Introduction to topological insulators

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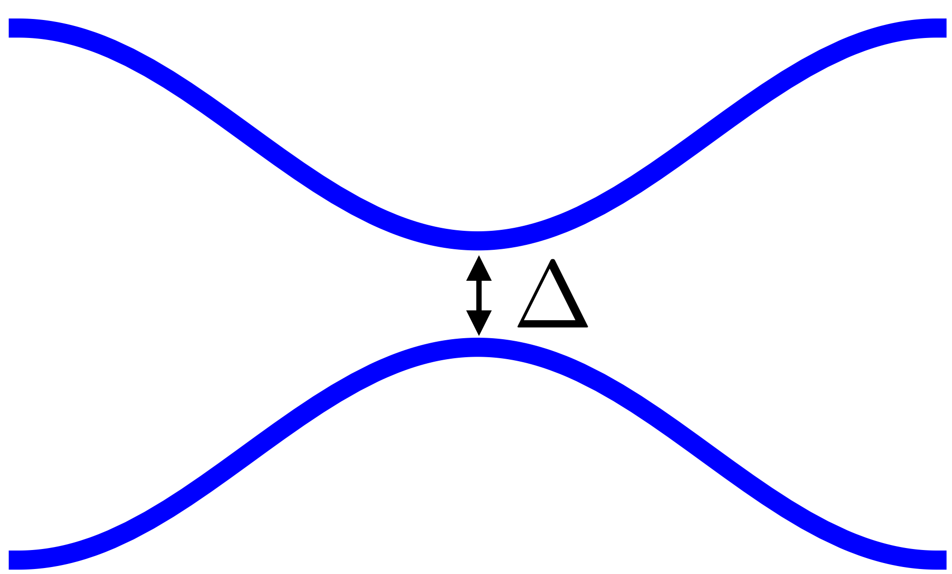
Adapted from Charlie Kane's Windsor Lectures: http://www.physics.upenn.edu/~kane/

Review article: Hasan & Kane Rev. Mod. Phys. 2010

What is an insulator?

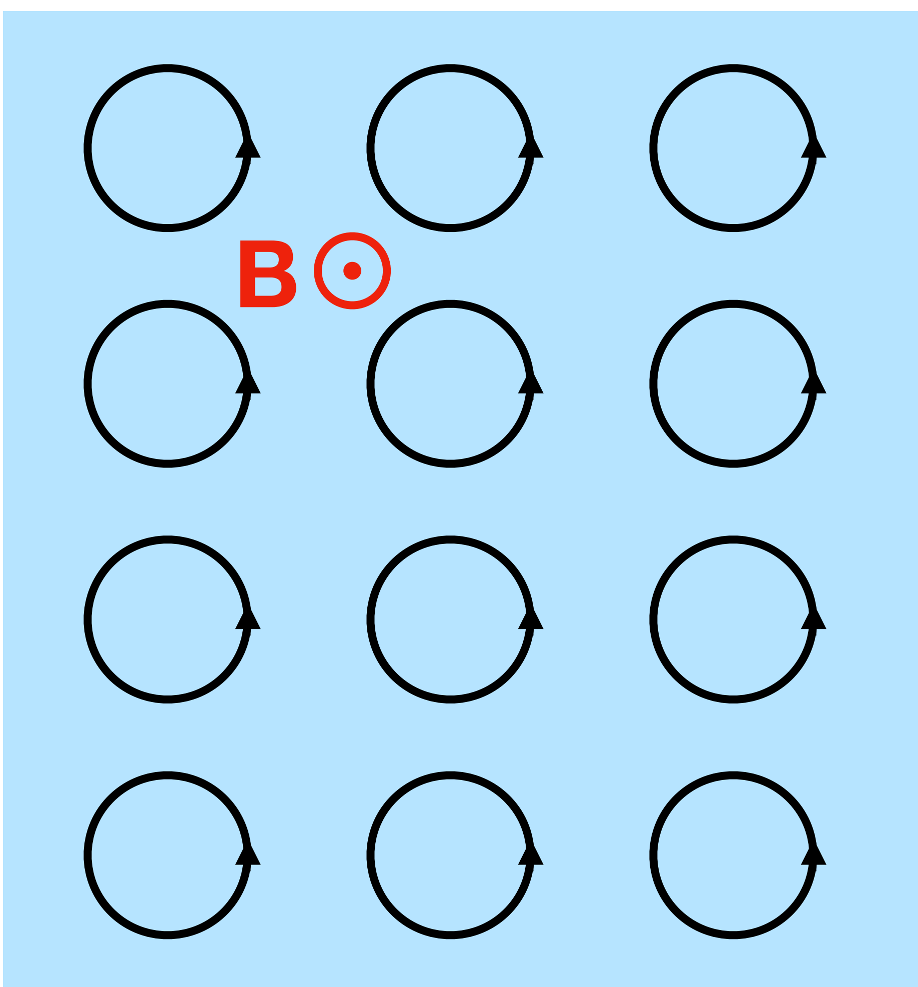
No low-energy excitations

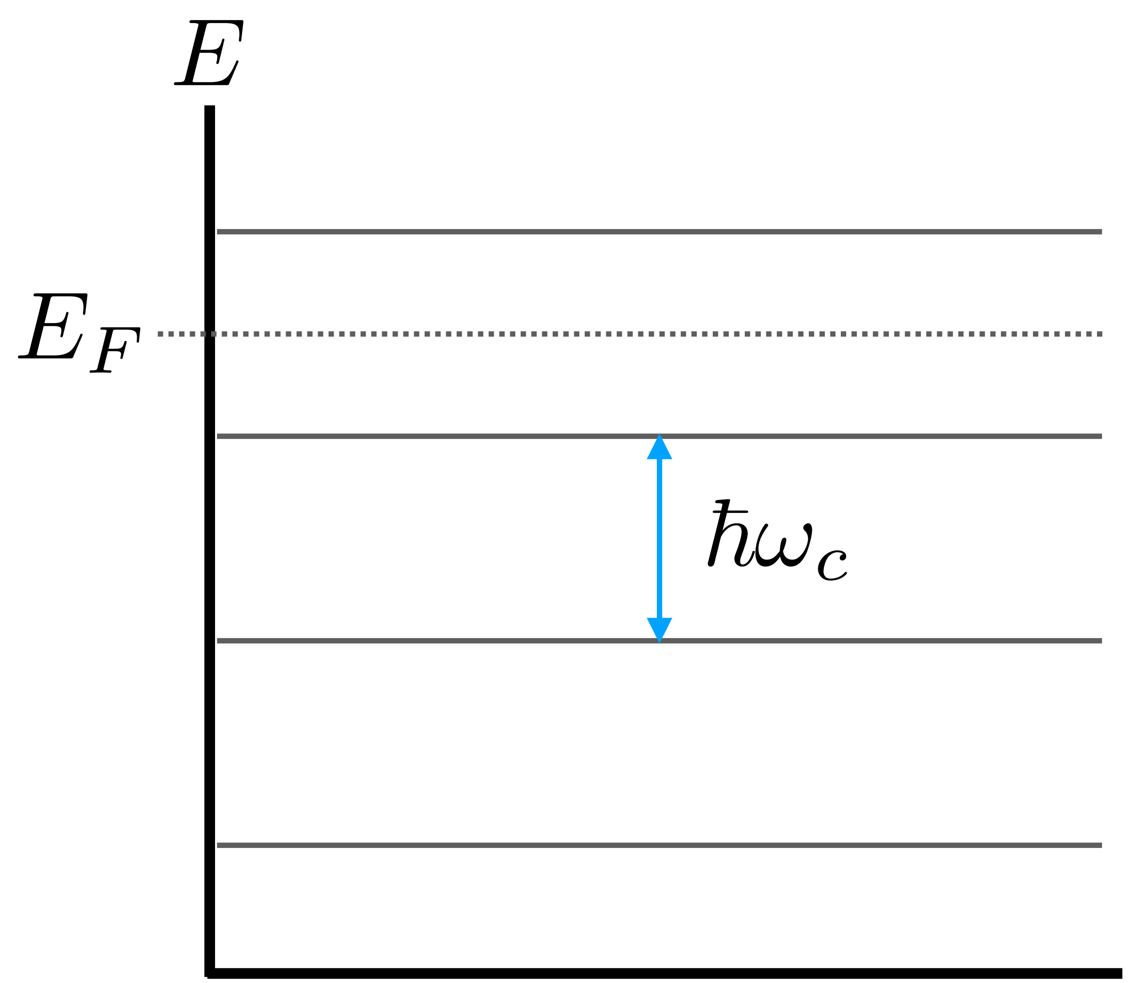


Electrical resistor

Not all insulators are the same: quantum Hall effect

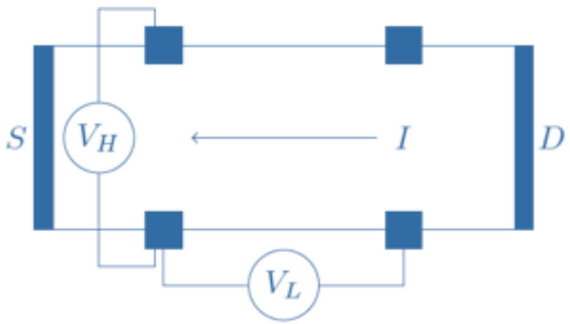
Electrons in a strong magnetic field

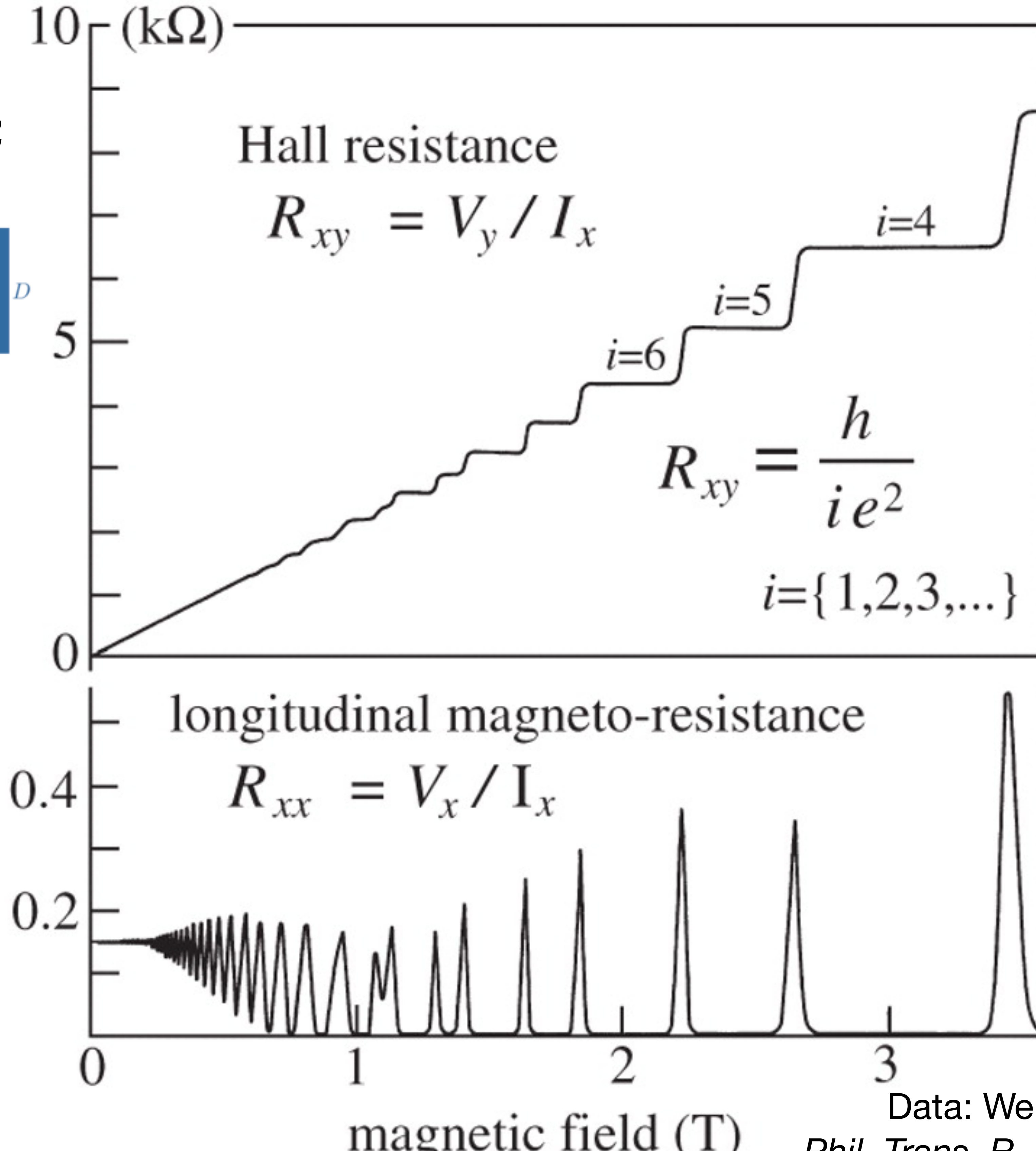




Quantum Hall devices are not insulating!!

