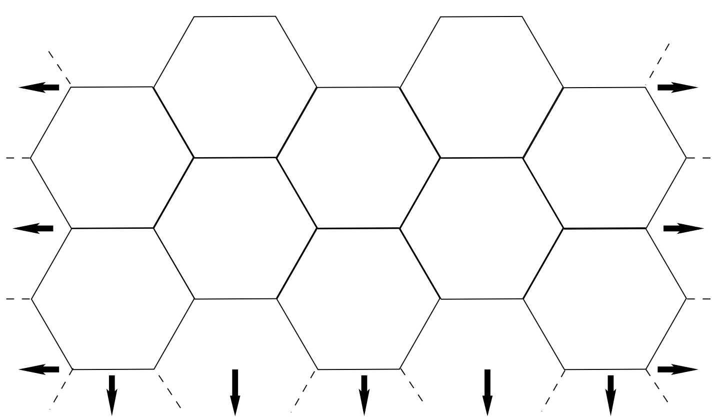
$$\theta|u_{II}(\mathbf{k})\rangle = -|u_I(-\mathbf{k})\rangle$$

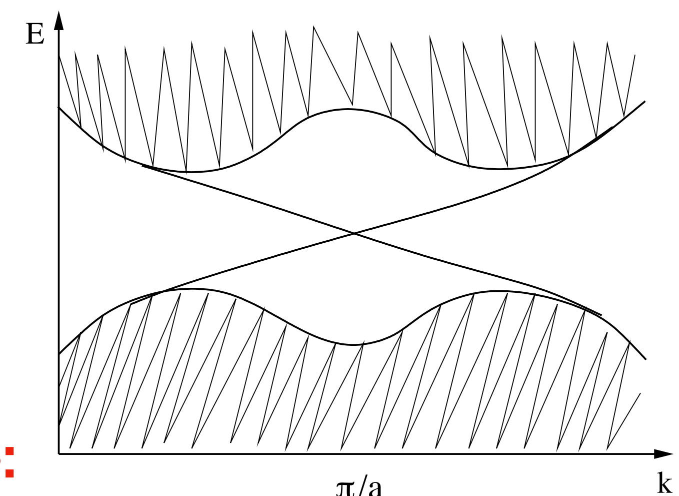
Individual Chern numbers:

$$c_I = +1$$
$$c_{II} = -1$$

$$C = c_I + c_{II} = 0 \quad \overset{\text{TRS}}{\Longleftrightarrow} \quad \sigma_{xy} = 0$$

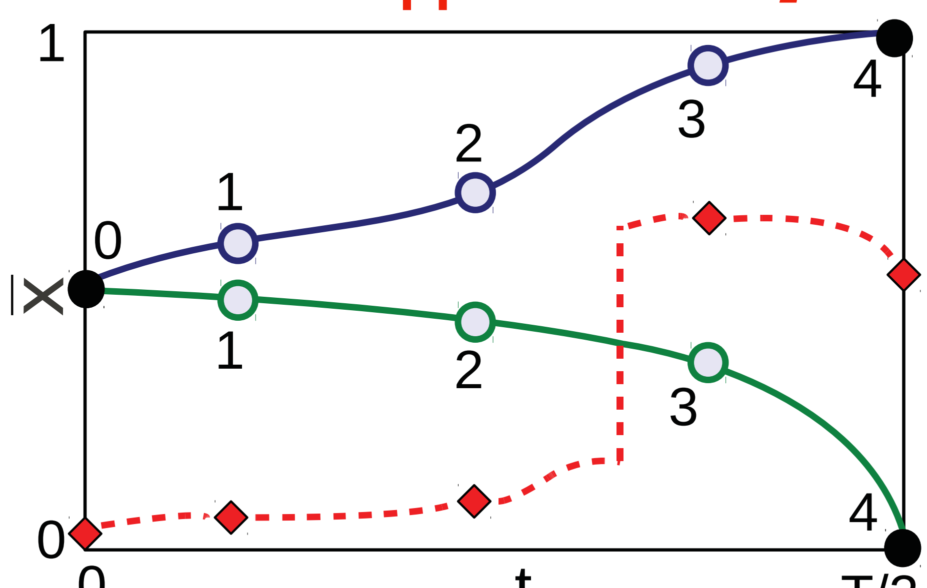
Meaning of Z_2: If c_i is odd, the phase is topological





Better approach for Z_2:

Symmetries constrain the hybrid Wannier center positions



Relaxing symmetry constraints on the Bloch states leads to hybridization of hybrid Wannier canters!!!

