乱れのある$\mathbf{Z}_2$トポロジカル絶縁体と非可換指数定理

桂 法称 (東大院理)
高麗 徹 (学習院大理)

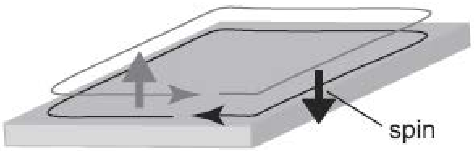
東京大学 THE UNIVERSITY OF TOKYO
学習院大学 GAKUSHUIN UNIVERSITY

- H. Katsura & T. Koma, *J. Math. Phys*. **57**, 021903 (2016).

2D class AII topological insulators

- Time-reversal $\Theta^2 = -1$, particle-hole 0, chiral 0

Robust edge states

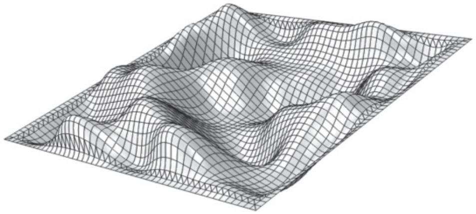


- Examples
  Kane-Mele, BHZ model, QSHE (HgTe quantum well)
- **Z**$_2$ index $\nu = 0,\ 1$ (*k*-space)

$$(-1)^{\nu} = \prod_{i=1}^{4} \frac{\mathrm{Pf}[w(\mathbf{\Gamma}_i)]}{\sqrt{\det[w(\mathbf{\Gamma}_i)]}}$$

Kane-Mele, *PRL* **95** (2005)
Fu-Kane, *PRB* **74** (2006).

Index in disordered systems?



- Niu-Thouless-Wu approach [*PRB* **31** (1985)]
  (k_x, k_y) → (θ_x, θ_y): boundary twists
  Essin-Moore, *PRB* **76**, 165307 (2007).
- **Noncommutative Geometry & IQHE**
  k-differentiation → Commutator in real space
  Avron, Seiler & Simon, *CMP* **159**, 399 ('94).

***Noncommutative ver. Z$_2$ index* (A → AII)**

Rigorous & practical!!

Time-reversal symmetry (TRS)

- Time reversal $\Theta = VK$ (*V*: unitary, *K*: complex conjugation)

  Antiunitary operation!

  Standard choice: $V = I \otimes (-i\sigma_y)$ with $\Theta^2 = -1$.

- TRS

  Hamiltonian *H* commutes with Θ, $[H, \Theta] = 0$.
  H has (i) even-TRS if $\Theta^2 = +1$, (ii) odd-TRS if $\Theta^2 = -1$.

Kramers' theorem

Consider a Hamiltonian *H* with odd-TRS. Every energy eigenvalue of *H* is at least two-fold degenerate (even deg.).

Proof) Let φ_1 be an eigenstate of *H.* φ_1 and φ_2=Θφ_1 have the same energy and $\langle \varphi_1, \varphi_2 \rangle = 0$, because

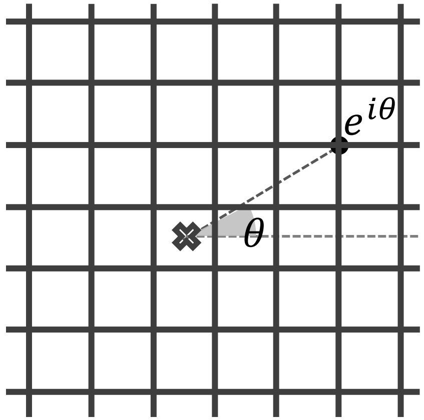
$$\langle \varphi_1, \varphi_2 \rangle = \langle \Theta\varphi_2, \Theta\varphi_1 \rangle = \langle \Theta^2 \varphi_1, \Theta\varphi_1 \rangle = -\langle \varphi_1, \Theta\varphi_2 \rangle = -\langle \varphi_1, \varphi_2 \rangle$$

