Topological insulators and superconductors

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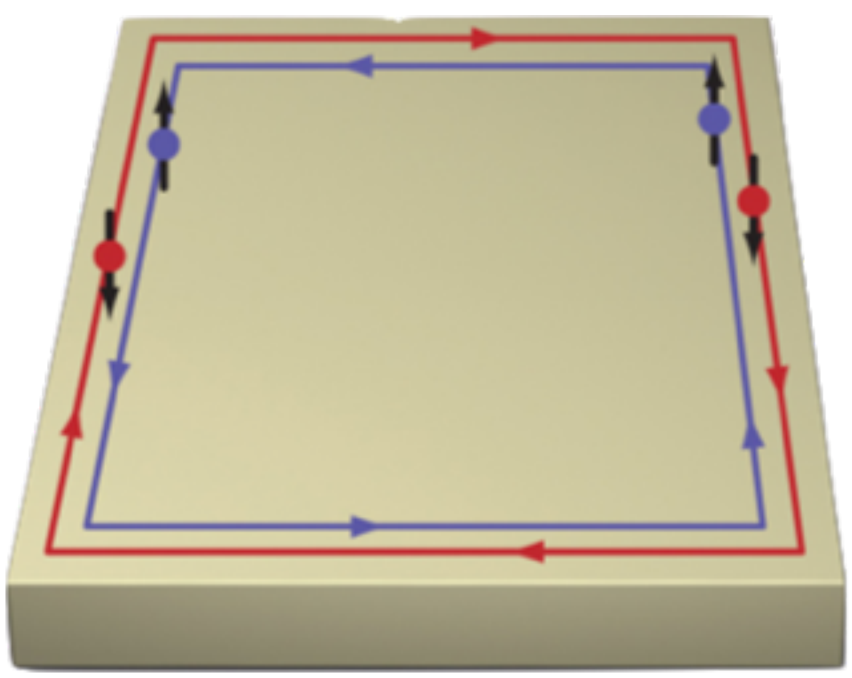
3rd lecture

1. Topological insulators w/ time-reversal symmetry
    - Time reversal symmetry and Kramers theorem
    - Quantum spin Hall state on square lattice
    - Z_2 surface invariant & Z_2 bulk invariant
    - 3D topological insulator



[picture courtesy S. Zhang et al.]

Time-reversal symmetry & Kramers theorem

Presence of time-reversal symmetry gives rise to new topological invariants **[Kane-Mele, PRL 05]**

$$\Theta : \quad t \to -t, \quad \mathbf{k} \to -\mathbf{k}, \quad \hat{S}^\mu \to -\hat{S}^\mu$$

Time-reversal symmetry implemented by anti-unitary operator:

$$\Theta = U_\mathrm{T} \mathcal{K} = e^{i\pi \hat{S}^y/\hbar} \mathcal{K}$$

complex conjugation operator

$$\Theta\, \psi = e^{i\pi \hat{S}^y/\hbar} \psi^*$$

For quadratic Hamiltonians in momentum space: $\Theta \mathcal{H}(\mathbf{k}) \Theta^{-1} = +\mathcal{H}(-\mathbf{k})$

For spin-$\frac{1}{2}$ particles: $\Theta^2 = -1 \qquad U_\mathrm{T} = -U_\mathrm{T}^T \qquad \Theta = i\sigma_y \mathcal{K} \qquad \Theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}$

Kramers theorem (for spin-1/2 particles): $\Theta^2 = -1 \quad \Rightarrow \langle \psi | \Theta \psi \rangle = -\langle \psi | \Theta \psi \rangle = 0$

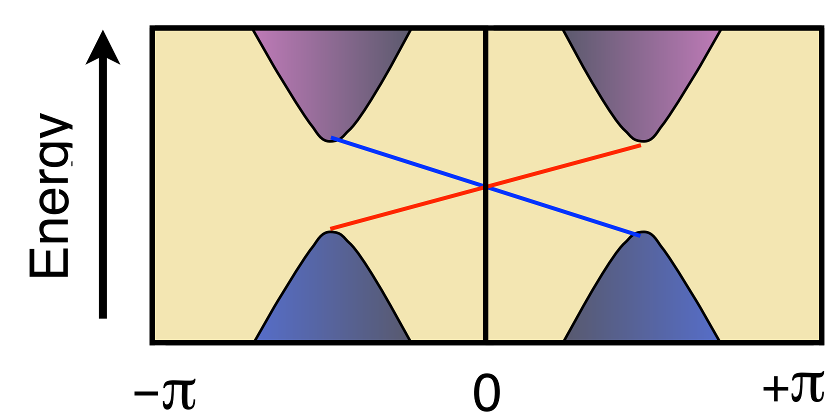
$\Longrightarrow$ all eigenstates are at least two-fold degenerate

$\Longrightarrow$ for Bloch functions in k-space:

$|u(\mathbf{k})\rangle$ and $|u(-\mathbf{k})\rangle$ have same energy; degeneracy at TRI momenta

Consequences for edge states:

— states at time-reversal invariant momenta are degenerate
— crossing of edge states is protected
— absence of backscattering from non-magnetic impurities



Time-reversal-invariant topological insulator

2D topological insulator

[Bernevig, Hughes, Zhang 2006]

(also known as Quantum Spin Hall insulator)

[Kane-Mele, PRL 05]

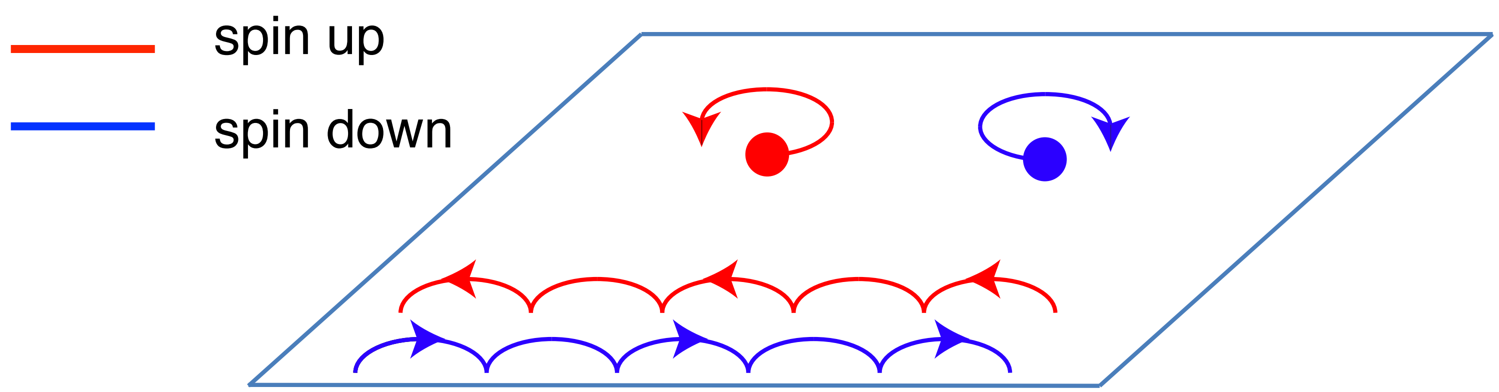
2D Bloch Hamiltonians in the presence of time-reversal symmetry:

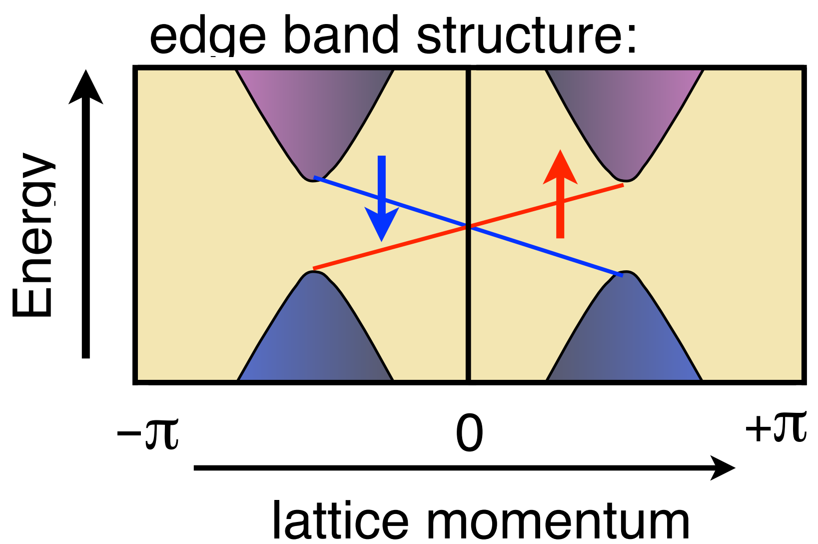
$$\boxed{\Theta \mathcal{H}(\mathbf{k}) \Theta^{-1} = +\mathcal{H}(-\mathbf{k})} \qquad \Theta = i\sigma_y \otimes \mathbb{1}\,\mathcal{K} \qquad \Theta^2 = -1$$

Simplest model:
(Chern insulator)^2

$$\mathcal{H}(k_x, k_y) = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{\mathrm{CI}}(\mathbf{k}) & 0 \\ 0 & H^*_{\mathrm{CI}}(-\mathbf{k}) \end{pmatrix}$$

S^z is conserved





Bulk energy gap but gapless edge: Spin filtered edge states

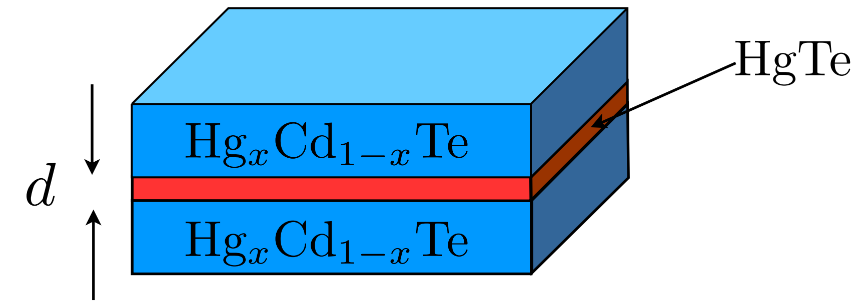
— protected by time-reversal symmetry
— half an ordinary 1D electron gas
— is realized in certain band insulators with strong spin-orbit coupling

TRI topological insulator: HgTe quantum wells

- observed in HgTe/(Hg,Cd) quantum wells

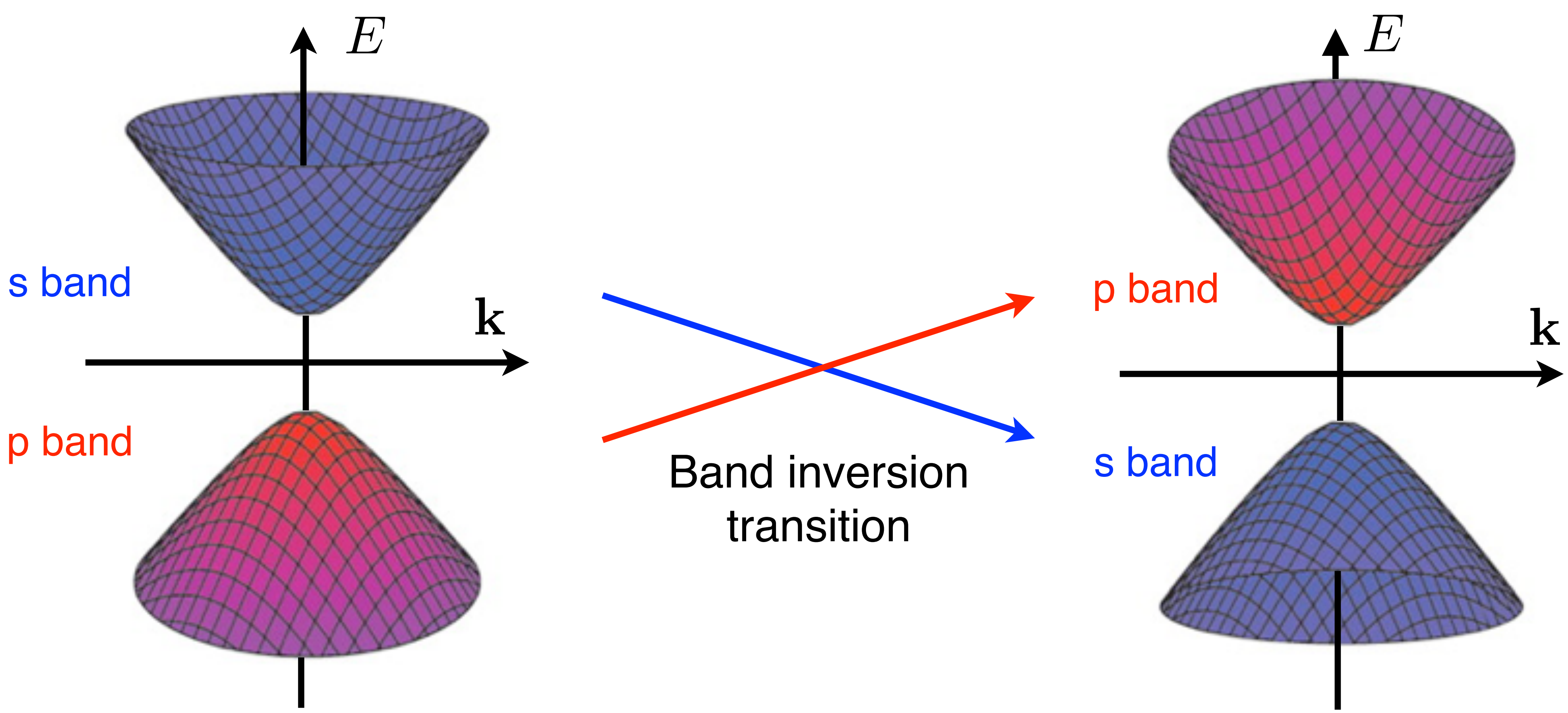
  [Bernevig, Hughes, Zhang Science 2006]

