Modern Topics in Solid-State Theory: Topological insulators and superconductors

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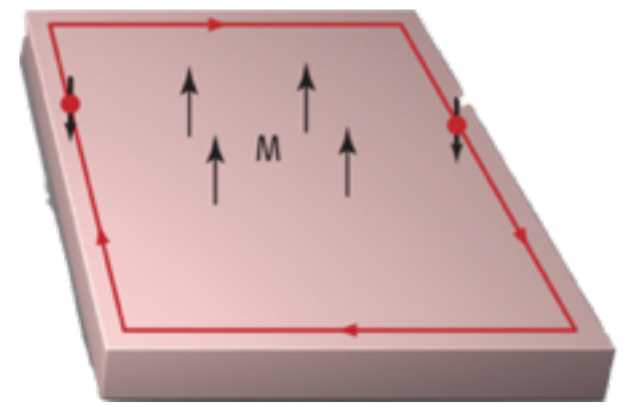
Lecture Two: Chern insulator & Quantum spin Hall state

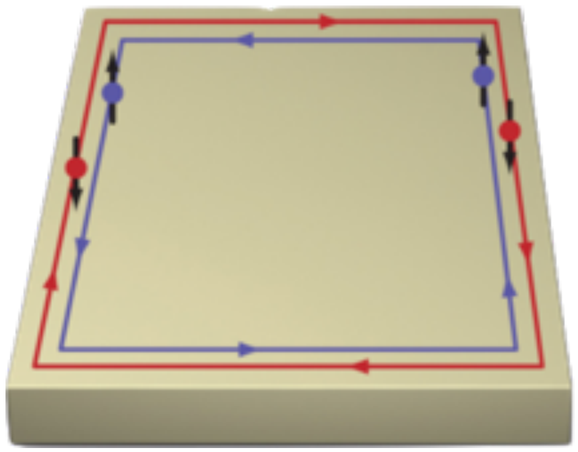
1. Chern insulator and IQHE

- Integer quantum Hall effect
- Chern insulator on square lattice
- Topological invariant



2. Quantum spin Hall state

- Time reversal symmetry
- QSH state on square lattice
- Z_2 surface invariant & Z_2 bulk invariant



[picture courtesy S. Zhang et al.]

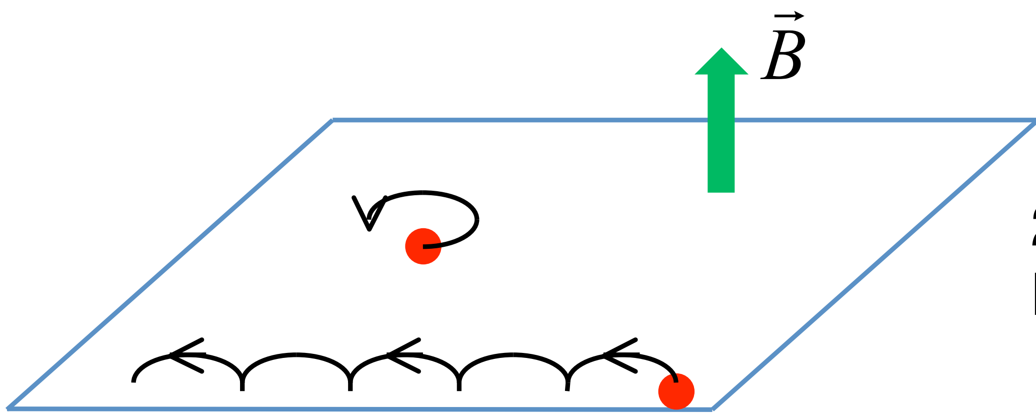
The Integer Quantum Hall State

Integer Quantum Hall State:

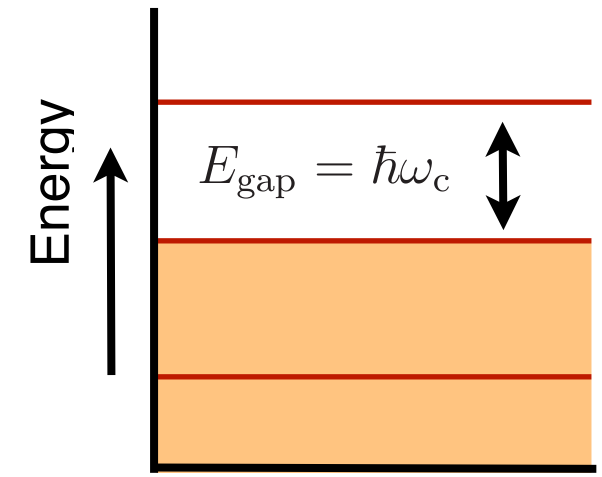
[von Klitzing '80]

First example of 2D topological material

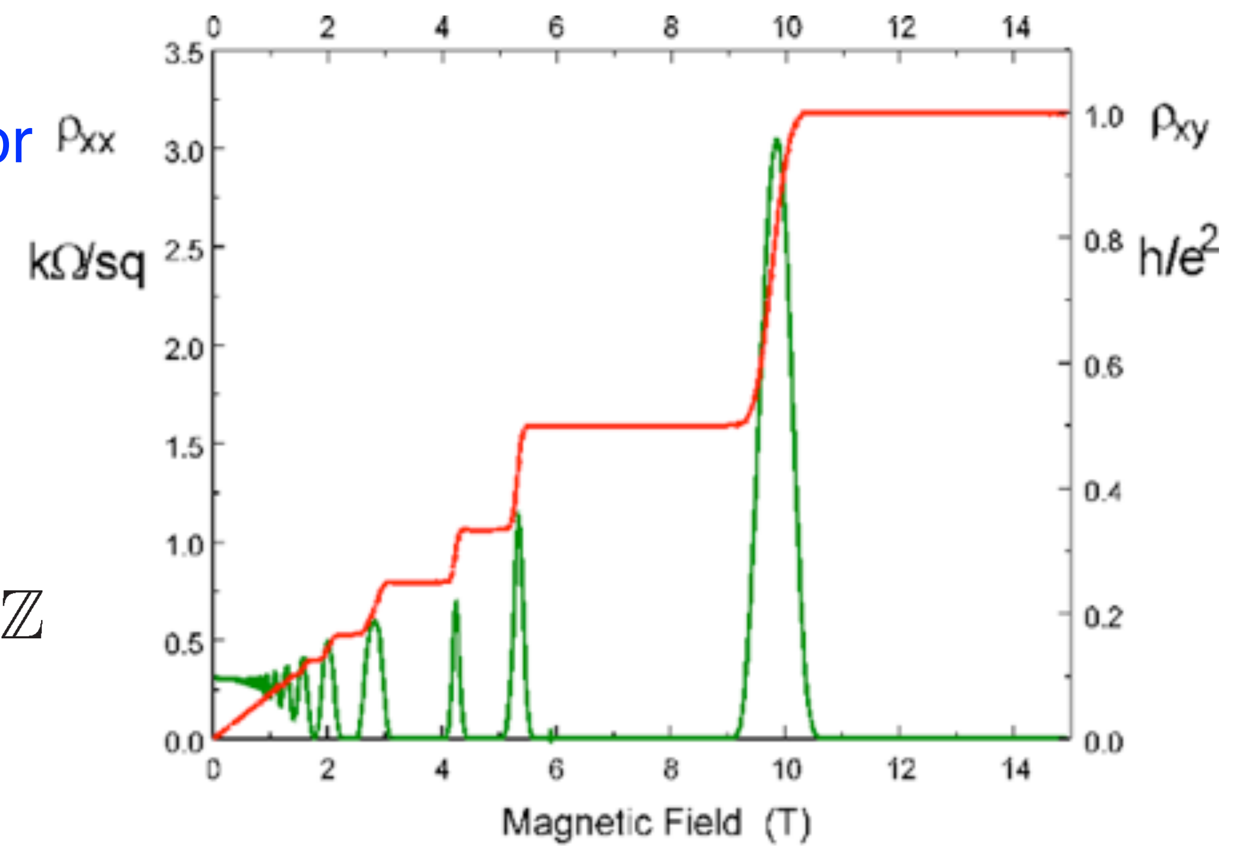
- 2D electron gas in large magnetic field, at low T



