Topological insulators, continued

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Recap from yesterday: topological invariants

Capture how valence band wave functions change as move around BZ

1D: Berry phase $\Rightarrow$ polarization

2D: Chern number = “winding” Berry phase $\Rightarrow$ edge states

Today: symmetry $+$ semimetals
Time-reversal symmetry forbids Chern number!

\[ \Theta^{-1} H(k) \Theta = H(-k) \]

\[ \Theta^2 = -\mathbb{I} \]

Degenerate Kramer’s pairs at
“Time-reversal-invariant-momenta” (TRIM) k=0, k=\( \pi \)

Conventional insulator

Topological insulator

Surface state: Kramers pair

This is usually what “topological insulator” refers to!

“Z_2” topological invariant \( \nu \): even vs odd bands cross \( E_F \) over half the BZ
Practical calculation of $Z_2$ invariant:

winding Berry phase around half Brillouin zone

Berry phase imitates surface spectrum (proof: Fidkowski, Jackson, Klich PRL 2011)

Yu, Qi, Bernevig, Fang, Dai PRB 84, 075119 (2011)

Berry phase imitates surface spectrum (proof: Fidkowski, Jackson, Klich PRL 2011)

2D TI in HgTe quantum wells

Theory: Bernevig, Hughes, Zhang Science 2006 “BH model”

- CdTe
- HgTe
- CdTe

\[ d < d_c \] normal band order
\[ d > d_c \] inverted (topological) band order
\[ d_c = 6.4 \text{nm} \]

Band inversion at \( k=0 \)
Experimental realization HgTe quantum wells

Experiment: Konig, Wiedmann, Brune, Roth, Buhmann, Molenkamp, Qi, Zhang Science 2007

G=0, d<d_c
Conventional insulator

G=2e^2/h, d>d_c
Topological insulator

Quantized conductance independent of sample width
Topological insulators in 3d

Four $\mathbb{Z}_2$ indices: $\left( \nu_0; \nu_1, \nu_2, \nu_3 \right)$

"Strong" index

k_y

Surface Brillouin zone

Ex: (1;000)

Ex: (0;100)

"Weak" indices

k_y

Bulk construction (not unique)

k=0 plane is 2D TI; k=\(\pi\) is conventional

Stacked 2D TIs

Refs:
Fu, Kane, Mele PRL 2007
Moore, Balents PRB 2007
Roy PRB 2009
Topological insulators in 3d

**Bi$_{1-x}$Sb$_x$**
- Band gap $\approx 0.03$ eV
- Theory: Fu & Kane PRL 2007

**Bi$_2$Se$_3$**
- Band gap $\approx 0.3$ eV

Figures from Hasan & Kane RMP
What comes after time-reversal symmetry?  
10-fold way classification


Classified by time-reversal and charge-conjugation symmetries

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- no symmetry
- Integer quantum Hall
- fermions w/ time-reversal
- 2d and 3d topological insulators (weak index not captured)
Crystal symmetries can protect topological phases

Point group symmetries: leave (at least) one point invariant
Consist of rotations, mirrors, inversion, and rotoinversion
32 crystallographic point groups

Translations: leave no point invariant
Generate one of the 14 Bravais lattices in 3D

Glide and screw symmetries: leave no point invariant, but also rotate/reflect

The 230 space groups enumerate all possible combinations of symmetries in 3D crystals
Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

Mirror symmetry: \( m_x : (x, y, z) \mapsto (-x, y, z) \)
Mirror Chern insulator: canonical TCI

Teo, Fu, Kane PRB 045426 (2008)

Mirror symmetry: \( m_x : (k_x, k_y, k_z) \mapsto (-k_x, k_y, k_z) \)

When \( k_x=0 \), \( m_x \) commutes with \( H(k_x=0, k_y, k_z) \) \( \Rightarrow \) bands labelled by \( m_x \) eigenvalue: +/- i

Define Chern number for each mirror sector: \( C_{\pm} \)

Mirror Chern number: \( C_m = \frac{1}{2}(C_+ - C_-) \)
Surface states of mirror Chern insulator

Teo, Fu, Kane PRB 045426 (2008)

New configurations with multiple Dirac cones, otherwise gapped

Crystal symmetries refine classification
SnTe predicted/observed mirror Chern insulator


Observation: Tanaka, et al, Nat. Phys. 8, 800 (2012), Ando group

ARPES

C_m=2

![Graph](image1)

![Graph](image2)

![Graph](image3)
Finding topological materials is challenging.