  [M. Koenig, Buhmann, Mohlenkamp, et al., Science 2007]



d < 6.3 nm: Normal band order

d > 6.3 nm: Inverted band order



$\nu = 0$: conventional insulator

$\nu = 1$: topological insulator

TRI topological insulator: HgTe quantum wells

[M. Koenig, Buhmann, Mohlenkamp, et al., Science 2007]

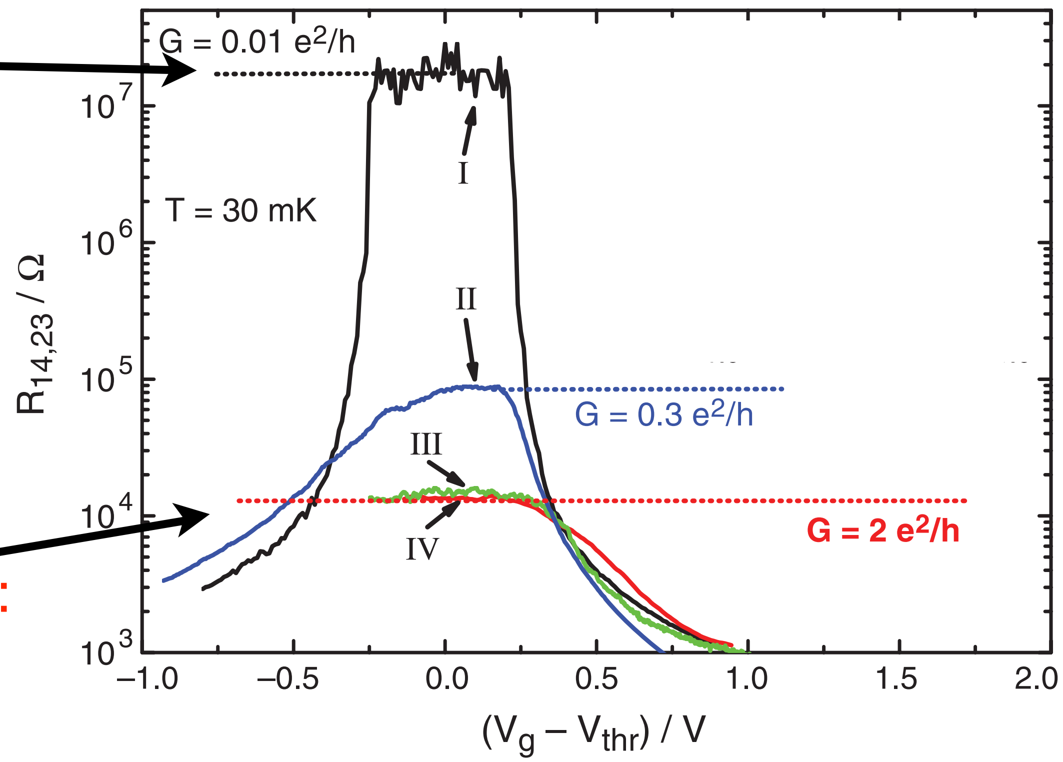
- observed in HgTe/(Hg,Cd) quantum wells

Measured conductance: $2e^2/h$ for short samples L < L_{mag}, L_{IS}

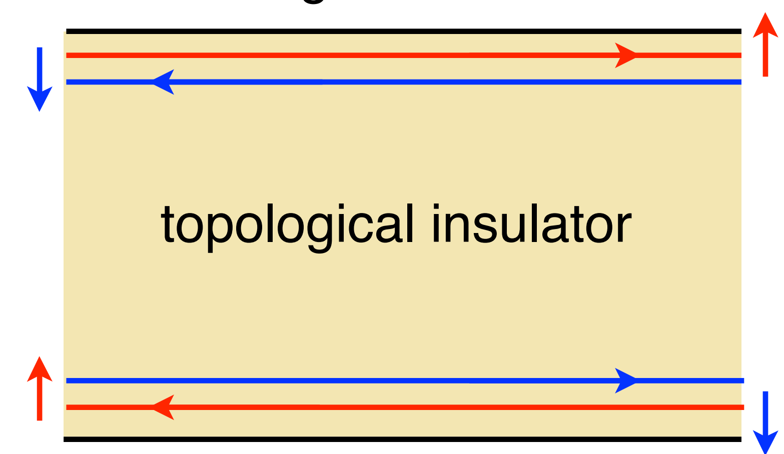
(two terminal conductance)

d < 6.3 nm
normal band order:
trivial

d > 6.3 nm
inverted band order:
topological



helical edge states:



Helical edge states are unique 1D electron conductor

- spin and momentum are locked
- no elastic backscattering from non-magnetic impurities
- perfect spin conductor!

2D topological insulator: Edge Z_2 invariant

[Kane Mele 05]

Time-reversal invariant insulators with $\Theta^2 = -1$

are classified by a **Z_2 topological invariant** ($\nu = 0,1$)

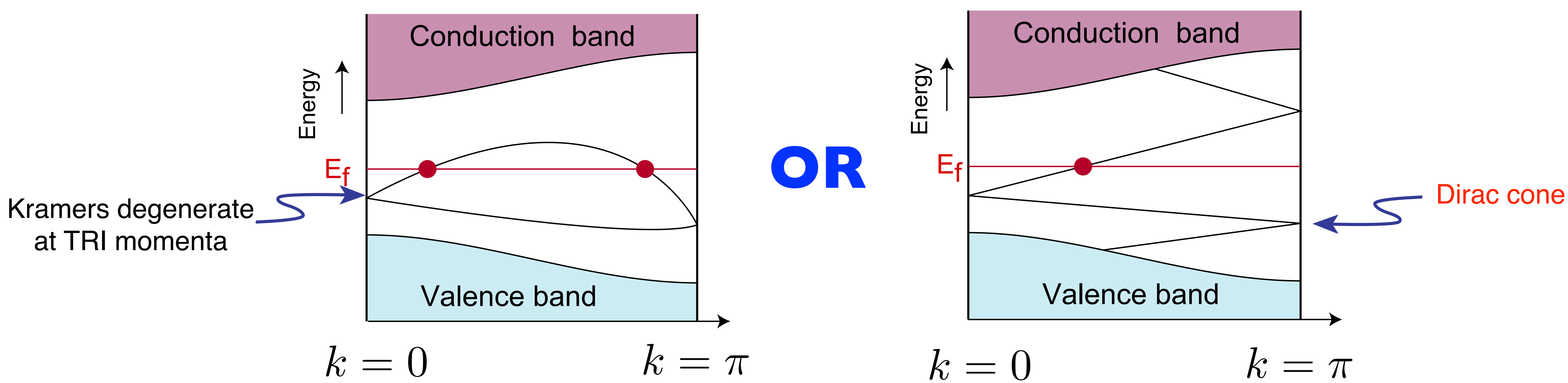
$$\boxed{\Theta \mathcal{H}(\mathbf{k}) \Theta^{-1} = +\mathcal{H}(-\mathbf{k})}$$

