#### Recent developments in topological materials

#### NHMFL Winter School January 6, 2014

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### Thanks

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#### Discussions

Berkeley:

Dung-Hai Lee, Joe Orenstein, Shinsei Ryu, R. Ramesh, Ivo Souza, Ashvin Vishwanath Special thanks also to

Duncan Haldane, Zahid Hasan, Charles Kane, Laurens Molenkamp, Shou-Cheng Zhang

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"An insulator's metallic side"

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"Quasiparticles do the twist"

### Outline of lectures

I. Overview of experimental background and idea of "topological order". Basic notions of topological insulators.Start on connection to magnetoelectric effect.



2. Berry phases in metals and insulators. Thouless-type order. Some current directions:

- A. Related topological phases.
- B. Emergent particles from adding superconductivity.
- C. Majoranas (versus Bogoliubov quasiparticles versus Laughlin quasiparticles.)



### Types of order

Much of condensed matter is about how different kinds of order emerge from interactions between many simple constituents.



Until 1980, all ordered phases could be understood as "symmetry breaking":

an ordered state appears at low temperature when the system spontaneously loses one of the symmetries present at high temperature.

#### Examples:

Crystals break the *translational* and *rotational* symmetries of free space. The "liquid crystal" in an LCD breaks *rotational* but not *translational* symmetry. Magnets break time-reversal symmetry and the rotational symmetry of spin space. Superfluids break an internal symmetry of quantum mechanics.

Types of order

At high temperature, entropy dominates and leads to a disordered state. At low temperature, energy dominates and leads to an ordered state.

In case this sounds too philosophical, there are testable results that come out of the "Landau theory" of symmetry-breaking:



Theory:  $\beta = 0.325 \pm 0.002$ 

"Universality" at continuous phase transitions (Wilson, Fisher, Kadanoff, ...)

Types of order

In 1980, the first ordered phase beyond symmetry breaking was discovered.

Electrons confined to a plane and in a strong magnetic field show, at low enough temperature, plateaus in the "Hall conductance":



Note I: the AC Josephson effect between superconductors similarly allows determination of *e*/*h*. Note II: there are also *fractional* plateaus, about which more later.

### Topological order

### What type of order causes the precise quantization in the Integer Quantum Hall Effect (IQHE)?

Definition I:

In a topologically ordered phase, some physical response function is given by a "topological invariant".

What is a topological invariant? How does this explain the observation?

Definition II:

A topological phase is insulating but always has metallic edges/surfaces when put next to vacuum or an ordinary phase.

What does this have to do with Definition I?

#### "Topological invariant" = quantity that does not change under continuous deformation

(A third definition: phase is described by a "topological field theory")

### Traditional picture: Landau levels

Normally the Hall ratio is (here *n* is a density)

$$R_H = \frac{I_x}{V_y B} = \frac{1}{nec} \Rightarrow \sigma_{xy} = \frac{nec}{B}$$

Then the value (now *n* is an integer)

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

corresponds to an areal density  $\frac{\pi}{2\pi\ell^2} = neB/hc.$ 

This is exactly the density of "Landau levels", the discrete spectrum of eigenstates of a 2D particle in an orbital magnetic field, spaced by the cyclotron energy. The only "surprise" is how precise the quantization is.

### Traditional picture: Landau levels and edge states

So a large system has massively degenerate Landau levels if there is no applied potential.

$$\sigma_{xy} = n \frac{e^2}{h} \qquad \qquad \frac{n}{2\pi\ell^2} = n eB/hc.$$

 $E = (n + 1/2)\hbar\omega_c, \quad \omega_c = \text{cyclotron frequency}$ 

Note: for a relativistic fermion, as in graphene, E goes as sqrt(B).

In a slowly varying applied potential, the local occupation changes; at some points Landau levels are fractionally filled and there are metallic "edge states".

Here we develop a different picture (Thouless): how do we understand the IQHE in a crystal?

### **Topological** invariants

Most topological invariants in physics arise as integrals of some geometric quantity.