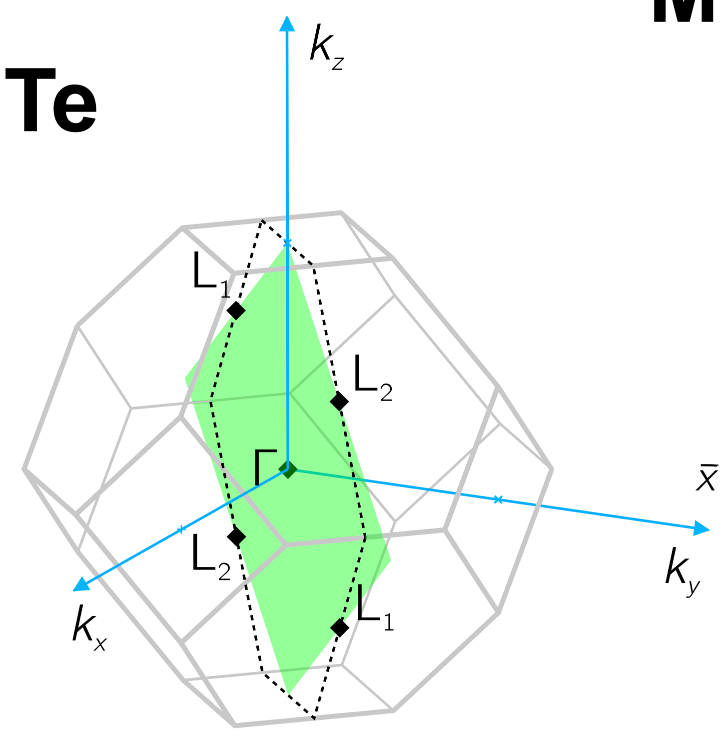
Soluyanov, Vanderbilt PRB'11
Yu, Qi, Bernevig, Fang, Dai PRB'11

