Z_2 Structure of the Quantum Spin Hall Effect

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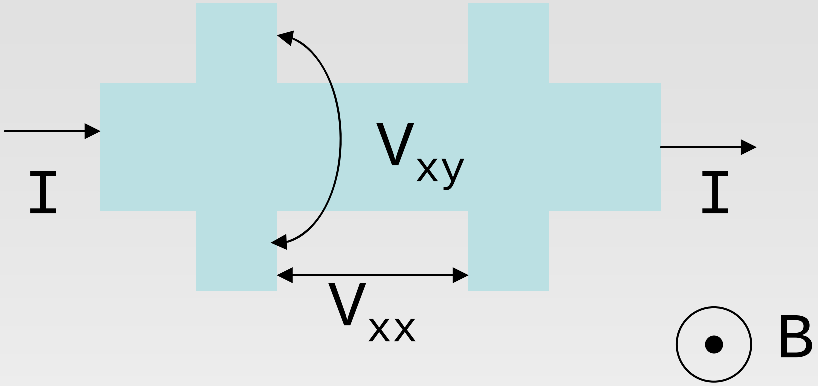
Summary

- 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 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



2DEG's in GaAs, Si, graphene (!)
In large B field.

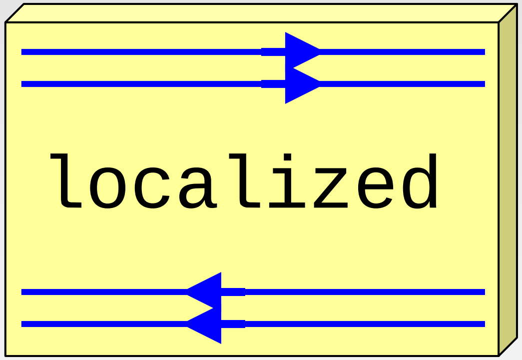
- Low temperature, observe plateaus:

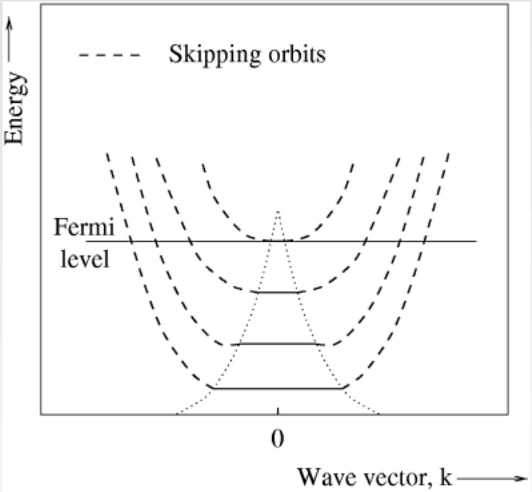
$$\sigma_{xx} = 0 \quad \sigma_{xy} = n\frac{e^2}{h}$$

- 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.

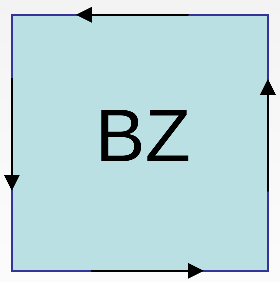
Topology of IQHE

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

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

- How to understand/interpret this?
  - Adiabatic Berry phase

$$\Phi = \int_{k_0}^{k_1} d\vec{k} \cdot \vec{A}(k) \qquad \vec{A}(k) = i\langle u|\vec{\nabla}_k|u\rangle$$



