

# Topological Band Theory

Amir Shapour Mohammadi

PHY 525  
Princeton University

December 2022

# Anomalous Quantum Hall Effect

Electron equation of motion

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_{\mathbf{k}} - \frac{d\mathbf{k}}{dt} \times \mathcal{B}(\mathbf{k}), \quad \frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \mathbf{E} \quad (1)$$

Current density

$$\mathbf{j} = \sigma \mathbf{E} + \sigma_{AH} \hat{\mathbf{n}} \times \mathbf{E} \quad (2)$$

Quantized anomalous Hall current (for band insulator)

$$\sigma_{AH}^n \hat{\mathbf{n}} = \frac{\sigma_0}{2\pi} \int_{BZ} d^2\mathbf{k} \, \mathcal{B}_n(\mathbf{k}) := \sigma_0 C_n \hat{\mathbf{n}}. \quad (3)$$

# Symmetries of Chern Number

Assuming time-reversal ( $\Theta |k\rangle = |-k\rangle$ ) symmetry, we have

$$\mathcal{B}(k) = \Theta^\dagger \mathcal{B}(k) \Theta = -\mathcal{B}(-k) \text{ (odd)}. \quad (4)$$

Assuming (space) inversion symmetry ( $\mathcal{I} |r\rangle = |-r\rangle, \mathcal{I} |k\rangle = |-k\rangle$ ), we have

$$\mathcal{B}(k) = \mathcal{I}^\dagger \mathcal{B}(k) \mathcal{I} = \mathcal{B}(-k) \text{ (even)}. \quad (5)$$

$\Theta +$  inversion symmetry implies  $\mathcal{B}(k)$  vanishes identically.

# Haldane Model (1988)

Goal: craft a Chern insulator (time-reversal breaking topological insulator), not the simplest model.

Recall the continuum model for graphene

$$H = v_F(\tau_z \sigma_x k_x + \sigma_y k_y) \quad (6)$$

where  $\sigma$  acts on sublattice space. We must break  $\Theta$  and/or chiral (sublattice,  $\mathcal{C}$ ) symmetry to open a band gap.

$$m_R \sigma_z \quad (\mathcal{C} \text{ broken}, \Theta \text{ obeyed}) \quad (7)$$

To yield non-zero Chern number, we must break  $\Theta$  symmetry (i.e. make the Berry curvature have the same sign at both Dirac points)

$$m_H \tau_z \sigma_z \quad (\mathcal{C}, \Theta \text{ broken}) \quad (8)$$

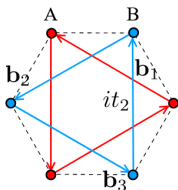
where  $\tau$  acts on the valley space.

# Haldane Model (tight-binding realization)

Haldane did this by adding an imaginary, or directional, (recall  $\Theta \propto \mathcal{K}$ ) next-to-nearest neighbor hopping induced by a magnetic field ( $\Phi_{net} = 0$ )

$$H = \Delta \sum_i (-1)^{\tau_i} c_i^\dagger c_i + t_1 \sum_{NN} (c_i^\dagger c_j + h.c.) + t_2 \sum_{NNN} (i c_i^\dagger c_j + h.c.). \quad (9)$$

The new term is restricted to  $\alpha\alpha$  sublattice hoppings.



Thus, we have a Chern insulator by modifying the graphene model. Can we find a topological insulator which obeys  $\Theta$  symmetry (i.e. not a Chern insulator)?

# Kane-Mele Model (2005), $\mathbb{Z}_2$ Index

Essentially, we consider two copies of Haldane's model, one per spin, induced by graphene's spin-orbit coupling

$$\lambda_{SO} s_z \tau_z \sigma_z \quad (10)$$

which is  $\Theta$  invariant ( $C = 0$ ). We use the Chern number of each spin system  $C_\sigma$  to define a topological index

$$\nu = \frac{1}{2}(C_\uparrow - C_\downarrow) \mod 2 \in \mathbb{Z}_2 \quad (11)$$

This model leads to the QSHE where there are counter-propagating electron spins on each edge (to obey  $\Theta$ ). However,  $\nu$  is not well-defined when we include Rashba spin-orbit coupling, and in general terms which are  $s_z$  non-conserving. We now aim at deriving a  $\mathbb{Z}_2$  index without the use of spin Chern numbers.

# Modern Theory of (Charge) Polarization

Polarization is hard to define. Total charge polarization (for 1D system)

$$\frac{dP(t)}{dt} = j(t), P = \sum_{n \text{ filled}} \int dx \langle W_{n0}(x) | \hat{x} | W_{n0}(x) \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \mathcal{A}(k) \quad (12)$$

where  $\mathcal{A}(k)$  is the summed over all filled bands.  $P$  only defined modulo  $eR/\Omega$  (lattice vector), but  $\Delta P$  (due to smooth change in parameters) is gauge-invariant

$$H(k_y = -\pi) \rightarrow H(k_y = \pi) \quad (13)$$

$$\Delta P = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_y \int_{-\pi}^{\pi} dk \mathcal{B}(k, k_y) = C \quad (14)$$

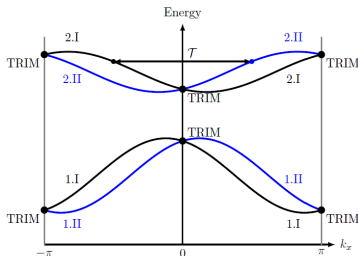
given a closed loop in parameter space. Note that  $\Delta P$  disappears in  $\Theta$  symmetry.

