Introduction to topological insulators
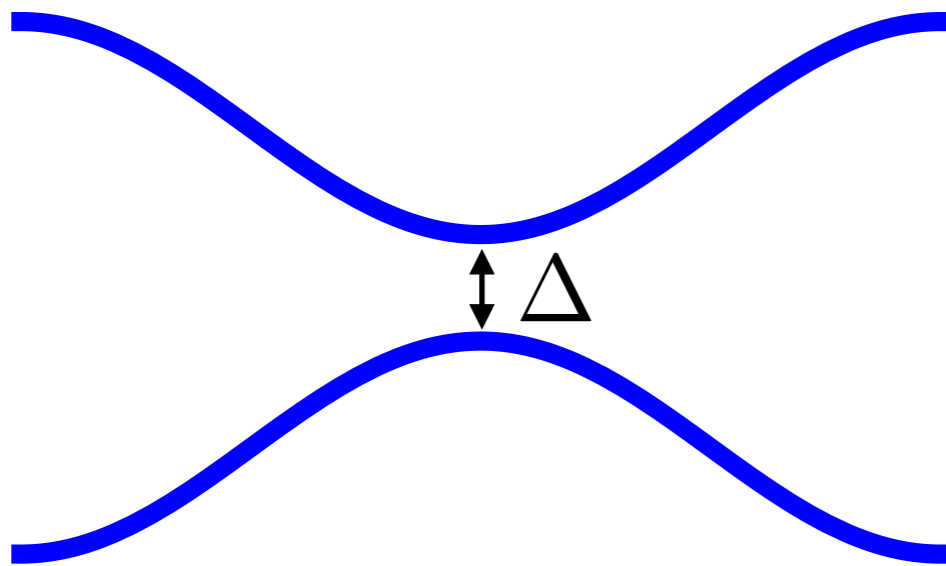
Jennifer Cano

Stony Brook University

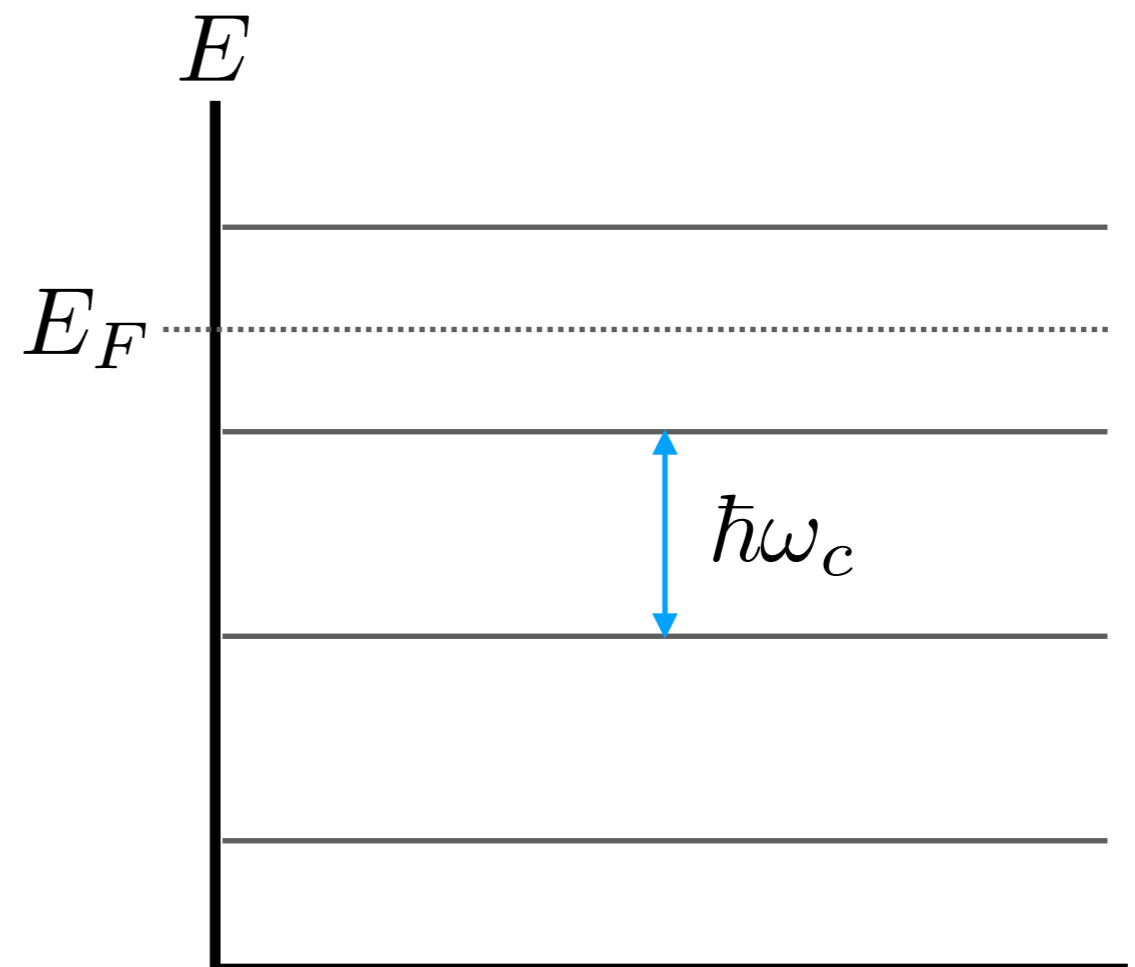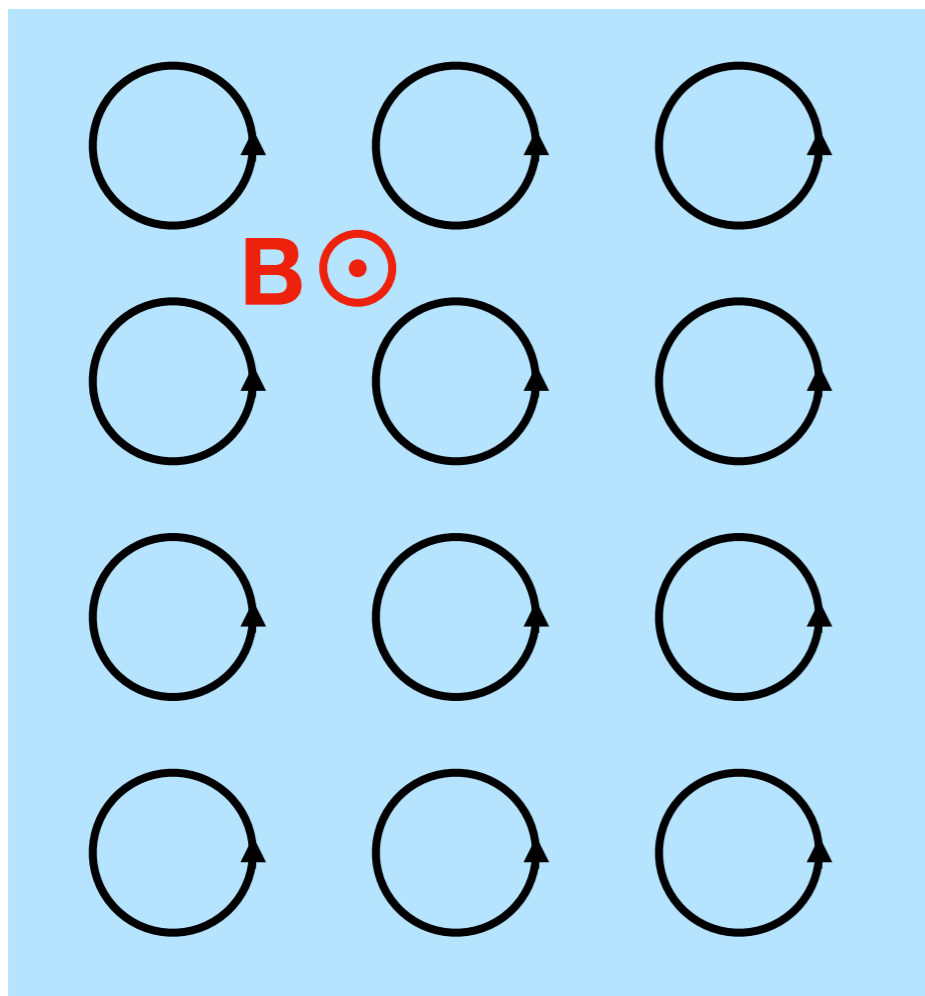FLATIRON INSTITUTE

What is an insulator?

No low-energy excitations
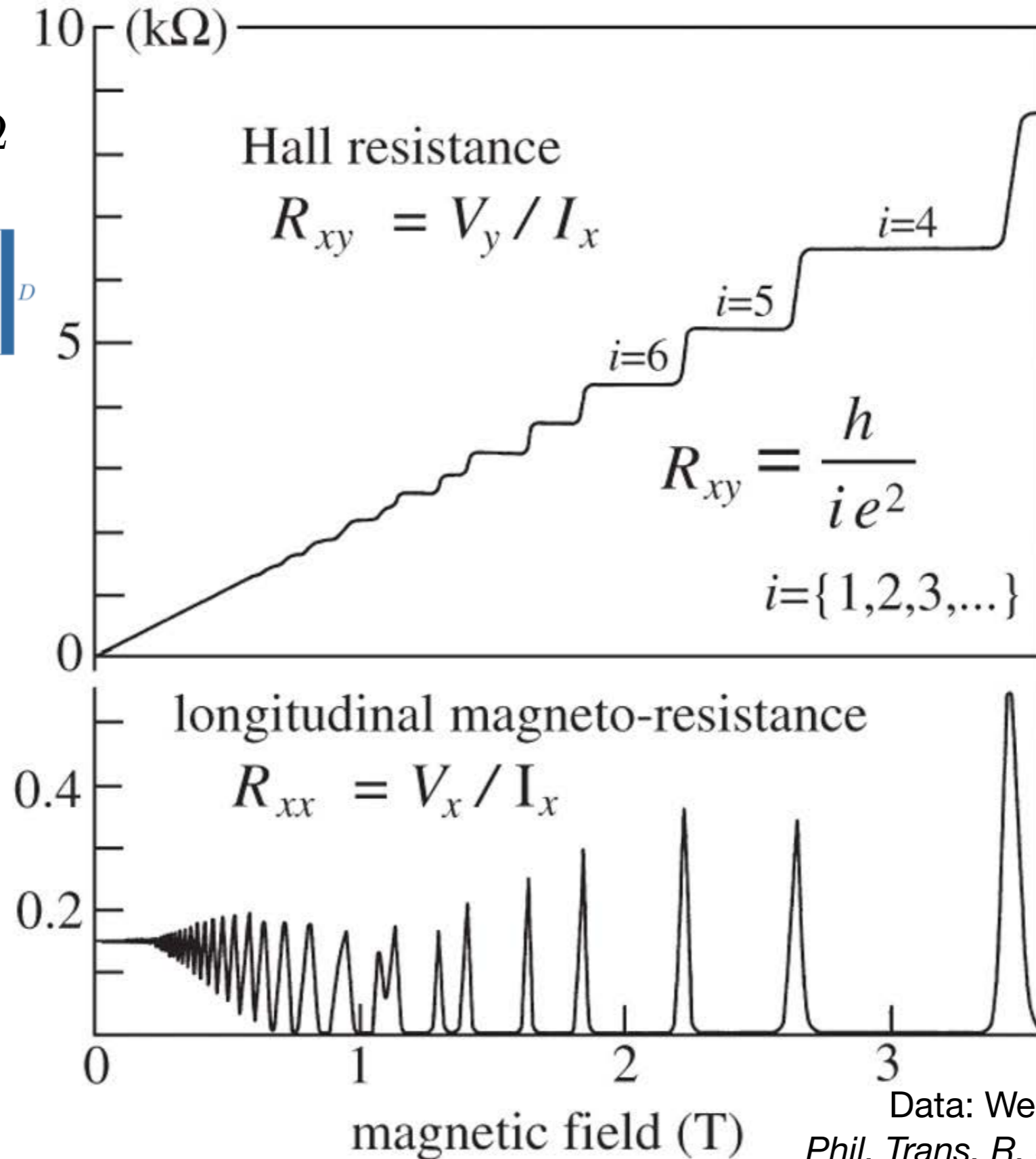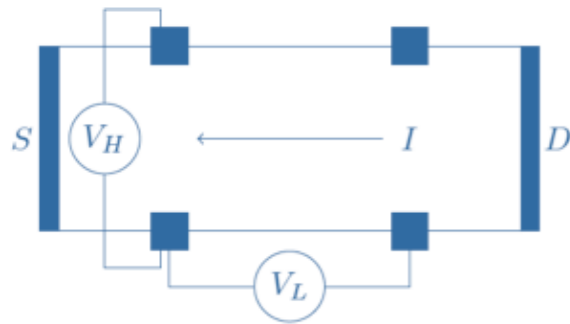