  - Gauge “symmetry” $|u\rangle \rightarrow e^{i\chi(k)}|u\rangle$

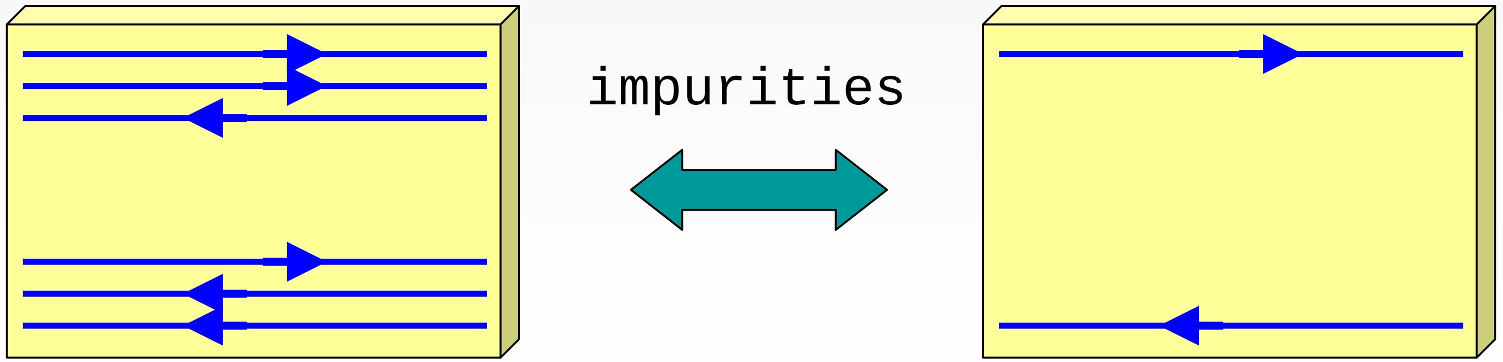
flux $\int d^2k \, \mathrm{curl}\, \vec{A} = \oint d\vec{k} \cdot \vec{A} = 2\pi n$

Not zero because phase is multivalued

How many topological classes?

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

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

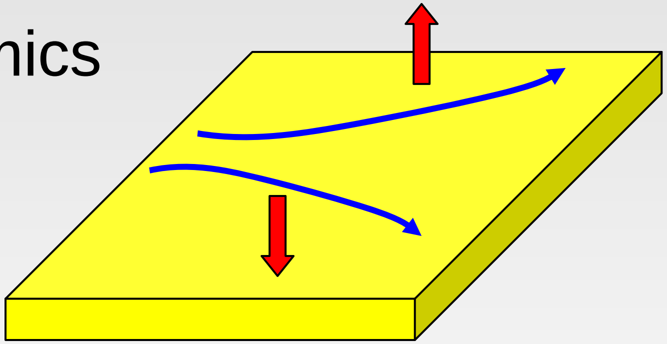


$n_1 = 1,\ n_2 = 1,\ n_3 = -1$ $\qquad$ $n_1 = 1,\ n_2 = 0,\ n_3 = 0$

“Semiclassical” Spin Hall Effect

- Idea: “opposite” Hall effects for opposite spins

- In a metal: semiclassical dynamics



$$\mathcal{J}_y^z = \sigma_{yx}^{SH} E_x$$

More generally $\mathcal{J}_\mu^i = \sigma_{\mu\nu}^i E_\nu$

- 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

Zhang, Nagaosa, Murakami, Bernevig

Kane,Mele, 2004

- A naïve view: same as before but in an *insulator*

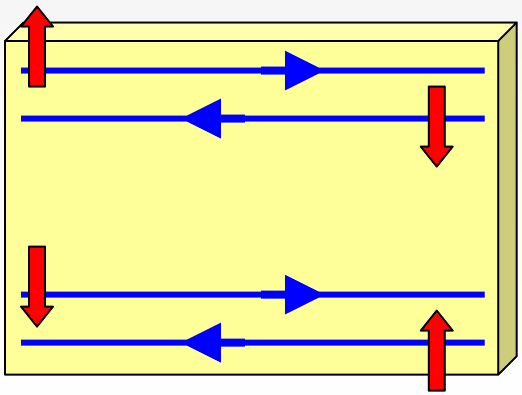
  -If spin is conserved, clearly *need* edge states to transport spin current

  -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)