# Kramer's Degeneracy

In  $d$  dimensions, there are  $2^d$   $\Theta$  invariant momenta at the center and boundary of the BZ ( $k_i = -k_i + G$ ). If our Hamiltonian is  $\Theta$  symmetric then

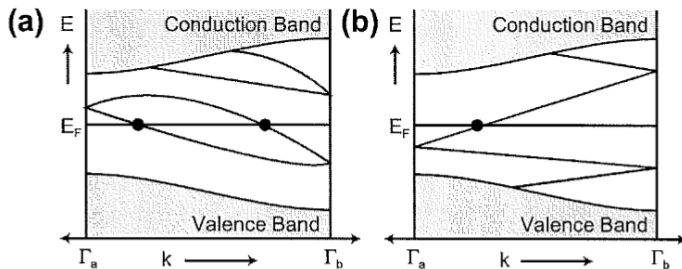
$$H|n\rangle = E|n\rangle \rightarrow H(\Theta|n\rangle) = E(\Theta|n\rangle) \quad (15)$$

In general,  $\Theta|n\rangle \neq |n\rangle$  (e.g.  $\perp$  for fermionic systems). We can apply this to get a picture of what we expect the band structure of a  $\Theta$  symmetric system to look like.





# Intuition for $\mathbb{Z}_2$ Invariant



# Time-reversal Polarization

We define the time-reversal polarizations

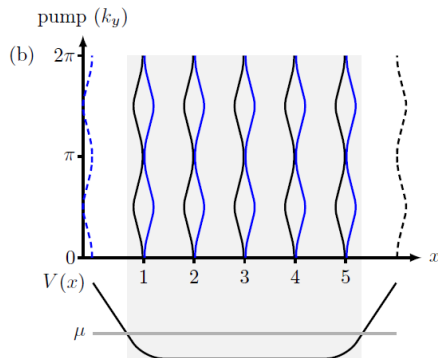
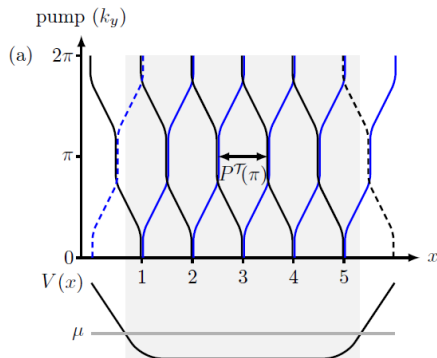
$$P^s = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk A^s(k) \quad (16)$$

where  $s = I, II$ . Due to  $\Theta$  symmetry,  $P = P^I + P^{II}$  will vanish, but the difference  $P^\Theta = P^I - P^{II}$  is generally non-zero and can be expressed

$$P^\Theta = \frac{1}{i\pi} \log \left( \frac{\sqrt{\det(B(\pi))}}{\text{Pf}(B(\pi))} \frac{\text{Pf}(B(0))}{\sqrt{\det(B(0))}} \right) \mod 2 \quad (17)$$

where  $B_{mn}(k) = \langle \phi_m(-k) | \Theta | \phi_n(k) \rangle$  is the sewing matrix. Note that  $P^\Theta$  is only dependent on the  $\Theta$  symmetric momenta. The expression simplifies greatly in the presence of inversion symmetry.

# Pair-switching

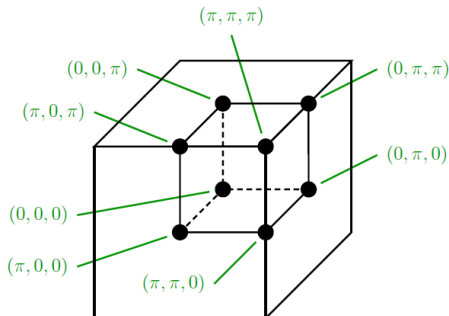


$$\nu = \prod_{l=1}^2 \frac{\sqrt{\det B(k_l)}}{\text{Pf}(B(k_l))}, v_k = \frac{1}{\hbar} \frac{\partial E_k}{\partial k} \hat{y} \quad (18)$$

# Generalization to Higher Dimension

In 3D (and higher dimensions), we can define weak and strong  $\mathbb{Z}_2$  topological indices respectively

$$\boldsymbol{\nu} = (\nu_s; \nu_x, \nu_y, \nu_z). \quad (19)$$



# Classification of Topological Insulators

Time-reversal ( $\Theta$ ), charge-conjugation ( $\Xi$ ), chiral symmetry ( $\Pi$ ).

Symmetry				$d$							
AZ	$\Theta$	$\Xi$	$\Pi$	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AD	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

Bernevig, B. Andrei, and Taylor L. Hughes. Topological Insulators and Topological Superconductors. Princeton University Press, 2013.

Links to lecture notes:

- <https://www.physics.upenn.edu/~kane/pubs/chap1.pdf>
- <https://ethz.ch/content/dam/ethz/special-interest/phys/theoretical-physics/cmtm-dam/documents/tqn/05.pdf>