Consider a two-dimensional surface.

At any point on the surface, there are two radii of curvature. We define the signed "Gaussian curvature"  $\kappa = (r_1 r_2)^{-1}$ 



from left to right, equators have negative, 0, positive Gaussian curvature

Now consider closed surfaces.





The area integral of the curvature over the whole surface is "quantized", and is a topological invariant (Gauss-Bonnet theorem).

$$\int_M \kappa \, dA = 2\pi \chi = 2\pi (2 - 2g)$$

where the "genus" g = 0 for sphere, I for torus, n for "n-holed torus".

### Topological invariants

Good news: for the invariants in the IQHE and topological insulators, we need one fact about solids

Bloch's theorem:

One-electron wavefunctions in a crystal (i.e., periodic potential) can be written

 $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$ 



where k is "crystal momentum" and u is periodic (the same in every unit cell).

Crystal momentum k can be restricted to the Brillouin zone, a region of k-space with periodic boundaries.

As k changes, we map out an "energy band". Set of all bands = "band structure".

The Brillouin zone will play the role of the "surface" as in the previous example,

and one property of quantum mechanics, the Berry phase

which will give us the "curvature".

### Berry phase

What kind of "curvature" can exist for electrons in a solid?

Consider a quantum-mechanical system in its (nondegenerate) ground state.

The adiabatic theorem in quantum mechanics implies that, if the Hamiltonian is now changed slowly, the system remains in its time-dependent ground state.

But this is actually very incomplete (Berry).

When the Hamiltonian goes around a closed loop k(t) in parameter space, there can be an irreducible phase

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}, \quad \mathcal{A} = \langle \psi_k | - i \nabla_k | \psi_k \rangle$$



Michael Berry

relative to the initial state.

Why do we write the phase in this form? Does it depend on the choice of reference wavefunctions?

### Berry phase

Why do we write the phase in this form? Does it depend on the choice of reference wavefunctions?

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}, \quad \mathcal{A} = \langle \psi_k | - i \nabla_k | \psi_k \rangle$$

If the ground state is non-degenerate, then the only freedom in the choice of reference functions is a local phase:

$$\psi_k \to e^{i\chi(k)}\psi_k$$

Under this change, the "Berry connection" A changes by a gradient,

$$\mathcal{A} 
ightarrow \mathcal{A} + 
abla_k \chi$$
 Michael Berry

just like the vector potential in electrodynamics.

So loop integrals of A will be gauge-invariant, as will the *curl* of A, which we call the "Berry curvature".

$$\mathcal{F} = \nabla \times \mathcal{A}$$

### Berry phase in solids

In a solid, the natural parameter space is electron momentum.

The change in the electron wavefunction within the unit cell leads to a Berry connection and Berry curvature:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$$
$$\mathcal{A} = \langle u_{\mathbf{k}} | -i\nabla_k | u_{\mathbf{k}} \rangle \qquad \mathcal{F} = \nabla \times \mathcal{A}$$

We keep finding more physical properties that are determined by these quantum geometric quantities.

The first was that the integer quantum Hall effect in a 2D crystal

follows from the integral of F (like Gauss-Bonnet!). Explicitly,



S. S. Chern

 $\nabla \times A$ 

$$n = \sum_{bands} \frac{i}{2\pi} \int d^2k \left( \left\langle \frac{\partial u}{\partial k_1} \middle| \frac{\partial u}{\partial k_2} \right\rangle - \left\langle \frac{\partial u}{\partial k_2} \middle| \frac{\partial u}{\partial k_1} \right\rangle \right) \quad \mathcal{F} = \sigma_{xy} = n \frac{e^2}{h} \qquad \text{TKNN, 1982} \quad \text{``first Chern number''}$$

### The importance of the edge

#### But wait a moment...

This invariant exists if we have energy bands that are either full or empty, i.e., a "band insulator".

How does an insulator conduct charge?

Answer: (Laughlin; Halperin)

There are *metallic* edges at the boundaries of our 2D electronic system, where the conduction occurs.