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





Nobel Prize 1985
Klaus von Klitzing

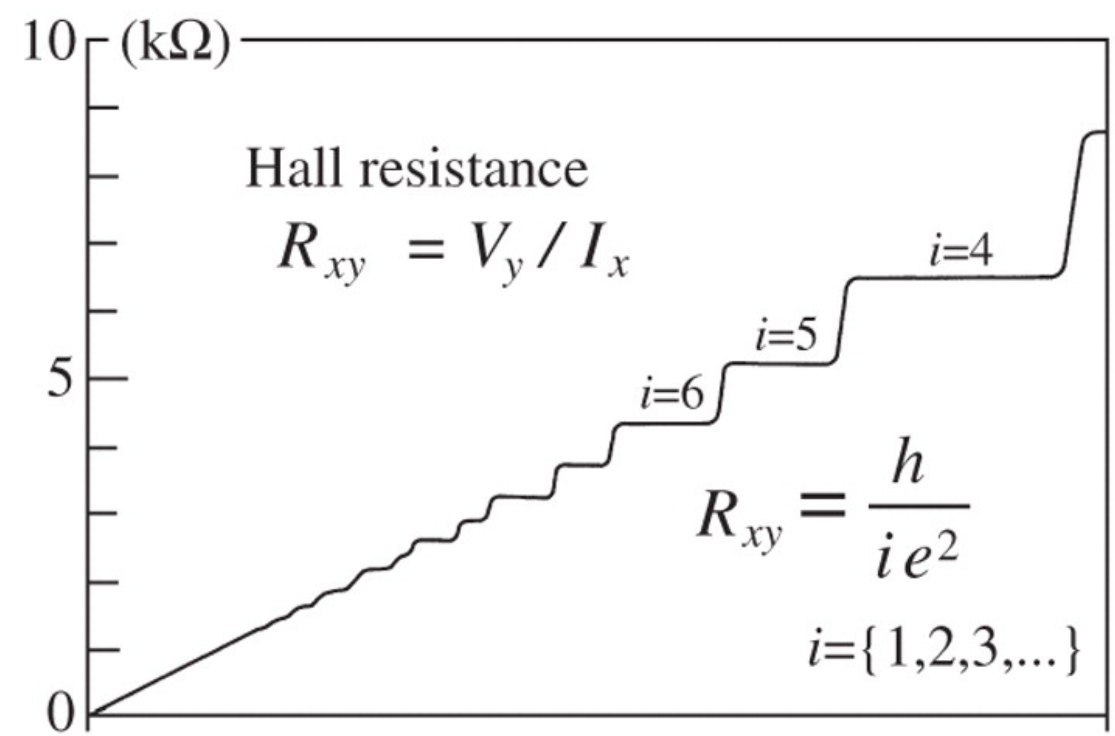
Data: Weis and von Klitzing,
Phil. Trans. R. Soc. A **369**, 3954 (2011)

Topological invariants do not change under smooth deformations

Example 1: genus

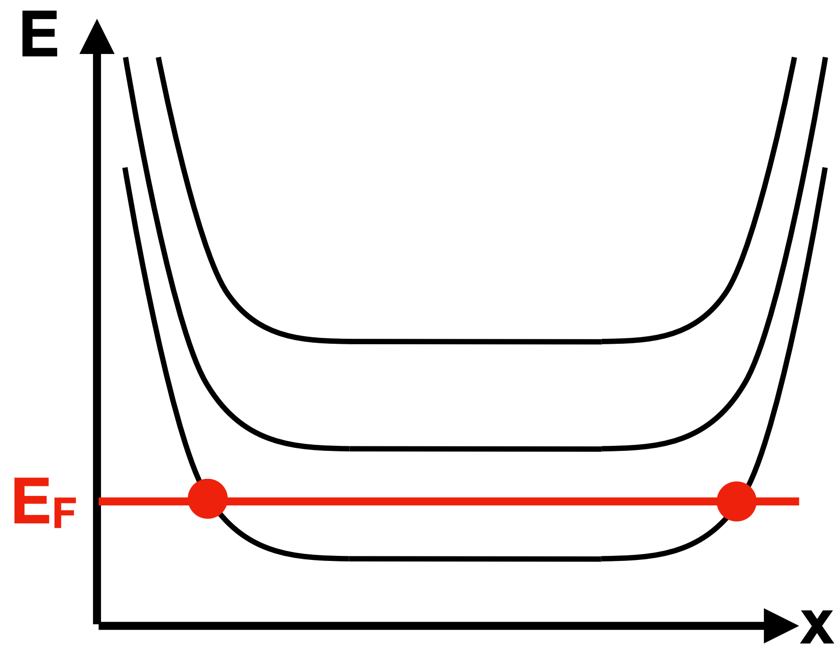
Example 2: Hall conductivity

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



Surface spectrum explains Hall conductivity

“Bulk-edge correspondence”



Landau levels bend up at edges

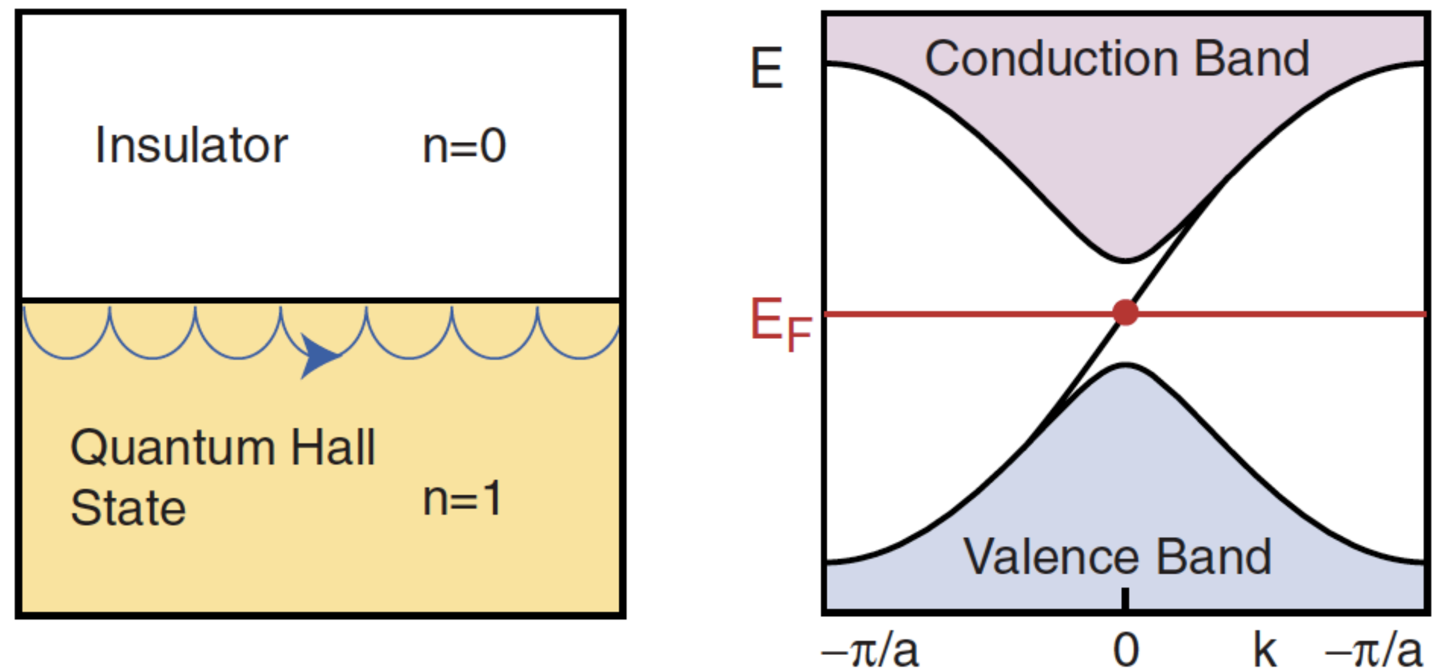
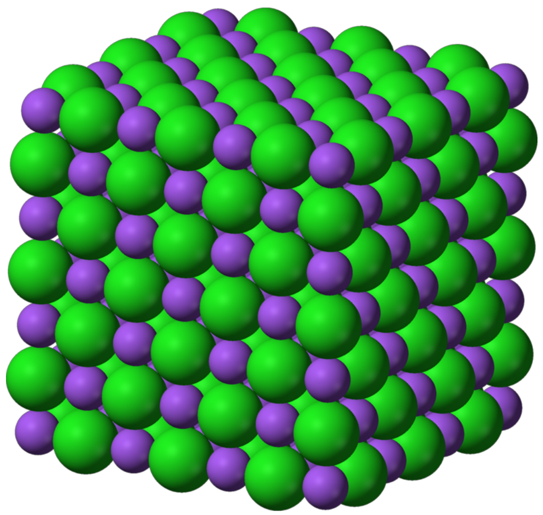


Image: Hasan & Kane RMP

Hall conductivity from bulk eigenstates: TKNN invariant
(Thouless, Kohmoto, Nightingale, den Nijs PRL 1982)

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

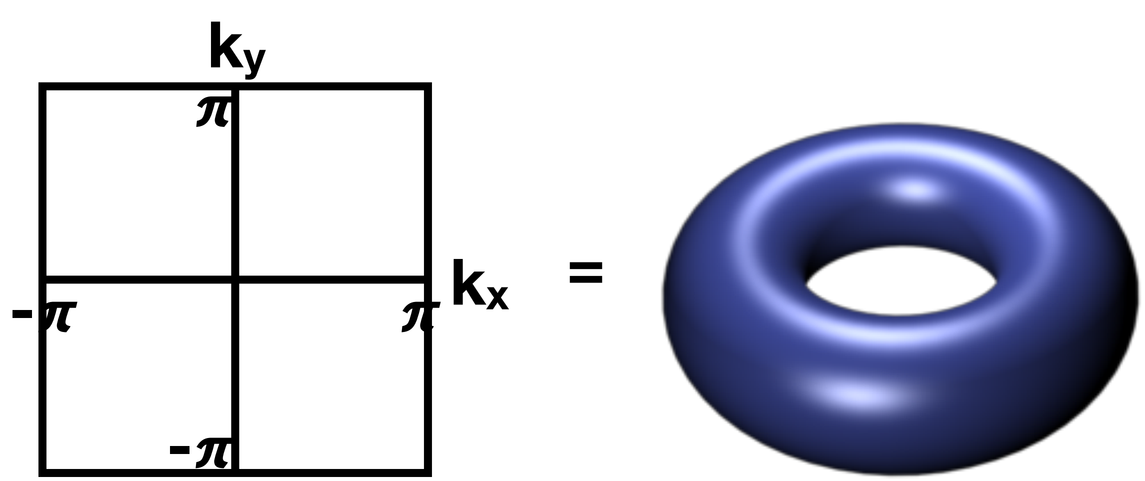
Energy eigenstates in a crystal are Bloch wavefunctions