$$\Theta^2 = -1$$

Lattice model

■ Setting

- Lattice $\mathbf{Z}^2$ (infinite square lattice), dual lattice $(\mathbf{Z}^2)^*$
- Wavefunction $\varphi_{a,\sigma}(x)$ (a=1,…,r, σ=↑, ↓, $x \in \mathbf{Z}^2$)
- Tight-binding Hamiltonian H with odd-TRS: $\Theta = VK, \quad \Theta^2 = -1$
  Short-ranged, may be inhomogeneous
- Flux operator U $\quad (U\varphi_{a,\sigma})(x) = e^{i\theta(x)}\varphi_{a,\sigma}(x)$

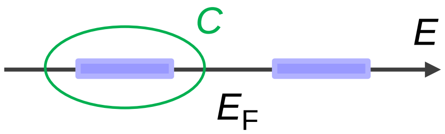


■ Pair of projections

- Assumptions
  (i) Fermi level E_F lies in the gap, (ii) $[V, U]=0$
- Fermi projection P_F
  Projection to the states below E_F. $(P_F)^2 = P_F$

$$P_F = \frac{1}{2\pi i}\oint_C (z-H)^{-1}dz$$

- Projection UP_FU^*
  $(UP_FU^*)^2 = UP_FU^*$, because $U^*U=1$ and $(P_F)^2=P_F$.



$\mathbf{Z}_2$ topological index (Noncommutative ver.)

$$\mathrm{Ind}(P_{\mathrm{F}}, UP_{\mathrm{F}}U^*) := \dim\ker\left(\underbrace{P_{\mathrm{F}} - UP_{\mathrm{F}}U^*}_{A} - 1\right) \mod 2$$

Index = The number of eigenstates of *A* with eigenvalue $\lambda = 1$ mod 2.

The index is 0 or 1, and

- Quantized without ensemble average
  Previous work: Prodan & Schulz-Baldes, 1402.5002, …
  requires the ergodicity of probability measure.
- Reduces to *k*-space $\mathbf{Z}_2$ index (translation invariant case)
- Robust against any odd-TRS perturbations
  Operator *A* is compact.
- But meaningful only in the infinite-volume limit
- A truncated version is useful in numerics

NOTE) Chern number Tr $A^3 = 0$ from TRS.

Outline of the proof

- Eigenvalues of $A = P_{\mathrm{F}} - U P_{\mathrm{F}} U^*$

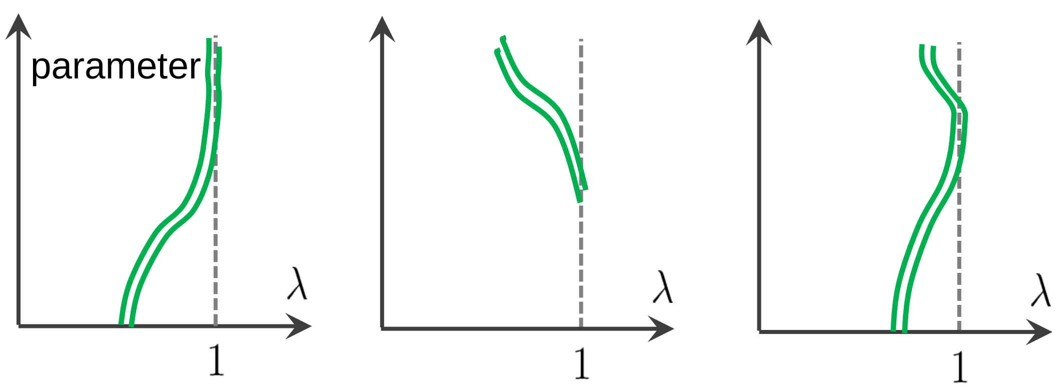
$A\varphi = \lambda\varphi$. The eigenvalues must satisfy $-1 \leq \lambda \leq 1$.

Kramers' theorem for *A*:
Multiplicity of λ must be **even** if $0 < |\lambda| < 1$.

