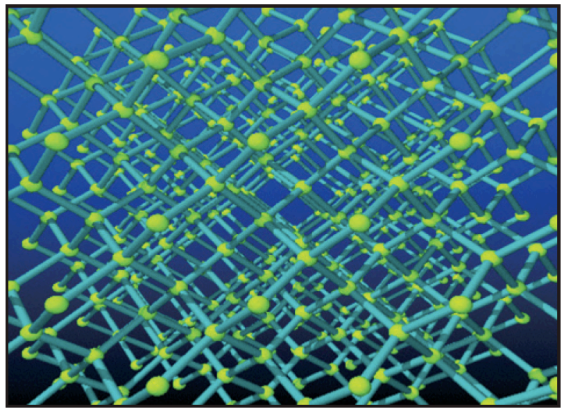
Lecture III: Topological phases

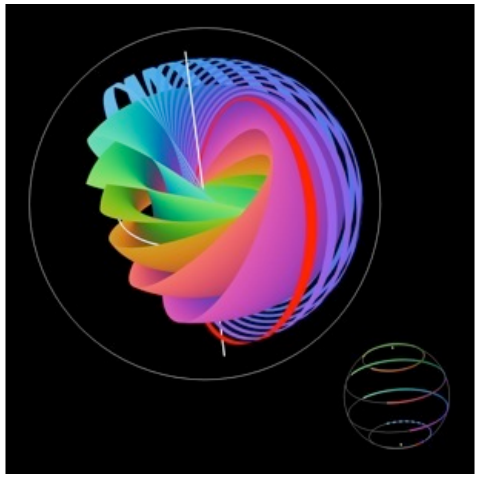
Ann Arbor, 11 August 2010



Joel Moore

University of California, Berkeley,

and Lawrence Berkeley National Laboratory



Western Institute of Nanoelectronics

Thanks

Collaborations

Berkeley students:
Andrew Essin
Roger Mong
Vasudha Shivamoggi
Cenke Xu (UCB→Harvard→UCSB)

Berkeley postdocs:
Pouyan Ghaemi
Ying Ran (UCB→Boston College)
Ari Turner

Leon Balents, Marcel Franz, Babak Seradjeh, David Vanderbilt, Xiao-Gang Wen

Discussions

Berkeley:
Dung-Hai Lee, Joe Orenstein, Shinsei Ryu, R. Ramesh, Ivo Souza, Ashvin Vishwanath
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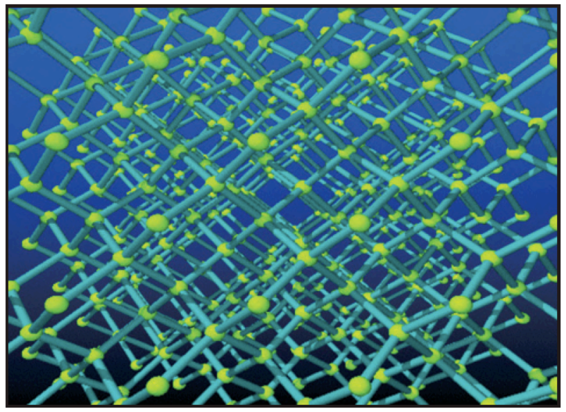
"An insulator's metallic side"
J. E. Moore, Physics **2**, 82 (2009)
"Quasiparticles do the twist"

Outline



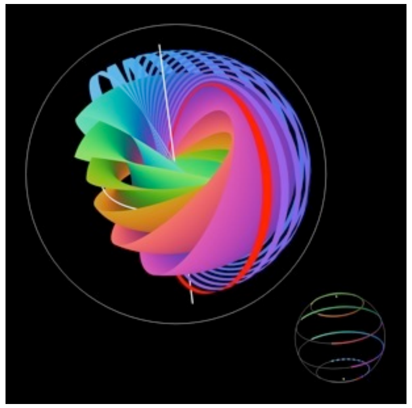
Introduction and overview

What is a topological phase?

How does topological order different from conventional order?

Are there topological phases in 3D materials and no applied field?
Yes — "topological insulators"
(experimental confirmation 2007 for 2D, 2008 for 3D)

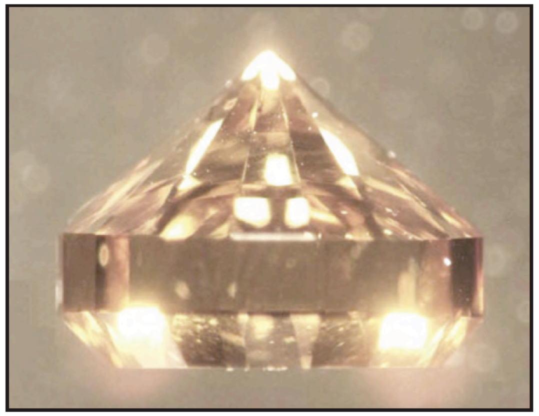
Which insulators are topological?