Translation symmetry: $$T(\mathbf{R})|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}|\psi\rangle$$

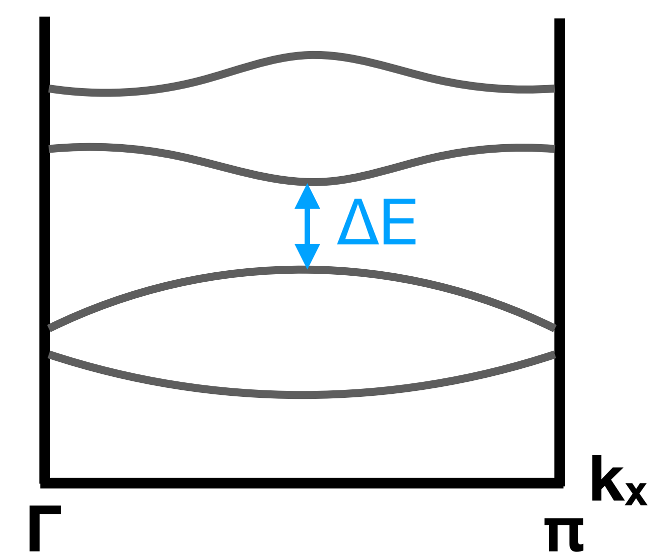
Bloch's theorem: $$|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u(\mathbf{k})\rangle$$

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

Berry phase

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 ⇒ Berry phase defined mod 2π:

$$|u(\mathbf{k})\rangle \to e^{i\phi(\mathbf{k})}|u(\mathbf{k})\rangle \qquad \mathbf{A} \to \mathbf{A} + \nabla_{\mathbf{k}}\phi(\mathbf{k})$$

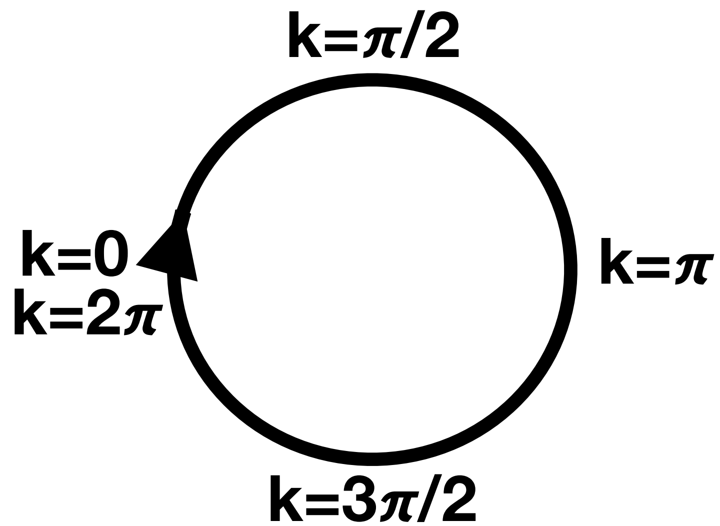
$$\gamma_C \to \gamma_C + \boxed{\oint_C \nabla_{\mathbf{k}}\phi(\mathbf{k})\cdot d\mathbf{k}}$$

$$2\pi n$$

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

Zak phase: Berry phase around Brillouin zone

Zak PRL 62, 2747 (1989)

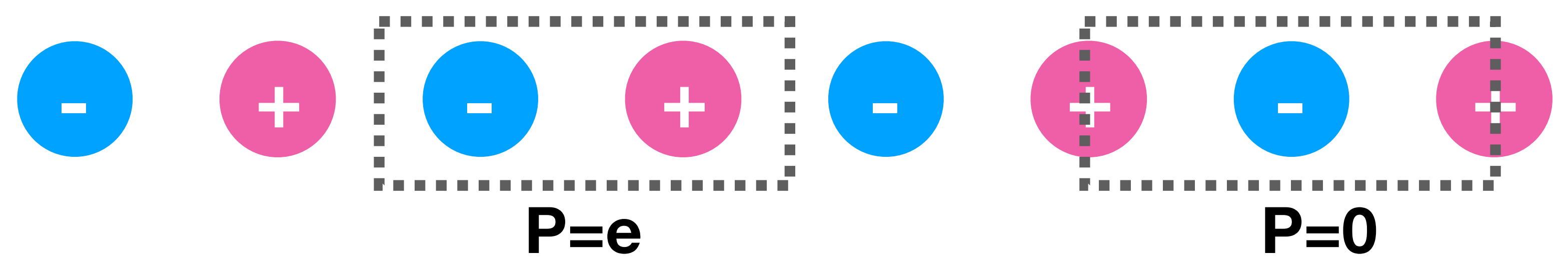


$$\gamma = \int_0^{2\pi} -i\langle u(k)|\partial_k|u(k)\rangle dk$$

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

$$i\partial_k \rightarrow x$$

Polarization of infinite crystal defined mod e:



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)

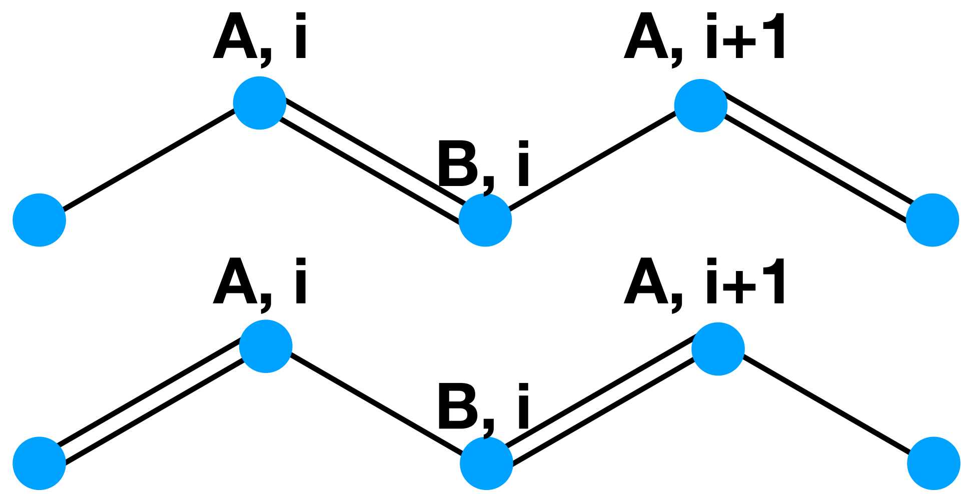
Berry phase in 1d: SSH model

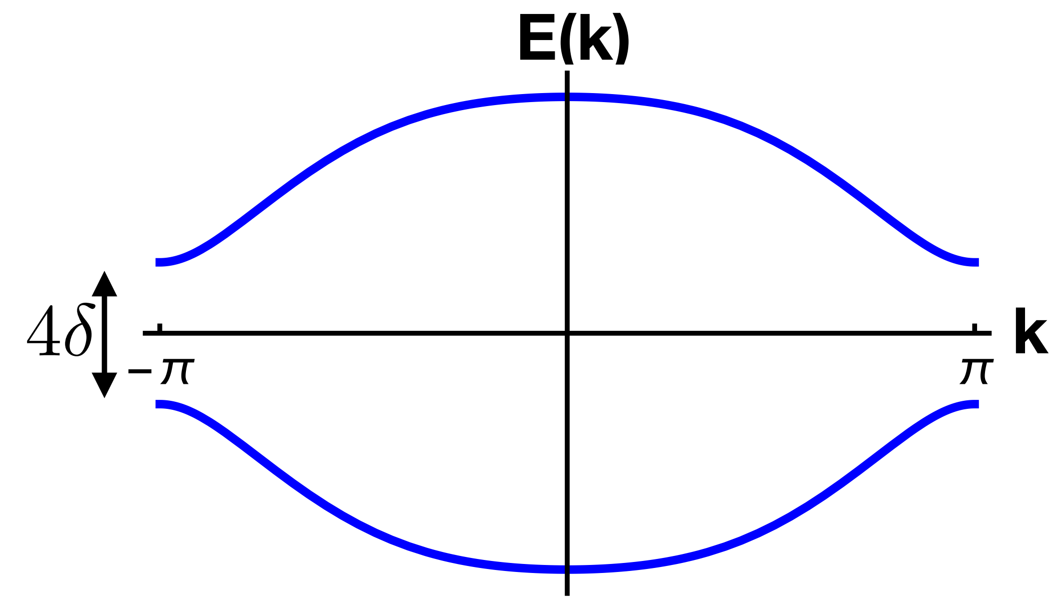
(Su, Schrieffer, Heeger PRL 1979)

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

$\delta > 0$

$\delta < 0$





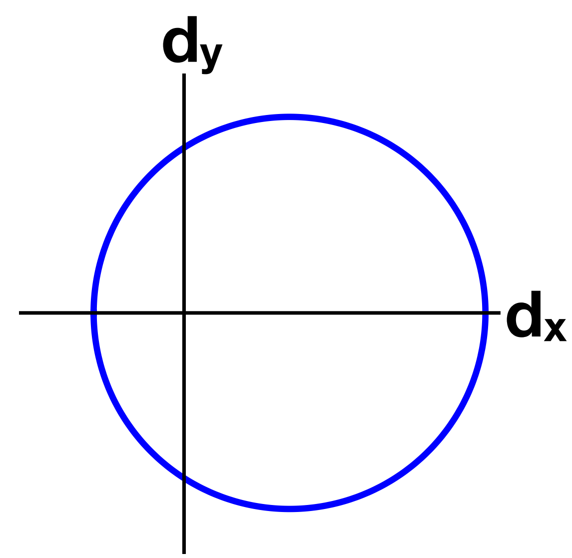
$$H(k) = d(k) \cdot \sigma$$

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

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

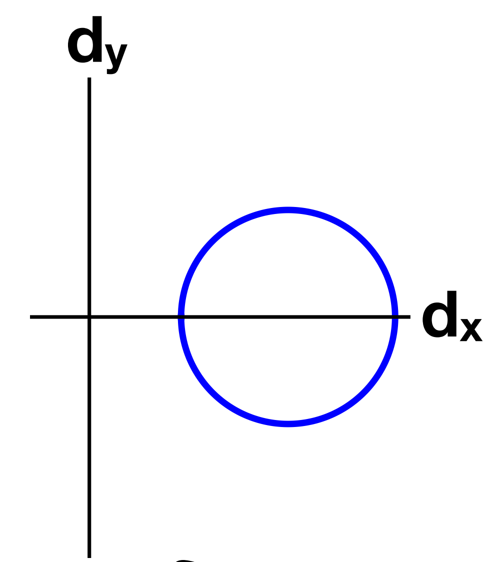
$$d_z(k) = 0$$

Symmetry enforces $d_z(k)=0$



$\delta < 0$

Berry phase π



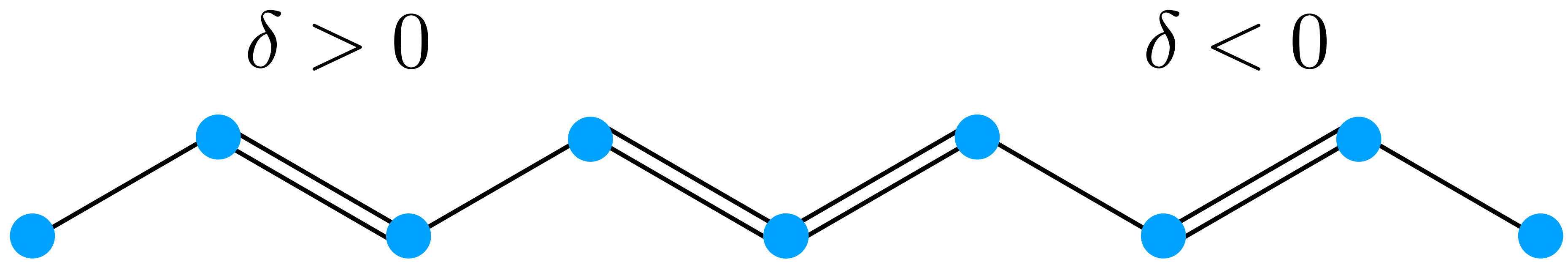
$\delta > 0$

Berry phase 0

Interpret difference in Berry phase as difference in polarization!!