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

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

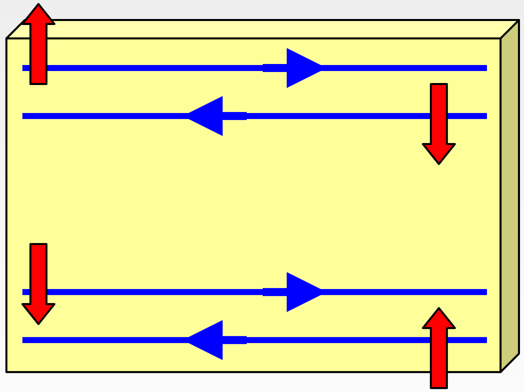


$\lambda_{SO} > \lambda_R$

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: $\begin{array}{l} \psi_R \rightarrow \psi_L \\ \psi_L \rightarrow -\psi_R \end{array}$

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: $u_{-k}(r,\sigma) = e^{i\chi(k)} \epsilon_{\sigma\sigma'} u_k^*(r,\sigma')$

$$\mathcal{B}_k \equiv (\text{curl}\,\vec{A})_k = -\mathcal{B}_{-k}$$

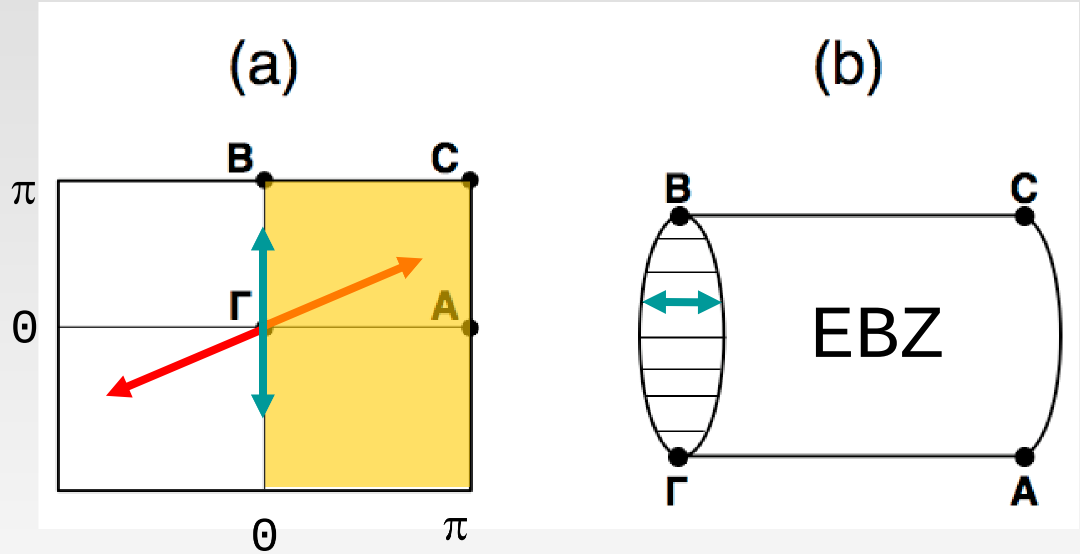
⇒ Chern number vanishes for each band.

- However, there is some 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 indepdent
- 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

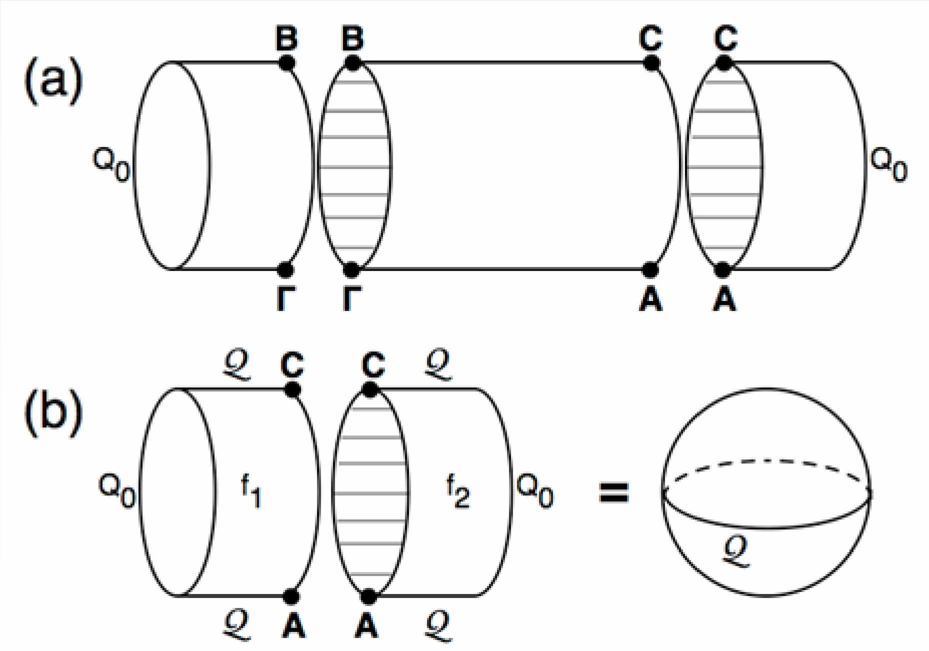
- Solution: “contract” the EBZ to a closed sphere (or torus)

