Z$_2$ Structure of the Quantum Spin Hall Effect

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Summary

- There are robust and distinct topological classes of time-reversal invariant band insulators in two and three dimensions, when spin-orbit interactions are taken into account.
- The important distinction between these classes has a $\mathbb{Z}_2$ character.
- One physical consequence is the existence of protected edge/surface states.
- There are many open questions, including some localization problems.
Quantum Hall Effect

- Low temperature, observe plateaus:

\[ \sigma_{xx} = 0 \quad \sigma_{xy} = n \frac{e^2}{h} \]

- QHE (especially integer) is robust
  - Hall resistance \( R_{xy} \) is quantized even in very messy samples with dirty edges, not so high mobility.
Why is QHE so stable?

• Edge states
  - No backscattering:
    - Edge states cannot localize

• Question: why are the edge states there at all?
  - We are lucky that for some simple models we can calculate the edge spectrum
  - c.f. FQHE: no simple non-interacting picture.
Topology of IQHE

• TKKN: Kubo formula for Hall conductivity gives integer topological invariant (Chern number):
  - w/o time-reversal, bands are generally non-degenerate.

\[ n = \sum_{\text{bands}} \frac{i}{2\pi} \int d^2 k \left( \left\langle \frac{\partial u}{\partial k_1} \right| \frac{\partial u}{\partial k_2} \right) - \left\langle \frac{\partial u}{\partial k_2} \right| \frac{\partial u}{\partial k_1} \right) \]

• How to understand/interpret this?
  - Adiabatic Berry phase
    \[ \Phi = \int_{k_0}^{k_1} d\vec{k} \cdot \vec{A}(k) \quad \vec{A}(k) = i\langle u | \vec{\nabla}_k | u \rangle \]
  - Gauge “symmetry” \[ |u \rangle \rightarrow e^{i\chi(k)} |u \rangle \]
  - Flux\[ \int d^2 k \text{ curl } \vec{A} = \oint d\vec{k} \cdot \vec{A} = 2\pi n \]

Not zero because phase is multivalued
How many topological classes?

• In ideal band theory, can define one TKKN integer \textit{per band}
  - Are there really this many different types of insulators? Could be even though only total integer is related to $\sigma_{xy}$

• NO! Real insulator has impurities and interactions
  - Useful to consider edge states:

$n_1 = 1, \ n_2 = 1, \ n_3 = -1$

$n_1 = 1, \ n_2 = 0, \ n_3 = 0$
“Semiclassical” Spin Hall Effect

- Idea: “opposite” Hall effects for opposite spins
- In a metal: semiclassical dynamics
  \[ J^z_y = \sigma^{SH}_{yx} E_x \]
  More generally \( J^i_\mu = \sigma^i_{\mu\nu} E_\nu \)

- Spin non-conservation = trouble?
  - no unique definition of spin current
  - boundary effects may be subtle

- It does exist! At least spin accumulation.
  - Theory complex: intrinsic/extrinsic…
Quantum Spin Hall Effect

- A naïve view: same as before but in an insulator
  - If spin is conserved, clearly need edge states to transport spin current
  - Since spin is not conserved in general, the edge states are more fundamental than spin Hall effect.

- Better name: $Z_2$ topological insulator

- Graphene (Kane/Mele)

$$H_0 = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \lambda_v \sum_i \xi_i c_{i\sigma}^\dagger c_{i\sigma}$$

$$H' = i\lambda_{SO} \sum_{\langle\langle ij\rangle\rangle} v_{ij} c_i^\dagger s^z c_j + i\lambda_R \sum_{\langle ij \rangle} c_i^\dagger (s \times \hat{d}_{ij})_z c_j$$

$\lambda_{SO} > \lambda_R$
Edge State Stability

• Time-reversal symmetry is sufficient to prevent backscattering!
  - (Kane and Mele, 2004; Xu and Moore, 2006; Wu, Bernevig, and Zhang, 2006)

\[ T: \begin{align*}
\psi_R &\rightarrow \psi_L \\
\psi_L &\rightarrow -\psi_R
\end{align*} \]

Kramer’s pair

More than 1 pair is not protected

• Strong enough interactions and/or impurities
  - Edge states gapped/localized
  - Time-reversal spontaneously broken at edge.
Bulk Topology

- Different starting points:
  - Conserved $S^z$ model: define “spin Chern number”
  - Inversion symmetric model: 2-fold degenerate bands
  - Only T-invariant model

- Chern numbers?
  - Time reversal: $u_{-k}(r, \sigma) = e^{i\chi(k)} \epsilon_{\sigma\sigma'} u^*_k(r, \sigma')$
    $$\mathcal{B}_k \equiv (\text{curl } \vec{A})_k = -\mathcal{B}_{-k}$$
    - Chern number vanishes for each band.