Domain wall states

(Su, Schrieffer, Heeger PRL 1979)

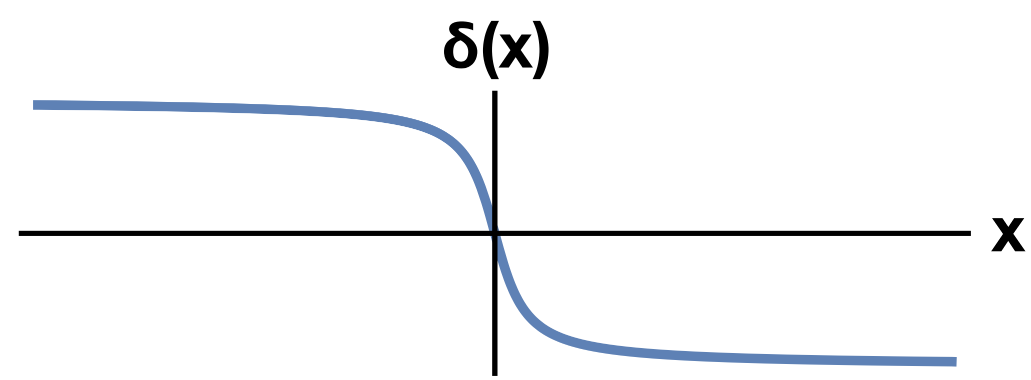


Low-energy continuum theory: $H = 2\delta\sigma_x - tk\sigma_y$

$(k \approx \pi, \delta \ll t)$

Domain wall: $\delta \to \delta(x)$

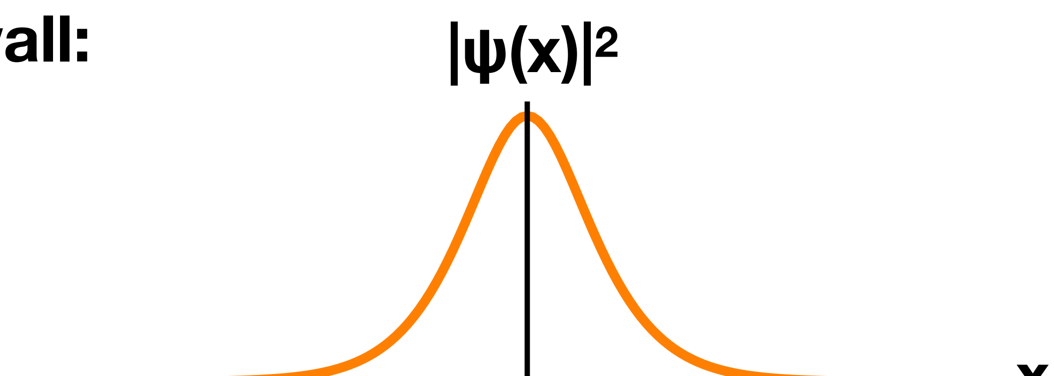
$k \to -i\partial_x$



Zero-energy state localized at domain wall:

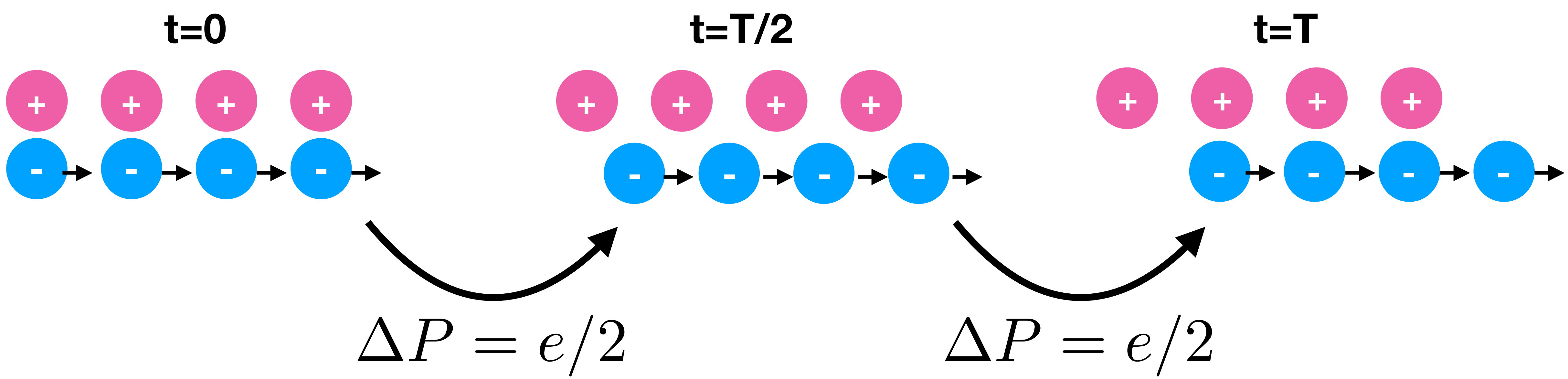
(Jackiw & Rebbi PRD 1976)

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



Thouless charge pump

(Thouless PRB 1983)

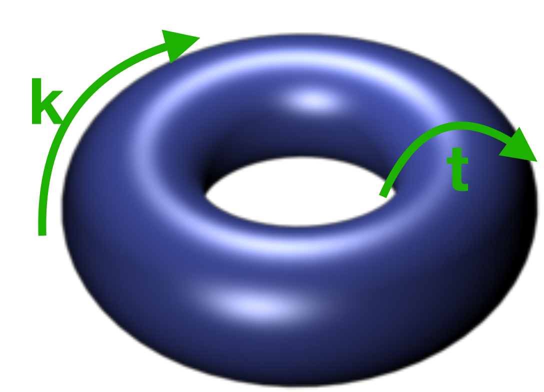


Integer charge pumped in one full cycle is a topological invariant:

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

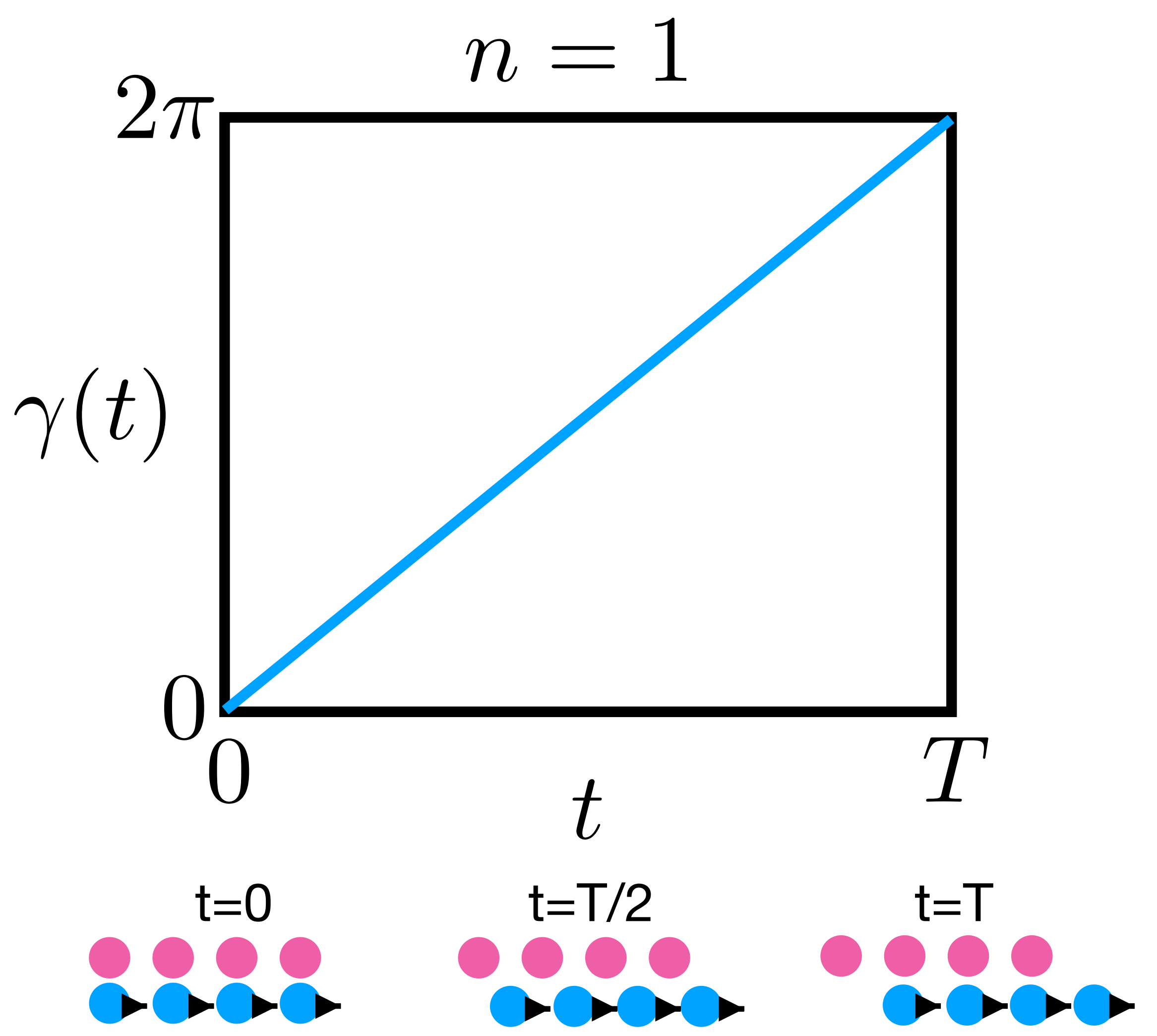
"Chern number"