These metallic edges are "chiral" quantum wires (one-way streets). Each wire gives one conductance quantum  $(e^2/h)$ .

The topological invariant of the *bulk* 2D material just tells how many wires there *have* to be at the boundaries of the system.

How does the bulk topological invariant "force" an edge mode?





### The importance of the edge

The topological invariant of the bulk 2D material just tells how many wires there have to be at the boundaries of the system.

How does the bulk topological invariant "force" an edge mode?

#### Answer:

Imagine a "smooth" edge where the system gradually evolves from IQHE to ordinary insulator. The topological invariant must change.

But the definition of our "topological invariant" means that, *if the system remains insulating* so that every band is either full or empty, the invariant cannot change.

 $\therefore$  the system must not remain insulating.





(What is "knotted" are the electron wavefunctions)

# 2005-present and "topological insulators"

The same idea will apply in the new topological phases discovered recently:

a "topological invariant", based on the Berry phase, leads to a nontrivial edge or surface state at any boundary to an ordinary insulator or vacuum.

However, the physical origin, dimensionality, and experiments are all different.



We discussed the IQHE so far in an unusual way. The magnetic field entered only through its effect on the Bloch wavefunctions (no Landau levels!).

This is not very natural for a magnetic field. It is ideal for spin-orbit coupling in a crystal.

### The "quantum spin Hall effect"

Spin-orbit coupling appears in nearly every atom and solid. Consider the standard atomic expression

 $H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$ 

For a given spin, this term leads to a momentumdependent force on the electron, somewhat like a magnetic field.

The spin-dependence means that the *time-reversal* symmetry of SO coupling (even) is different from a real magnetic field (odd).

It is possible to design lattice models where spin-orbit coupling has a remarkable effect: (Murakami, Nagaosa, Zhang 04; Kane, Mele 05)

spin-up and spin-down electrons are in IQHE states, with opposite "effective magnetic fields".

![](_page_17_Picture_7.jpeg)

![](_page_17_Figure_8.jpeg)

### The "quantum spin Hall effect"

In this type of model, electron spin is conserved, and there can be a "spin current".

An applied electrical field causes oppositely directed Hall currents of up and down spins.

The charge current is zero, but the "spin current" is nonzero, and even quantized!

![](_page_18_Picture_4.jpeg)

 $\mathcal{J}_{i}^{i} = \sigma_{H}^{s} \epsilon_{ijk} E_{k}$ 

#### However...

I. In real solids there is no conserved direction of spin.

2. So in real solids, it was expected that "up" and "down" would always mix and the edge to disappear.

3. The theory of the above model state is just two copies of the IQHE.

### The 2D topological insulator

It was shown in 2005 (Kane and Mele) that, in real solids with all spins mixed and no "spin current", something of this physics does survive.

In a material with only spin-orbit, the "Chern number" mentioned before always vanishes.

Kane and Mele found a new topological invariant in time-reversal-invariant systems of fermions.

But it isn't an integer! It is a Chern *parity* ("odd" or "even"), or a "Z2 invariant".

![](_page_19_Picture_5.jpeg)

Systems in the "odd" class are "2D topological insulators"

I.Where does this "odd-even" effect come from?2.What is the Berry phase expression of the invariant?3. How can this edge be seen?

# The "Chern insulator" and QSHE

Haldane showed that although *broken time-reversal* is necessary for the QHE, it is not necessary to have a net magnetic flux.

Imagine constructing a system ("model graphene") for which spin-up electrons feel a pseudofield along z, and spin-down electrons feel a pseudofield along -z.

Then SU(2) (spin rotation symmetry) is broken, but timereversal symmetry is not:

an edge will have (in the simplest case) a clockwise-moving spin-up mode and a counterclockwise-moving spin-down mode (Murakami, Nagaosa, Zhang, '04)

![](_page_20_Picture_5.jpeg)

#### Example: Kane-Mele-Haldane model for graphene

The spin-independent part consists of a tight-binding term on the honeycomb lattice, plus possibly a sublattice staggering

![](_page_21_Figure_2.jpeg)

The first term gives a semimetal with Dirac nodes (as in graphene).