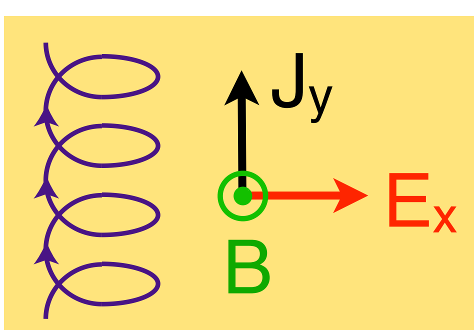
2D cyclotron motion
Landau levels



- There is an energy gap, but it is not an insulator



▶ Quantized Hall conductivity: $J_y = \sigma_{xy} E_x$

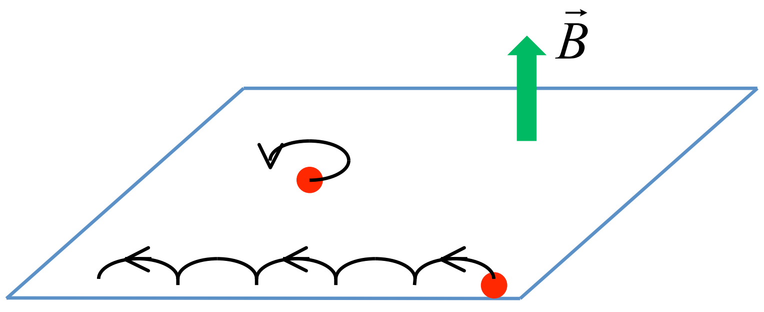


$$\sigma_{xy} = n\frac{e^2}{h} \qquad n \in \mathbb{Z}$$

- Plateaus in resistivity $\rho_{xy} = \frac{1}{n}\frac{h}{e^2}$

The Integer Quantum Hall State

What causes the precise quantization in IQHE?



Explanation One: Edge state transport

IQHE has an energy gap in the bulk:

— charge cannot flow in bulk; only along 1D channels at edges (chiral edge states)

— chiral edge state cannot be localized by disorder (no backscattering)

— edge states are perfect charge conductor!

Explanation Two: Topological band theory

Distinction between the integer quantum Hall state and a conventional insulator is a topological property of the band structure ***[Thouless et al, 84]***

$\mathcal{H}(\mathbf{k})$: Brillouin zone $\longmapsto$ Hamiltonians with energy gap

Classified by Chern number: $n = \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k$ (= topological invariant) $n \in \mathbb{Z}$

Kubo formula: $\sigma_{xy} = \frac{e^2}{h} \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k$

$\Longrightarrow$ does not change under smooth deformations, as long as bulk energy gap is not closed

Bulk-boundary correspondence

topological invariant $$n = \frac{i}{2\pi} \sum_{\substack{\text{filled} \\ \text{states}}} \int \mathcal{F} d^2k \qquad n \in \mathbb{Z}$$

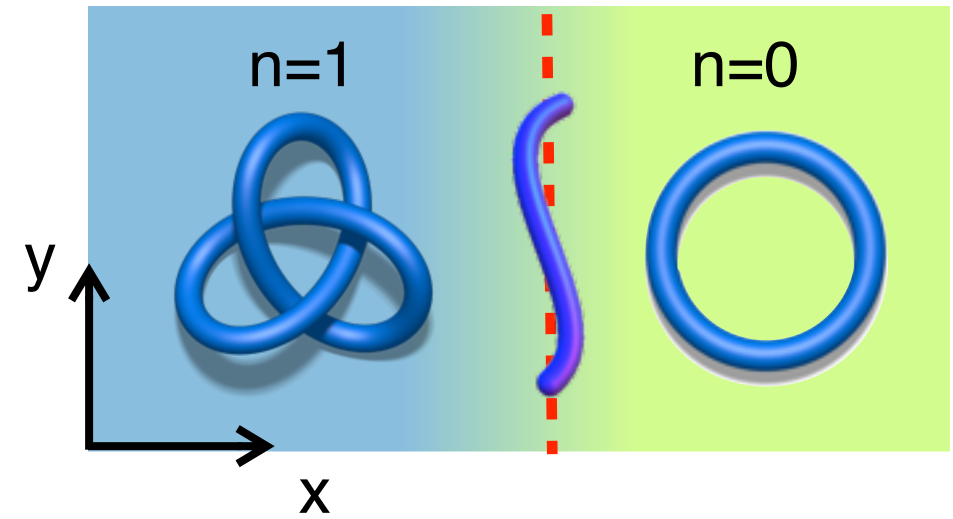
Bulk-boundary correspondence:

Zero-energy states must exist at the interface between two different topological phases

Follows from the quantization of the topological invariant.

$\Delta n = |n_\mathrm{L} - n_\mathrm{R}|$ = number or edge modes

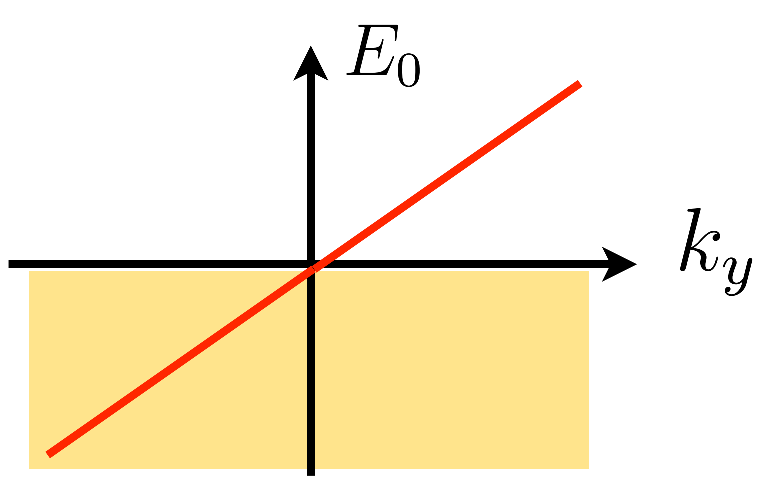
Zero-energy state at interface



Stable gapless edge states:

- robust to smooth deformations (respect symmetries of the system)
- insensitive to disorder, impossible to localize
- cannot exist in a purely 1D system (Fermion doubling theorem)