This can be understood via the bulk-boundary correspondence:

$\Rightarrow$ consider edge states in half of the edge Brillouin zone (other half is related by TRS)

Edge Z_2 invariant:

$\nu = 0$: conventional insulator $\qquad$ $\nu = 1$: topological insulator



trivial phase
even # Dirac cones

non-trivial phase
odd # Dirac cones

$\Rightarrow$ **Edge Z_2 invariant** distinguishes between even / odd number of Kramers pairs of edge states

[after Hasan & Kane, RMP 2010]

2D topological insulator: First bulk Z_2 invariant

[Kane Mele 05]

[Fu and Kane]

Bulk Z_2 invariant as an obstruction to define a "TR-smooth gauge":

– $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs
– TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta|u_n^{(2)}(\mathbf{k})\rangle$

$\Longrightarrow$ consider anti-symmetric "t-*matrix*":

$$\boxed{t_{mn}(\mathbf{k}) = \left\langle u_m^-(\mathbf{k})\right| \Theta \left|u_n^-(\mathbf{k})\right\rangle}$$

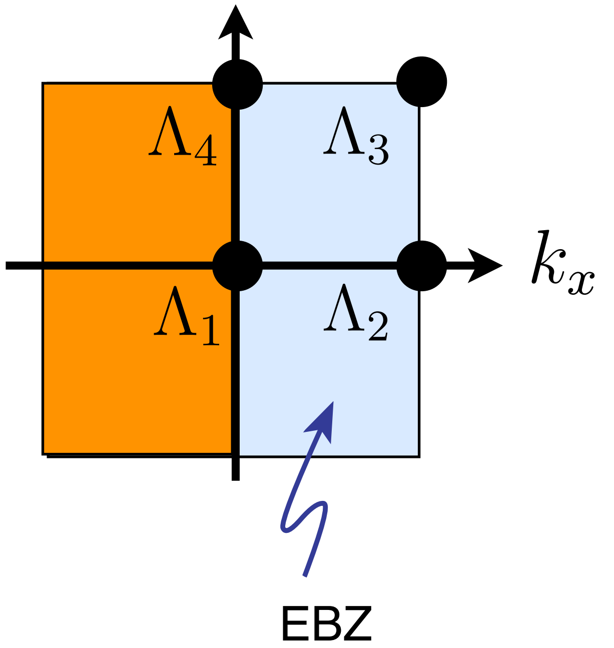
antisymmetry property: $t^{\mathrm{T}}(\mathbf{k}) = -t(\mathbf{k})$

$\Longrightarrow$ Pfaffian can be defined: $\mathrm{Pf}\left[t(\mathbf{k})\right]$

e.g.: $\mathrm{Pf}\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z$

$$(\mathrm{Pf}\left[\omega(\Lambda_a)\right])^2 = \det\left[\omega(\Lambda_a)\right]$$

▶ Zeroes of $\mathrm{Pf}\left[t(\mathbf{k})\right]$ occur in isolated points, carry phase winding



▶ Due to time-reversal symmetry:

(i) $|\mathrm{Pf}[t(\mathbf{k})]| = |\mathrm{Pf}[t(-\mathbf{k})]| \Rightarrow$ zeros come in pairs

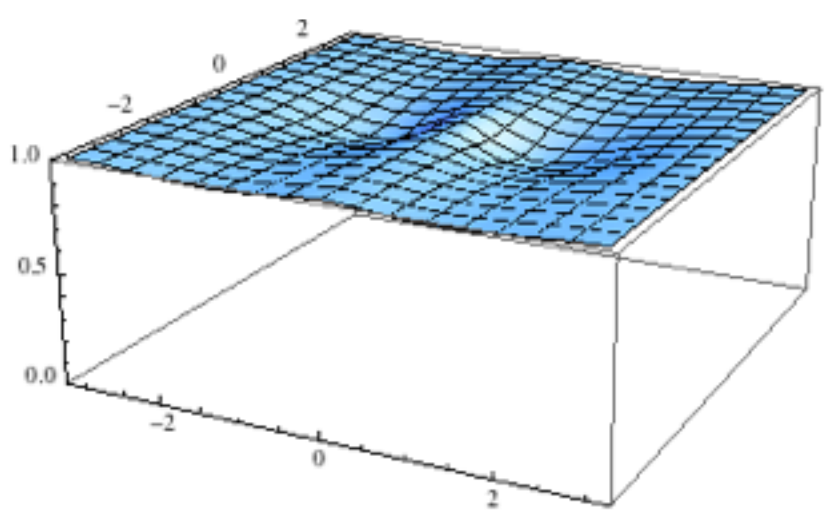
(ii) At TRI momenta Λ_a we have $|\mathrm{Pf}[t(\Lambda_a)]| = 1$

$\Rightarrow$ zeros cannot be brought to TRI momenta

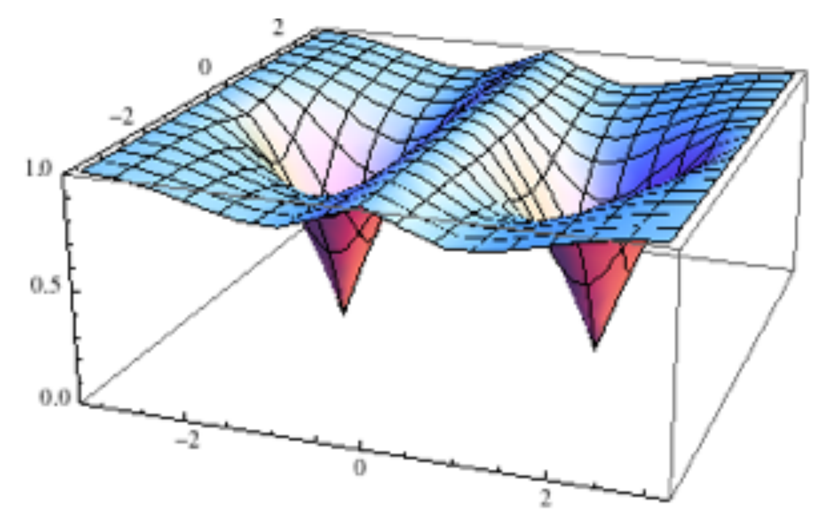
2D topological insulator: First bulk Z_2 invariant