The second term, which appears if the sublattices are inequivalent (e.g., BN), opens up a (spin-independent) gap.

When the Fermi level is in this gap, we have an ordinary band insulator.

#### Example: Kane-Mele-Haldane model for graphene

The spin-independent part consists of a tight-binding term on the honeycomb lattice, plus possibly a sublattice staggering

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

The spin-dependent part contains two SO couplings

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

The first spin-orbit term is the key: it involves second-neighbor hopping ( $v_{ij}$  is ±1 depending on the sites) and Sz. It opens a gap in the bulk and acts as the desired "pseudofield" if large enough.  $v_{ij} \propto (\mathbf{d_1} \times \mathbf{d_2})_z$ 

Claim: the system with an SO-induced gap is fundamentally different from the system with a sublattice gap: it is in a different phase. It has gapless edge states for *any* edge (not just zigzag).

#### Example: Kane-Mele-Haldane model for graphene

$$H_{0} = -t \sum_{\langle ij \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + \lambda_{v} \sum_{i} \xi_{i} c_{i\sigma}^{\dagger} c_{i\sigma}$$
$$H' = i\lambda_{SO} \sum_{\langle \langle ij \rangle \rangle} v_{ij} c_{i}^{\dagger} s^{z} c_{j} + i\lambda_{R} \sum_{\langle ij \rangle} c_{i}^{\dagger} (\mathbf{s} \times \hat{\mathbf{d}}_{ij})_{z} c_{j}$$

Without Rashba term (second SO coupling), have two copies of Haldane's IQHE model. All physics is the same as IQHE physics.

The Rashba term violates conservation of Sz--how does this change the phase? Why should it be stable once up and down spins mix?

### Invariants in T-invariant systems?

If a quantum number (e.g., Sz) can be used to divide bands into "up" and "down", then with T invariance, one can define a "spin Chern integer" that counts the number of Kramers pairs of edge modes:

$$n_{\uparrow} + n_{\downarrow} = 0, n_{\uparrow} - n_{\downarrow} = 2n_s$$

### What about T-invariant systems?

If a quantum number (e.g., Sz) can be used to divide bands into "up" and "down", then with T invariance, one can define a "spin Chern number" that counts the number of Kramers pairs of edge modes:

$$n_{\uparrow} + n_{\downarrow} = 0, n_{\uparrow} - n_{\downarrow} = 2n_s$$

For general spin-orbit coupling, there is no conserved quantity that can be used to classify bands in this way, and no integer topological invariant.

Instead, a fairly technical analysis shows

I. each pair of spin-orbit-coupled bands in 2D has a Z2 invariant (is either "even" or "odd"), essentially as an integral over half the Brillouin zone;

2. the state is given by the overall Z2 sum of occupied bands: if the sum is odd, then the system is in the "topological insulator" phase

#### Goudsmit and Uhlenbeck, 1927: electrons have spin 1/2

![](_page_26_Picture_1.jpeg)

Kramers, 1930: integer-spin and spin-half particles behave very differently under time reversal

### The 2D topological insulator

#### I.Where does this "odd-even" effect come from?

In a time-reversal-invariant system of electrons, all energy eigenstates come in degenerate pairs.

The two states in a pair cannot be mixed by any Tinvariant perturbation. (disorder)

So an edge with a single Kramers pair of modes is perturbatively stable (C. Xu-JEM, C. Wu et al., 2006).

![](_page_27_Figure_5.jpeg)

### The 2D topological insulator

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![](_page_28_Figure_5.jpeg)

But this rule does not protect an ordinary quantum wire with 2 Kramers pairs:

![](_page_28_Figure_7.jpeg)

The topological vs. ordinary distinction depends on time-reversal symmetry.

### Experimental signatures

Key physics of the edges: robust to disorder and hence good *charge* conductors .