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



Chern number = winding Berry phase

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

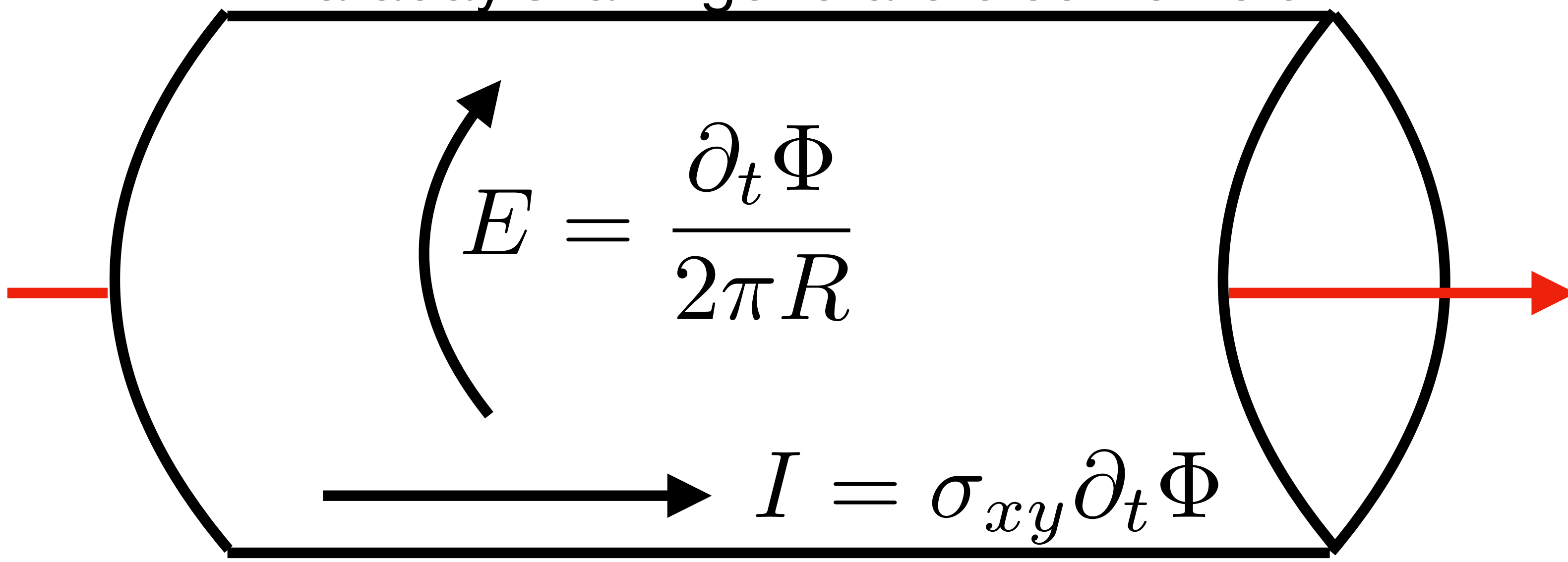


Practical way to compute Chern number

Integer quantum Hall: Laughlin flux argument

Laughlin PRB 1981

2. Faraday’s law: generate electric field



1. Thread flux quantum

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

3. Hall conductance determines current

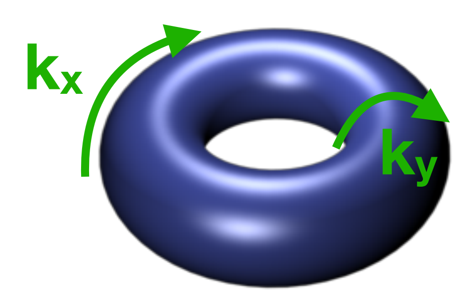
4. Charge pumping: $\Delta Q = \int_0^T I(t) dt = \sigma_{xy} \frac{h}{e}$

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

Thouless pump!

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

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

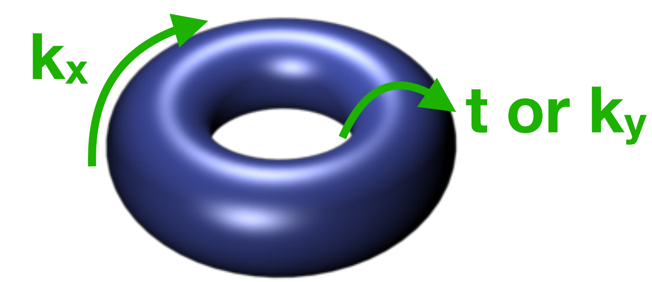


Chern number with t → k_y

Chern number ⇒ surface state

Topological invariant: TKNN or Chern number

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



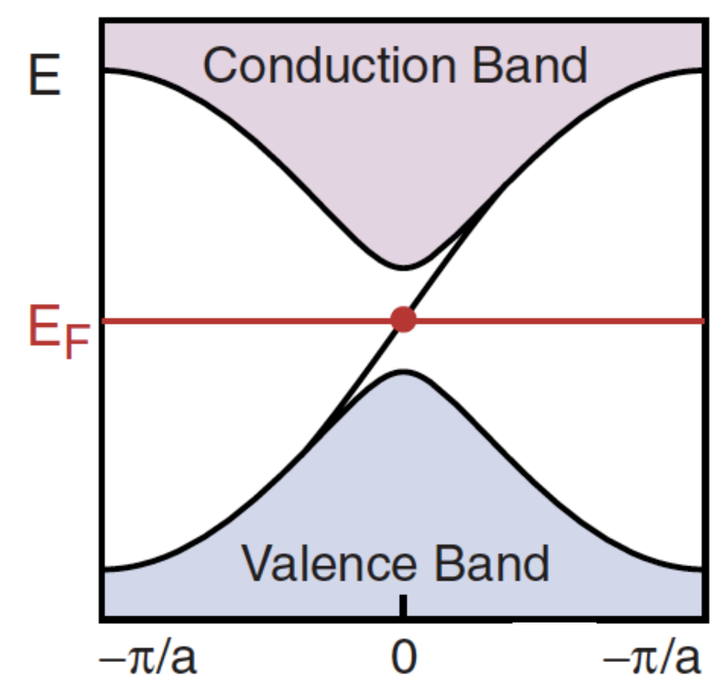
Bulk diagnosis

↕

Bulk-edge correspondence

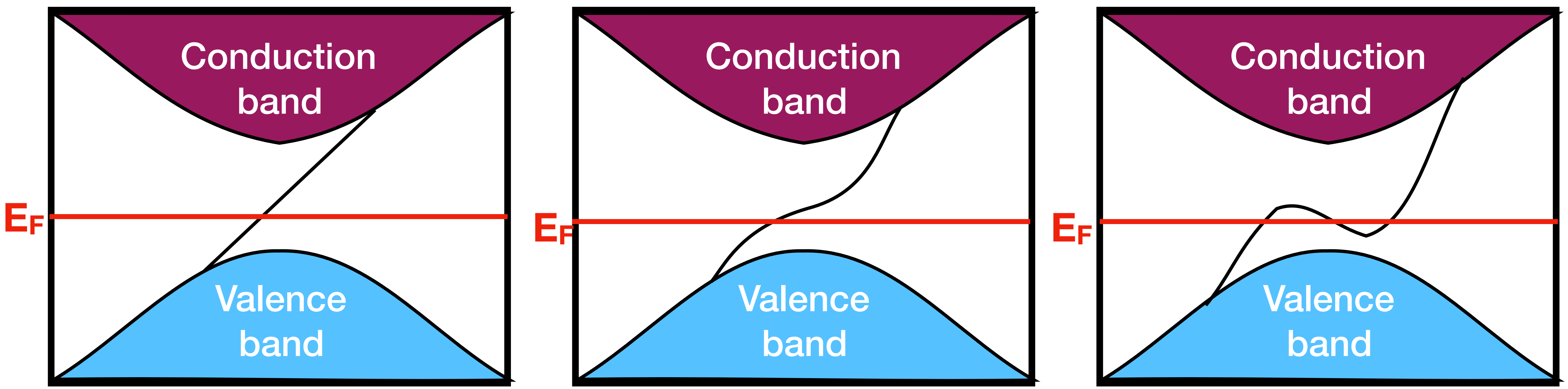
Surface diagnosis

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



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

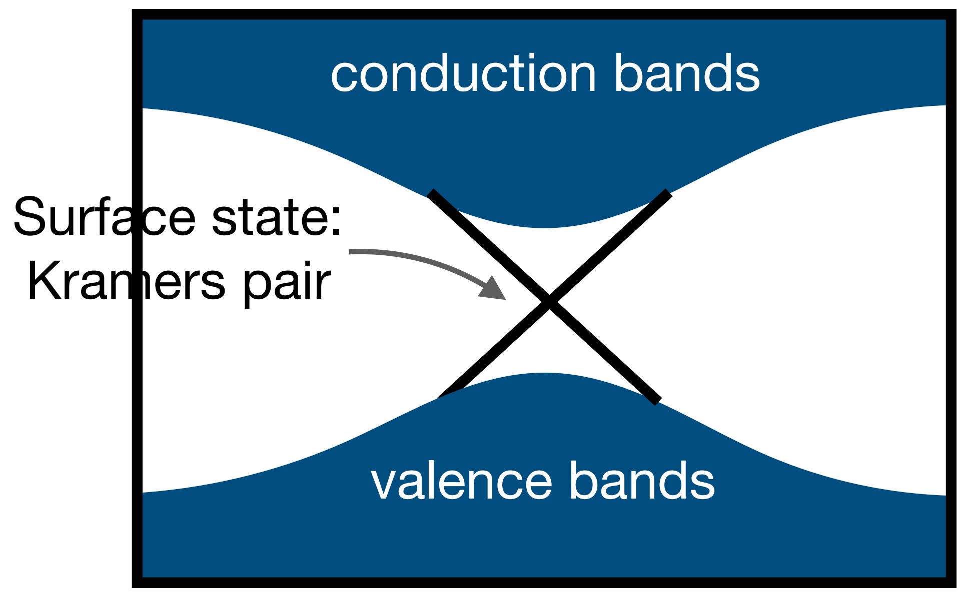
Chern number = $n_+ - n_-$

Time-reversal symmetry

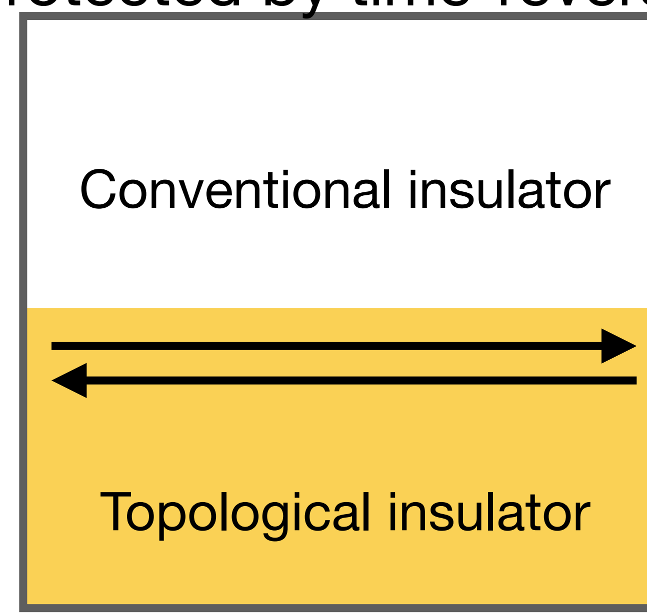
$$\Theta^{-1} H(\mathbf{k}) \Theta = H(-\mathbf{k}) \qquad \Theta^2 = -\mathbb{I}$$

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

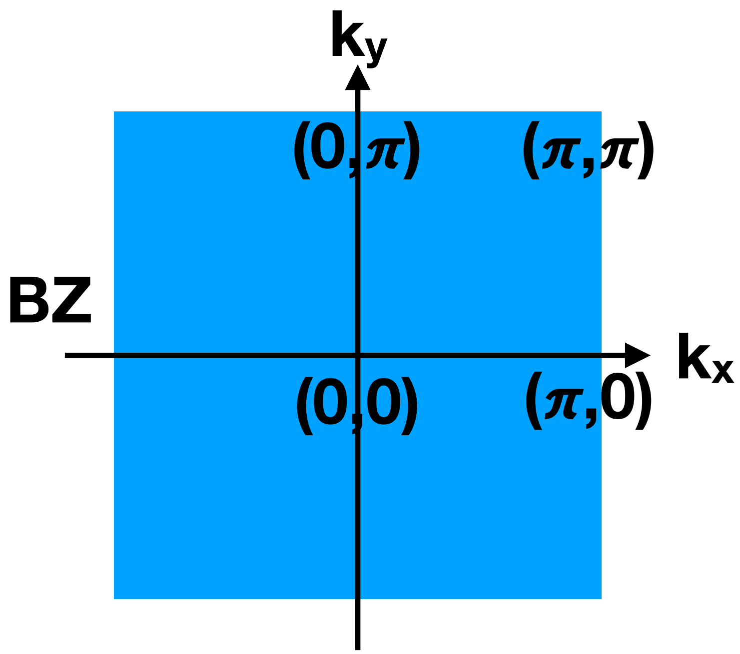


“Z_2” topological invariant ν: even vs odd bands cross E_F over *half* the BZ

Fermion parity pump

Bulk Z_2 invariant

Kane & Mele PRL 95, 146802 (2005)