Multiplicity is finite except for $\lambda = 0$.

"Kramers" pair: $\boxed{\varphi_1,\ \varphi_2 = BU\Theta\varphi_1}$ $\quad B := 1 - P_{\mathrm{F}} - U P_{\mathrm{F}} U^*$

Algebraic relations $\{A, B\} = 0, \quad A^2 + B^2 = 1, \quad [U, V] = 0$
ensure that i) φ_2 is nonvanishing, ii) φ_1 and φ_2 are orthogonal.



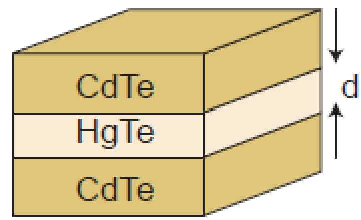
λ=1 is always pair-created or pair-annihilated!
Abrupt change of λ is not allowed

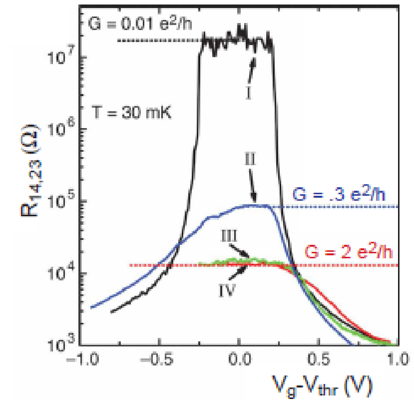
Stability (continuity of λ) can be proved using min-max theorem.

Bernevig-Hughes-Zhang model

Effective model for QSHE in HgTe quantum well

BHZ, *Science* **314** (06),
Konig *et al*., *Science* **318** (07).
First experimental realization!





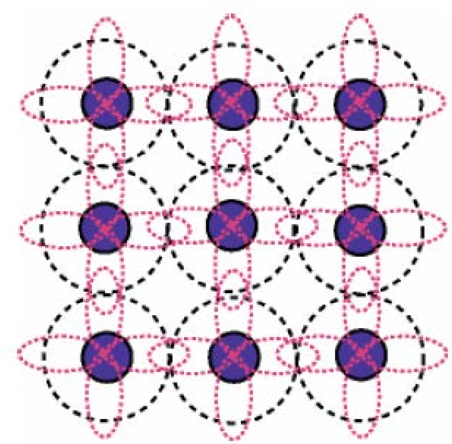
■ Lattice model

- Lattice **Z**^{2} (square lattice)
- Wavefunction $\varphi_{a,\sigma}(x)$ (*a*=*s*,*p*, *σ*=↑,↓, *x*∈ **Z**^{2})
- Tight-binding Hamiltonian *H*

a. On-site potential $\epsilon_a \quad (a = s, p)$

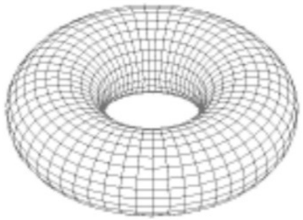
b. Hopping in *x* or *y* *s-p mixing (spin-orbit)*

$$t_{\mu,\sigma} = \begin{pmatrix} t_{ss} & t_{sp}e^{i\sigma\theta_\mu} \\ t_{sp}e^{-i\sigma\theta_\mu} & -t_{pp} \end{pmatrix} \quad (\mu = \pm x, \pm y)$$



A simple case: $\epsilon_s = m,\ \epsilon_p = -m, \quad t_{ss} = t_{pp} = t_{sp} = t,$
Z$_2$ index in *k*-space is ***nontrivial*** if |*m*/*t*|<2.