The topological insulator is therefore detectable by measuring the two-terminal conductance of a finite sample: should see maximal ID conductance.  $G = \frac{2e^2}{h}$ 

In other words, spin transport does not have to be measured to observe the phase.

Materials recently proposed: Bi, InSb, strained Sn (3d), HgTe (2d) (Bernevig, Hughes, and Zhang, Science (2006); experiments by Molenkamp et al. (2007) see an edge with approximate quantization)

### The 2D topological insulator

Key: the topological invariant predicts the "number of quantum wires".

While the wires are not one-way, so the Hall conductance is zero, they still contribute to the *ordinary* (two-terminal) conductance.

There should be a low-temperature edge conductance from one spin channel at each edge:

![](_page_30_Figure_4.jpeg)

![](_page_30_Picture_5.jpeg)

Laurens Molenkamp

This appears in (Hg,Cd)Te quantum wells as a quantum Hall-like plateau in zero magnetic field.

#### Review of 3D facts

The 2D conclusion is that band insulators come in two classes: ordinary insulators (with an even number of edge modes, generally 0) "topological insulators" (with an odd number of Kramers pairs of edge modes, generally 1).

What about 3D? The only 3D IQHE states are essentially layered versions of 2D states: Mathematically, there are three Chern integers:

#### Cxy (for xy planes in the 3D Brillouin torus), Cyz, Cxz

There are similar layered versions of the topological insulator, but these are not very stable; intuitively, adding parities from different layers is not as stable as adding integers.

However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

General description of invariant from JEM and L. Balents, PRB RC 2007. The connection to physical consequences in inversion-symmetric case (proposal of BiSb, Dirac surface state): Fu, Kane, Mele, PRL 2007. See also R. Roy, arXiv.

#### Build 3D from 2D

Note that only at special momenta like k=0 is the "Bloch Hamiltonian" time-reversal invariant: rather, k and -k have T-conjugate Hamiltonians. Imagine a square BZ:

![](_page_32_Figure_2.jpeg)

In 3D, we can take the BZ to be a cube (with periodic boundary conditions):

think about xy planes

2 inequivalent planes look like 2D problem

![](_page_32_Figure_6.jpeg)

3D "strong topological insulators" go from an 2D ordinary insulator to a 2D topological insulator (or vice versa) in going from  $k_z=0$  to  $k_z=\pm\pi/a$ .

This is allowed because intermediate planes have no time-reversal constraint.

### Topological insulators in 3D

I. This fourth invariant gives a robust 3D "strong topological insulator" whose metallic surface state in the simplest case is a single "Dirac fermion" (Fu-Kane-Mele, 2007)

![](_page_33_Figure_2.jpeg)

2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

#### Claim:

Certain insulators will always have metallic surfaces with strongly spin-dependent structure

How can we look at the metallic surface state of a 3D material to test this prediction?

### ARPES of topological insulators

Imagine carrying out a "photoelectric effect" experiment very carefully.

![](_page_34_Figure_2.jpeg)

Measure as many properties as possible of the outgoing electron to deduce the momentum, energy, and spin it had while still in the solid.

This is "angle-resolved photoemission spectroscopy", or ARPES.

### ARPES of topological insulators

First observation by D. Hsieh et al. (Z. Hasan group), Princeton/LBL, 2008.

This is later data on  $Bi_2Se_3$  from the same group in 2009:

![](_page_35_Figure_3.jpeg)

The states shown are in the "energy gap" of the bulk material--in general no states would be expected, and especially not the Dirac-conical shape.

### STM of topological insulators

The surface of a simple topological insulator like  $Bi_2Se_3$  is "1/4 of graphene": it has the Dirac cone but no valley or spin degeneracies.

Scanning tunneling microscopy image (Roushan et al., Yazdani group, 2009)

![](_page_36_Figure_3.jpeg)

STM can see the absence of scattering within a Kramers pair (cf. analysis of superconductors using quasiparticle interference, D.-H. Lee and S. Davis).