Electrical resistor

Not all insulators are the same: quantum Hall effect

Electrons in a strong magnetic field

Quantum Hall devices are not insulating!!

$$h/e^2 = 25.8\text{k}\Omega$$

Nobel Prize 1985
Klaus von Klitzing

Hall resistance
$$R_{xy} = V_y / I_x$$

$i=4$

$i=5$

$i=6$

$$R_{xy} = \frac{h}{i\,e^2}$$

$$i=\{1,2,3,...\}$$

longitudinal magneto-resistance
$$R_{xx} = V_x / I_x$$

magnetic field (T)

Data: Weis and von Klitzing,
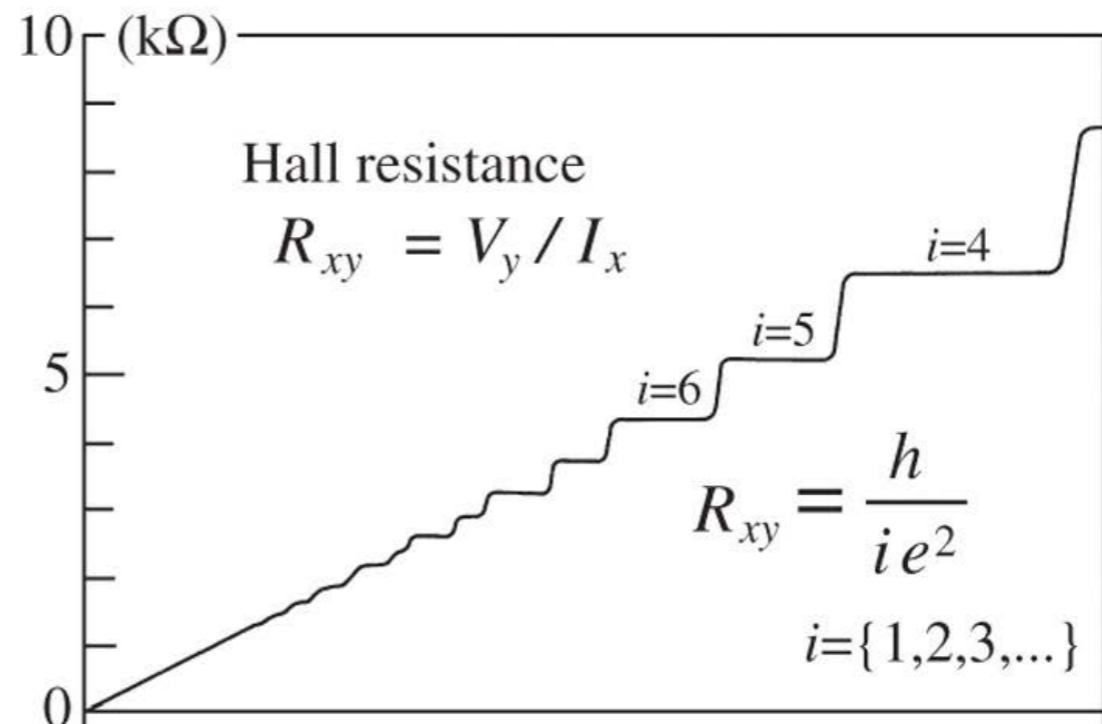*Phil. Trans. R. Soc. A* **369**, 3954 (2011)

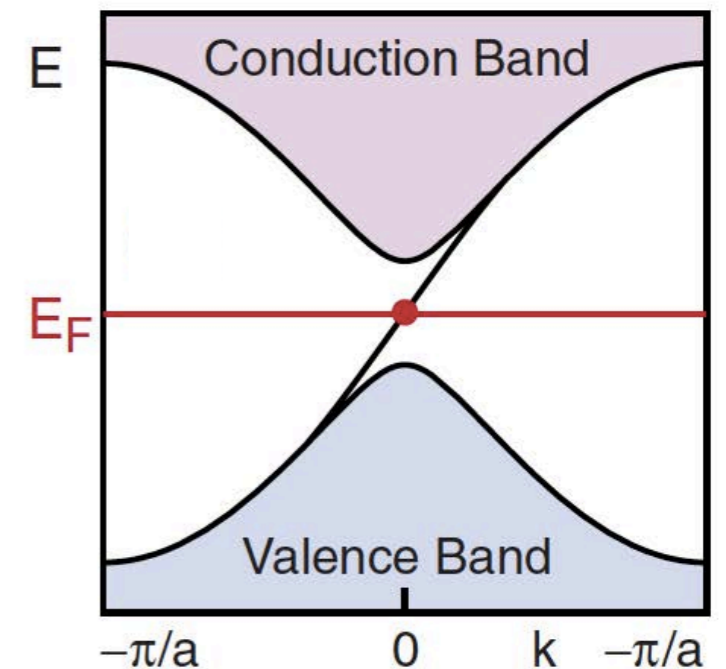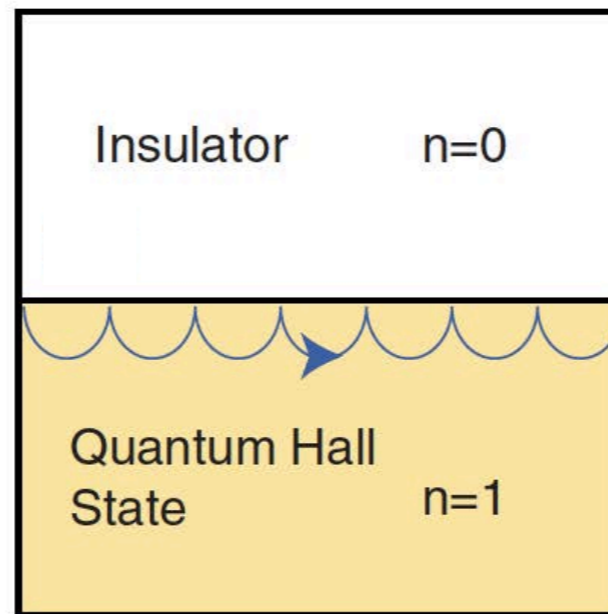# Topological invariants do not change under smooth deformations

Example 1: genus

Example 2: Hall conductivity

$$\sigma_{xy} = Ne^2/h$$

Hall resistance
$R_{xy} = V_y / I_x$

$10 - (k\Omega)$

$i=4$

$i=5$

$i=6$

5

$R_{xy} = \dfrac{h}{i\,e^2}$

$i=\{1,2,3,...\}$

0

Surface spectrum explains Hall conductivity

"Bulk-edge correspondence"
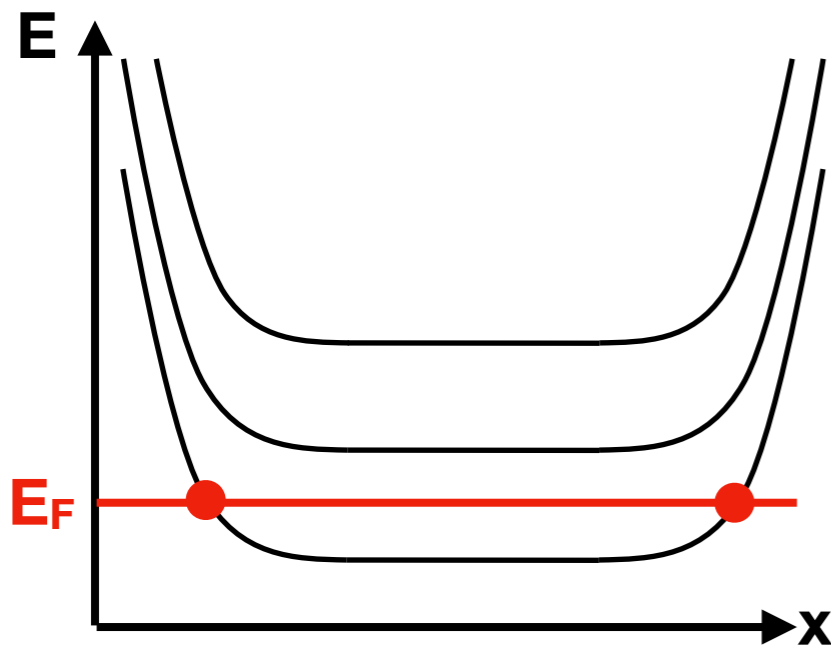
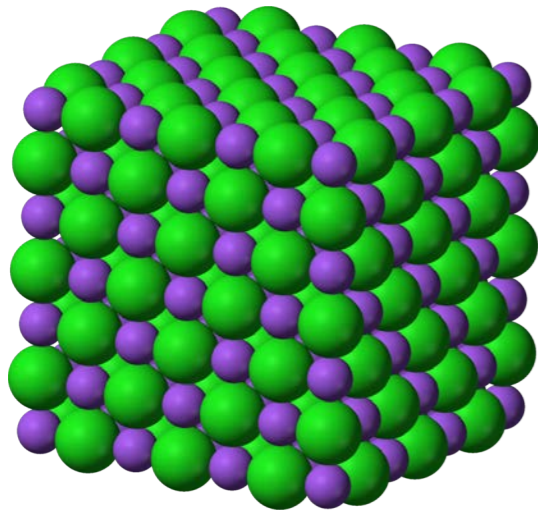Landau levels bend up at edges

Image: Hasan & Kane RMP

Don't need to look at surface!
Hall conductivity from bulk eigenstates: TKNN invariant
(Thouless, Kohmoto, Nightingale, den Nijs PRL 1982)

$$\sigma_{\mathrm{H}} = \frac{ie^2}{2\pi h} \sum \int d^2k \int d^2r \left(\frac{\partial u^*}{\partial k_1} \frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2} \frac{\partial u}{\partial k_1} \right)$$

We will build up to this…

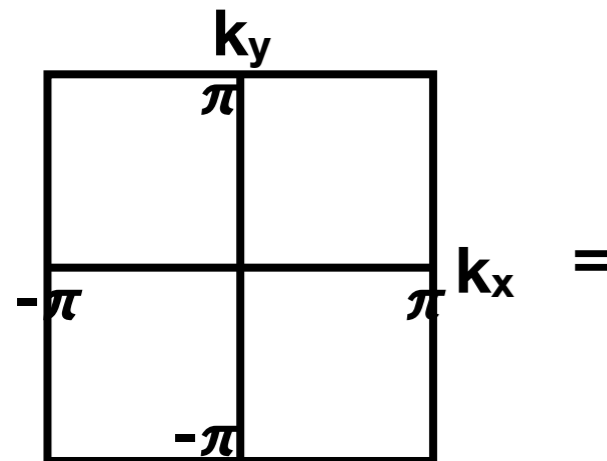# Energy eigenstates in a crystal are Bloch wavefunctions

Translation symmetry:
$$T(\mathbf{R})|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}|\psi\rangle$$
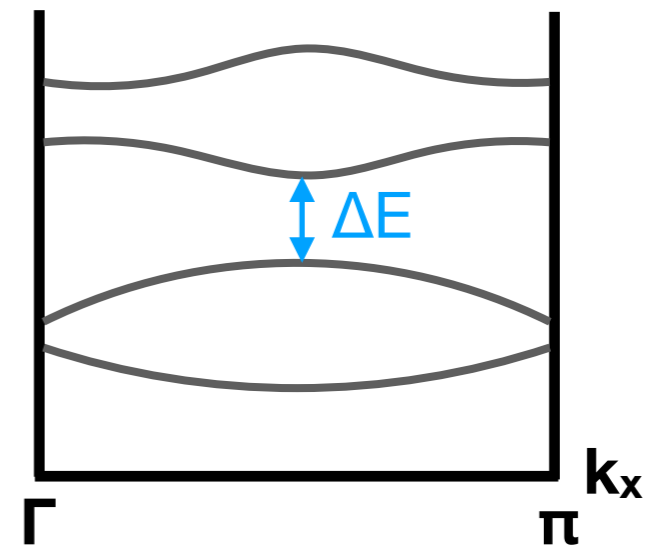
Bloch's theorem:
$$|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u(\mathbf{k})\rangle$$