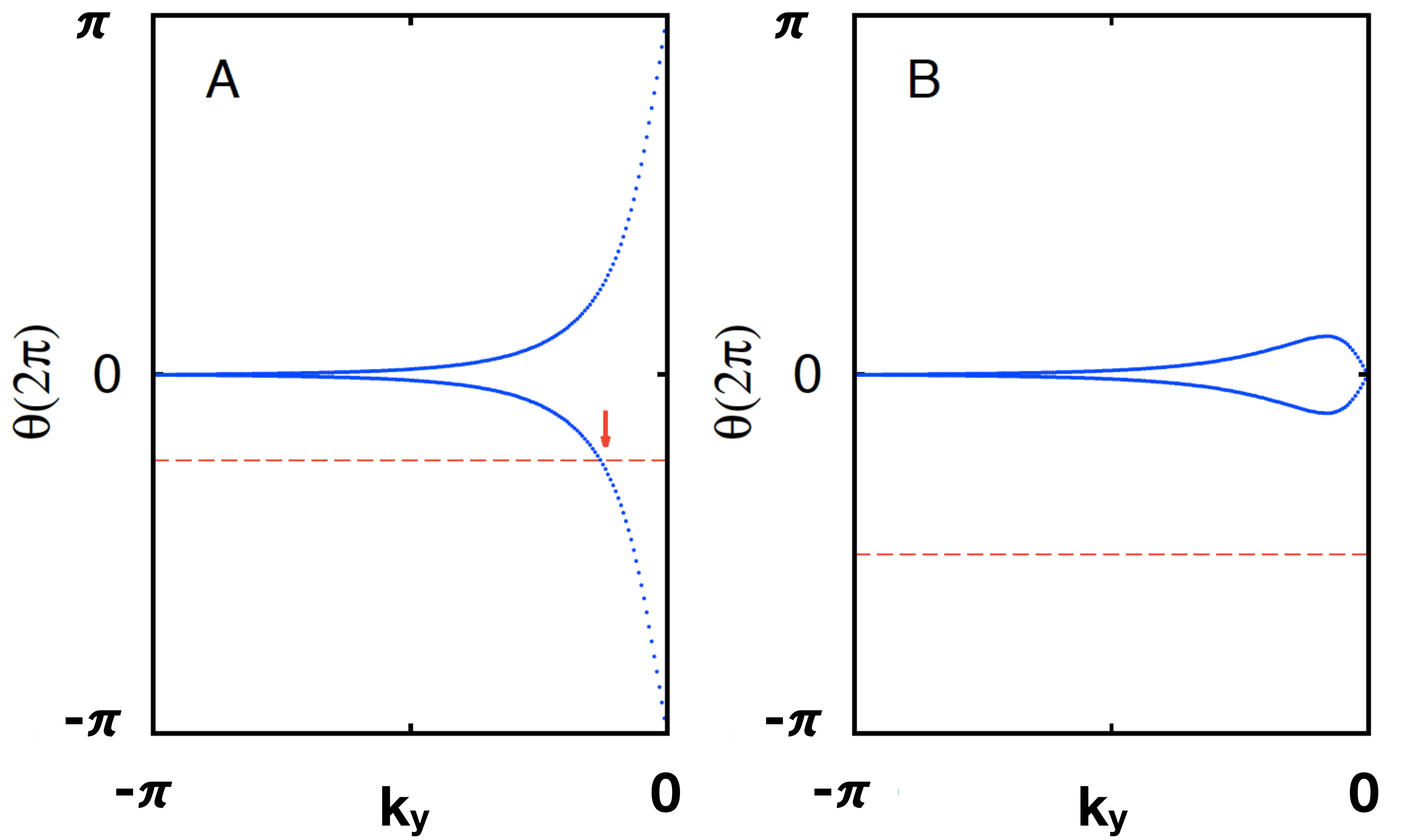
$$(-1)^{\nu} = \prod_{\Lambda_a \in \mathrm{TRIM}} \frac{\mathrm{Pf}[w(\Lambda_a)]}{\sqrt{\mathrm{Det}[w(\Lambda_a)]}} = \pm 1$$

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

Gauge invariant but must choose continuous gauge

In practice, difficult to compute

Practical calculation of Z_2 invariant: winding Berry phase



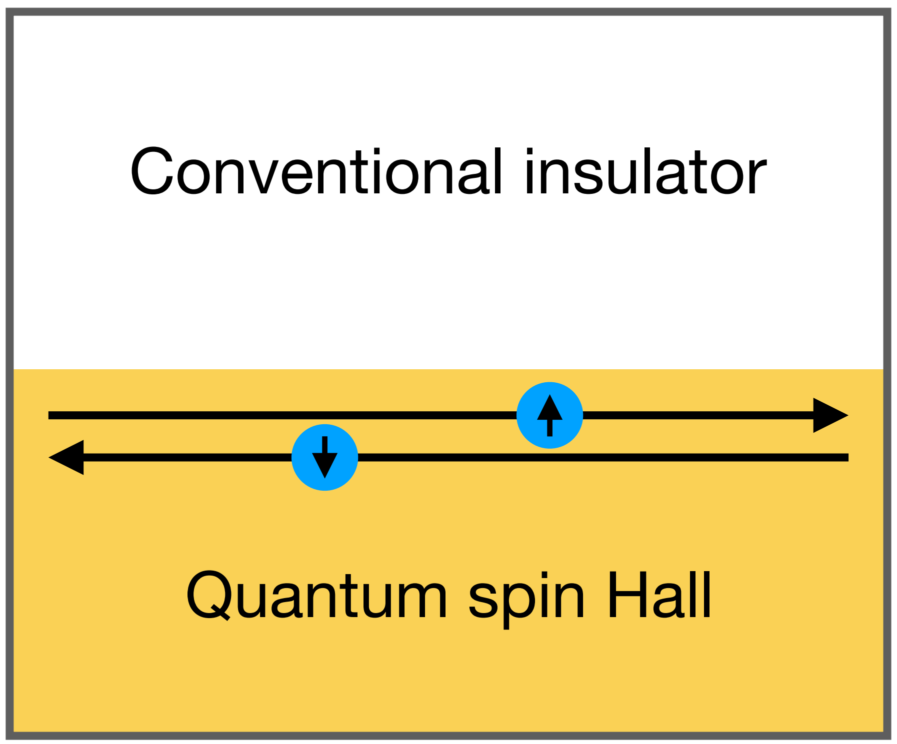
Yu, Qi, Bernevig, Fang, Dai PRB 84, 075119 (2011)
Soluyanov and Vanderbilt Phys. Rev. B 83, 235401 (2011)

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

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

Easier computation of Z_2 invariant with symmetry

Spin conservation:
"quantum spin Hall effect"



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)

Inversion symmetry

Z_2 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)

Quantum spin Hall effect in graphene with spin orbit coupling

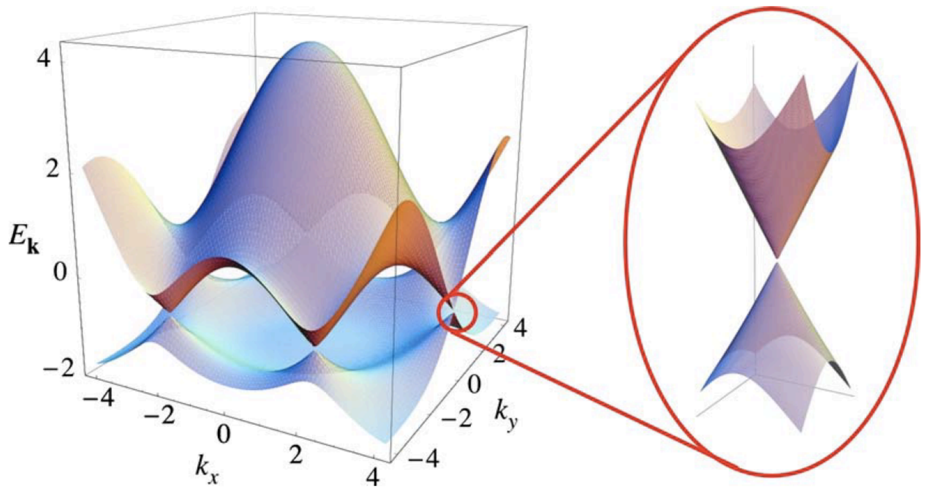
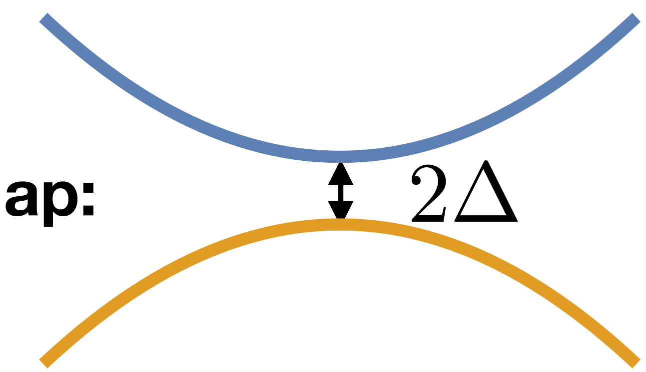


Fig: Castro Neto, et al, RMP (2009)

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

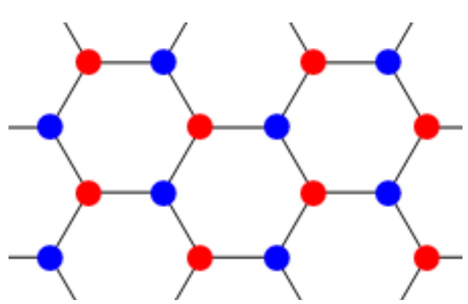
$\sigma_z = \text{sublattice} \quad \tau_z = \text{valley} \quad s_z = \text{spin}$

Three ways to open energy gap:



1. Sublattice potential (hBN)

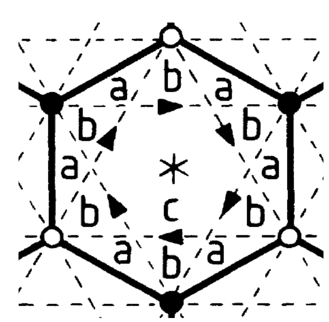
$$\Delta_{\text{hBN}}\sigma_z$$



Breaks inversion symmetry

2. Staggered flux
Haldane PRL 1988

$$\Delta_{\text{Haldane}}\sigma_z\tau_z$$



Breaks time-reversal
Quantum Hall effect

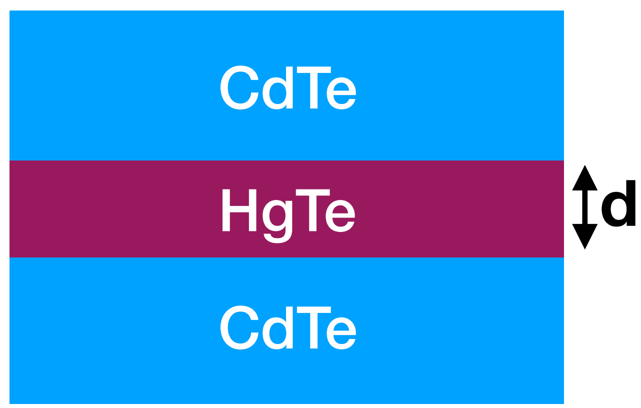
3. Spin-orbit coupling
Kane and Mele PRL 1995

$$\Delta_{\text{SOC}}\sigma_z\tau_z s_z$$

Preserves all symmetries
Quantum spin Hall effect

Quantum spin Hall in HgTe quantum wells

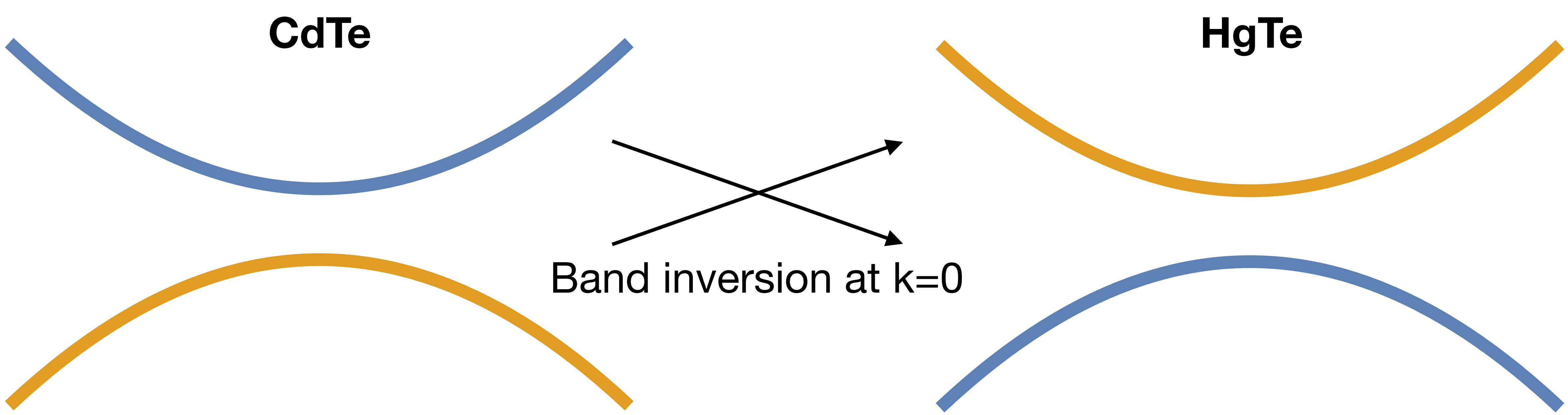
Theory: Bernevig, Hughes, Zhang Science 2006 “BHZ model”



$d<d_c$ normal band order

$d>d_c$ inverted (topological) band order

d_c = 6.4nm

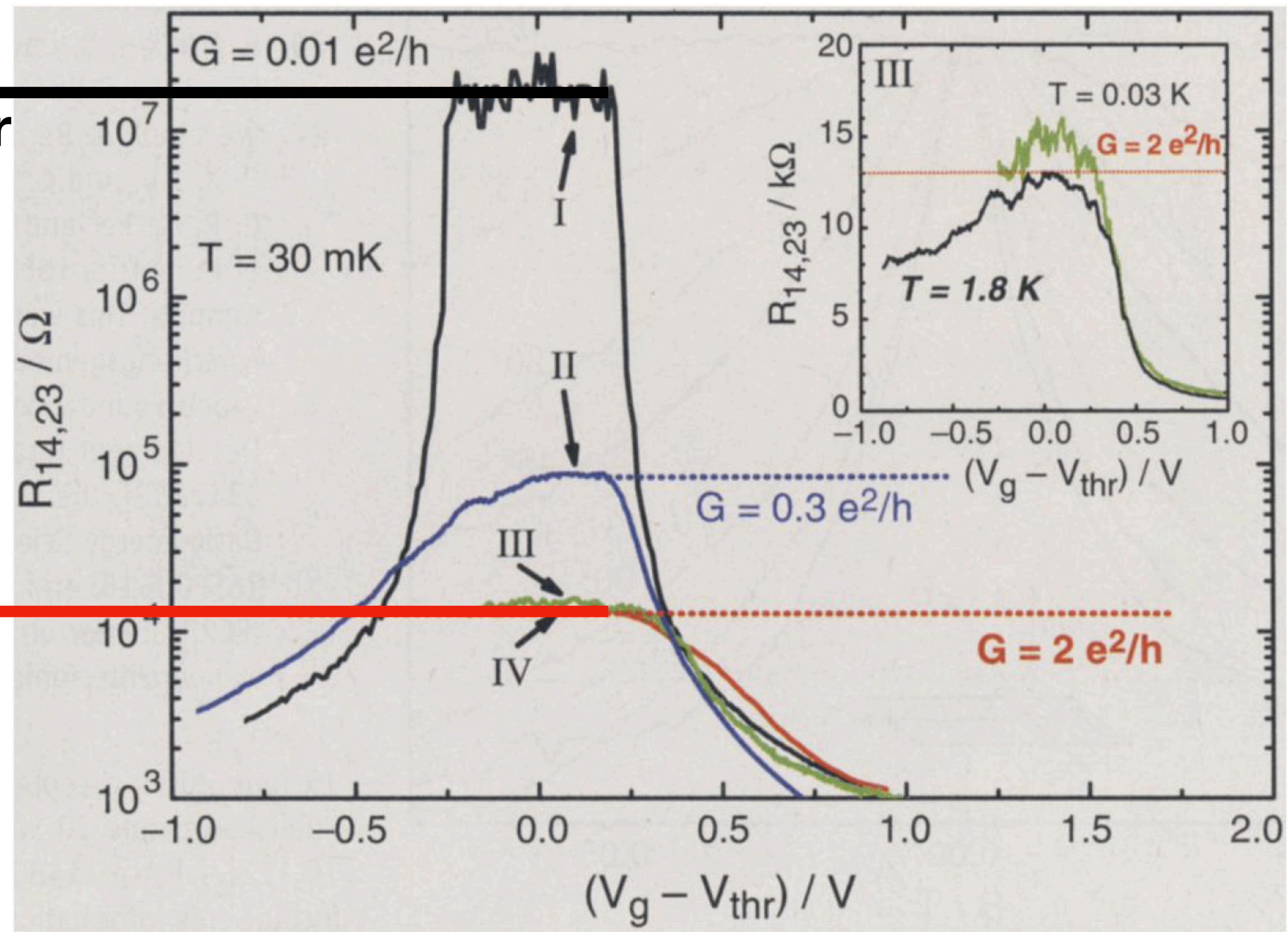


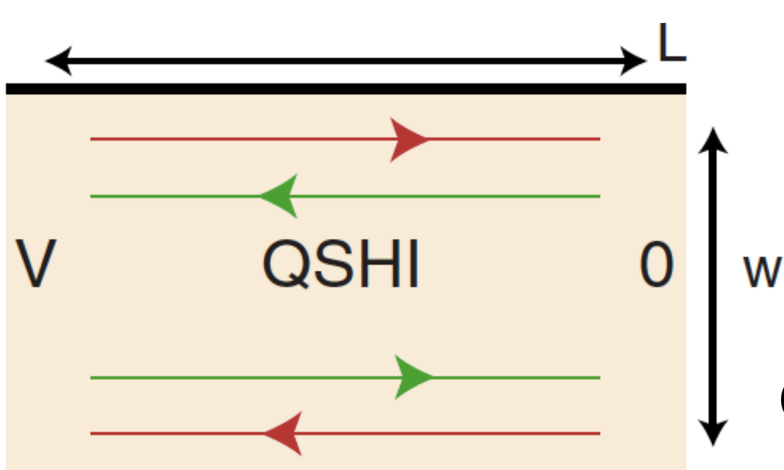
Experimental realization HgTe quantum wells

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

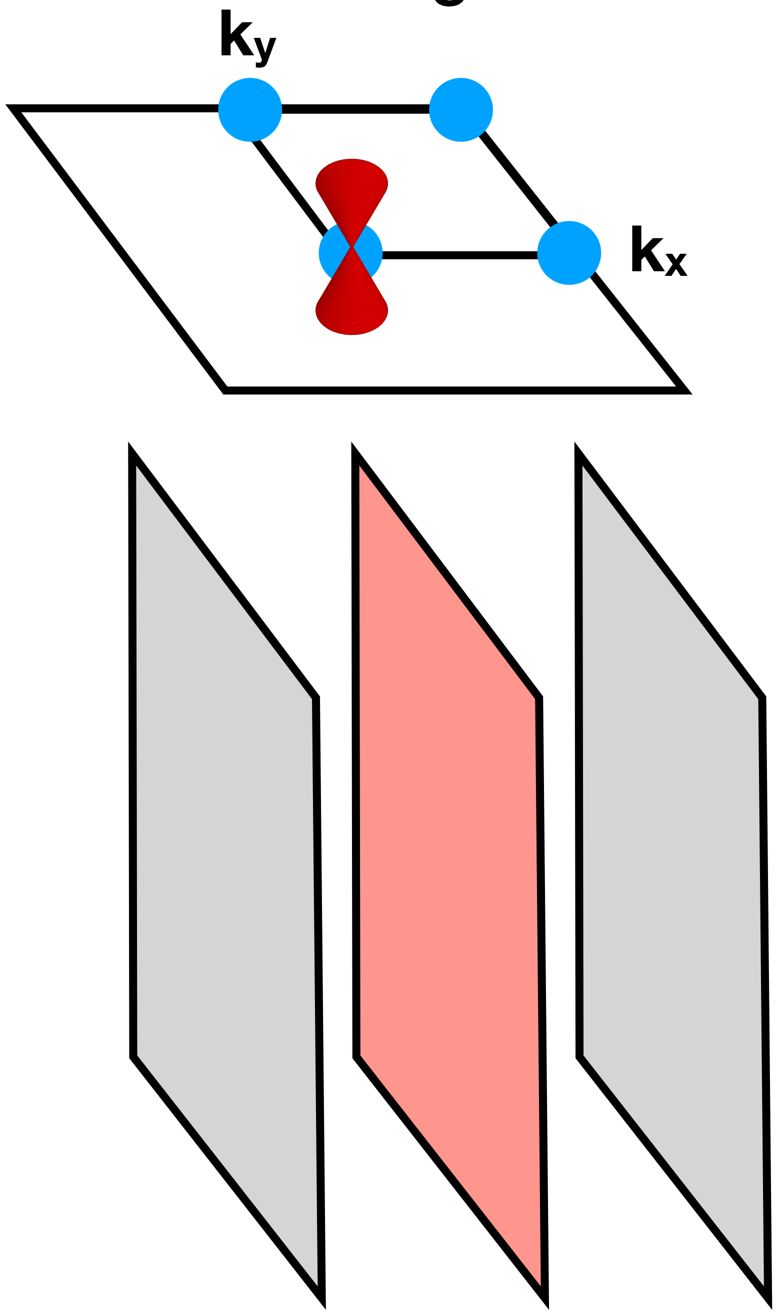
Topological insulators in 3d

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

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

"Strong" index

Ex:
(1;000)