Topological invariant = number or zeros of $\mathrm{Pf}\left[t(\mathbf{k})\right]$ in EBZ modulo 2

conventional insulator



topological insulator



$$I = \frac{1}{2\pi i}\int_{\partial(\mathrm{EBZ})} d\mathbf{k}\cdot\nabla\log\left(\mathrm{Pf}\left[\langle u_m^-(\mathbf{k})|\Theta|u_n^-(\mathbf{k})\rangle\right]\right) \mod 2$$

It follows from **bulk-boundary correspondence**: edge Z_2 invariant = bulk Z_2 invariant

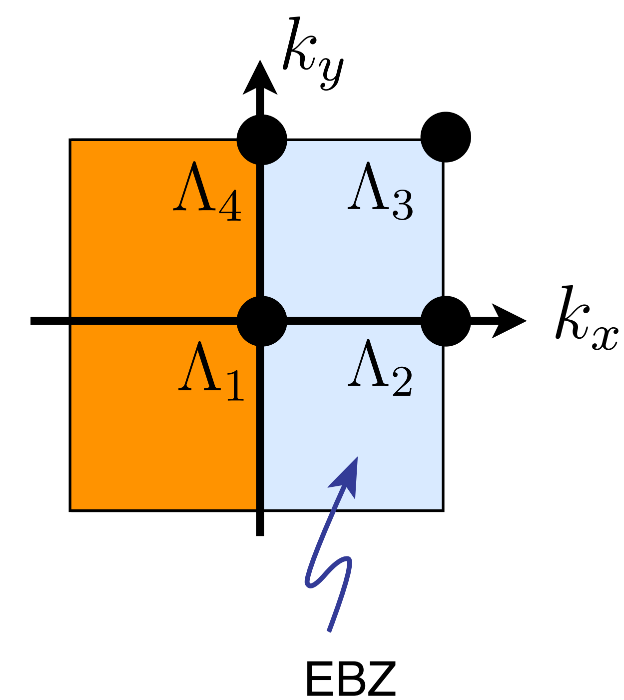
2D topological insulator: Second bulk Z_2 invariant

[Kane Mele 05]

[Fu and Kane]

Bulk Z_2 invariant as an obstruction to define a “TR-smooth gauge”:

- $|u_n^{(1)}(\mathbf{k})\rangle$ and $|u_n^{(2)}(\mathbf{k})\rangle$ denote gauge choices in the two EBZs
- TR-smooth gauge: $|u_n^{(1)}(-\mathbf{k})\rangle = \Theta|u_n^{(2)}(\mathbf{k})\rangle$



$\Rightarrow$ consider unitary *sewing matrix:*

$$\boxed{\omega_{mn}(\mathbf{k}) = \langle u_m^-(-\mathbf{k})|\Theta|u_n^-(\mathbf{k})\rangle}$$

antisymmetry property: $\omega^T(\mathbf{k}) = -\omega(-\mathbf{k})$

at TRI momenta: $\Lambda_a = -\Lambda_a \Rightarrow \omega^T(\Lambda_a) = -\omega(\Lambda_a)$ is antisymmetric

$\Rightarrow$ Pfaffian can be defined: $\mathrm{Pf}\,[\omega(\Lambda_a)]$ e.g.: $\mathrm{Pf}\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z$

$$(\mathrm{Pf}\,[\omega(\Lambda_a)])^2 = \det\,[\omega(\Lambda_a)]$$

Bulk Z_2 invariant (ν= 0,1):

$$\boxed{(-1)^\nu = \prod_{a=1}^{4} \frac{\mathrm{Pf}\,[\omega(\Lambda_a)]}{\sqrt{\det\,[\omega(\Lambda_a)]}} = \pm 1}$$

(gauge invariant, but smooth gauge needed)

It follows from **bulk-boundary correspondence**: edge Z_2 invariant = bulk Z_2 invariant

2D topological insulator: Bulk Z_2 invariants

Three equivalent definitions for **bulk Z_2 topological invariant:**

(A) in terms of sewing matrix:

$$\boxed{(-1)^{\nu} = \prod_{a=1}^{4} \frac{\mathrm{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} = \pm 1}$$

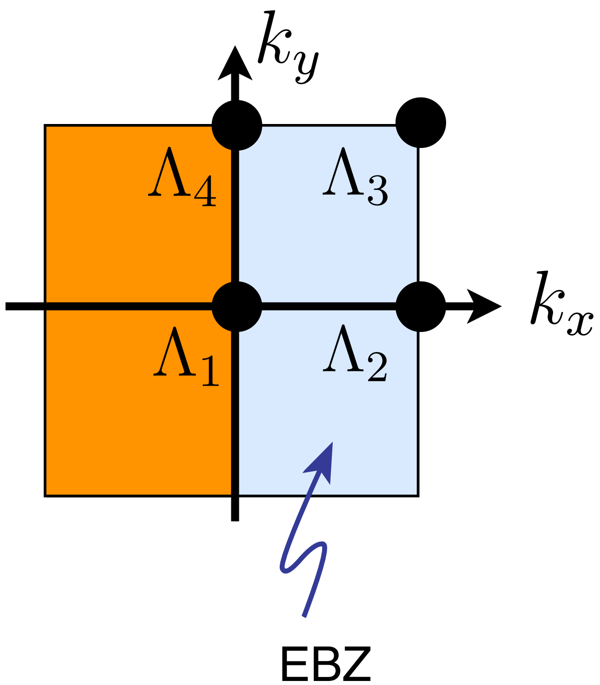
(gauge invariant, but smooth gauge needed)

sewing matrix: $\omega_{mn}(\mathbf{k}) = \langle u_m^-(-\mathbf{k})|\Theta|u_n^-(\mathbf{k})\rangle$ (is unitary, and anti-symmetric at TRI momenta)

(B) count number of zeroes of $\mathrm{Pf}\left[\langle u_m^-(\mathbf{k})|\Theta|u_n^-(\mathbf{k})\right]$ in EBZ

$$I = \frac{1}{2\pi i}\int_{\partial(\mathrm{EBZ})} d\mathbf{k}\cdot\nabla \log\left(\mathrm{Pf}\left[\underbrace{\langle u_m^-(\mathbf{k})|\Theta|u_n^-(\mathbf{k})}\right]\right) \mod 2$$