IQHE: chiral Dirac Fermion



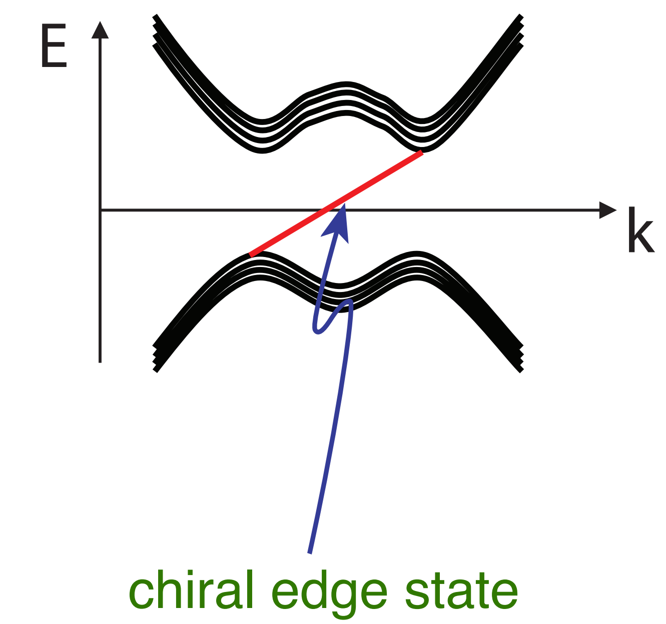
Chern insulator ("integer quantum Hall state on a lattice")

Experimental realization: Cr-doped $(Bi,Sb)_2Te_3$ **[D. Haldane PRL '88] [Chang et al. Science '13]**

Tight-binding model: $H_{\rm CI} = \begin{pmatrix} c^\dagger_{s,\mathbf{k}} & c^\dagger_{p,\mathbf{k}} \end{pmatrix} \mathcal{H}_{\rm CI} \begin{pmatrix} c_{s,\mathbf{k}} \\ c_{p,\mathbf{k}} \end{pmatrix}$ $\quad \mathcal{H}_{\rm CI} = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma} + \epsilon_0(\mathbf{k})\sigma_0$

$$d_x(\mathbf{k}) = \sin k_x \qquad d_y(\mathbf{k}) = \sin k_y \qquad d_z(\mathbf{k}) = (2 + M - \cos k_x - \cos k_y)$$

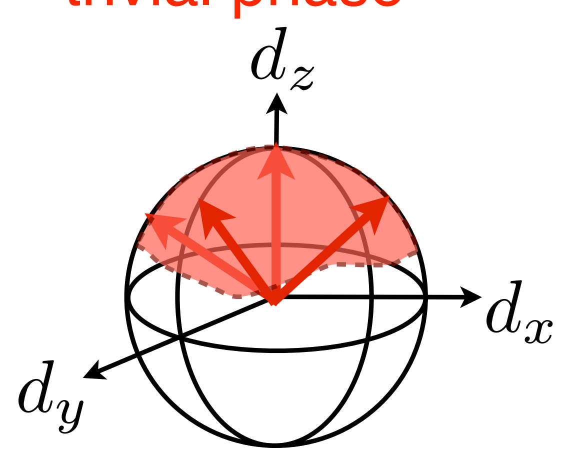
$E_\pm = \pm |\mathbf{d}(\mathbf{k})|$ $\quad$ Spectrum flattening: $\hat{\mathbf{d}}(\mathbf{k}) = \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|}$



trivial phase

$M > 0$

$n_{\mathbb{Z}} = 0$

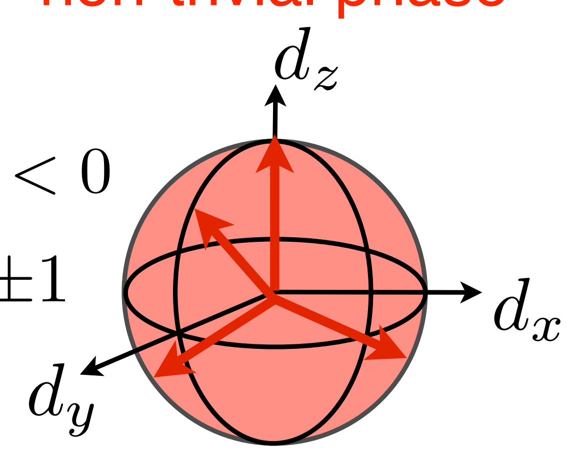


no edge state

non-trivial phase

$-4 < M < 0$

$n_{\mathbb{Z}} = \pm 1$



chiral edge state

Chern number: $n_{\mathbb{Z}} = \frac{1}{8\pi} \int_{\rm BZ} d^2\mathbf{k}\, \epsilon^{\mu\nu} \hat{\mathbf{d}} \cdot \left[\partial_{k_\mu} \hat{\mathbf{d}} \times \partial_{k_\nu} \hat{\mathbf{d}} \right]$ $\quad$ quantized Hall effect $\sigma_{xy} = \frac{e^2}{h} n$

Mapping $\quad \hat{\mathbf{d}}(\mathbf{k})$: Brillouin zone $\longmapsto \hat{\mathbf{d}}(\mathbf{k}) \in S^2$ $\qquad$ "$\pi_2(S^2) = \mathbb{Z}$"

Chern insulator ("integer quantum Hall state on a lattice")

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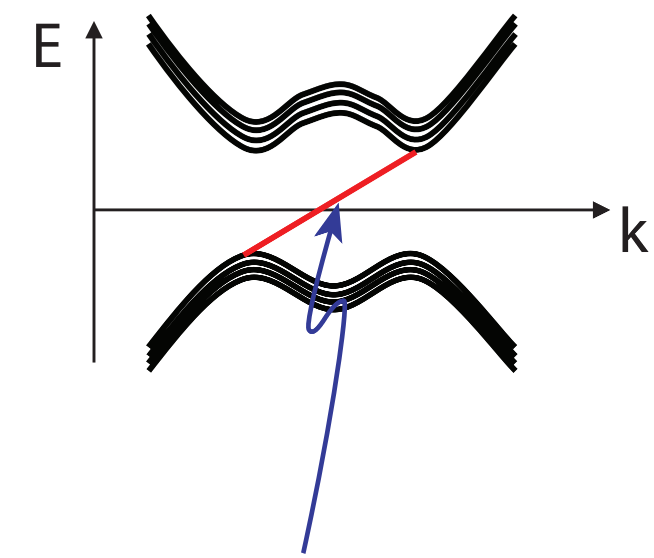
Tight-binding model: $H_{\mathrm{CI}} = \begin{pmatrix} c^\dagger_{s,\mathbf{k}} & c^\dagger_{p,\mathbf{k}} \end{pmatrix} \mathcal{H}_{\mathrm{CI}} \begin{pmatrix} c_{s,\mathbf{k}} \\ c_{p,\mathbf{k}} \end{pmatrix}$ $\quad \mathcal{H}_{\mathrm{CI}} = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma} + \epsilon_0(\mathbf{k})\sigma_0$

$$d_x(\mathbf{k}) = \sin k_x \qquad d_y(\mathbf{k}) = \sin k_y \qquad d_z(\mathbf{k}) = (2 + M - \cos k_x - \cos k_y)$$

$$E_\pm = \pm |\mathbf{d}(\mathbf{k})|$$

Spectrum flattening: $\hat{\mathbf{d}}(\mathbf{k}) = \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|}$