  - *Arbitrary* extension of H(k) (or Bloch states) preserving T-identifications

    -Chern number *does* depend on this “contraction”

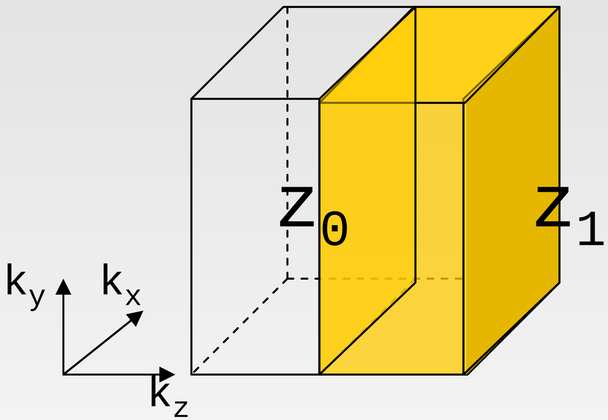
    -But evenness/oddness of Chern number is preserved!

- Z_2 invariant: $x=(-1)^C$



Two contractions differ by a “sphere”

3D bulk topology



3D EBZ

2d “cylindrical” EBZs

- 2 Z_2 invariants

Periodic 2-tori like 2d BZ

- 2 Z_2 invariants

+

= 4 Z_2 invariants

(16 “phases”)

- a more symmetric counting:

$x_0 = \pm 1$, $x_1 = \pm 1$ etc.