Brillouin zone contains distinct **k**

Eigenvalues of Hamiltonian form band structure

$$H(\mathbf{k})|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})|u_n(\mathbf{k})\rangle$$

Two band structures are topologically equivalent if they can be deformed into each other without closing energy gap

Zak phase: Berry phase around Brillouin zone

Berry connection:
$$\mathbf{A} = -i\langle u(\mathbf{k})|\nabla_{\mathbf{k}}|u(\mathbf{k})\rangle$$

Berry phase:
$$\gamma_C = \oint_C \mathbf{A} \cdot d\mathbf{k}$$

Wave function phase ambiguity $\Rightarrow$ Berry phase defined mod 2π:

$$|u(\mathbf{k})\rangle \rightarrow e^{i\phi(\mathbf{k})}|u(\mathbf{k})\rangle \qquad \mathbf{A} \rightarrow \mathbf{A} + \nabla_{\mathbf{k}}\phi(\mathbf{k})$$
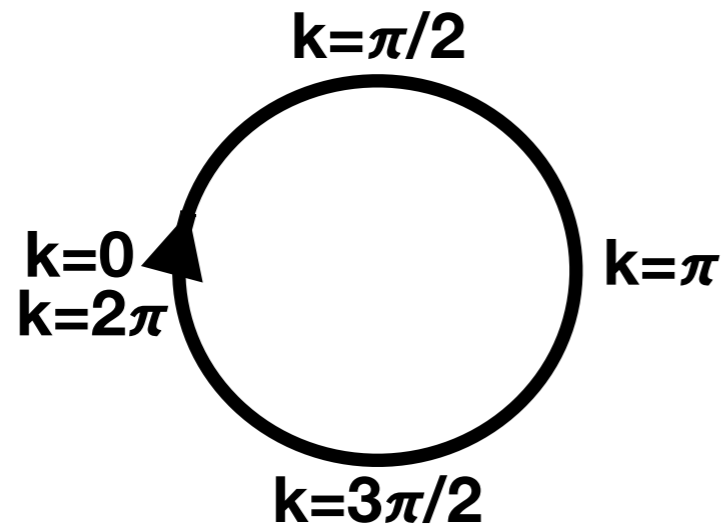
$$\gamma_C \rightarrow \gamma_C + \boxed{\oint_C \nabla_{\mathbf{k}}\phi(\mathbf{k}) \cdot d\mathbf{k}}$$
$$2\pi n$$

Berry curvature: $\quad \mathbf{F} = \nabla_{\mathbf{k}} \times \mathbf{A} \qquad$ gauge invariant!

Berry phase in 1D gives polarization
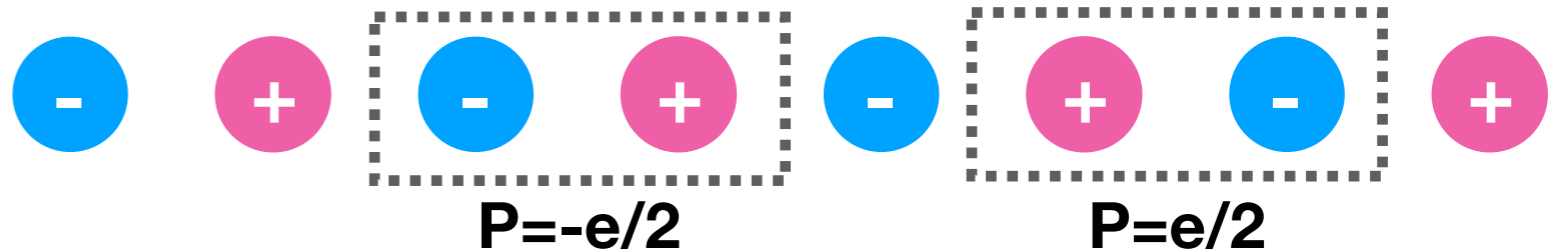

$$\gamma = \int_0^{2\pi} -i\langle u(k)|\partial_k|u(k)\rangle dk$$

$$P = \frac{e}{2\pi}\oint A(k)dk$$

$$i\partial_k \to x$$

Polarization of infinite crystal defined mod e:

P=-e/2   **P=e/2**

Differences in polarization are well-defined:

$$\Delta P = \int \partial_t P(t)dt = \frac{e}{2\pi}\iint dtdk \boxed{\nabla \times \mathbf{A}}$$
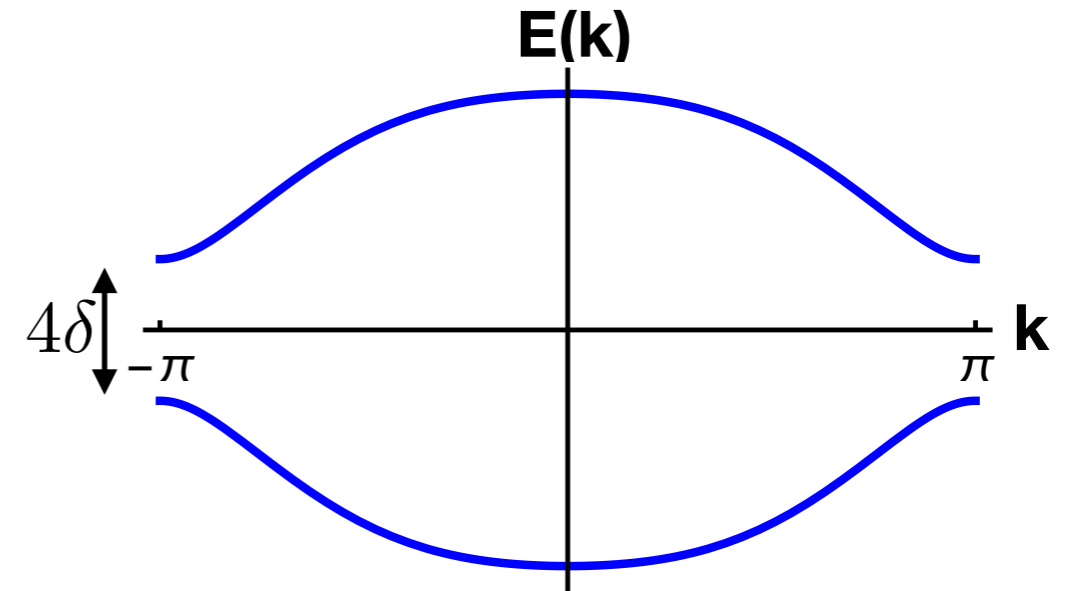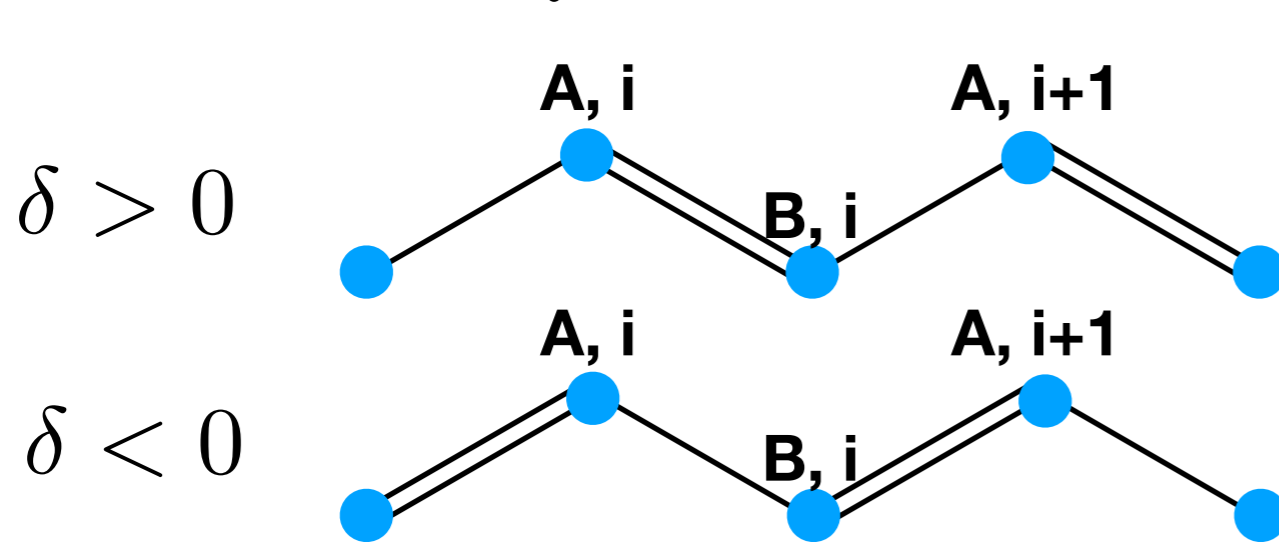
"Modern theory of polarization"

King-Smith & Vanderbilt PRB (1993)
Resta Ferroelectrics 136, 51 (1992)

SSH model: example of topological transition

(Su, Schrieffer, Heeger PRL 1979)

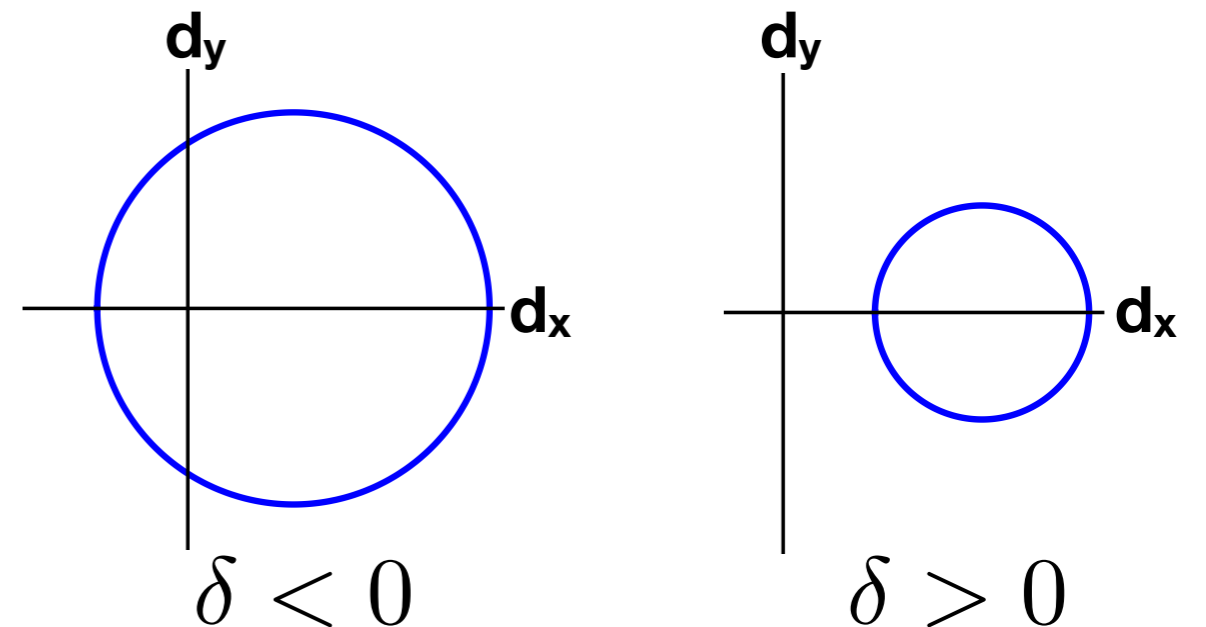$$H = \sum_i (t + \delta)c^{\dagger}_{A,i}c_{B,i} + (t - \delta)c^{\dagger}_{A,i+1}c_{B,i} + \text{h.c.}$$