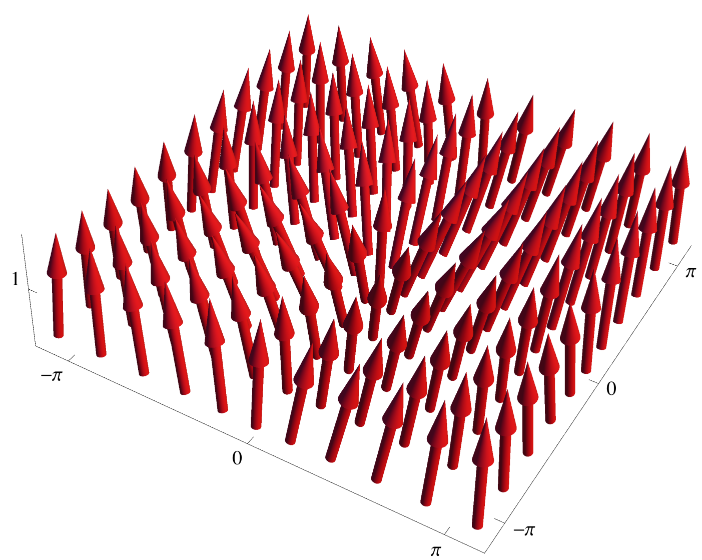


chiral edge state

Texture of unit vector $\hat{\mathbf{d}}(\mathbf{k})$

trivial phase

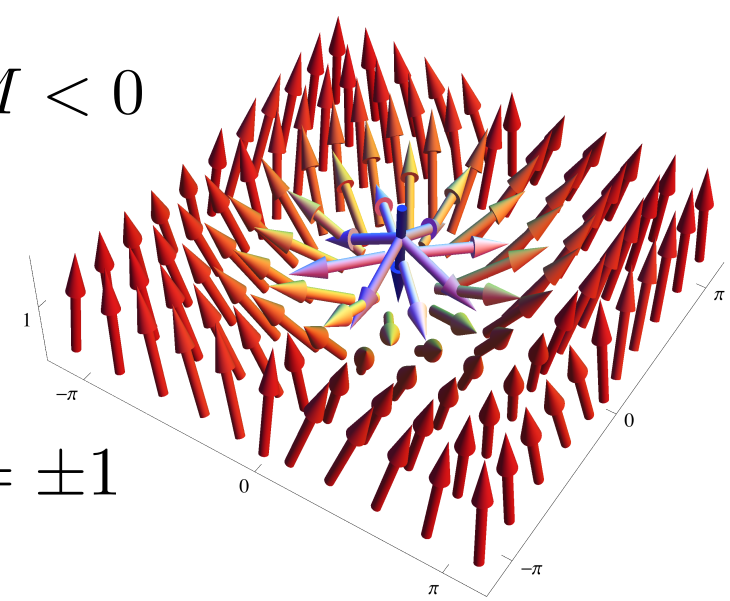
$M > 0$



$n_{\mathbb{Z}} = 0$

non-trivial phase

$-4 < M < 0$



$n_{\mathbb{Z}} = \pm 1$

Chern number: $n_{\mathbb{Z}} = \frac{1}{8\pi} \int_{\mathrm{BZ}} d^2\mathbf{k}\, \epsilon^{\mu\nu} \hat{\mathbf{d}} \cdot \left[\partial_{k_\mu} \hat{\mathbf{d}} \times \partial_{k_\nu} \hat{\mathbf{d}} \right]$

Chern insulator on square lattice

Chern insulator on square lattice: $\mathcal{H}_{\mathrm{CI}} = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma} + \epsilon_0(\mathbf{k})\sigma_0$

$$d_x(\mathbf{k}) = \sin k_x \qquad d_y(\mathbf{k}) = \sin k_y \qquad d_z(\mathbf{k}) = (2 + M - \cos k_x - \cos k_y)$$

Effective low-energy continuum theory for M=0: (expand around $\mathbf{k} = 0$; σ_0 term can be neglected)

$$H_{\mathrm{CI}} = k_x\sigma_x + k_y\sigma_y + M\sigma_z$$

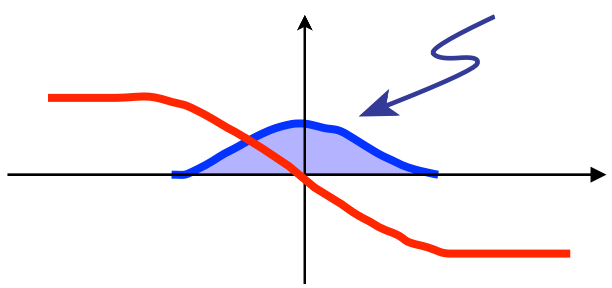
two eigenfunctions with energies: $E_\pm = \pm\lambda = \pm\sqrt{\mathbf{k}^2 + M^2}$

$$|u_{\mathbf{k}}^+\rangle = \frac{1}{\sqrt{2\lambda(\lambda - M)}}\begin{pmatrix} k_x - ik_y \\ \lambda - M \end{pmatrix} \qquad |u_{\mathbf{k}}^-\rangle = \frac{1}{\sqrt{2\lambda(\lambda + M)}}\begin{pmatrix} -k_x + ik_y \\ \lambda + M \end{pmatrix}$$

Berry curvature: $F_{xy} = \partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x} = +\frac{M}{2\lambda^3}$

gives nonzero Chern number
(= Hall conductance σ_{xy})

$$n = \frac{1}{2\pi}\int d^2k\, F_{xy} = \frac{1}{2}\mathrm{sgn}(M)$$



NB: Chern number must be integer for integrals over compact manifolds.
Proper regularization of Dirac Hamiltonian will lead to $n \in \mathbb{Z}$

Chiral edge state at boundary between two Chern insulators with different n

$$\psi_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ik_y y} e^{-\int_0^x M(x')dx'}$$

Experimental realisation of Chern insulator

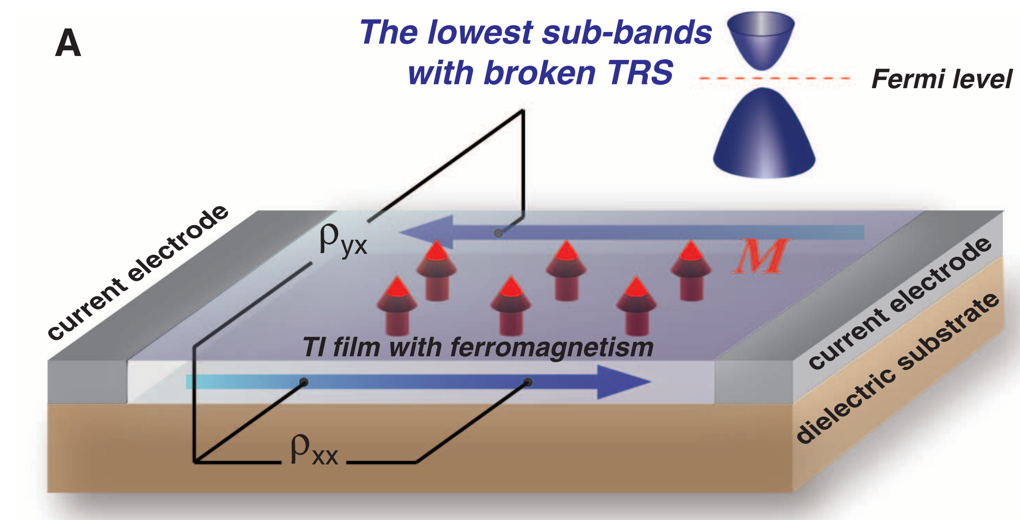
[Chang et al. Science '13]

- Cr-doped $(Bi,Sb)_2Te_3$

— Thin layer of topological insulator, which has helical surface states

— States on top surface are gapped out by finite size quantization

— Time-reversal symmetry is broken by magnetic ad-atoms (Cr or V)