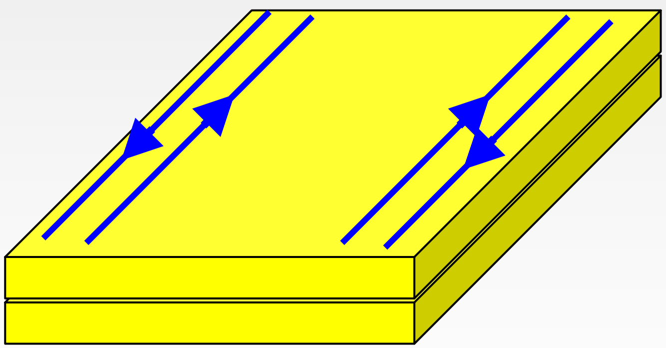
$$\boxed{x_0 x_1 = y_0 y_1 = z_0 z_1}$$

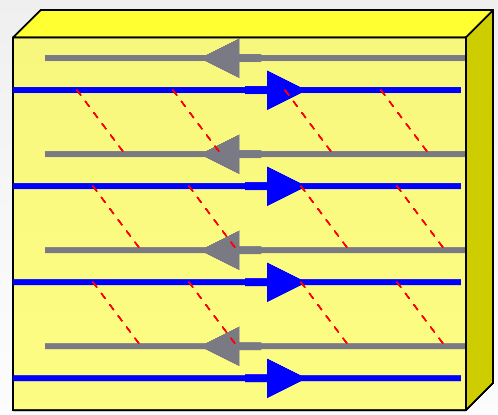
Robustness and Phases

- 8 of 16 “phases” are *not* robust

$$x_0 x_1 = y_0 y_1 = z_0 z_1 = +1$$

- Can be realized by stacking 2d QSH systems





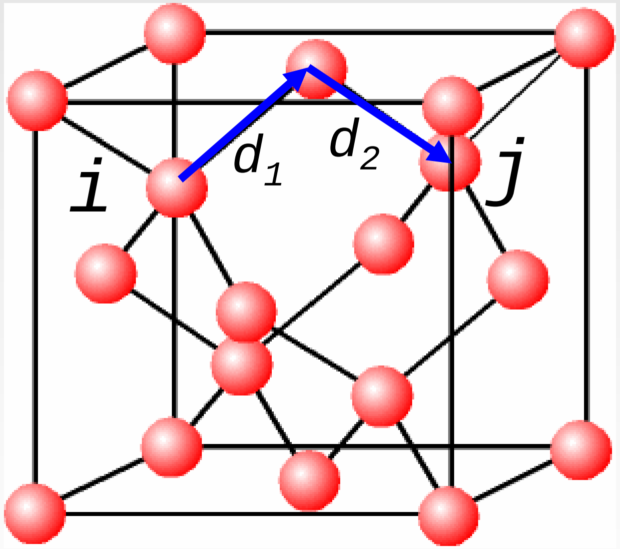
Disorder can backscatter between layers

- Qualitatively distinct: $x_0 x_1 = y_0 y_1 = z_0 z_1 = -1$
  - Fu/Kane/Mele: $x_0 x_1 = +1$: “Weak Topological Insulators”

3D topological insulator

- Fu/Kane/Mele model (2006):

cond-mat/0607699
(Our paper: cond-mat/0607314)



diamond lattice

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

e.g.

$$t_{i,i+d_1} = (1+\delta)t$$

$$t_{i,i+d_\mu} = t \qquad \mu = 2,3,4$$

δ=0: 3 3D Dirac points
δ>0: topological insulator
δ<0: "WTI"=trivial insulator

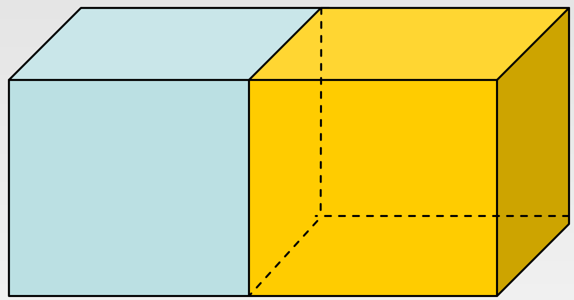
- with appropriate sign convention:

$$\boxed{x_0 x_1 = \text{sign}(m_X m_Y m_Z)}$$

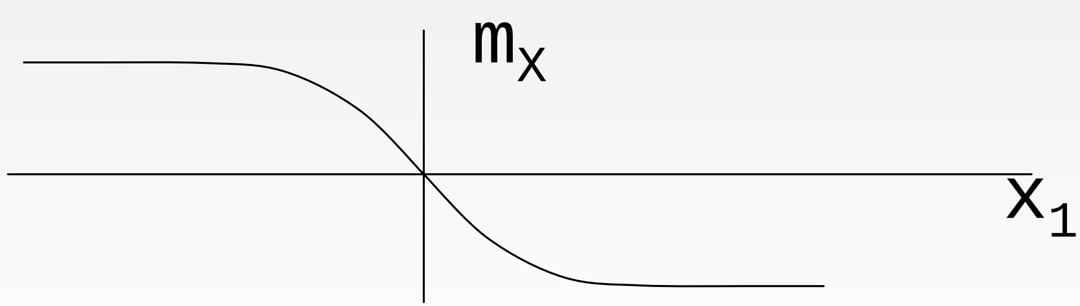
Surface States

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

trivial insulator (WTI)