$H(k) = d(k) \cdot \sigma$

$d_x(k) = (t + \delta) + (t - \delta)\cos(k)$

$d_y(k) = (t - \delta)\sin(k)$

$d_z(k) = 0$

Symmetry enforces $d_z(k) = 0$

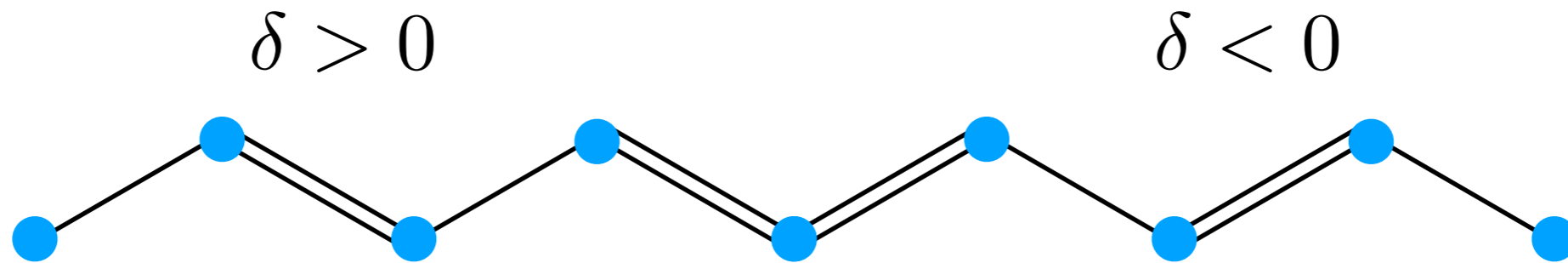$\delta > 0$

$\delta < 0$

E(k)

4δ $-\pi$ π k

d_y d_x $\delta < 0$ **Berry phase π**

d_y d_x $\delta > 0$ **Berry phase 0**

Interpret difference in Berry phase as difference in polarization!!
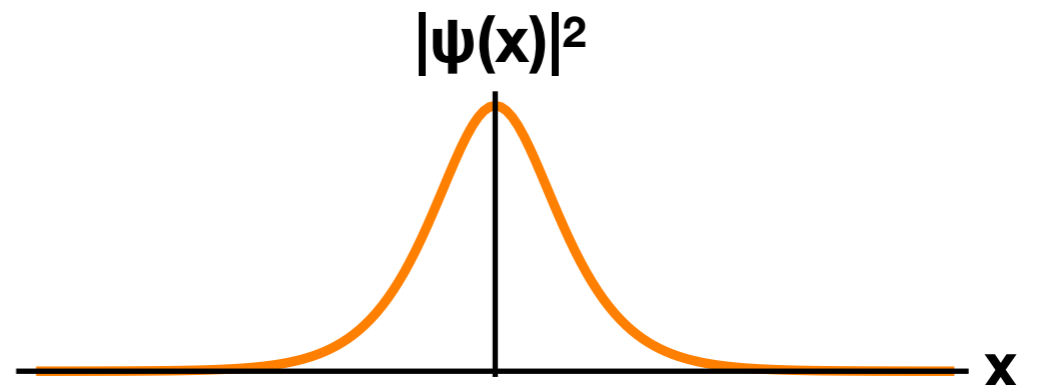
Domain wall states
(Su, Schrieffer, Heeger PRL 1979)

$$\delta > 0 \qquad\qquad \delta < 0$$

Low-energy continuum theory: $\quad H = 2\delta\sigma_x - tk\sigma_y$
$$(k \approx \pi, \delta \ll t)$$

Domain wall: $\quad \delta \to \delta(x)$
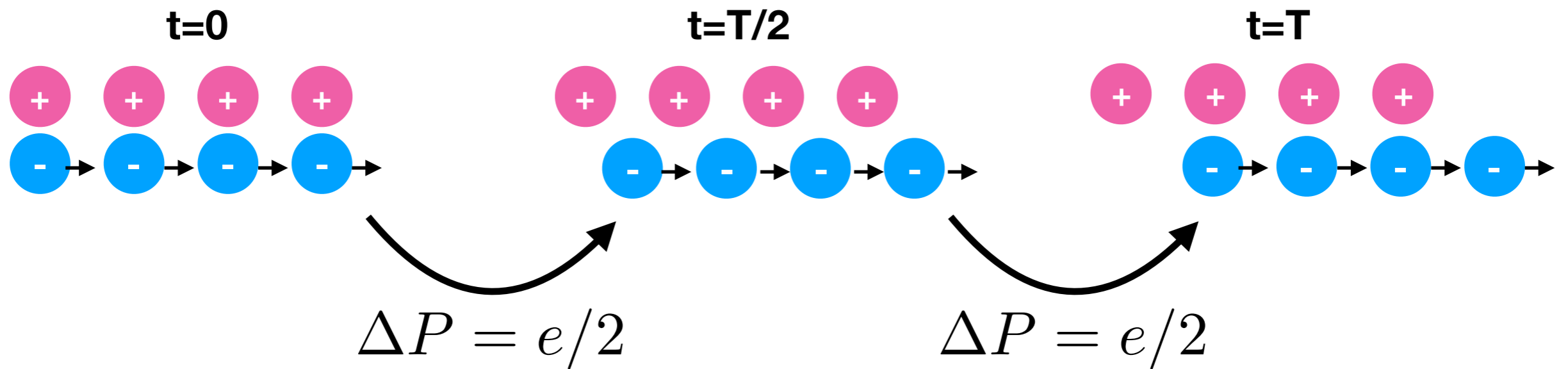
$$k \to -i\partial_x$$
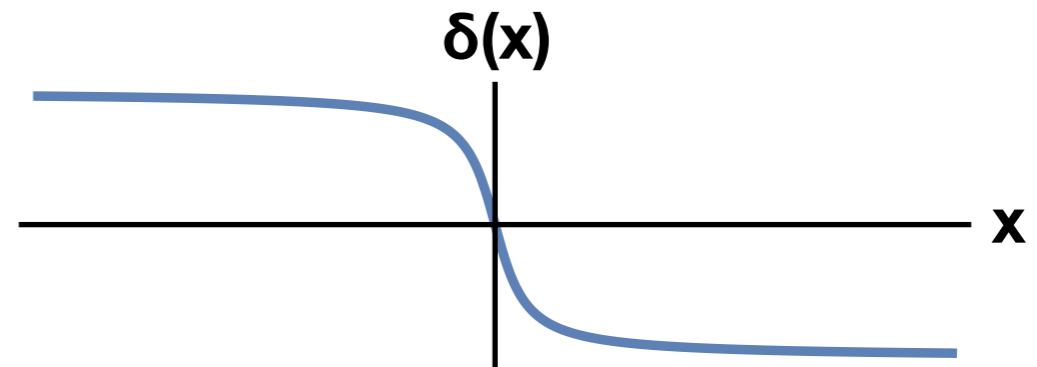
E=0 state localized at domain wall:
(Jackiw & Rebbi PRD 1976)

$$\psi(x) = e^{\int^x dx' \frac{2\delta(x')}{t}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

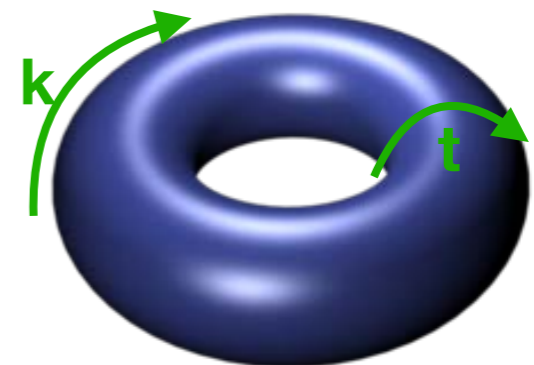# Thouless charge pump

(Thouless PRB 1983)

t=0

t=T/2

t=T

$$\Delta P = e/2 \qquad\qquad \Delta P = e/2$$

Integer charge pumped in one full cycle is a topological invariant:

$$\Delta P = \int_0^T \partial_t P(t)dt = \left(\frac{1}{2\pi} \int_0^T dt \int_0^{2\pi} dk \nabla \times \mathbf{A} \right) e = ne$$
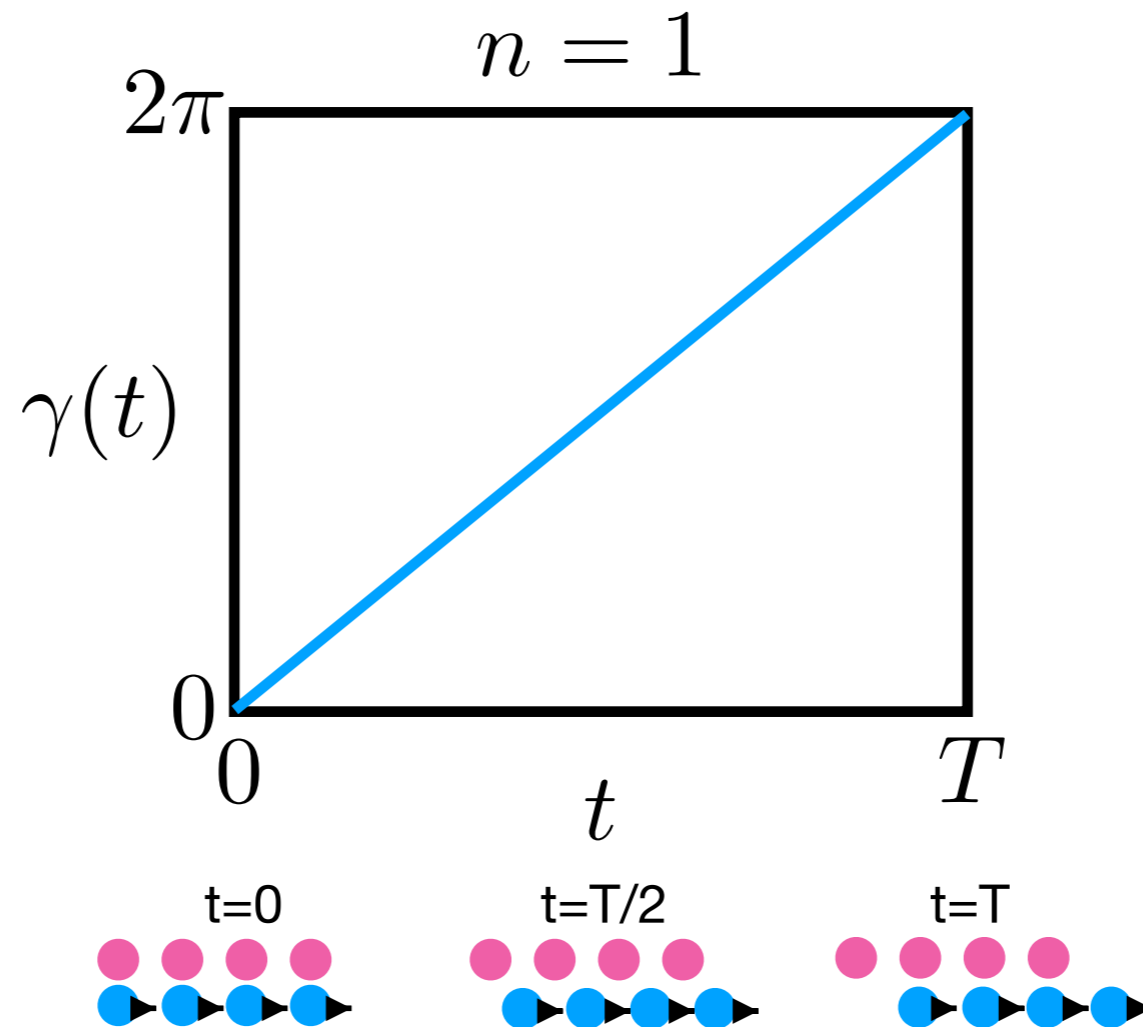
"Chern number"