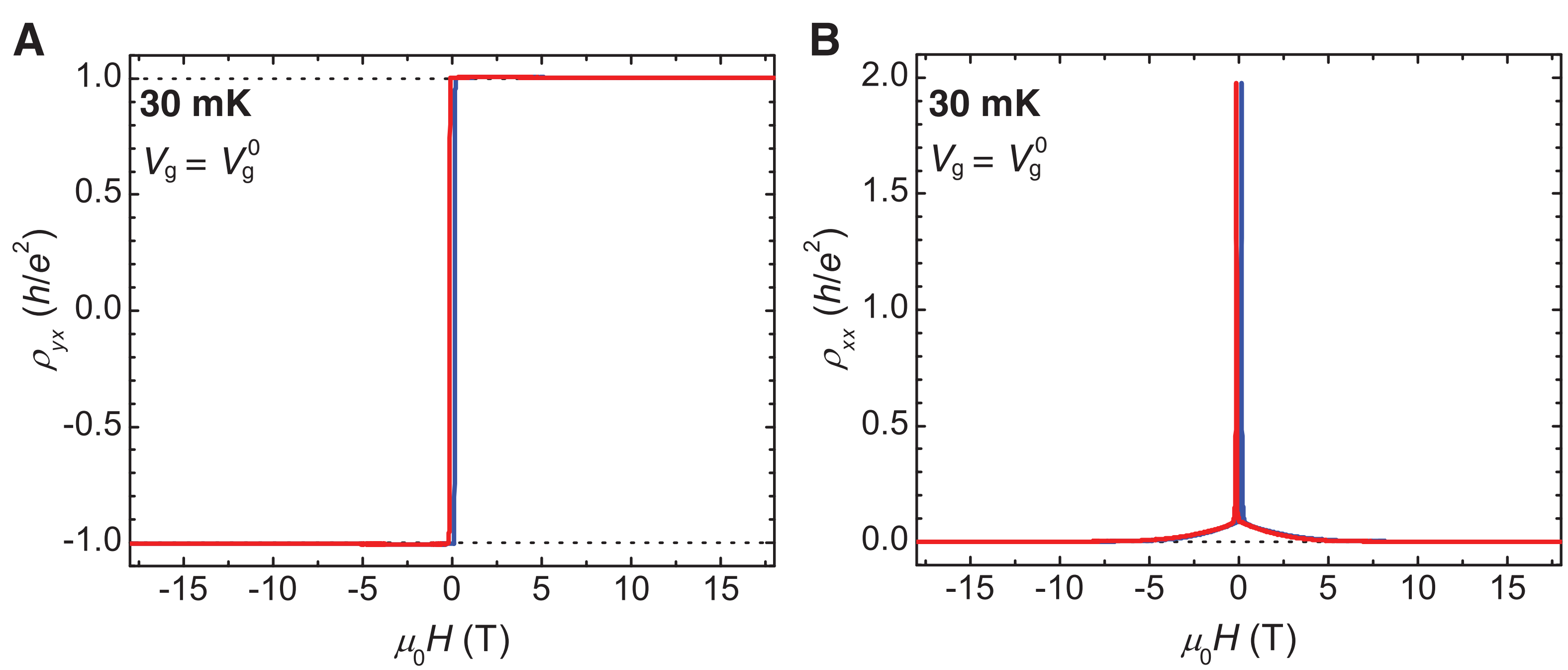
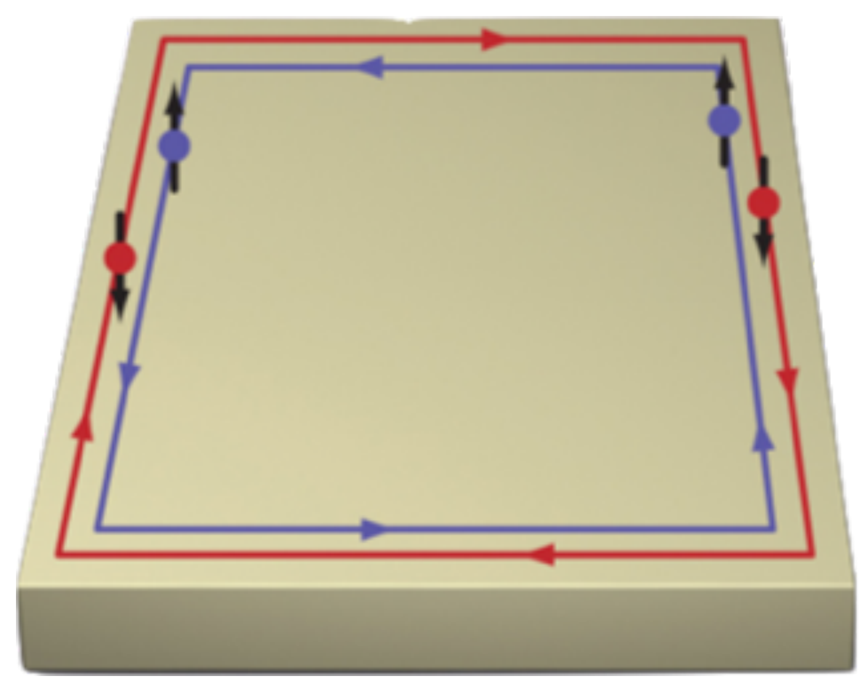


Fig. 3. The QAH effect under strong magnetic field measured at 30 mK. (**A**) Magnetic field dependence of ρ_{yx} at V_g^0. (**B**) Magnetic field dependence of ρ_{xx} at V_g^0. The blue and red lines in (A) and (B) indicate the data taken with increasing and decreasing fields, respectively.

Quantum spin Hall state



[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: $\Theta^2 = -1 \quad U_{\mathrm{T}} = -U_{\mathrm{T}}^T \quad \Theta = i\sigma_y \mathcal{K} \quad \Theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}$

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

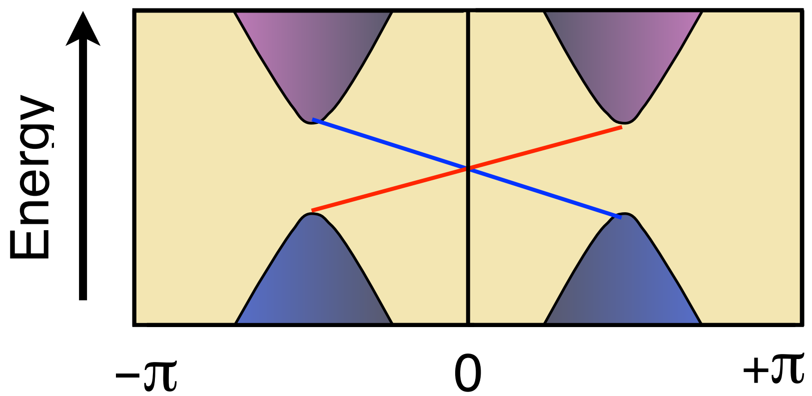
$\Rightarrow$ all eigenstates are at least two-fold degenerate

$\Rightarrow$ 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

(also known as Quantum Spin Hall insulator)

[Bernevig, Hughes, Zhang 2006]

[Kane-Mele, PRL 05]