Ad hoc symmetry classification.

Crystals classified in real space, but topology classified in momentum space.
Topological Quantum Chemistry.org (Bernevig group):
Materiae Database http://materiae.iphy.ac.cn (Chen Fang group)
Topological semimetals
Topology of Weyl fermions

\[ H = k \cdot \sigma \]

Does not require any symmetry

Movable but un-removable:

\[ k \cdot \sigma - m\sigma_z = (k - k_0) \cdot \sigma, \quad k_0 = (0,0,m) \]

Fermi surface \( E_F^2 = k_x^2 + k_y^2 + k_z^2 \) is a sphere with a Chern number!

\[ C = \frac{1}{2\pi} \int_{FS} (\nabla \times A) \cdot dS = \frac{1}{2\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \frac{\sin \theta}{2} = 1 \]

Source/sink of Berry curvature
Bulk-boundary correspondence: Weyl fermions exhibit surface Fermi arcs

Wan, Turner, Vishwanath, Savrasov PRB 83, 205101 (2011)

Recall: Chern number implies gapless surface state

Chern number jumps across Weyl point \( \Rightarrow \) gapless surface states
Bulk-boundary correspondence: Weyl fermions exhibit surface Fermi arcs

TaAs data from Hasan group: Science 349, 613 (2015)
(Some) Experimental signatures of Weyl fermions

Topology gives rise to Fermi arcs, chiral anomaly, and unusual quantum oscillations


Fig: Xiong, et al, Science 2015

Potter, Kimchi, Vishwanath, Nat. Comm. 2014


Crystal symmetry protects zoo of band crossings

Dirac fermions

Multifold fermions

JC, Bradlyn, Vergniory: APL Materials 7, 101125 (2019)

Double, triple Weyl fermions


Line nodes

Burkov, Hook, Balents PRB 2011

Are symmetry-protected band crossings topological?

Yes for “chiral” fermions, which are a source/sink of Berry curvature

Weyl fermions and some (but not all) multifold fermions are chiral

Dirac fermions are *not* chiral!
Are Dirac fermions topological?

Argument against: lack of Fermi arc

Kargarian, Randeria, Lu PNAS 2016, PRB 2018
Is a Dirac fermion topological?

Argument for: applied field splits into two Weyl fermions

Chiral anomaly in Na$_3$Bi
Xiong, et al, Science 2015

“Chiral anomaly factory”
JC et al, PRB 95, 161306 (2017)

Distinct scaling of magnetoresistance
We propose a “bulk-hinge correspondence” for Dirac fermions via higher order topological insulator.
Higher order topological insulator: gapped surfaces but gapless hinges

Fig: Wieder, Bradlyn, JC et al Nature Reviews Materials (2021)
Higher order topology elucidates “bulk-hinge correspondence” for Dirac semimetals

**Weyl fermion:** critical point between 2D trivial and topological insulators

**Dirac fermion:** critical point between 2D higher order and trivial insulators

Fang and Cano PRB 103, 165109 (2021)
Fang and Cano PRB 104, 245101 (2021)
Materials: Dirac fermions with hinge arcs

α''-Cd₃As₂

KMgBi

Summary: topological insulators are classified by bulk topological invariants

Topological invariant determined by symmetry and dimensionality

Topological invariant of bulk crystal determines surface spectrum: “bulk-edge correspondence”

Topological semimetals classified by invariants on lower-dimensional gapped sub manifolds

Topological materials classified at TopologicalQuantumChemistry.org

My group @ Stony Brook

Signatures of higher order topological insulators and semimetals
Queiroz PRL 123, 266802 (2019); Fang PRB 103, 165109 (2021); Fang ArXiv: 2109.01670

Manipulating topological surface states
Cano PRB 103, 155157 (2021); Chou PRB 104, L201113 (2021)

Moire: tunable topology + correlations
Wang PRR 3, 023155 (2021); Wang 2105.07491 -> PRL; Zang 104, 075150 (2021); Wang 2110.14570