- However, there is some $\mathbb{Z}_2$ structure instead
  - Kane+Mele 2005: Pfaffian = zero counting
  - Roy 2005: band-touching picture
  - J.Moore+LB 2006: relation to Chern numbers+3d story
Avoiding T-reversal cancellation

- 2d BZ is a torus

Coordinates along RLV directions:

- Bloch states at \( k + -k \) are not independent
- Independent states of a band found in “Effective BZ” (EBZ)
- Cancellation comes from adding “flux” from EBZ and its T-conjugate
  - Why not just integrate Berry curvature in EBZ?
Closing the EBZ

- Problem: the EBZ is “cylindrical”: not closed
  - No quantization of Berry curvature

- Solution: “contract” the EBZ to a closed sphere (or torus)

- Arbitrary extension of H(k) (or Bloch states) preserving T-identifications
  - Chern number does depend on this “contraction”
  - But evenness/oddness of Chern number is preserved!

- $\mathbb{Z}_2$ invariant: $x = (-1)^C$

Two contractions differ by a “sphere”
3D bulk topology

2d “cylindrical” EBZs
- 2 $\mathbb{Z}_2$ invariants

Periodic 2-tori like 2d BZ
- 2 $\mathbb{Z}_2$ invariants

• a more symmetric counting:
  \[ x_0 = \pm 1, \quad x_1 = \pm 1 \text{ etc.} \]

\[ x_0 x_1 = y_0 y_1 = z_0 z_1 \]

= 4 $\mathbb{Z}_2$ invariants
(16 “phases”)
Robustness and Phases

- 8 of 16 “phases” are not robust

\[ x_0x_1 = y_0y_1 = z_0z_1 = +1 \]

- Can be realized by stacking 2d QSH systems

- Qualitatively distinct: \[ x_0x_1 = y_0y_1 = z_0z_1 = -1 \]

- Fu/Kane/Mele: \( x_0x_1 = +1 \): “Weak Topological Insulators”
3D topological insulator

- Fu/Kane/Mele model (2006): cond-mat/0607699
  (Our paper: cond-mat/0607314)

\[ H = \sum_{ij} t_{ij} c_i^\dagger c_j + i \lambda \sum_{\langle ij \rangle} c_i^\dagger \vec{\sigma} \cdot (\vec{d}_1 \times \vec{d}_2) c_j \]

e.g. \[ t_{i,i+d_1} = (1+\delta)t \]
\[ t_{i,i+d_\mu} = t \quad \mu = 2, 3, 4 \]

- \( \delta = 0 \): 3 3D Dirac points
- \( \delta > 0 \): topological insulator
- \( \delta < 0 \): "WTI"=trivial insulator

\[ x_0 x_1 = \text{sign}(m_X m_Y m_Z) \]
Surface States

• “Domain wall fermions” (c.f. Lattice gauge theory)

• trivial insulator (WTI)

• topological insulator

\[
\left[ \sum_{j=1}^{3} i\gamma_j \partial_j + m_X(x_1)\gamma_4 \right] \psi = \epsilon \psi
\]

• chiral Dirac fermion:

\[
\psi = e^{\int_{0}^{x_1} dx' m_X(x')}{\phi(x_2, x_3)}
\]

\[
\gamma_j \partial_j \phi = \epsilon \phi
\]

\[
\gamma_{41} \phi = \phi
\]
“Topological metal”

- The surface \textit{must} be metallic

- 2d Fermi surface

- Dirac point generates Berry phase of \( \pi \) for Fermi surface

\[
T : u_k(r, \sigma) = \zeta_k \epsilon_{\sigma \sigma'} u^*_{-k}(-r, \sigma') \\
|\zeta_k| = 1 \quad \int d\vec{k} \cdot \zeta_k^* \nabla_k \zeta_k = \pm 2\pi i
\]
Question 1

• What is a material?
  – No “exotic” requirements!
  – Can search amongst insulators with “substantial spin orbit”
    • n.b. even GaAs has 0.34eV=3400K “spin orbit” splitting (split-off band)
  – Understanding of bulk topological structure enables theoretical search by first principles techniques
  – Perhaps elemental Bi is “close” to being a topological insulator (actually semi-metal)?

Murakami Fu et al
Question 2

• What is a smoking gun?
  – Surface state could be accidental
  – Photoemission in principle can determine even/odd number of surface Dirac points (ugly)
  – Suggestion (vague): response to non-magnetic impurities?
    • This is related to localization questions
Question 3

• Localization transition at surface?
  – *Weak disorder*: symplectic class $\Rightarrow$ anti-
    localization
  – Strong disorder: clearly can localize
    • But due to Kramer’s structure, this *must* break T-
      reversal: i.e. accompanied by spontaneous surface
      magnetism
    • Guess: strong non-magnetic impurity creates local
      moment?
  – Two scenarios:
    • Direct transition from metal to magnetic insulator
      – Universality class? Different from “usual” symplectic
        transition?
    • Intermediate magnetic metal phase?
Question 4

- Bulk transition
  - For clean system, *direct* transition from topological to trivial insulator is described by a single massless 3+1-dimensional Dirac fermion
  - Two disorder scenarios
    - Direct transition. Strange insulator-insulator critical point?
    - Intermediate metallic phase. Two metal-insulator transitions. Are they the same?
  - N.B. in 2D QSH, numerical evidence (Nagaosa *et al*) for new universality class
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