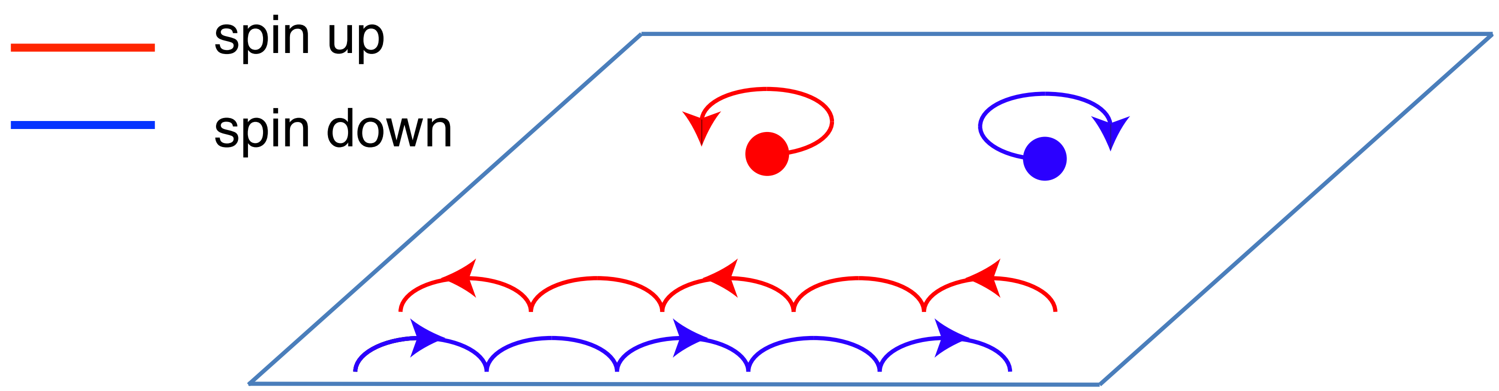
2D Bloch Hamiltonians in the presence of time-reversal symmetry:

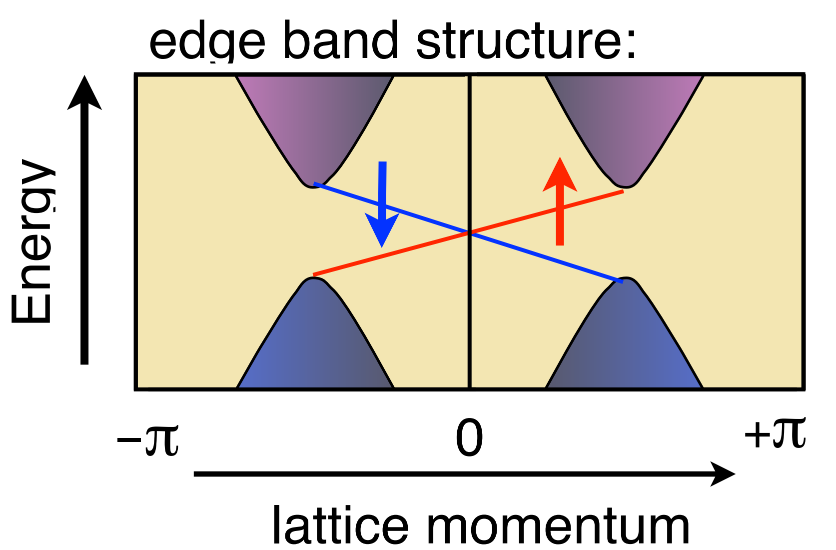
$$\boxed{\Theta\mathcal{H}(\mathbf{k})\Theta^{-1} = +\mathcal{H}(-\mathbf{k})} \qquad \Theta = i\sigma_y \otimes \mathbb{1}\,\mathcal{K} \qquad \Theta^2 = -1$$

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

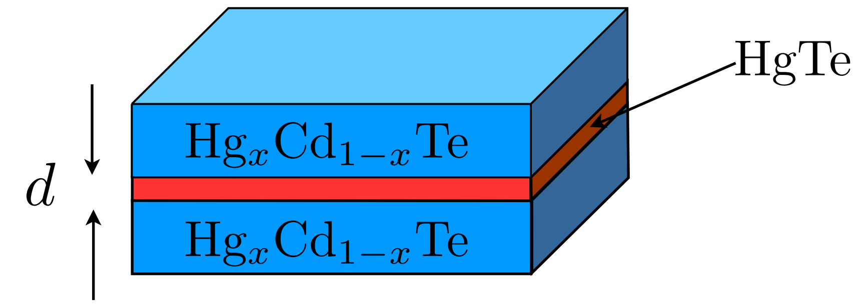
— protected by time-reversal symmetry
— half an ordinary 1D electron gas
— is realized in certain band insulators with strong spin-orbit coupling

TRI topological insulator: HgTe quantum wells

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

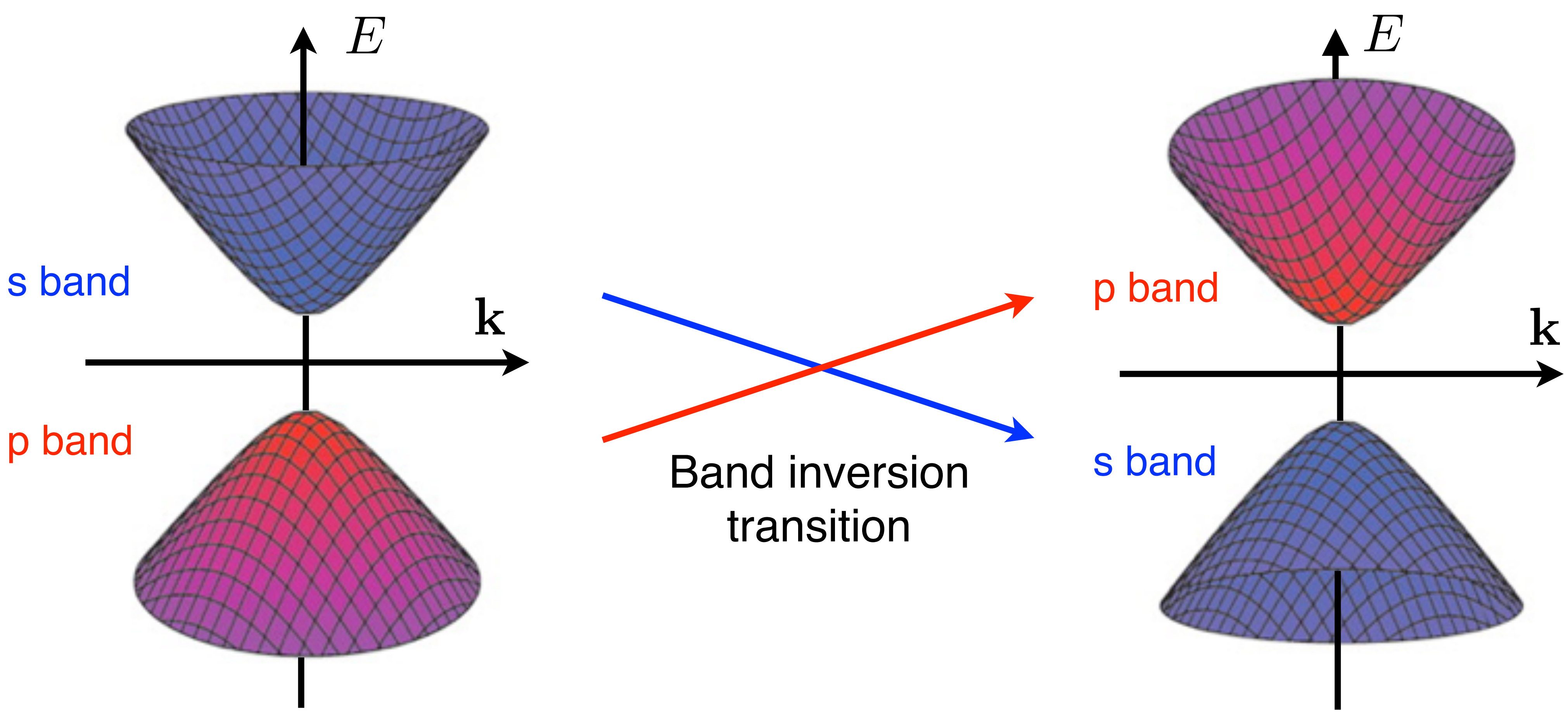
  [Bernevig, Hughes, Zhang Science 2006]