Crystalline Topological Insulators: Mirror

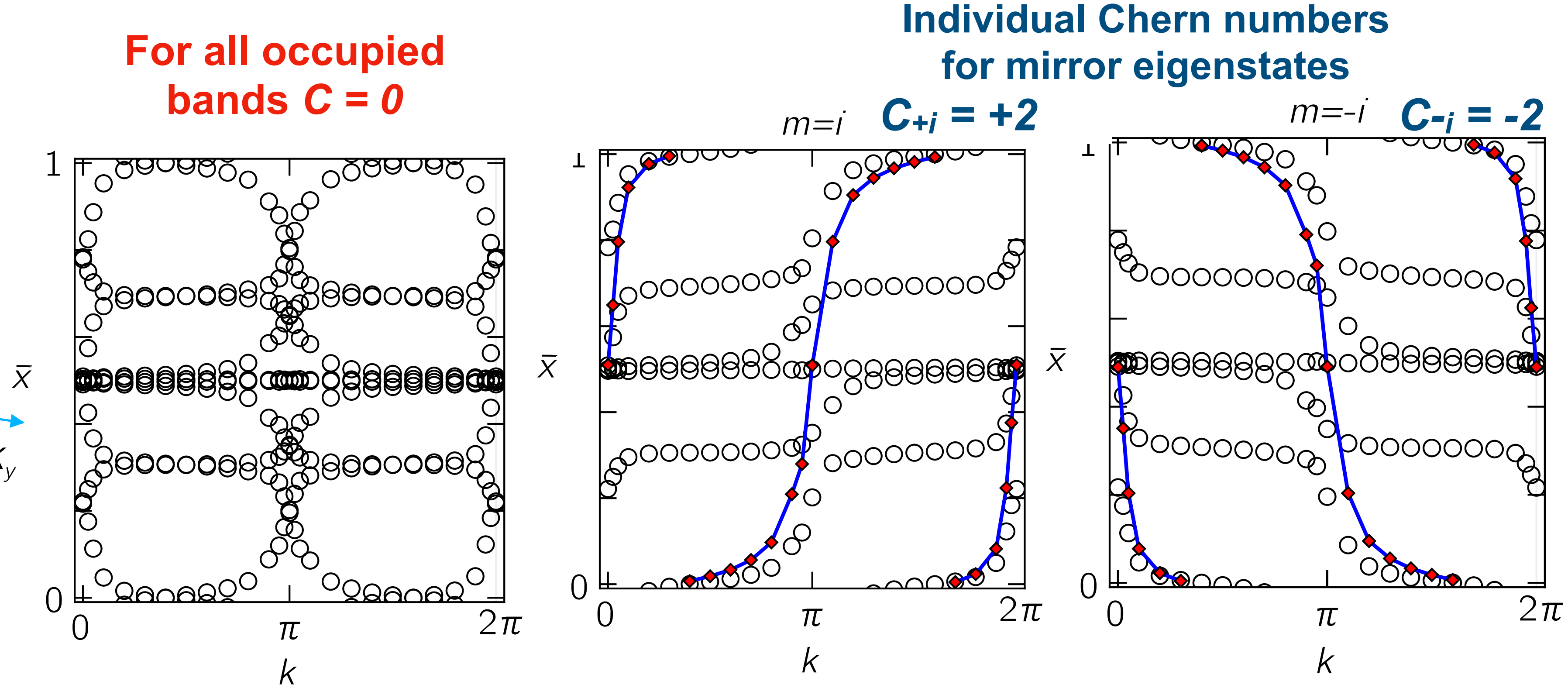
Mirror Chern numbers

Teo, Fu, Kane PRB'08,

SnTe



Hsieh *et al* Nature Comm'12



How to obtain symmetry eigenstates?

With symmetrized Wannier-based tight-binding models!

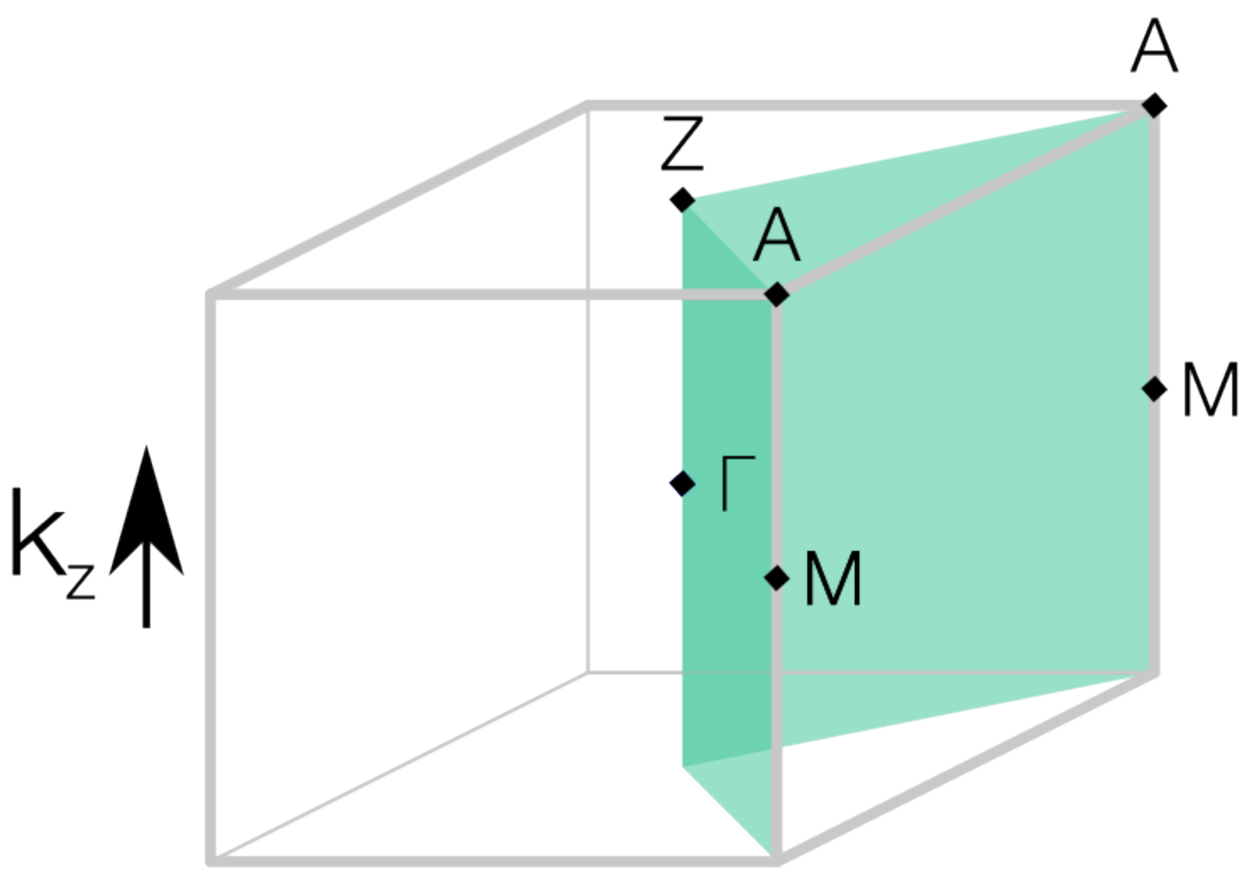
PHYSICAL REVIEW MATERIALS **2**, 103805 (2018)