Chern number is an integer topological invariant characterizing Bloch wavefunctions of two variables
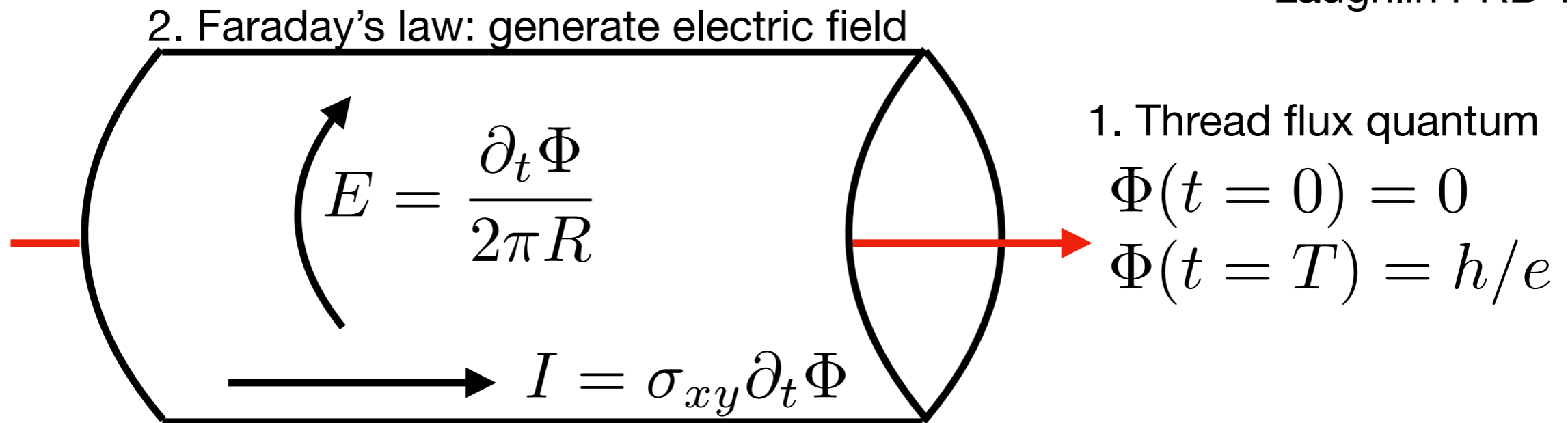
k

t

Chern number = winding Berry phase

$$\frac{2\pi}{e}\Delta P = \int_0^T \partial_t \gamma(t)dt = \gamma(T) - \gamma(0) = 2\pi n$$

Practical way to compute Chern number

Integer quantum Hall: Laughlin flux argument

2. Faraday's law: generate electric field

$$E = \frac{\partial_t \Phi}{2\pi R}$$

1. Thread flux quantum

$$\Phi(t=0) = 0$$
$$\Phi(t=T) = h/e$$

$$I = \sigma_{xy}\partial_t \Phi$$

3. Hall conductance determines current
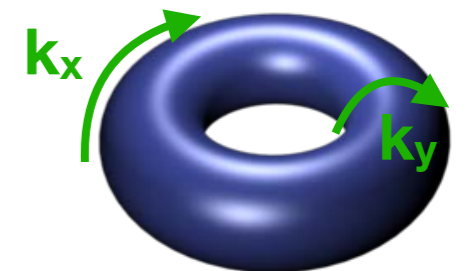
4. Charge pumping: $\Delta Q = \int_0^T I(t)dt = \sigma_{xy}\dfrac{h}{e}$

5. Energy gap $\Rightarrow \Delta Q = ne$

Thouless pump!

$$\sigma_{xy} = n\frac{e^2}{h}$$

Comparison to TKNN invariant: $n = \dfrac{1}{2\pi}\displaystyle\int d^2k \, \nabla \times \mathbf{A}$

k_x k_y
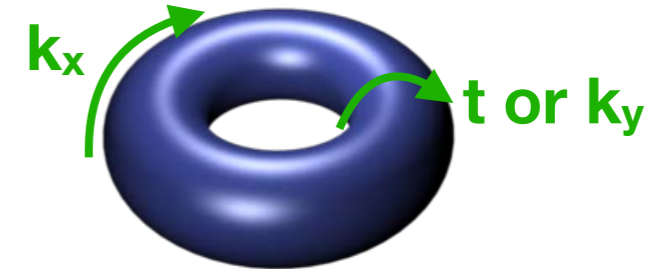
Chern number with t → k_y

Chern number ⇒ surface state

Topological invariant: TKNN or Chern number

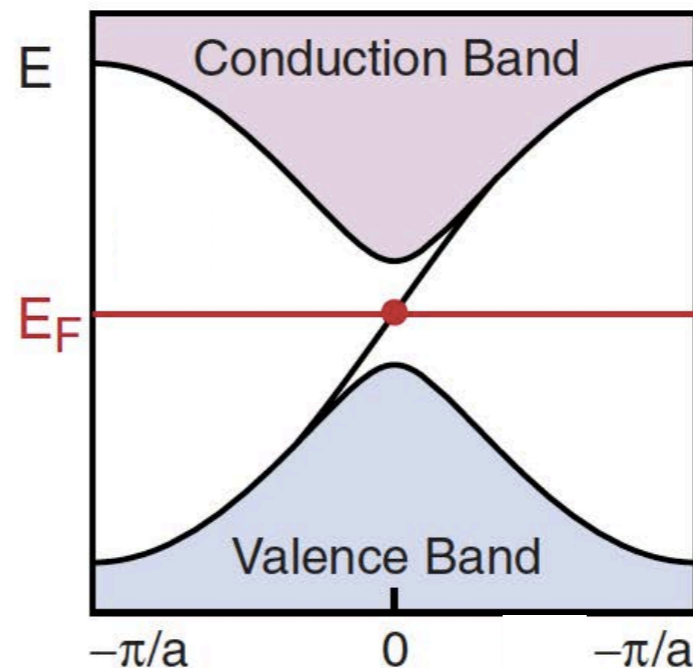$$n = \frac{1}{2\pi} \int d^2 k \, \nabla \times \mathbf{A}$$

k_x

t or k_y

Bulk diagnosis

Bulk-edge correspondence

If x-axis is time: 1d Thouless pump
If x-axis is k: Laughlin argument

Surface diagnosis

E

Conduction Band

E_F

Valence Band

$-\pi/a$ 0 $-\pi/a$

Bulk-edge correspondence

Surface states are required but dispersion is determined by microscopics
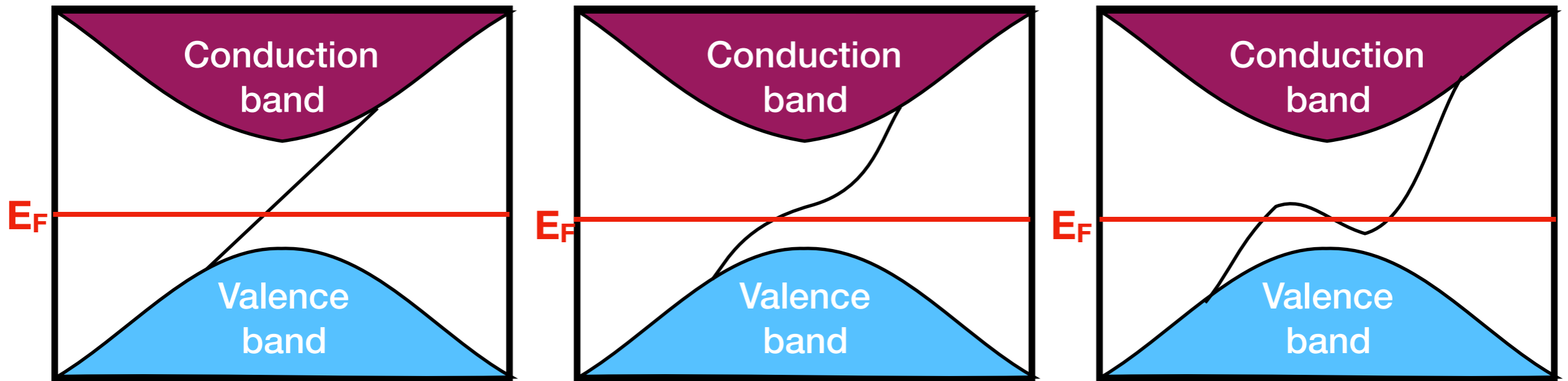
n_+ = # bands with positive slope that cross E_F
n_- = # bands with negative slope that cross E_F
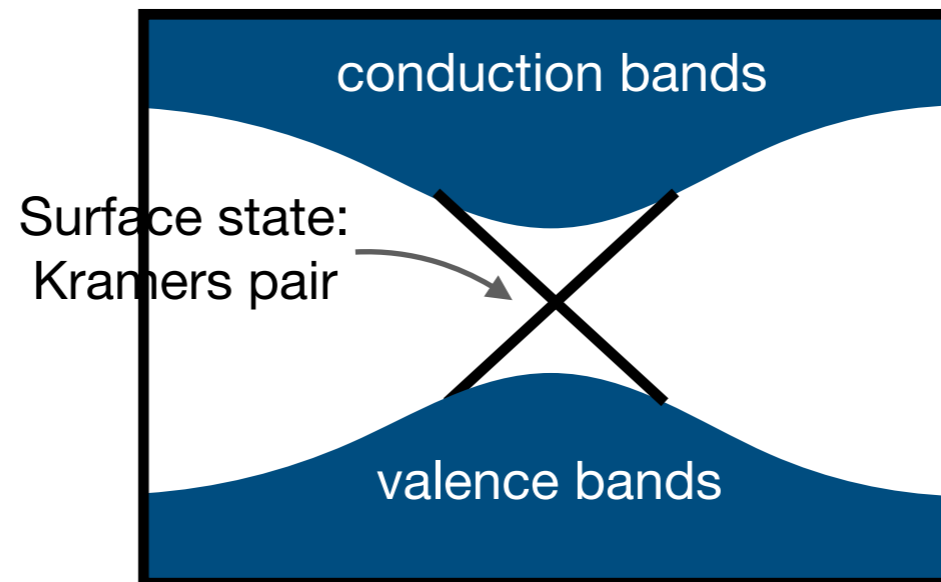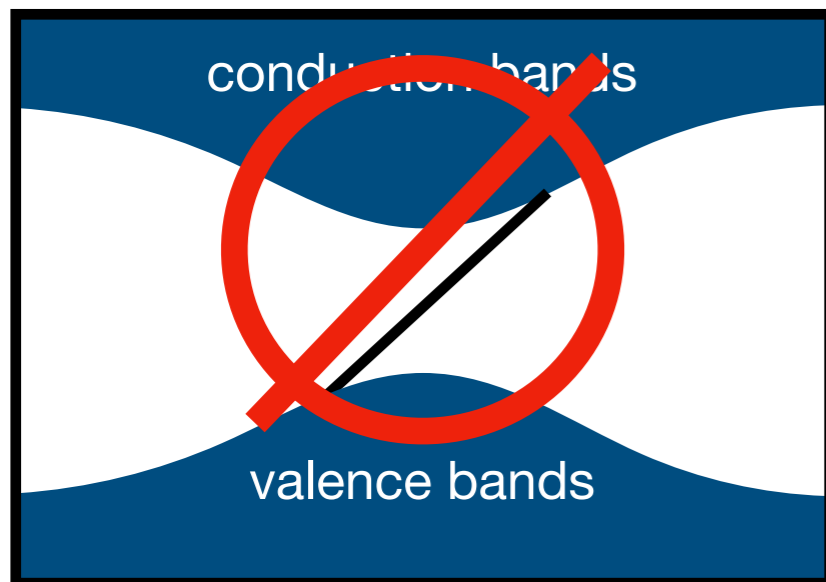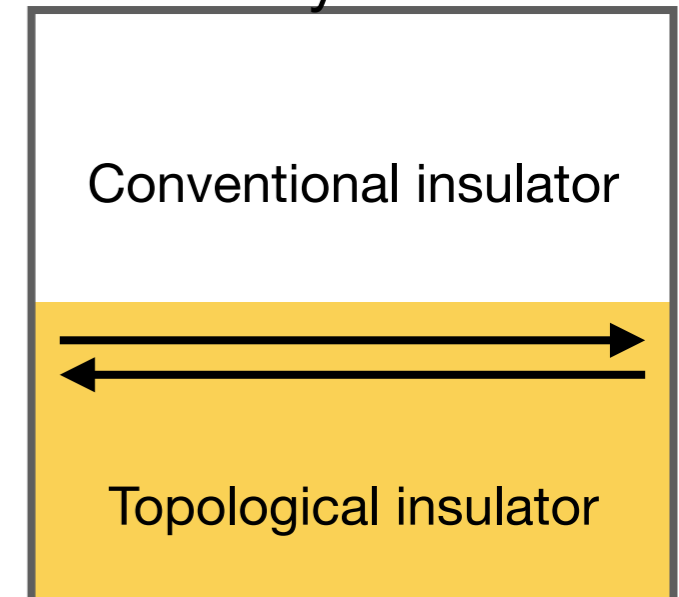
Chern number = $n_+ - n_-$

Time-reversal symmetry

$$\Theta^{-1}H(\mathbf{k})\Theta = H(-\mathbf{k}) \qquad \Theta^2 = -\mathbb{I}$$

Degenerate Kramer's pairs at
"Time-reversal-invariant-momenta" (TRIM) k=0, k=$\boldsymbol{\pi}$

Time-reversal forbids Chern number!