  [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

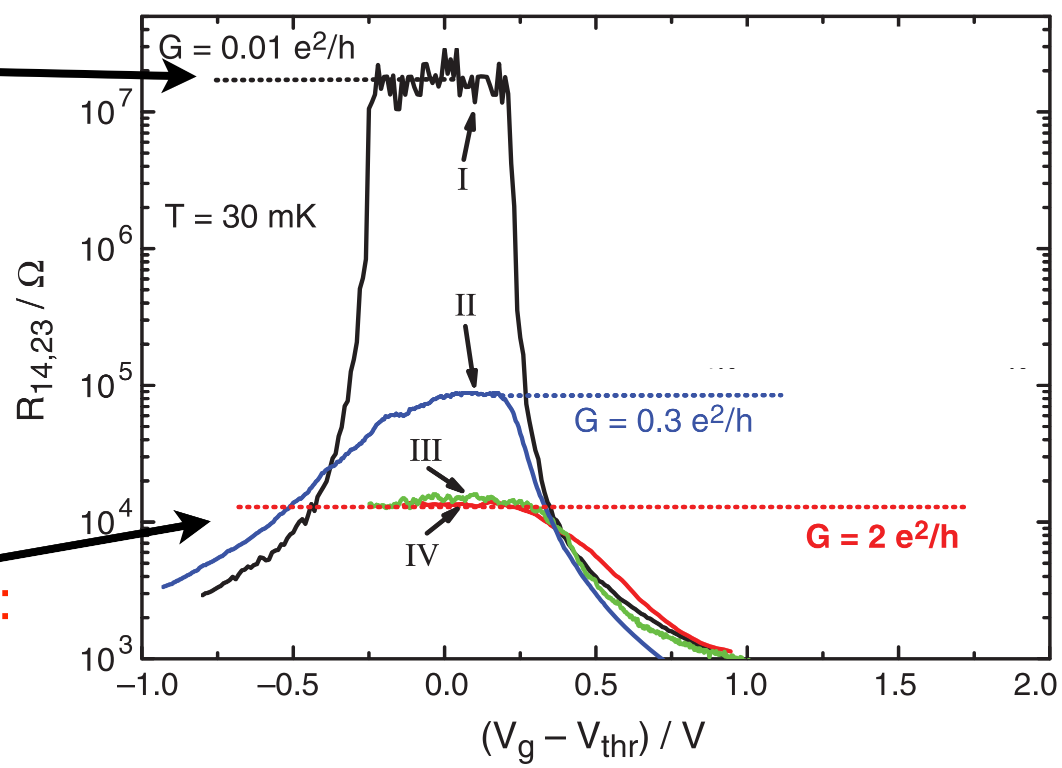
[M. Koenig, Buhmann, Mohlenkamp, et al., Science 2007]

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

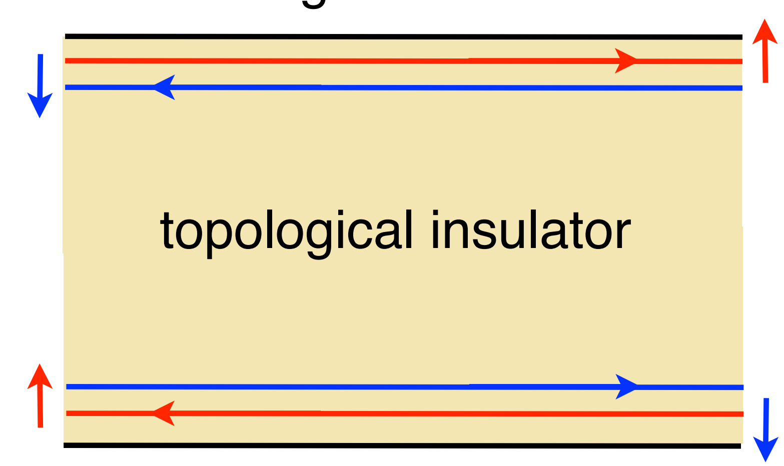
Measured conductance: $2e^2/h$ for short samples L < L_{mag}, L_{IS}
(two terminal conductance)

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** ($\nu = 0,1$)

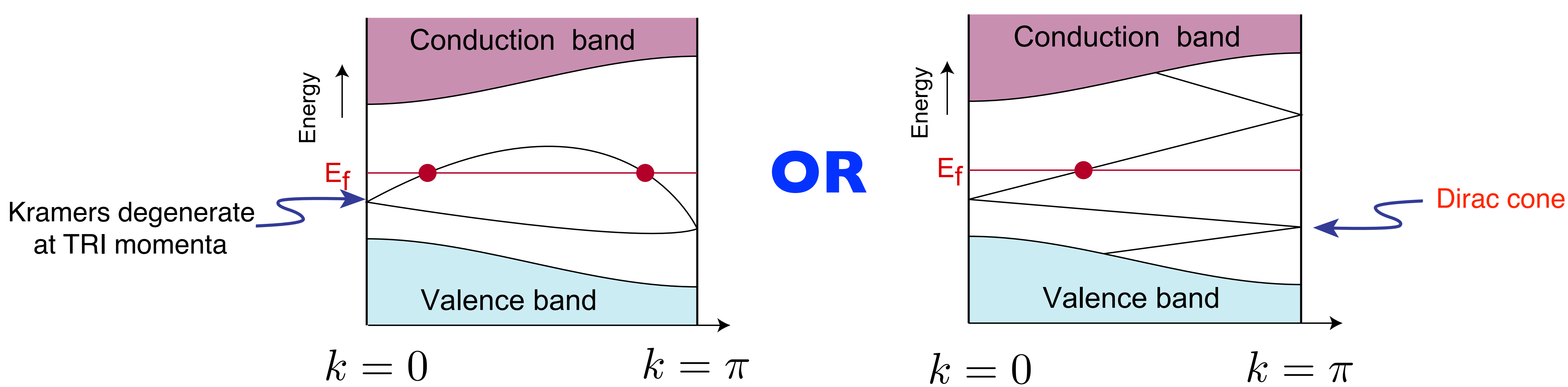
$$\Theta \mathcal{H}(\mathbf{k}) \Theta^{-1} = +\mathcal{H}(-\mathbf{k})$$

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*":