Automated construction of symmetrized Wannier-like tight-binding models from *ab initio* calculations

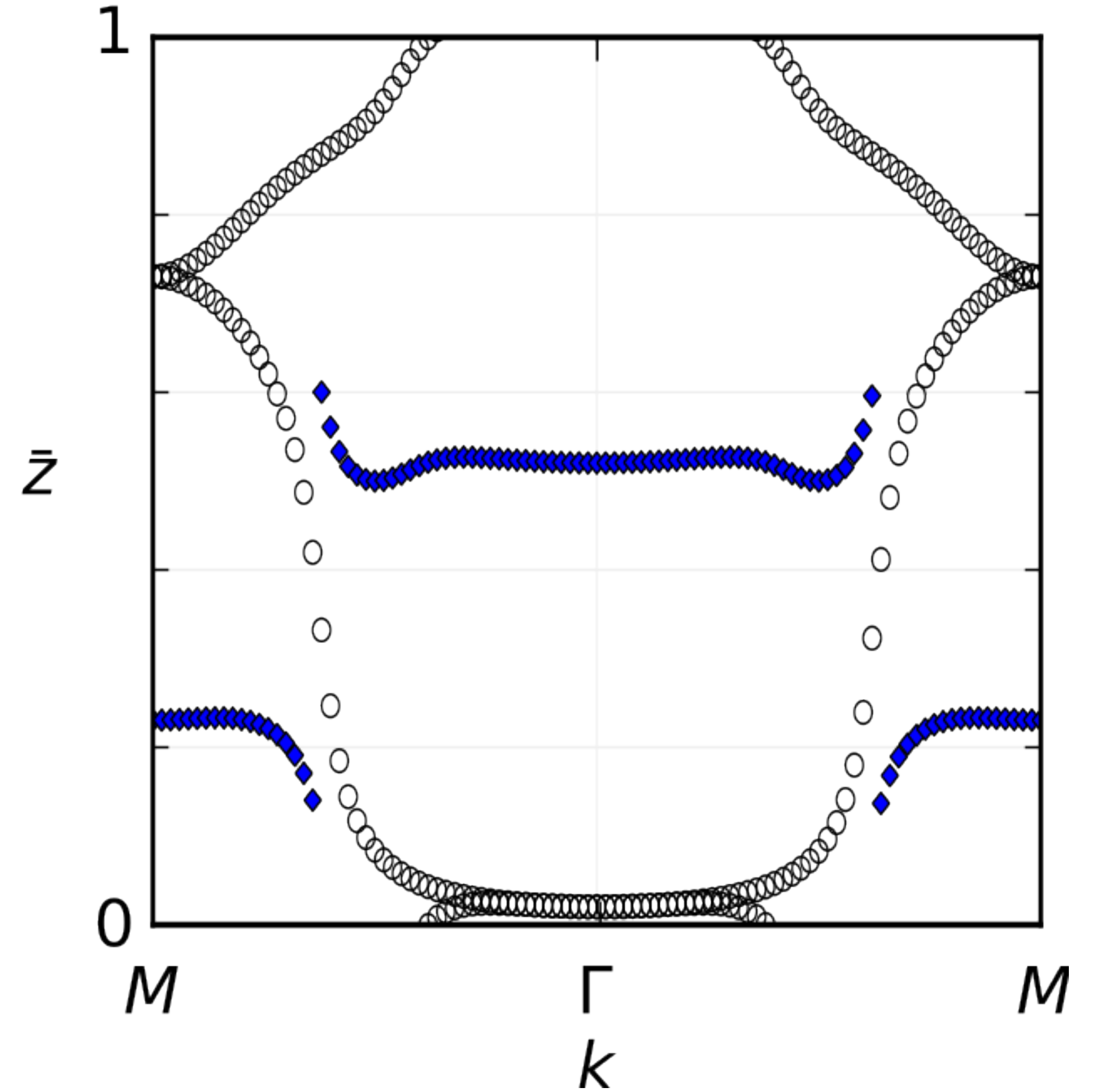
Dominik Gresch,[1] QuanSheng Wu,[2,*] Georg W. Winkler,[3,*] Rico Häuselmann,[4] Matthias Troyer,[1,5] and Alexey A. Soluyanov[1,6,7]