Two surface states,
protected by time-reversal

conduction bands

valence bands

conduction bands

Surface state:
Kramers pair

valence bands

Conventional insulator

Topological insulator
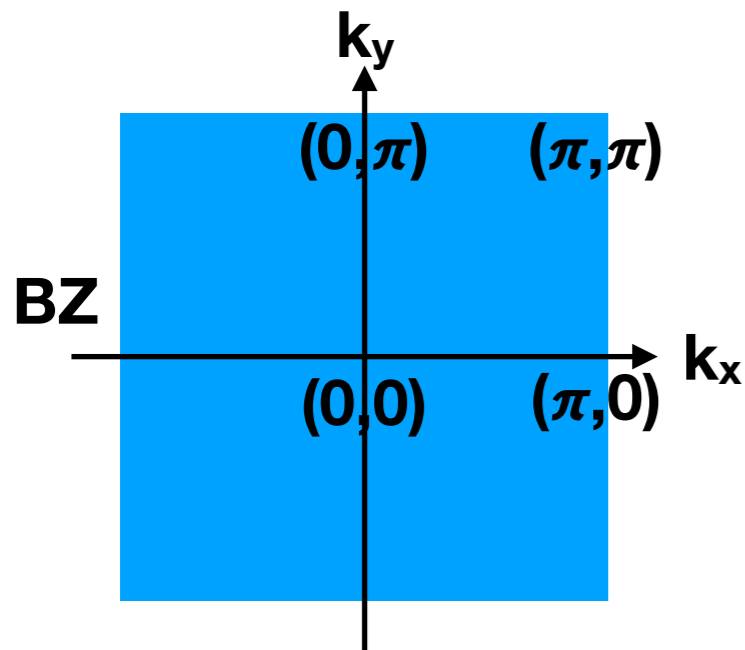
"Z$_2$" topological invariant v: even vs odd bands cross E$_F$ over *half* the BZ

Fermion parity pump
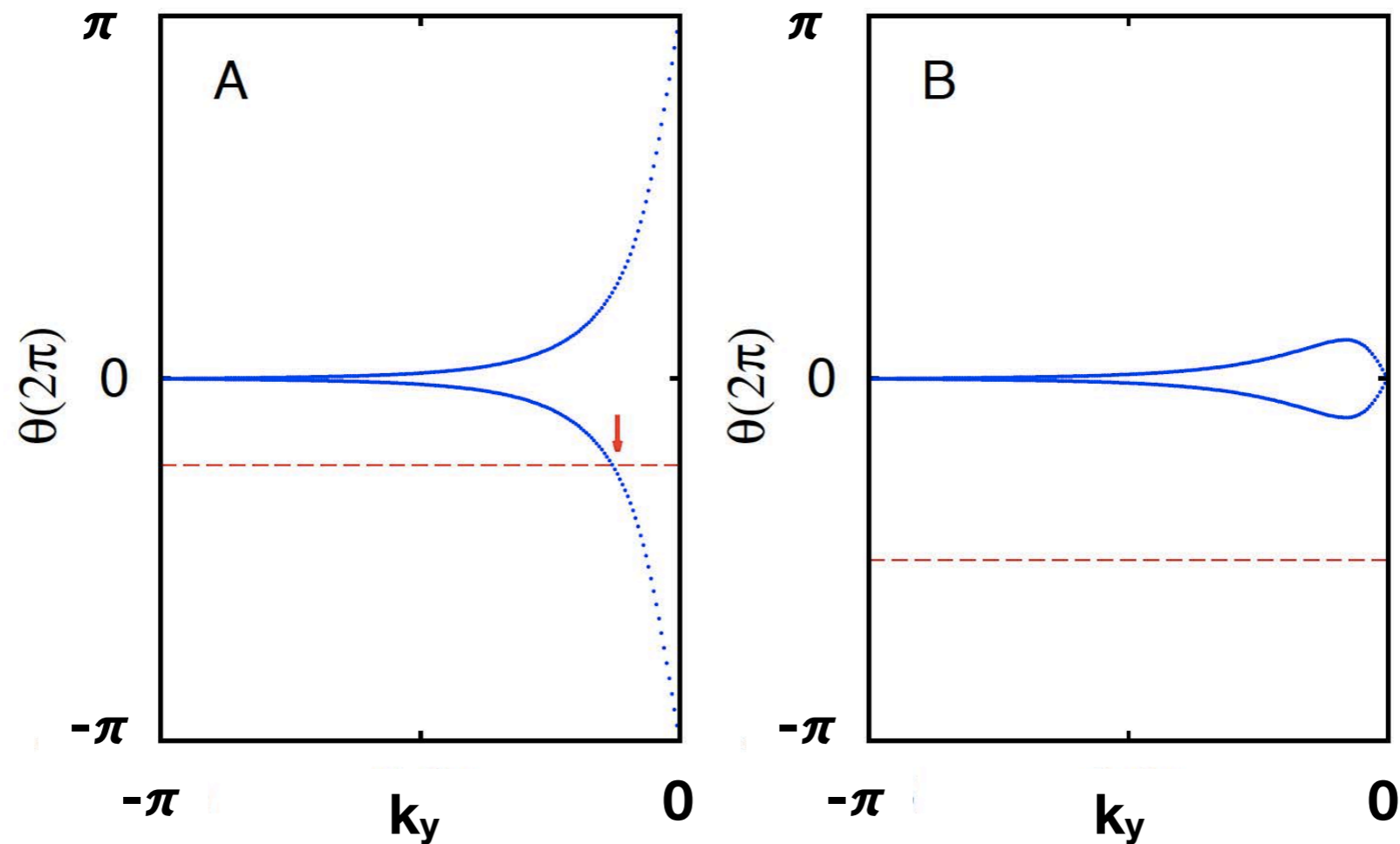
Bulk Z₂ invariant

Kane & Mele PRL 95, 146802 (2005)

$$(-1)^{\nu} = \prod_{\Lambda_a \in \mathrm{TRIM}} \frac{\mathrm{Pf}[w(\Lambda_a)]}{\sqrt{\mathrm{Det}[w(\Lambda_a)]}} = \pm 1$$

$$w_{mn}(k) = \langle u_{-k,m} | \Theta | u_{k,n} \rangle$$

Gauge invariant but must choose continuous gauge

In practice, difficult to compute

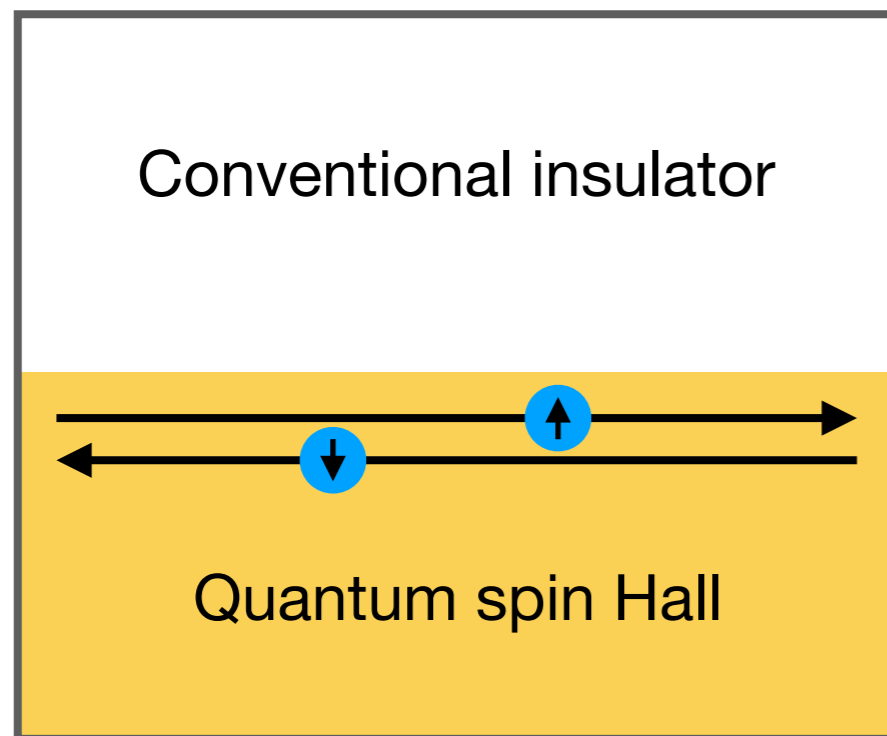# Practical calculation of Z₂ invariant: winding Berry phase

Yu, Qi, Bernevig, Fang, Dai PRB 84, 075119 (2011)
Soluyanov and Vanderbilt Phys. Rev. B 83, 235401 (2011)

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

Z2Pack software package: Gresch, et al, PRB 95, 075146 (2017)

Easier computation of Z₂ invariant with symmetry

Spin conservation: "quantum spin Hall effect"

Inversion symmetry

Conventional insulator

Quantum spin Hall

Z₂ invariant given by product of inversion eigenvalues of occupied bands:

$$(-1)^\nu = \prod_{\Lambda_a \in \mathrm{TRIM}} \prod_i \xi_{2i}(\Lambda_a)$$

Fu & Kane PRB 76, 045302 (2007)

Each spin has Chern number: $n_\uparrow = -n_\downarrow$

$\nu = n_\uparrow \bmod 2$

Kane & Mele PRL 95, 146802 (2005),
Bernevig & Zhang PRL 96, 106802 (2006)

Quantum spin Hall effect in graphene with spin orbit coupling
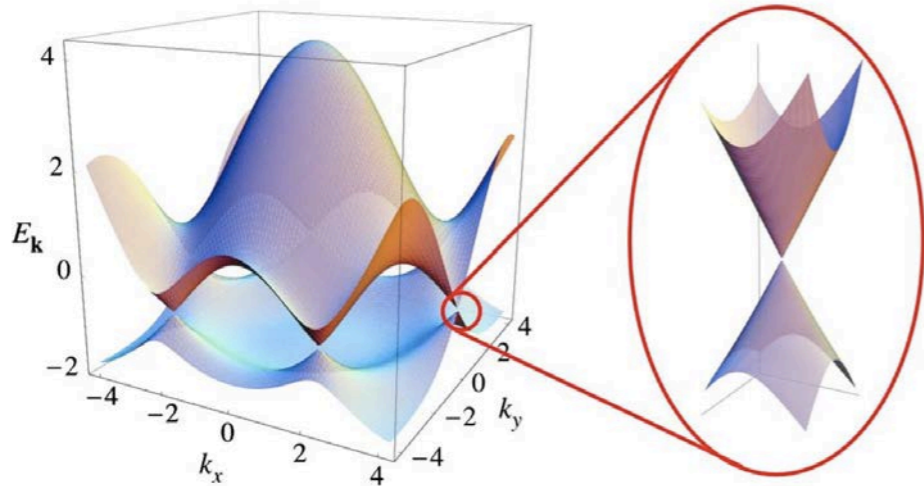
Fig: Castro Neto, et al, RMP (2009)

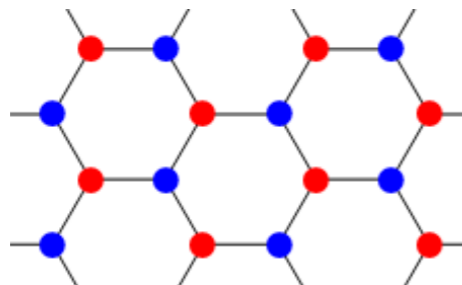$$\mathcal{H}_0 = -i\hbar v_F \psi^\dagger (\sigma_x \tau_z \partial_x + \sigma_y \partial_y)\psi$$

$$\sigma_z = \text{sublattice} \quad \tau_z = \text{valley} \quad s_z = \text{spin}$$

Three ways to open energy gap:

2Δ
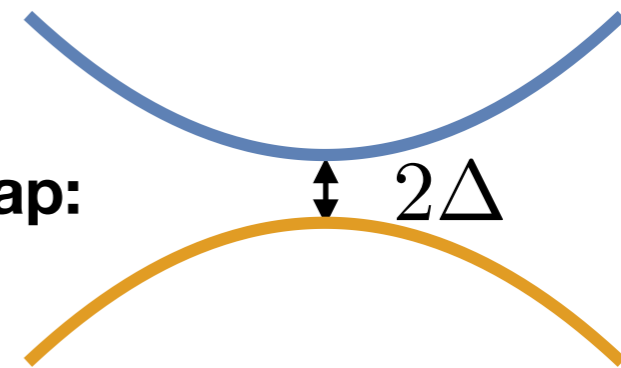
1. Sublattice potential (hBN)

$$\Delta_{\text{hBN}}\sigma_z$$

Breaks inversion symmetry

2. Staggered flux Haldane PRL 1988

$$\Delta_{\text{Haldane}}\sigma_z \tau_z$$
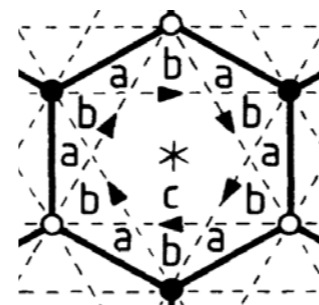
Breaks time-reversal Quantum Hall effect

3. Spin-orbit coupling Kane and Mele PRL 1995
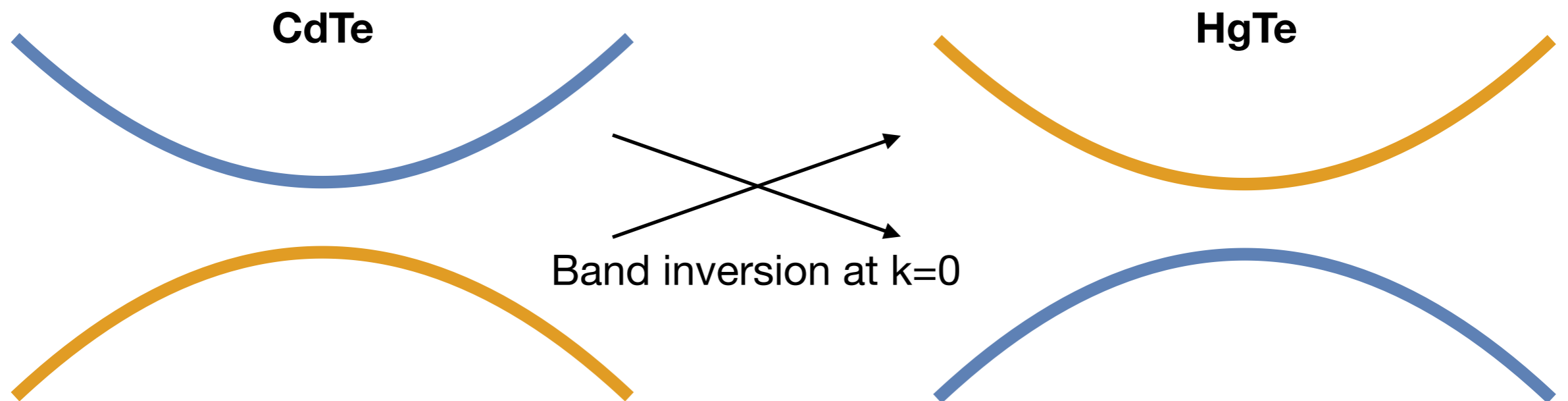
$$\Delta_{\text{SOC}}\sigma_z \tau_z s_z$$

Preserves all symmetries Quantum spin Hall effect

Quantum spin Hall in HgTe quantum wells

Theory: Bernevig, Hughes, Zhang Science 2006 "BHZ model"

CdTe

HgTe $\updownarrow$ **d**

CdTe
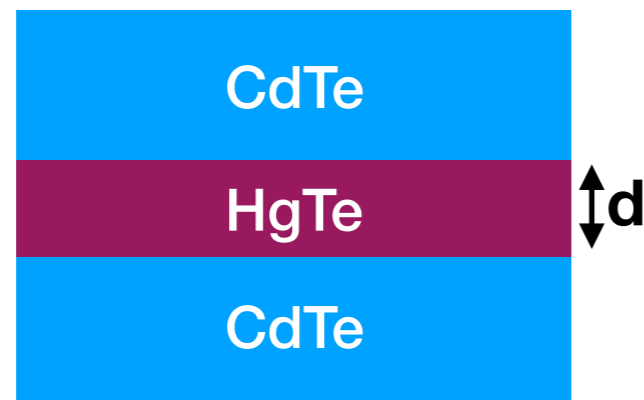
d<d$_c$ normal band order
d>d$_c$ inverted (topological) band order
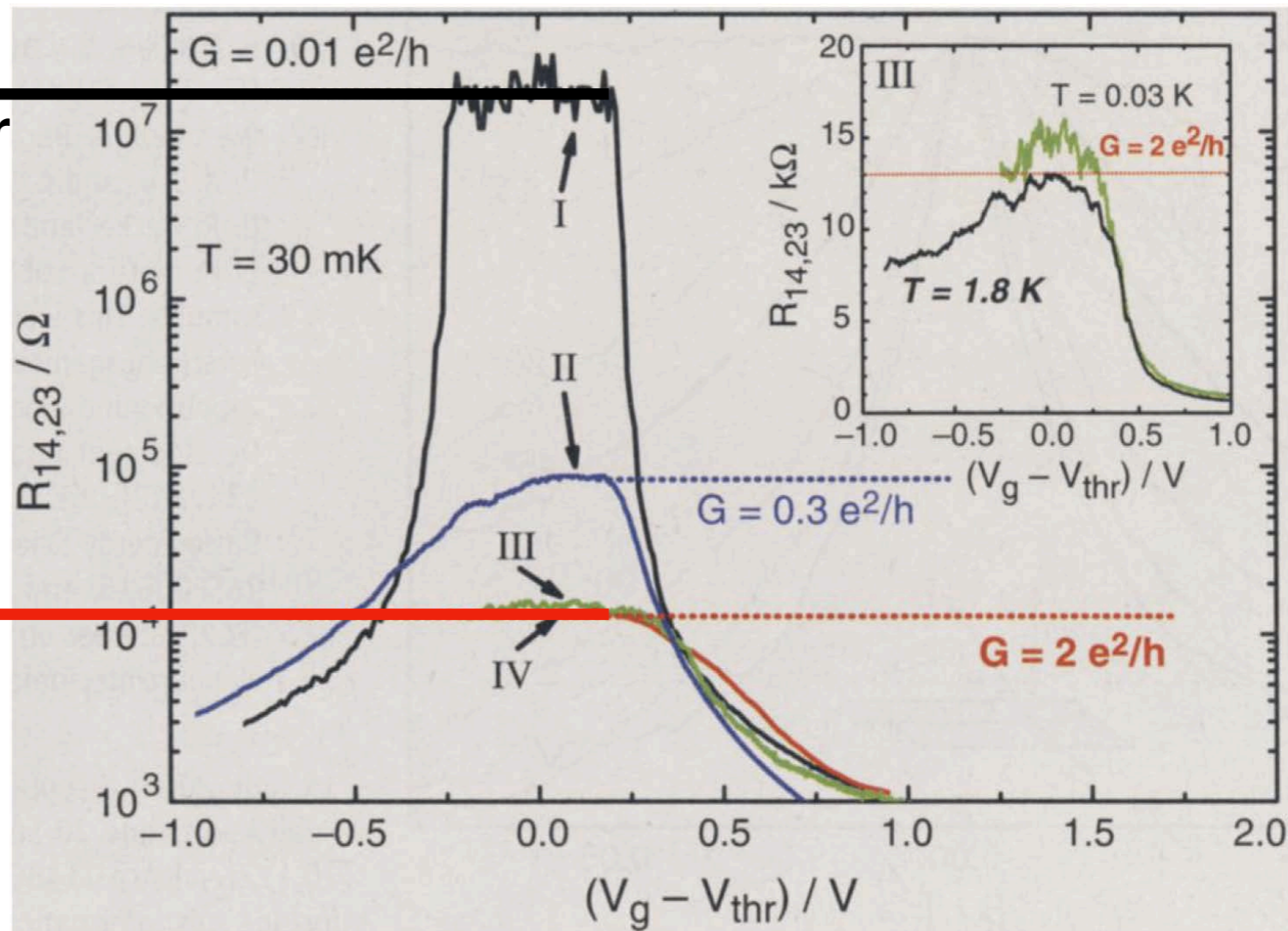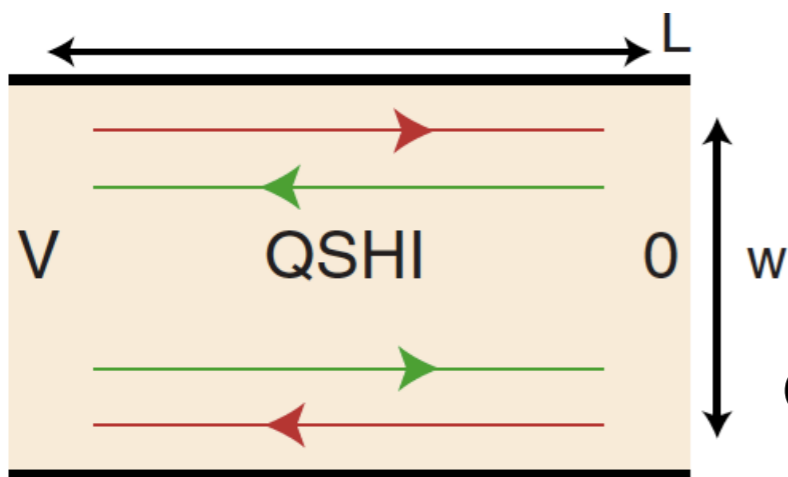**d$_c$ = 6.4nm**

CdTe

HgTe

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

Refs:
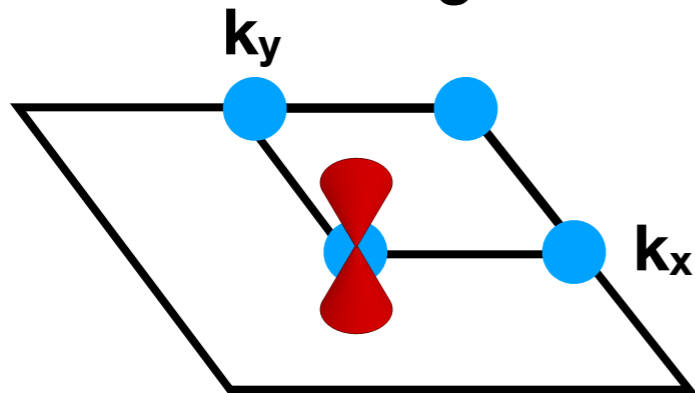Fu, Kane, Mele PRL 2007
Moore, Balents PRB 2007
Roy PRB 2009

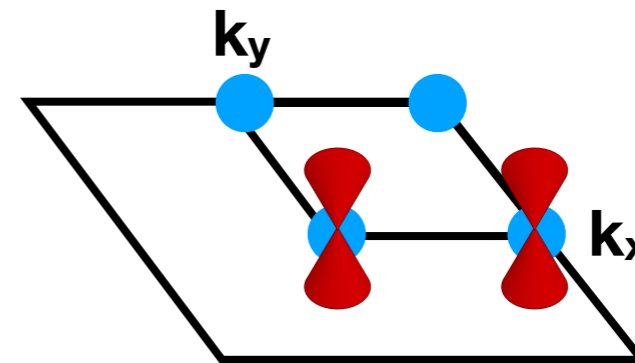Four Z_2 indices: $(\nu_0; \nu_1, \nu_2, \nu_3)$

"Strong" index

"Weak" indices

k_y

k_x

k_y

k_x

Ex: (1;000)