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

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

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

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

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

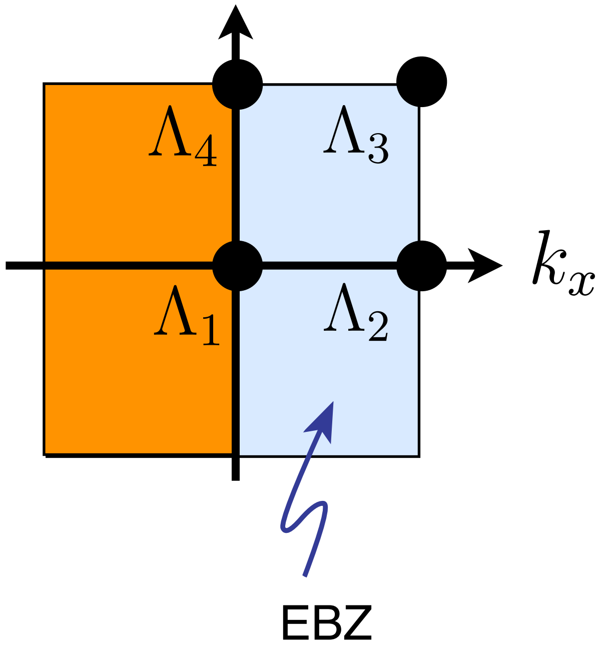
▶ Zeroes of $\mathrm{Pf}\,[t(\mathbf{k})]$ occur in isolated points, carry phase winding

▶ 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 $|\mathrm{Pf}[t(\Lambda_a)]| = 1$

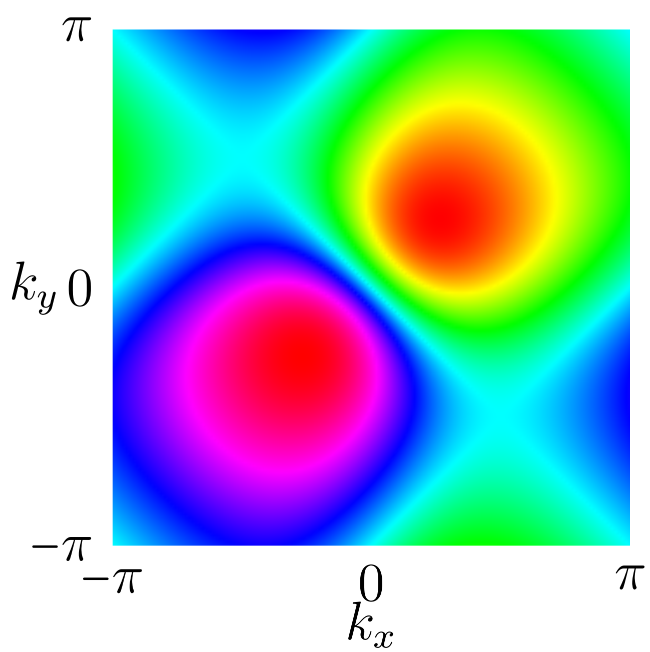
$\Rightarrow$ zeros cannot be brought to TRI momenta



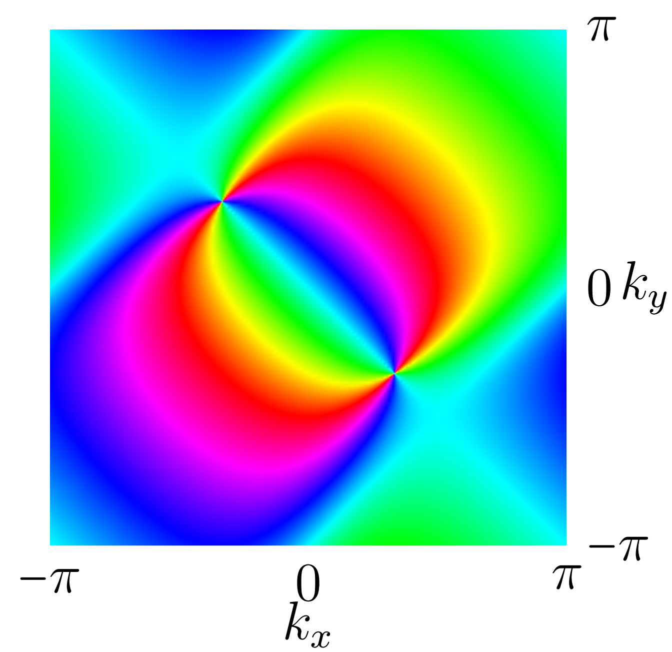
2D topological insulator: First bulk Z_2 invariant

Topological invariant = number or zeros of $\mathrm{Pf}\,[t(\mathbf{k})]$ 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

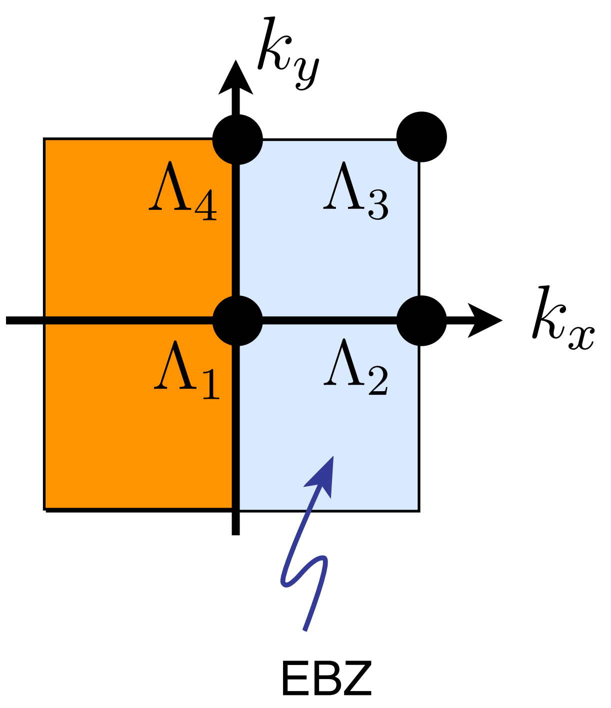
2D topological insulator: Second bulk Z_2 invariant

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

[Kane Mele 05]

[Fu and Kane]

- $|u_n^{(1)}(\mathbf{k})\rangle$ 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 unitary *sewing matrix:*

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

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

$\Longrightarrow$ 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 ($\nu = 0,1$):

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

(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:

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

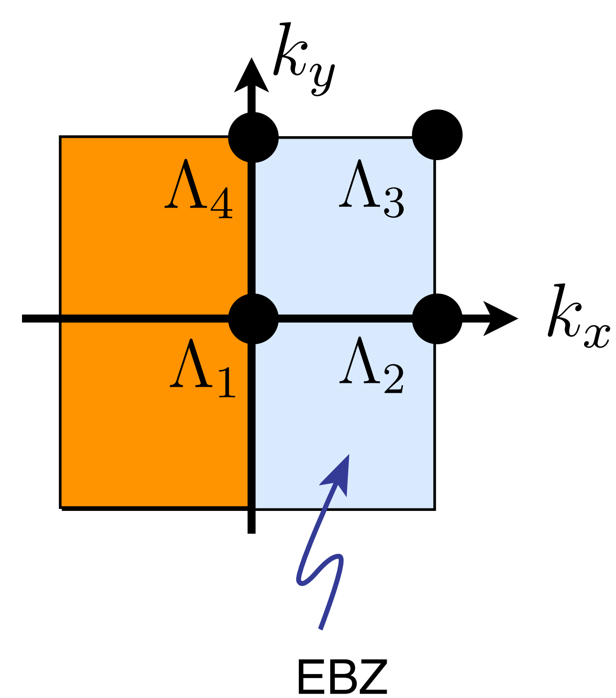
(gauge invariant, but smooth gauge needed)

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:

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