### Spintronic applications of 3D TIs

This is a very active area on the archive, but most of what is discussed is very simple:

![](_page_37_Figure_2.jpeg)

a charge current at one TI surface has a nonzero average spin. The same is true for a Rashba quantum well, where the two electron sheets almost cancel; in a TI there is only one sheet and the effect is much stronger.

### Stability, or Phases versus points

True quantum phases in condensed matter systems should be robust to *disorder* and *interactions*.

#### Examples:

The Fermi gas is robust to repulsive interactions in 2D and 3D (the "Fermi liquid") but *not* in ID. In ID, conventional metallic behavior is only seen at one fine-tuned point in the space of interactions.

The Fermi gas is robust to disorder in 3D but not in 1D or 2D (Anderson localization): the clean system is only a point in phase space in 1D or 2D.

The IQHE is a phase robust to both disorder and interactions.

What about the QSHE? Is it a new phase of condensed matter?

## Remark on simple generalization of IQHE topology

TKNN, 1982: the Hall conductance is related to an integral over the magnetic Brillouin zone:  $\sigma_{xy} = n \frac{e^2}{h}$ 

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

Niu, Thouless, Wu, 1985: many-body generalization more generally, introducing "twist angles" around the two circles of a torus and considering the (assumed unique) ground state as a function of these angles,

$$n = \int_{0}^{2\pi} \int_{0}^{2\pi} d\theta \, d\varphi \, \frac{1}{2\pi i} \left| \left\langle \frac{\partial \phi_0}{\partial \varphi} \middle| \frac{\partial \phi_0}{\partial \theta} \right\rangle - \left\langle \frac{\partial \phi_0}{\partial \theta} \middle| \frac{\partial \phi_0}{\partial \varphi} \right\rangle \right|$$

This quantity is an integer. For T-invariant systems, all ordinary Chern numbers are zero.

## Redefining the Berry phase with disorder

Suppose that the parameters in H do not have exact lattice periodicity.

Imagine adding boundary phases to a finite system, or alternately considering a "supercell". Limit of large supercells -> disordered system.

Effect of boundary phase is to shift k: alternate picture of topological invariant is in terms of half the  $(\Phi_1, \Phi_2)$  torus.  $\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\$ 

Can define Chern parities by pumping, analogous to Chern numbers, and study phase diagram w/disorder

#### The 2D topological insulator with disorder

Spin-orbit T=0 phase diagram (fix spin-independent part): instead of a point transition between ordinary and topological insulators, have a symplectic metal in between.

![](_page_41_Figure_2.jpeg)

What about interactions? It turns out that a more interesting approach is required than in the IQHE case.

### Summary of I-particle results

I. There are now more than 3 strong topological insulators that have been seen experimentally  $(Bi_xSb_{1-x}, Bi_2Se_3, Bi_2Te_3, ...)$ . SmB<sub>6</sub>??? (Kondo insulator)

2. Their metallic surfaces exist in zero field and have the predicted form.

3. These are fairly common bulk 3D materials (and also <sup>3</sup>He B).

4. The temperature over which topological behavior is observed can extend up to room temperature or so.

### What's left

What is the physical effect or response that defines a topological insulator beyond single electrons?

What are they good for?

### Ways to define a 3D TI

I. The spin-orbit coupling must be strong enough that a bulk metallic phase transition is passed through as the spin-orbit coupling is increased from zero.

"An odd number of bands must be inverted"

Suggests we look at heavy, small-bandgap semiconductors.

2. Compute Z2 invariants in 2 time-reversal invariant planes.

3. With inversion symmetry (Fu and Kane, 2007): the Z2 invariant reduces to the product of parity eigenvalues at the 8 points where k = -k.

Definitions beyond band structure:

4.A material with an odd number of surface Dirac fermions.

5. (A material with a quantized magnetoelectric effect when  $\frac{2}{3}$  its surface is gapped--next section)

![](_page_43_Figure_9.jpeg)