topological insulator



$m_Y, m_Z > 0$

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

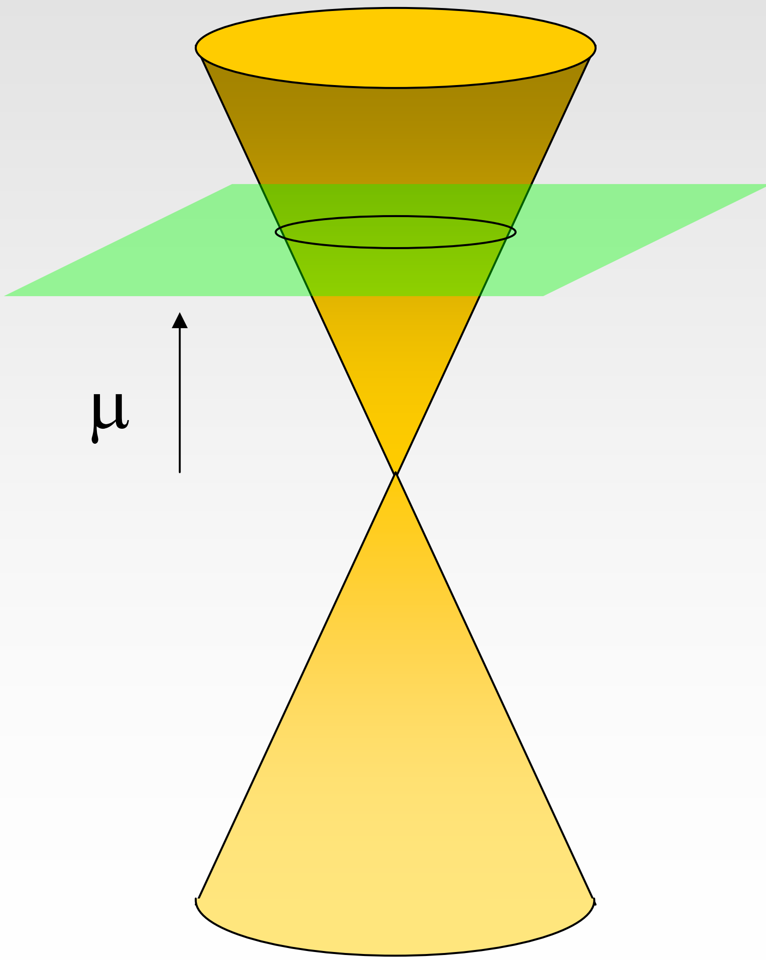
$$\gamma_j\partial_j\phi = \epsilon\phi$$

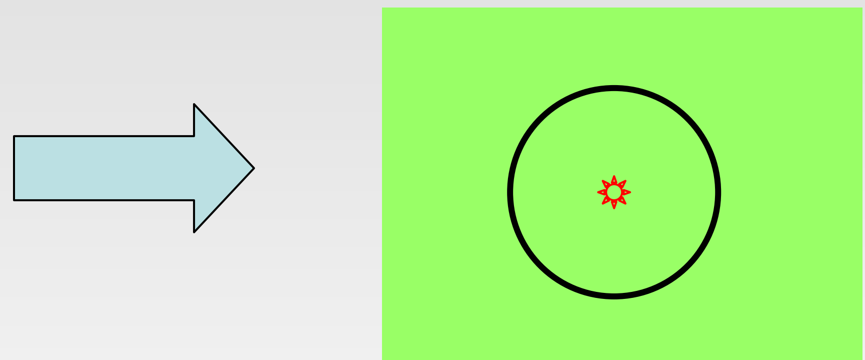
- chiral Dirac fermion: $\psi = e^{\int_0^{x_1} dx' m_X(x')}\phi(x_2, x_3)$

$$\gamma_{41}\phi = \phi$$

“Topological metal”

- The surface *must* be metallic





- 2d Fermi surface

- Dirac point generates Berry phase of π for Fermi surface

$$T: \;\; u_k(r,\sigma) = \zeta_k \epsilon_{\sigma\sigma'} u^*_{-k}(-r,\sigma')$$

$$|\zeta_k| = 1 \qquad\qquad \oint d\vec{k}\cdot \zeta_k^* \vec{\nabla}_k \zeta_k = \pm 2\pi i$$

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

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 Z_2 character.
- One physical consequence is the existence of protected *edge/surface states.*
- There are many open questions, including some localization problems