Ex: (0;100)
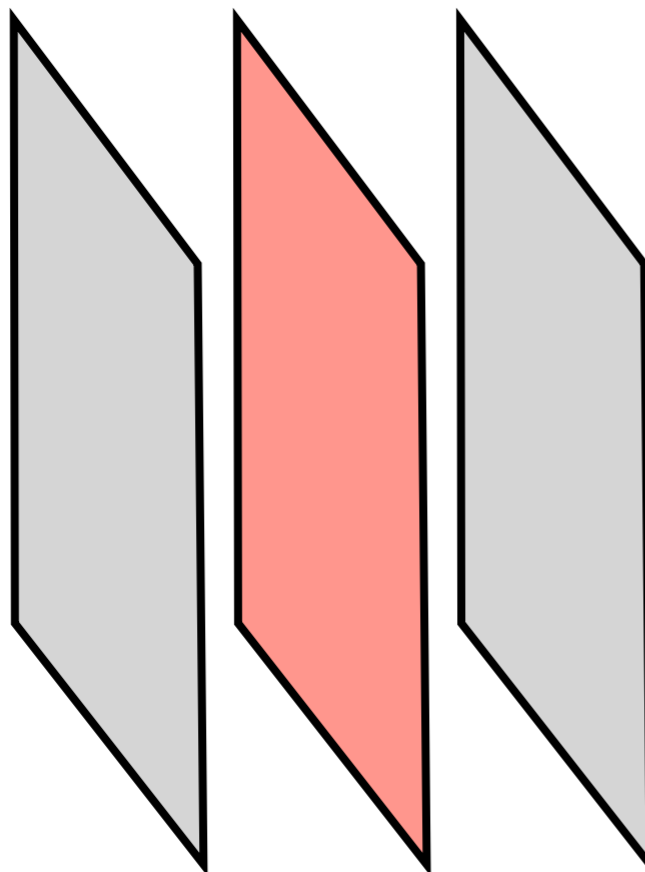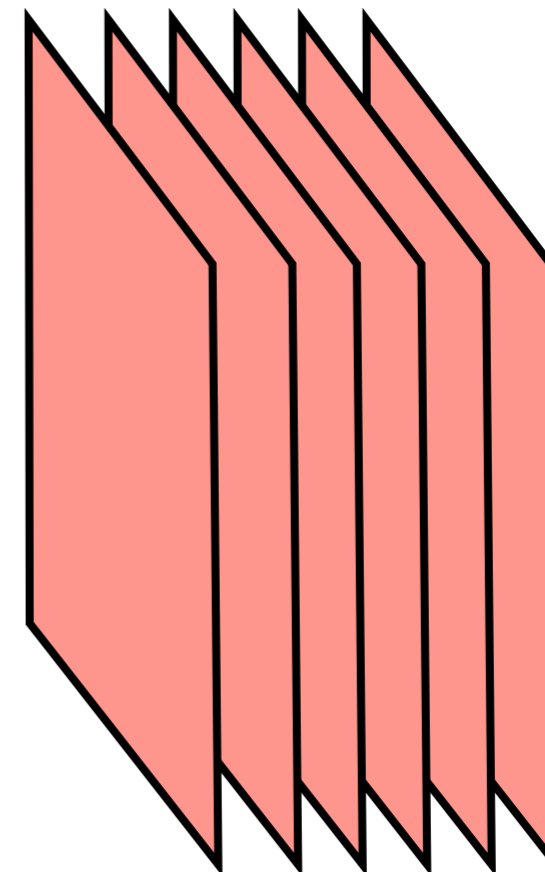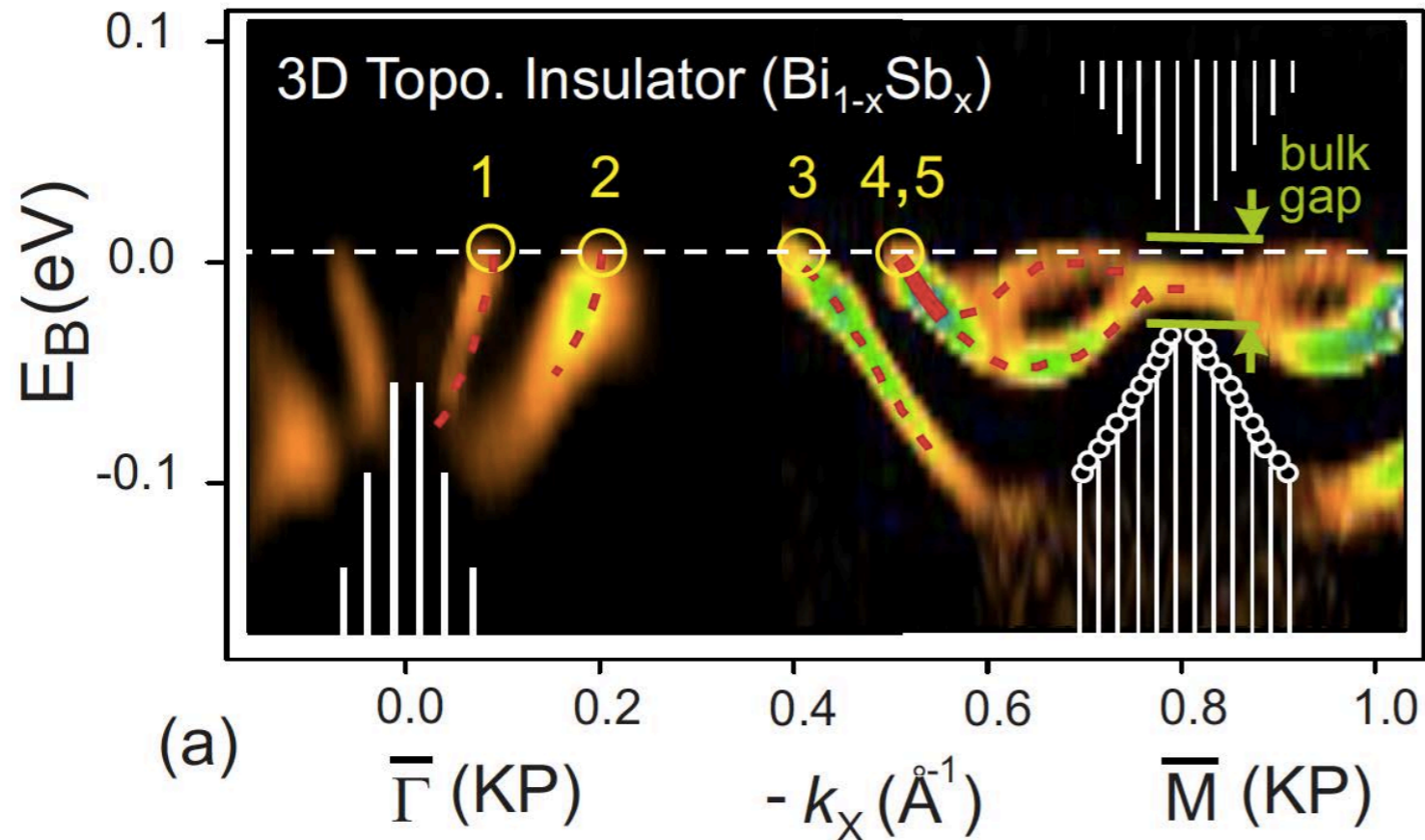
Surface Brillouin zone

Bulk construction (not unique)

k=0 plane is 2D TI; k=π is conventional
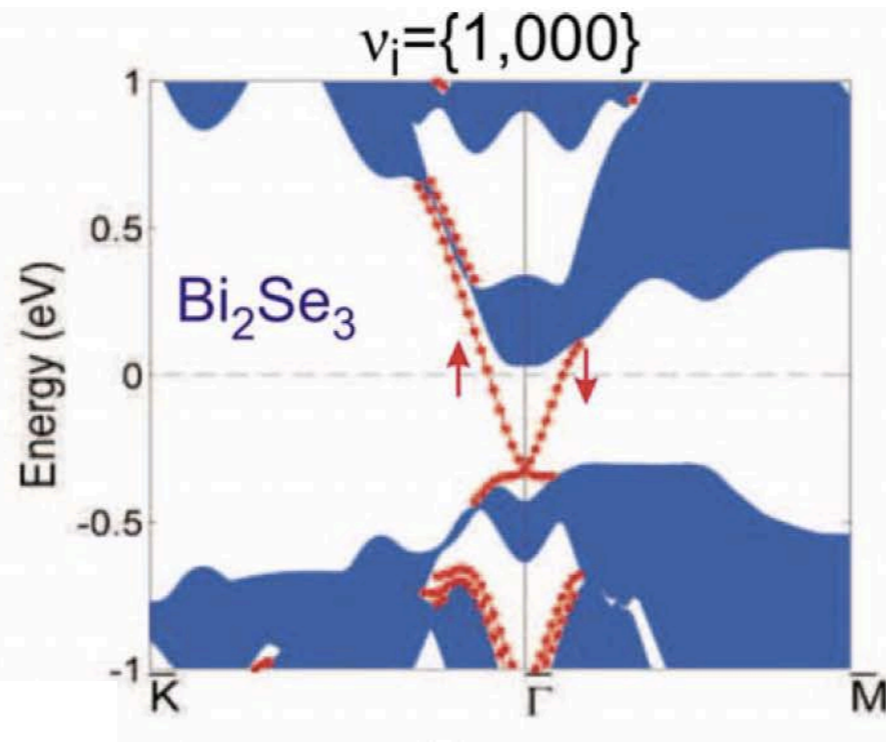
Stacked 2D TIs

Topological insulators in 3d
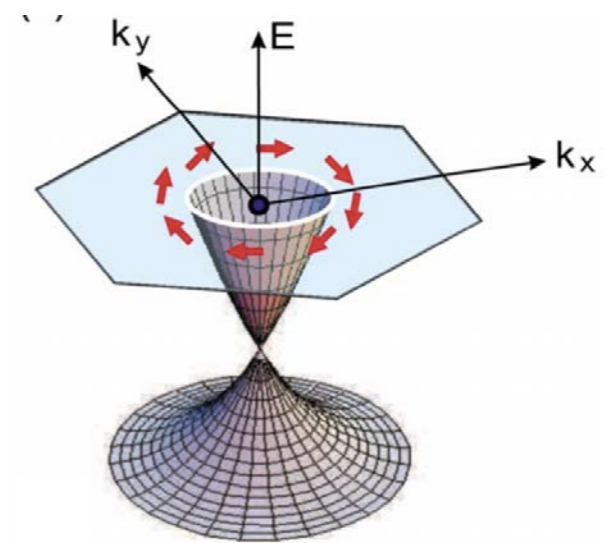
Figures from Hasan & Kane RMP
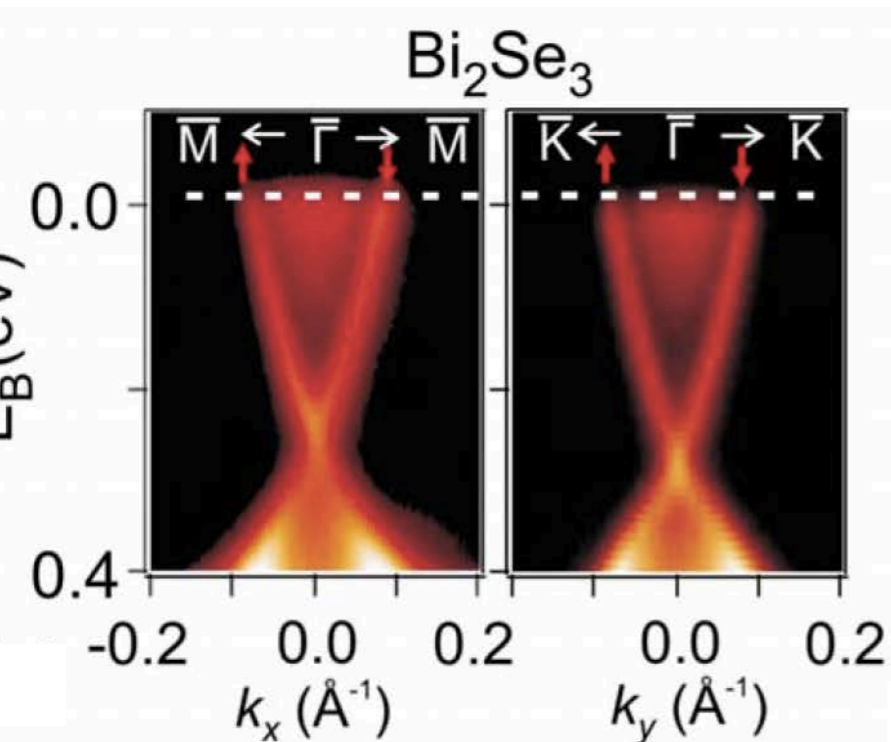
What comes after time-reversal symmetry? 10-fold way classification

Ryu, Schnyder, Furusaki, Ludwig, New J. Phys. (2010)

Classified by time-reversal and charge-conjugation symmetries

complex case:

Cartan\$\backslash d$	0	1	2	3	4	5	6	7	8	9	10	11	$\cdots$
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$

no symmetry $\longrightarrow$ A

Integer quantum Hall

real case:

Cartan\$\backslash d$	0	1	2	3	4	5	6	7	8	9	10	11	$\cdots$
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$

fermions w/ time-reversal $\longrightarrow$ AII

2d and 3d topological insulators (weak index not captured)