Crystalline Topological Insulators: C_4

Not yet found C4-topological insulators



Alexandradinata *et al* PRB'14

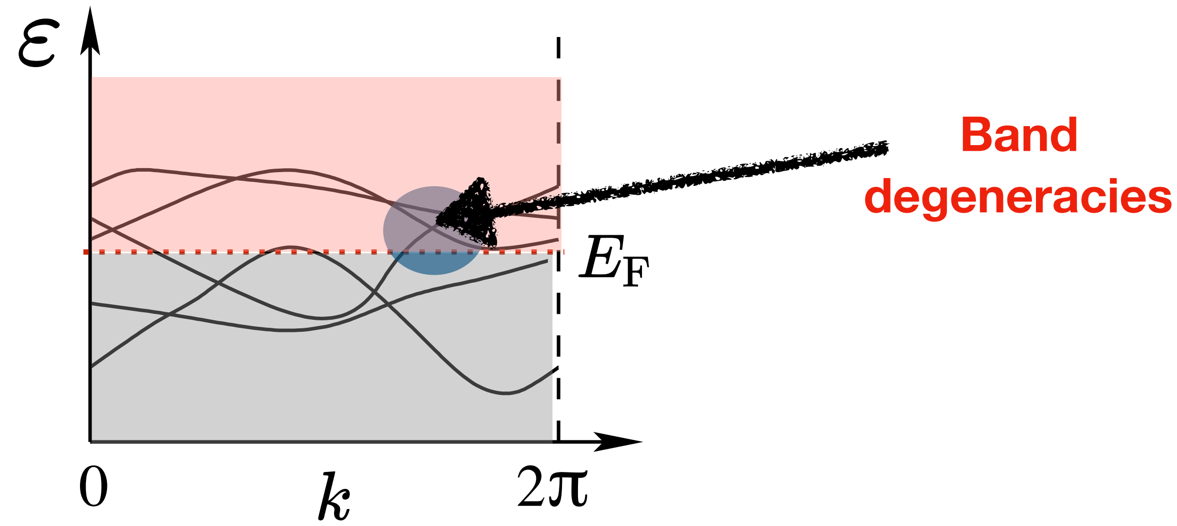


$$c_\alpha = -c_\beta = 1$$

$$C = 0$$

Topological (Semi-) Metals

How to define topology and Chern numbers in metals?



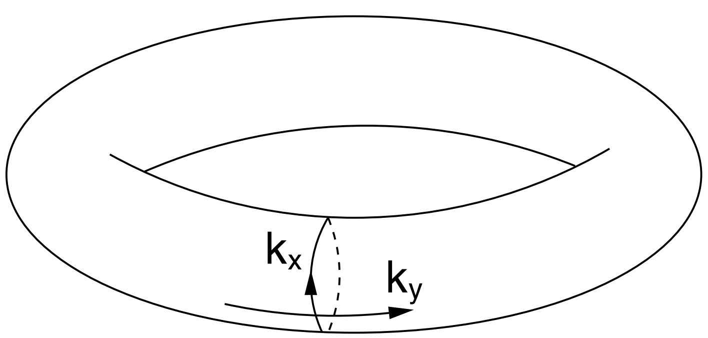
Brief overview via the analogy to Chern and Z_2 insulators

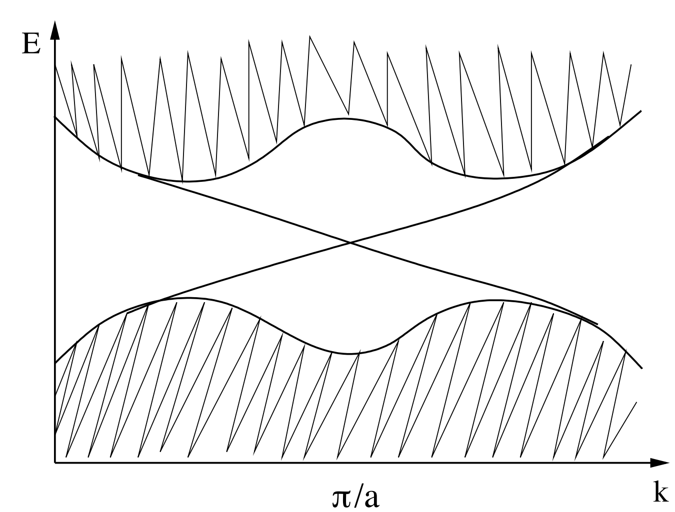
$$C = \frac{1}{2\pi}\int_{BZ} dk_x dk_y \left[\partial_{k_x}\langle u_{n\mathbf{k}}|\partial_{k_y}|u_{n\mathbf{k}}\rangle - \partial_{k_y}\langle u_{n\mathbf{k}}|\partial_{k_x}|u_{n\mathbf{k}}\rangle\right]$$

$$\mathbb{Z}_2 \approx C_\uparrow - C_\downarrow$$

Berry curvature flux through a BZ torus:

***C* counts the number of monopoles inside the torus**



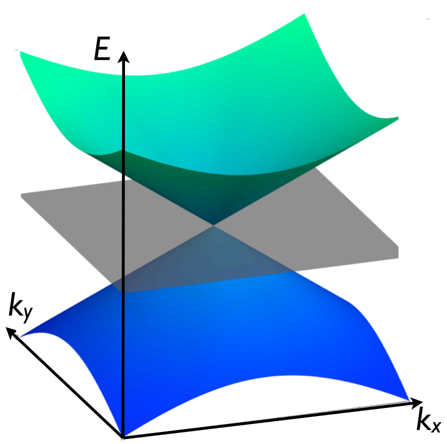


Weyl Semimetals

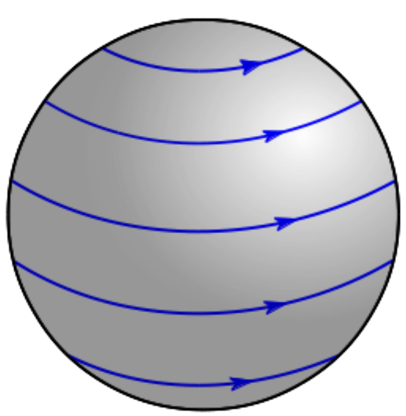
A linear crossing of two bands: $H = (\boldsymbol{v} \cdot \boldsymbol{k})I + \boldsymbol{k} \cdot \boldsymbol{\sigma}$