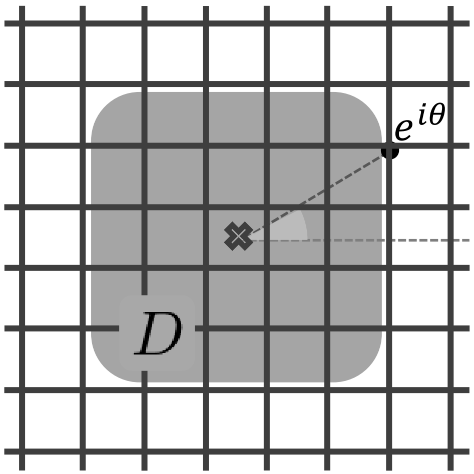
Finite-size approximation of index



■ Numerical procedure

- Consider a lattice torus (N by N) with PBC
- Fermi projection $$P_{\mathrm{F}} = \sum_{E_n < E_{\mathrm{F}}} |\psi_n\rangle\langle\psi_n|$$
- Calculate projection $A = P_{\mathrm{F}} - U P_{\mathrm{F}} U^*$
- Truncated A supported in domain D

  $A \to A_D$ *D* is chosen, e.g. *N*/2 by *N*/2.
- Compute eigenvalues of A_D



■ Uniform case (Warm-up)

Linear size: N = 36 (# of states = 5184)
Parameters: m =1.0, t =1.0 (E_{F}=0)

Desired result!
dim ker (A-1) mod 2 = 1

(First few) largest eigenvalues of A_D

$\{\mathbf{0.99999}, 0.52116, 0.52116, 0.394446, 0.394446, \ldots\}$

Disordered case

■ On-site disorder (odd-TRS)

$$\epsilon_s = -\epsilon_p = m \quad \Rightarrow \quad m_x = m + W\,\delta m_x \qquad \delta m_x \in [-0.5, 0.5]$$

- ***m* =1.0**, *t* =1.0, *W* =0.3 (*N*=32)
  Eigenvalues of A_D :
  $\{\mathbf{0.99999}, 0.52860, 0.52860, 0.39644, 0.39644, \ldots\}$

Topological!
Z_2 index =1

- ***m* =4.0**, *t* =1.0, *W* =0.3 (*N*=32)
  Eigenvalues of A_D :
  $\{0.23380, 0.23380, 0.16879, 0.16879, 0.08973, 0.08973, \ldots\}$

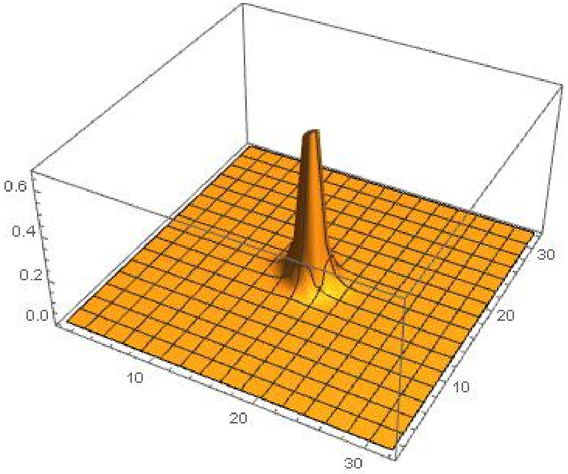
Trivial…
Z_2 index =0

Excellent quantization! (At least for weak disorder)

■ Spatial profile of ker (A_D -1)

The corresponding state is ***localized*** at the center of the flux operator *U*.

Seems like an analog of edge state.



Summary

- Studied 2D disordered insulators with time-reversal symmetry
- Operator theoretic definition of $\mathbf{Z}_2$ topological index

$$\mathrm{Ind}(P_{\mathrm{F}}, UP_{\mathrm{F}}U^*) = \dim\ker\left(P_{\mathrm{F}} - UP_{\mathrm{F}}U^* - 1\right) \mod 2$$

- Proved quantization and robustness
- Application to Bernevig-Hughes-Zhang model

Future directions

- Phase diagrams of disordered TI
  Reproduce Yamakage *et al*., *PRB* **87** (‘13)?
- What is the index for **3D** TI with disorder?
  Strong or weak? Metallic surface v.s. dark side
- Can exhaust all possible cases in periodic table?
  Work in progress…