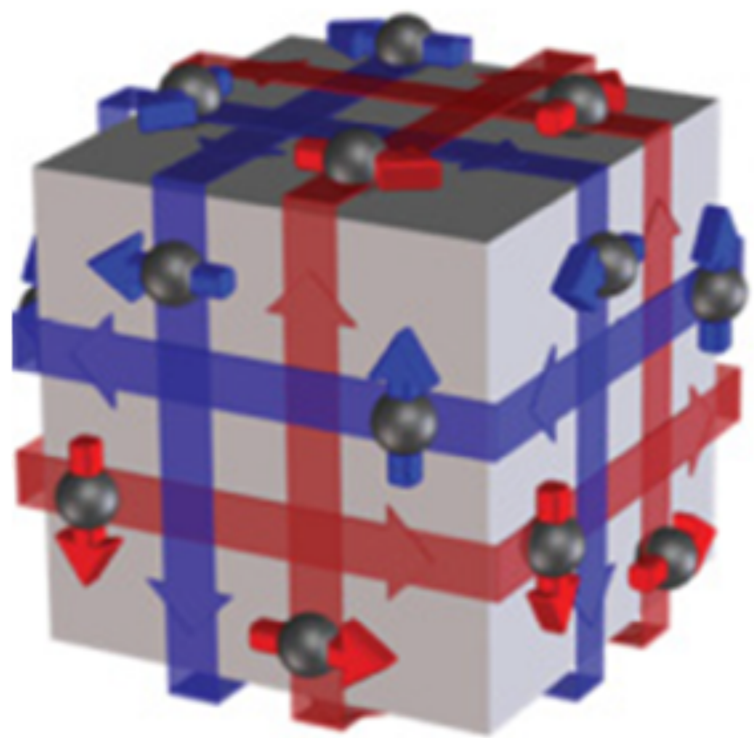
(antisymmetric at all momenta, but not unitary)



(C) in terms of Berry connection:

$$\nu = \frac{1}{2\pi}\left[\oint_{\partial(EBZ)} d\boldsymbol{k}\cdot\mathcal{A} - \int_{\mathrm{EBZ}} d^2\boldsymbol{k}\,\mathcal{F}\right] \mathrm{mod}\;\; 2$$

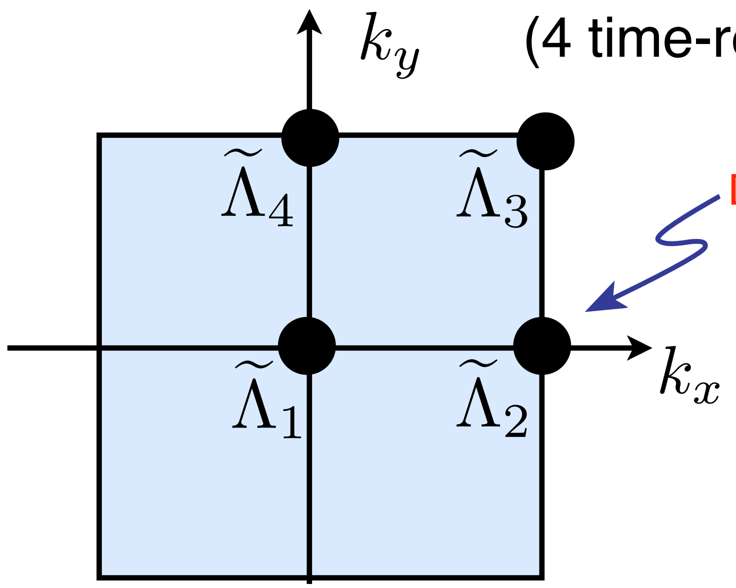
Three-dimensional topological insulators



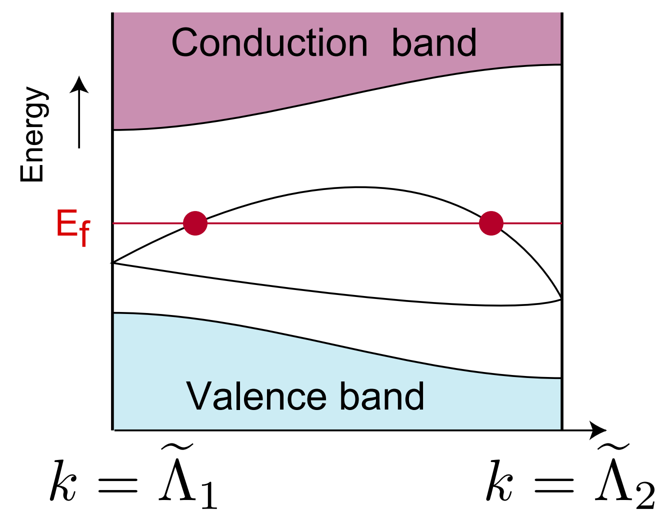
3D topological insulator: Surface Z_2 invariant

- How do surface states connect between TRI momenta? **[after Hasan & Kane, RMP 2010]**

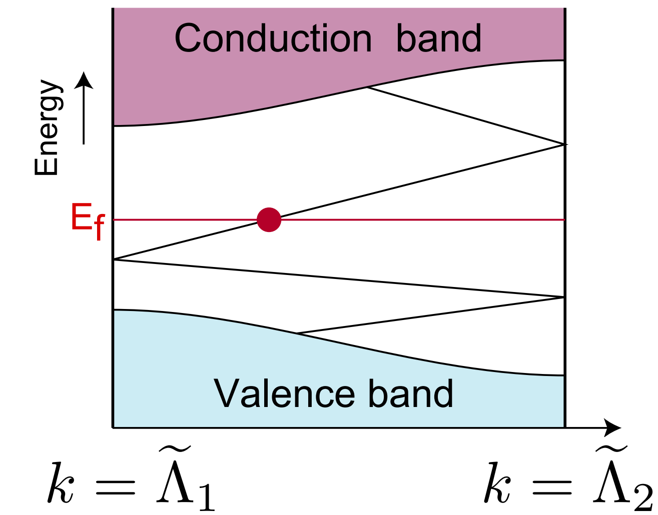
(4 time-reversal invariant momenta in surface BZ)