$v = 0$

Weyl fermion-point

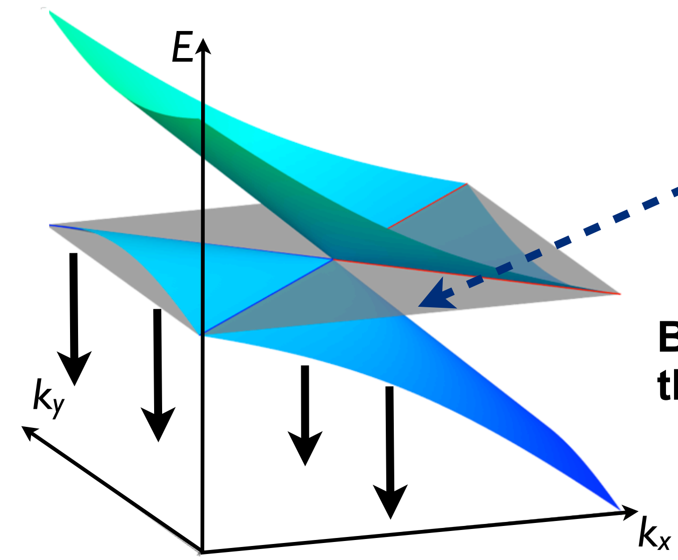


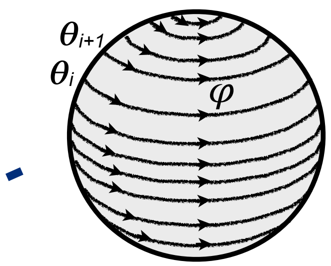
Insulator on a sphere in *k*-space



$|v| > 1$

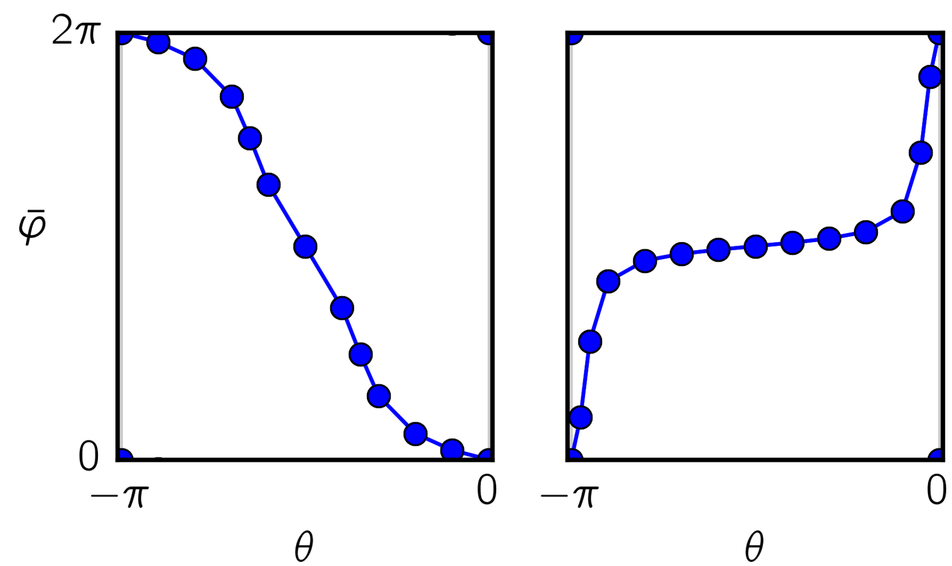
Non-relativistic Weyl fermion-point





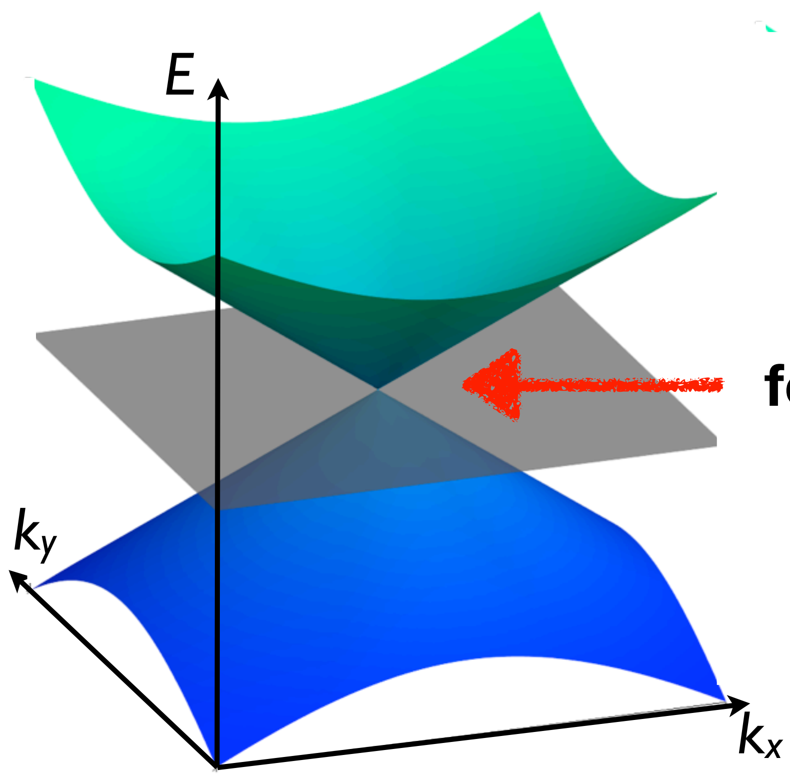
Berry curvature of these bands is used

Weyl fermion chirality= Chern number on a sphere



Dirac Semimetals

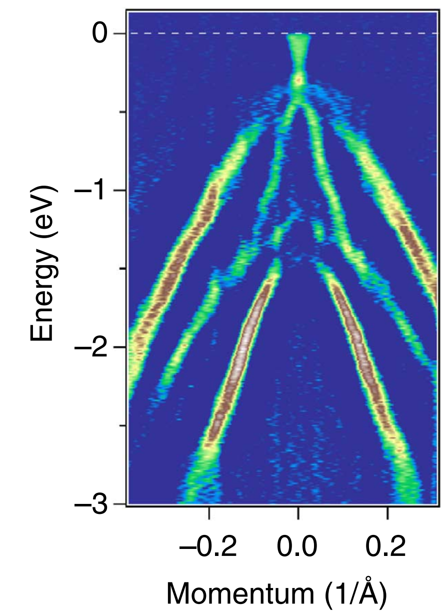
In *PT*-symmetric compounds all bands are spin-degenerate