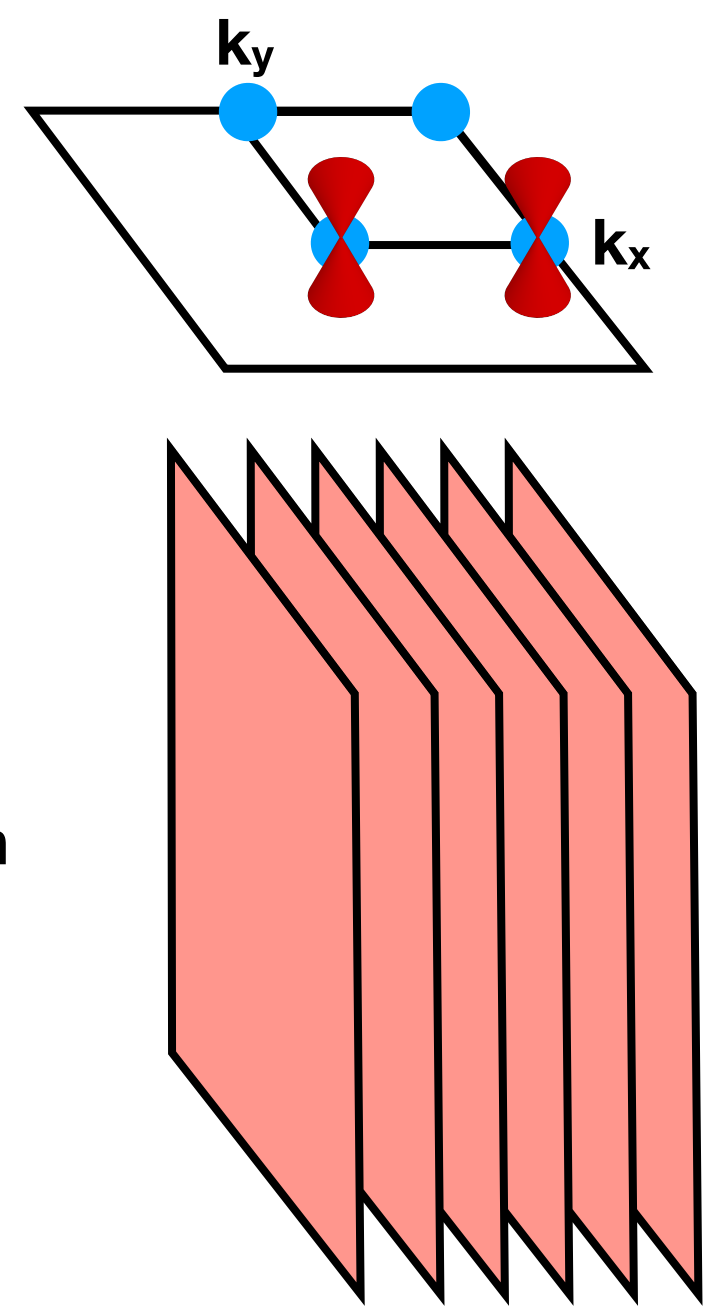
Surface Brillouin zone

Bulk construction
(not unique)

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

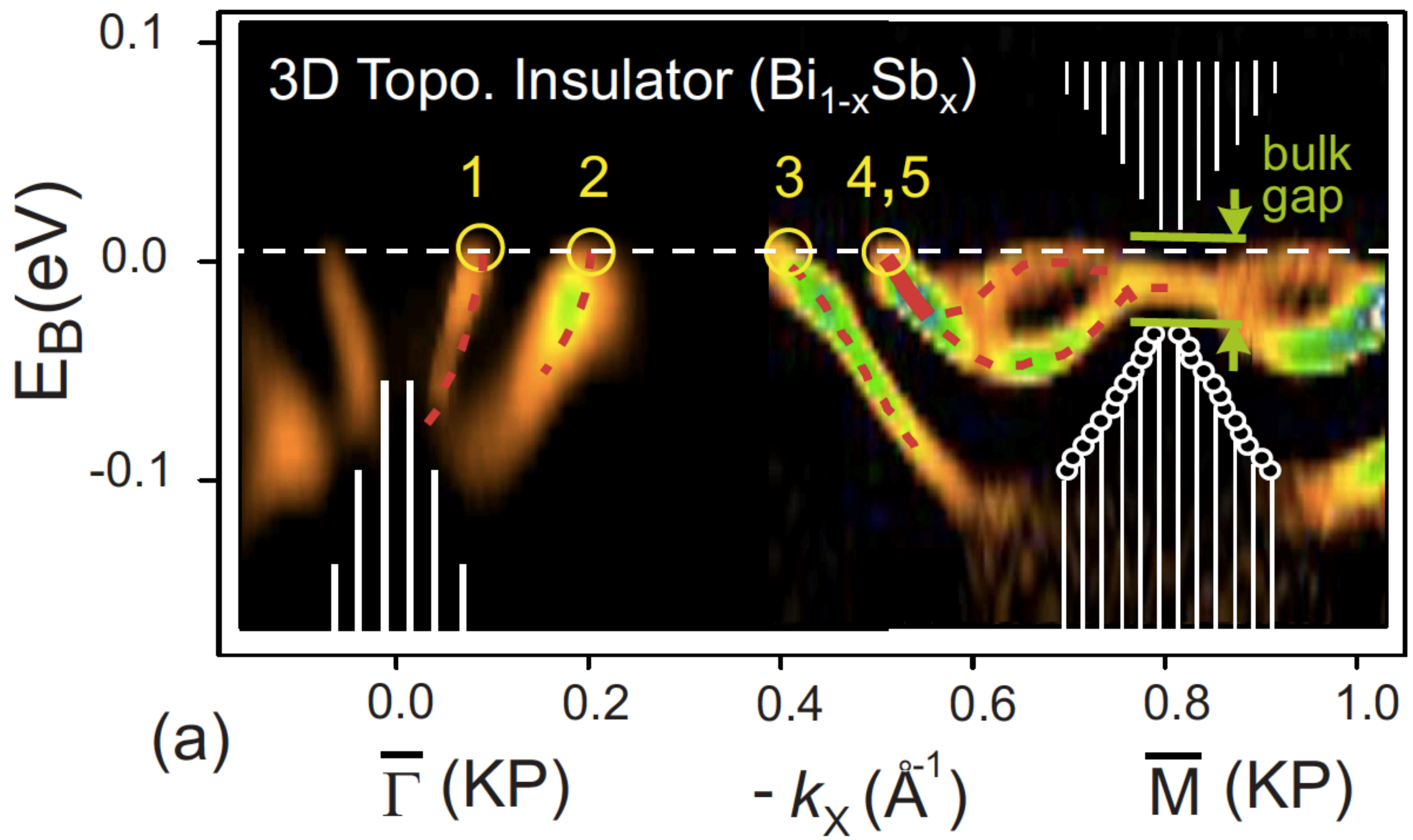
"Weak" indices

Ex:
(0;100)

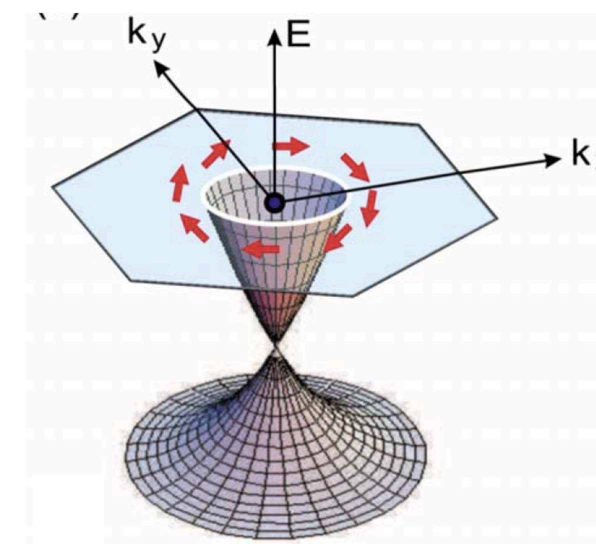


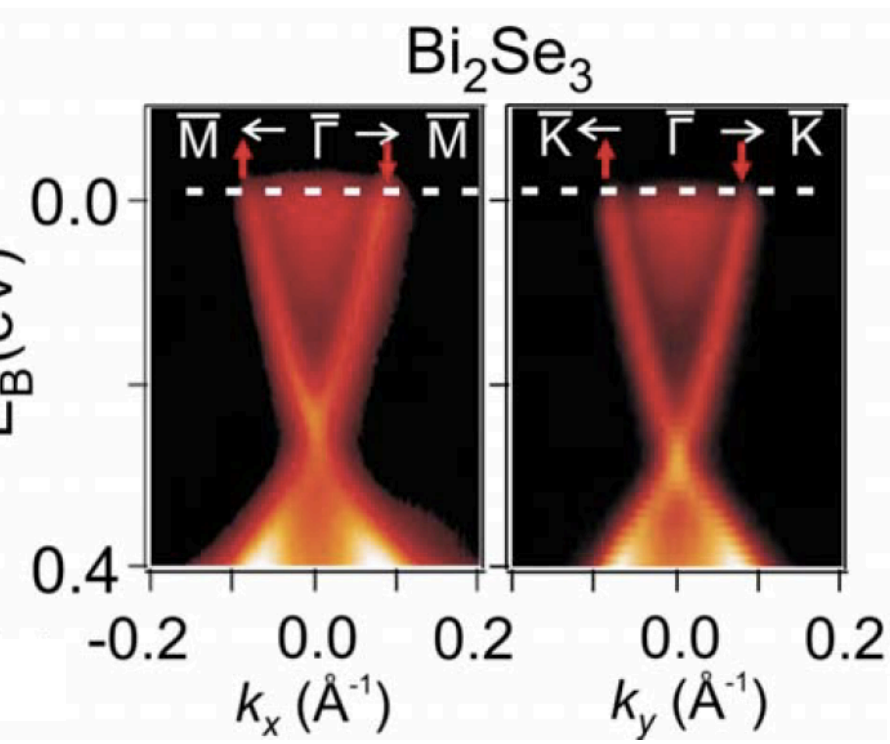
Stacked 2D TIs

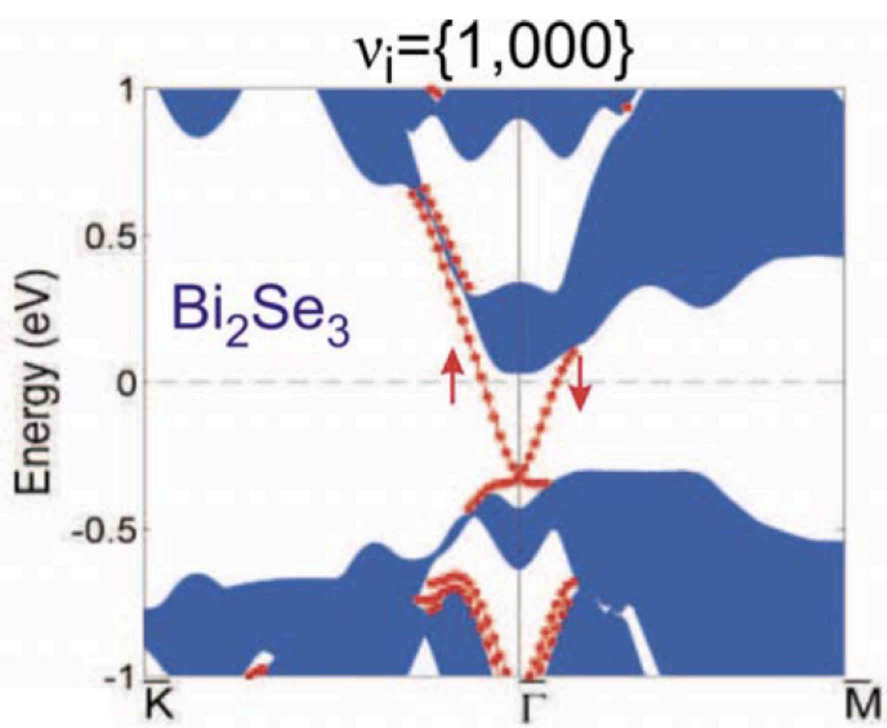
Topological insulators in 3d



$\underline{Bi_{1-x}Sb_x}$
Band gap ~ .03eV
Theory: Fu & Kane PRL 2007
Expt: Hsieh, et al, Nature 2008







$\underline{Bi_2Se_3}$
Band gap ~ .3eV
Theory: Zhang, et al,
Nat. Phys. 2009
Expt: Xia et al, Nat. Phys. 2009

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

no symmetry → A

Integer quantum Hall

real case:

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

fermions w/ time-reversal → AII

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