surface Brillouin zone



OR



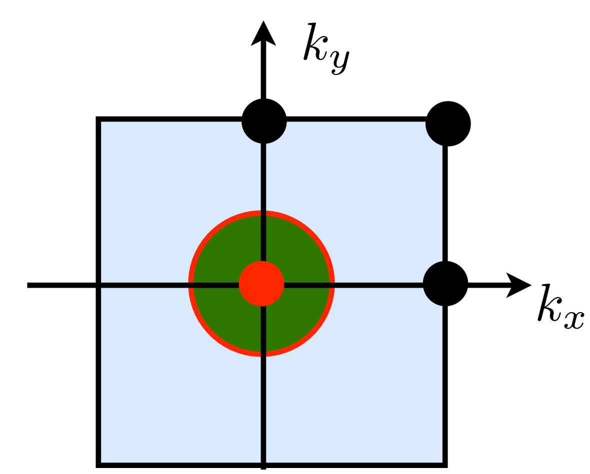
- **Surface Z_2 invariant:**

$\nu = 1$: **Strong topological insulator**

— Fermi surface encloses *odd* number of TRI momenta

— independent of surface orientation

— protected by time-reversal symmetry

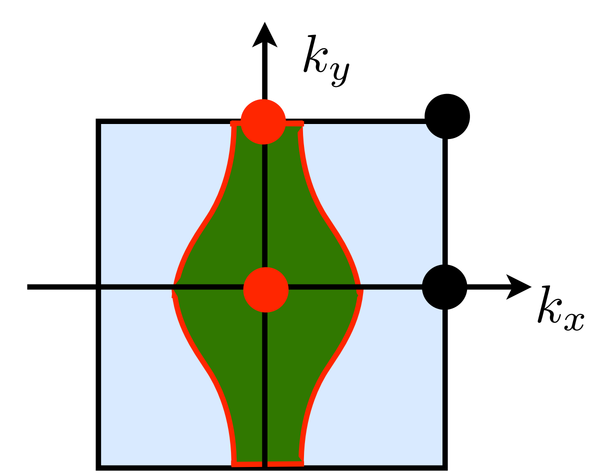


$\nu = 0$: **Weak topological insulator**

— Fermi surface encloses *even* number of TRI momenta

— depends on surface orientation (quasi-2D topological insulator)

— protected by time-reversal *and* translation symmetry



3D topological insulator: Bulk Z_2 invariant

[Kane-Mele, Moore-Balents, Roy, Fu-Kane-Mele (06-07)]

- **Bulk Z_2 invariant:**

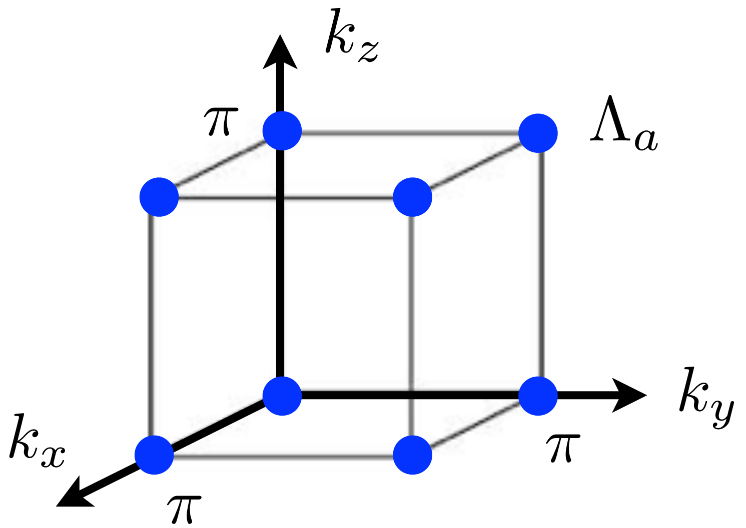
$$\boxed{t_{mn}(\mathbf{k}) = \left\langle u_m^-(\mathbf{k}) \right| \Theta \left| u_n^-(\mathbf{k}) \right\rangle}$$

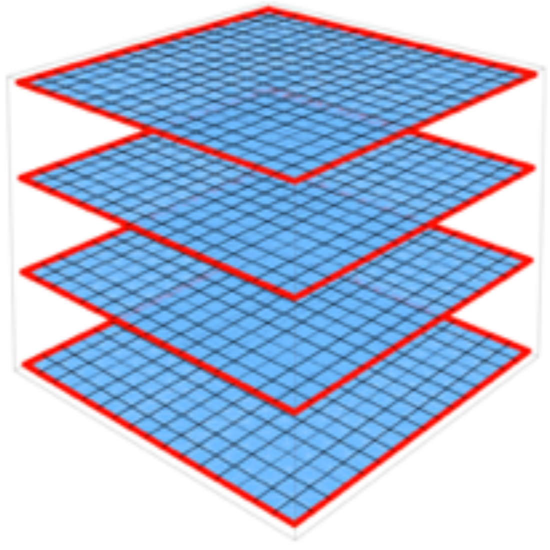
– Zeros of $\mathrm{Pf}[t(\mathbf{k})]$ are lines

– Due to time-reversal symmetry there are only 16 possibilities for the arrangement of the lines:

$$(\nu_0; \nu_1, \nu_2, \nu_3)$$

8 TRI momenta in bulk BZ





– Strong Z_2 invariant

$$(-1)^{\nu_0} = \prod_{a=1}^{8} \frac{\mathrm{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}} = \pm 1$$

– Weak Z_2 invariant

$$(-1)^{\nu_i} = \prod_{a=1}^{4} \frac{\mathrm{Pf}\left[\omega(\Lambda_a)\right]}{\sqrt{\det\left[\omega(\Lambda_a)\right]}}\Bigg|_{k_i=0}$$

Bulk-boundary correspondence: edge Z_2 invariant = bulk Z_2 invariant

Experimental detection of 3D topological insulators

▶ observed in certain band insulators with strong spin-orbit coupling

BiSb alloy, Bi_2Se_3, Bi_2Te_3, $TlBiTe_2$, $TlSbSe_2$, etc ....