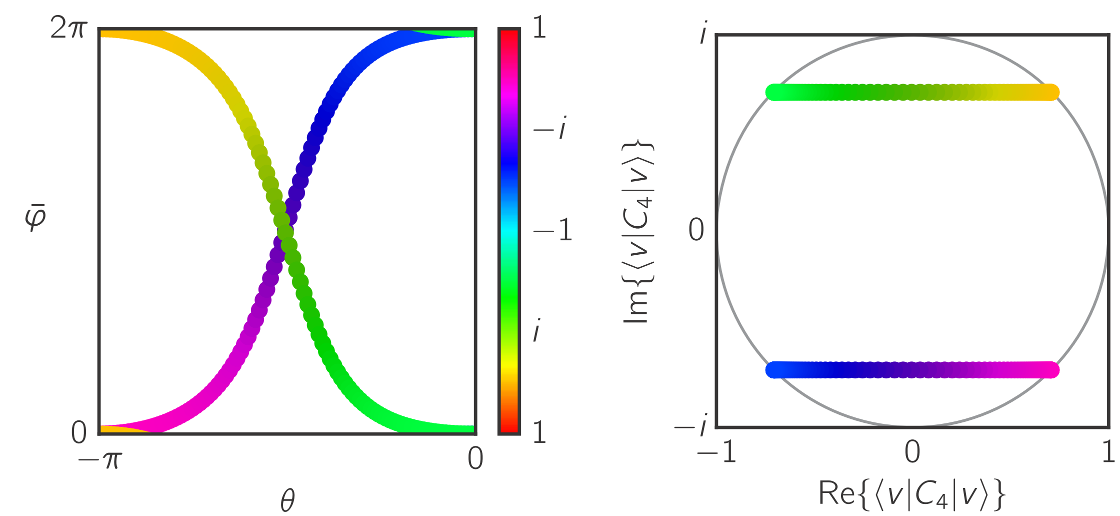


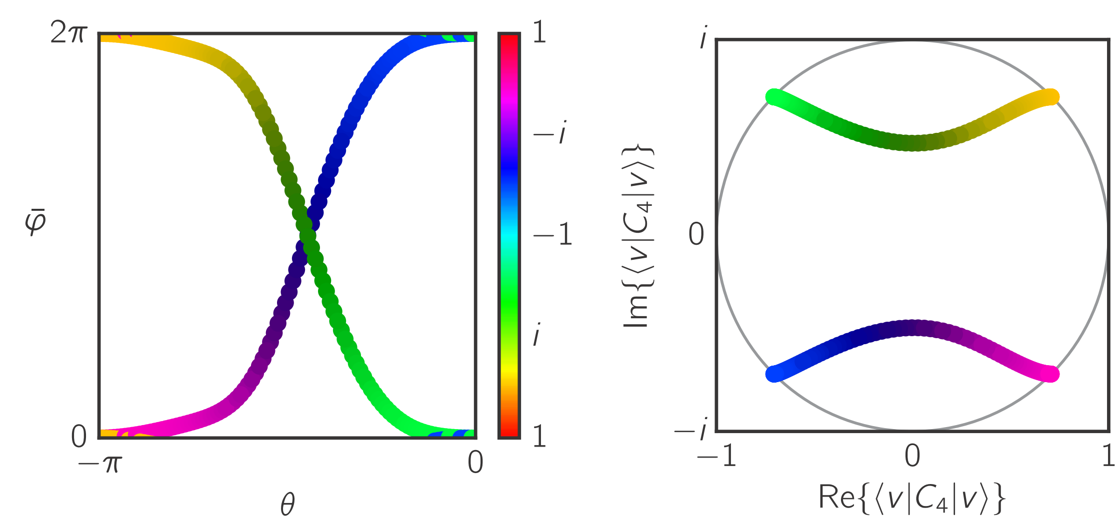
four-fold degeneracy

$$\mathbb{Z}_2 = C_\uparrow - C_\downarrow$$

Cd$_3$As$_2$







Z2Pack Software

PHYSICAL REVIEW B **95**, 075146 (2017)

Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials

Dominik Gresch,[1] Gabriel Autès,[2,3] Oleg V. Yazyev,[2,3] Matthias Troyer,[1] David Vanderbilt,[4]
B. Andrei Bernevig,[5] and Alexey A. Soluyanov[1,6]

Z2Pack

http://z2pack.ethz.ch

Dominik Gresch

A framework to identify topological phases in materials

allows one to

1. *Automatically identify material candidates for topological insulator/semimetal phases*
2. *Do a high-throughput search and classification of topologies in existing materials*
3. *Identify novel topological phases in weakly correlated materials*

Z2Pack works with first-principles, tight-binding and k.p models

Abinit → $M_{mn}^{(\mathbf{k},\mathbf{k}+\delta\mathbf{k})} = \langle u_{m,\mathbf{k}} | u_{n,\mathbf{k}+\delta\mathbf{k}} \rangle$ → WANNIER90 → Z2Pack → Topological invariant