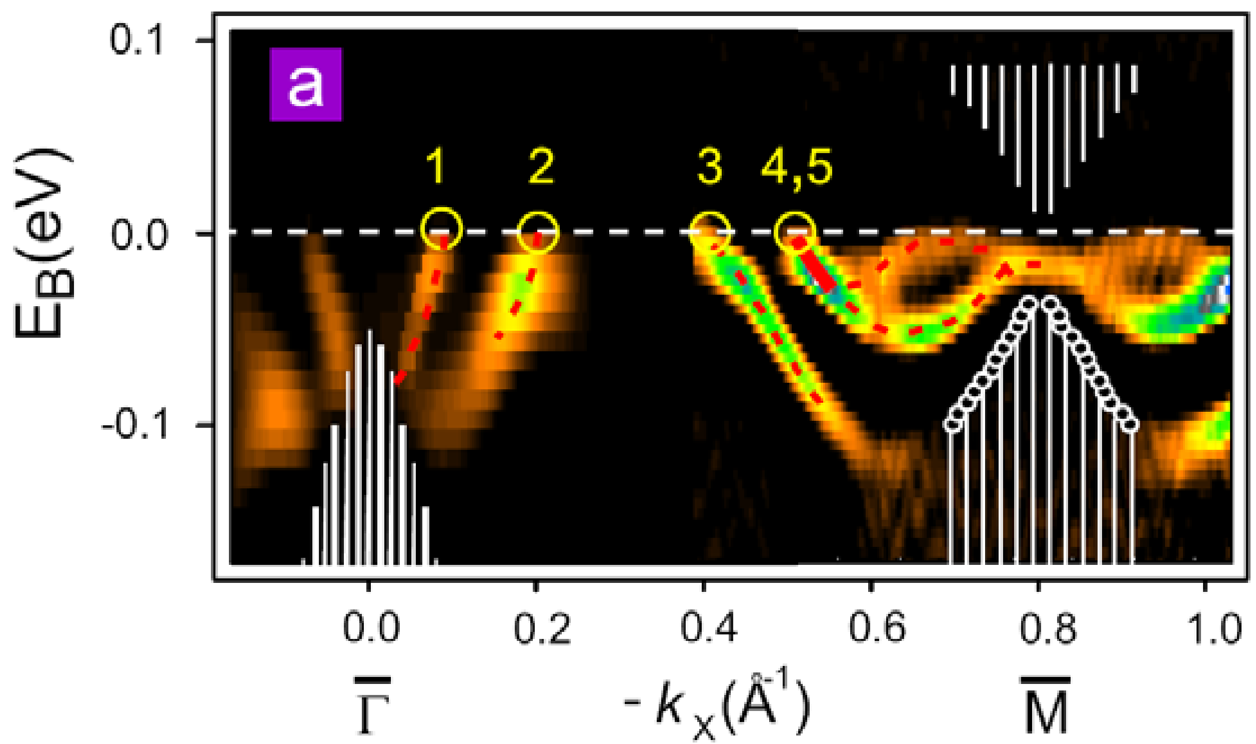
stable surface states cross a gap, that is opened up by spin-orbit coupling

- $\mathrm{Bi}_{1-x}\ \mathrm{Sb}_x$:

[Fu, Kane, PRL 2007]

[Hsieh, Hasan et al, Nature 2008]

momentum resolved photoemission (ARPES)



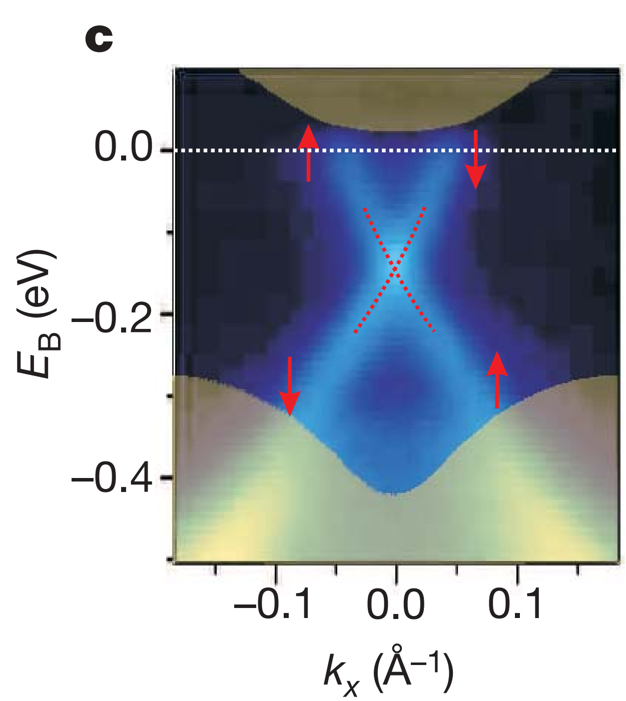
five surface state bands cross E_F between TRI momenta $\bar{\Gamma}$ and $\bar{\mathrm{M}}$

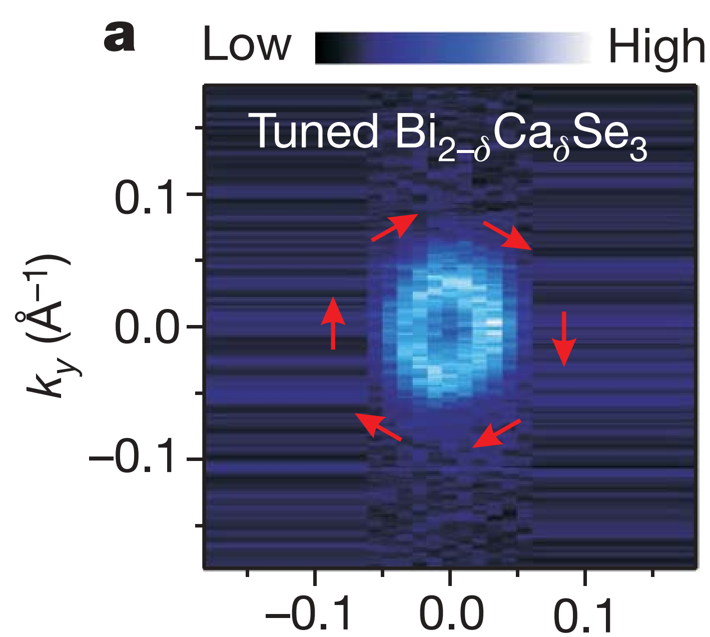
$\Rightarrow$ strong topological insulator

Experimental detection of 3D topological insulators

- $\mathrm{Bi_2\ Se_3}$:

spin resolved and momentum resolved photoemission (ARPES)

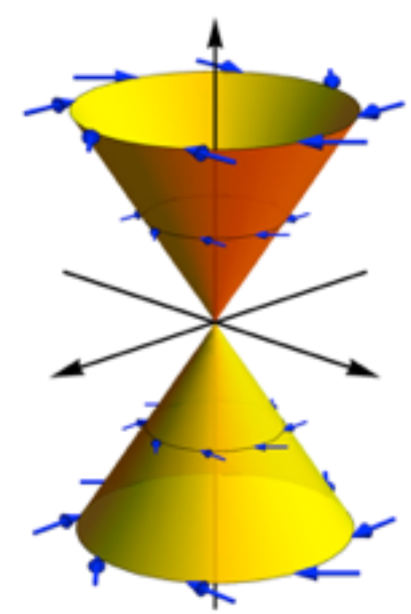




[H. Zhang et al., Nat Phys 2009]

[Hsieh, Hasan et al, Nature 2009]

simple surface state structure, similar to graphene



Unique properties of helical surface states:

- spin and momentum are locked
- half of an ordinary 2DEG, “1/4 of graphene”
- robust to disorder, impossible to localize