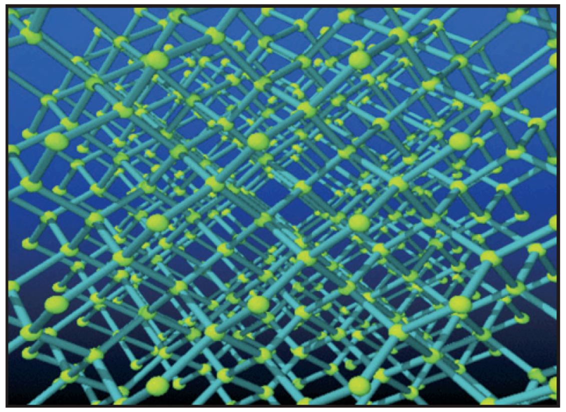


Possible applications...

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":

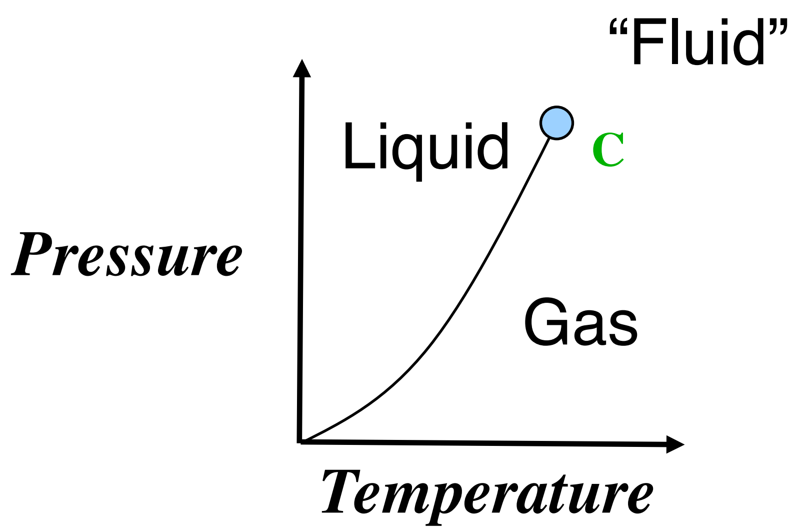
an ordered state appears at low temperature when the system spontaneously loses one of the symmetries present at high temperature.

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.

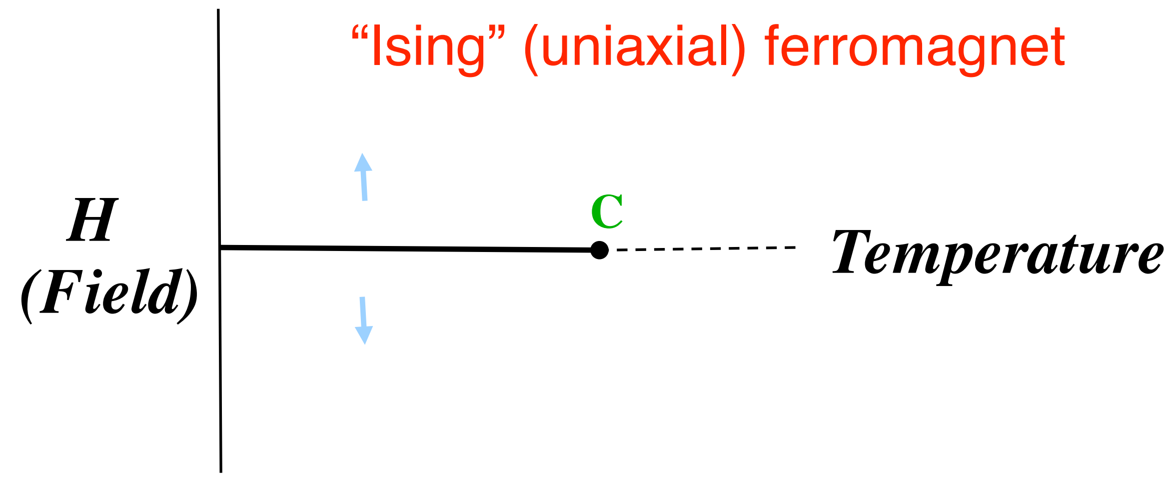
Types of order

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:



$$\rho_L - \rho_G \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$



$$M_{\uparrow} - M_{\downarrow} \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$

$$\text{Experiment}: \quad \beta = 0.322 \pm 0.005$$

$$\text{Theory}: \quad \beta = 0.325 \pm 0.002$$

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

Types of order

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

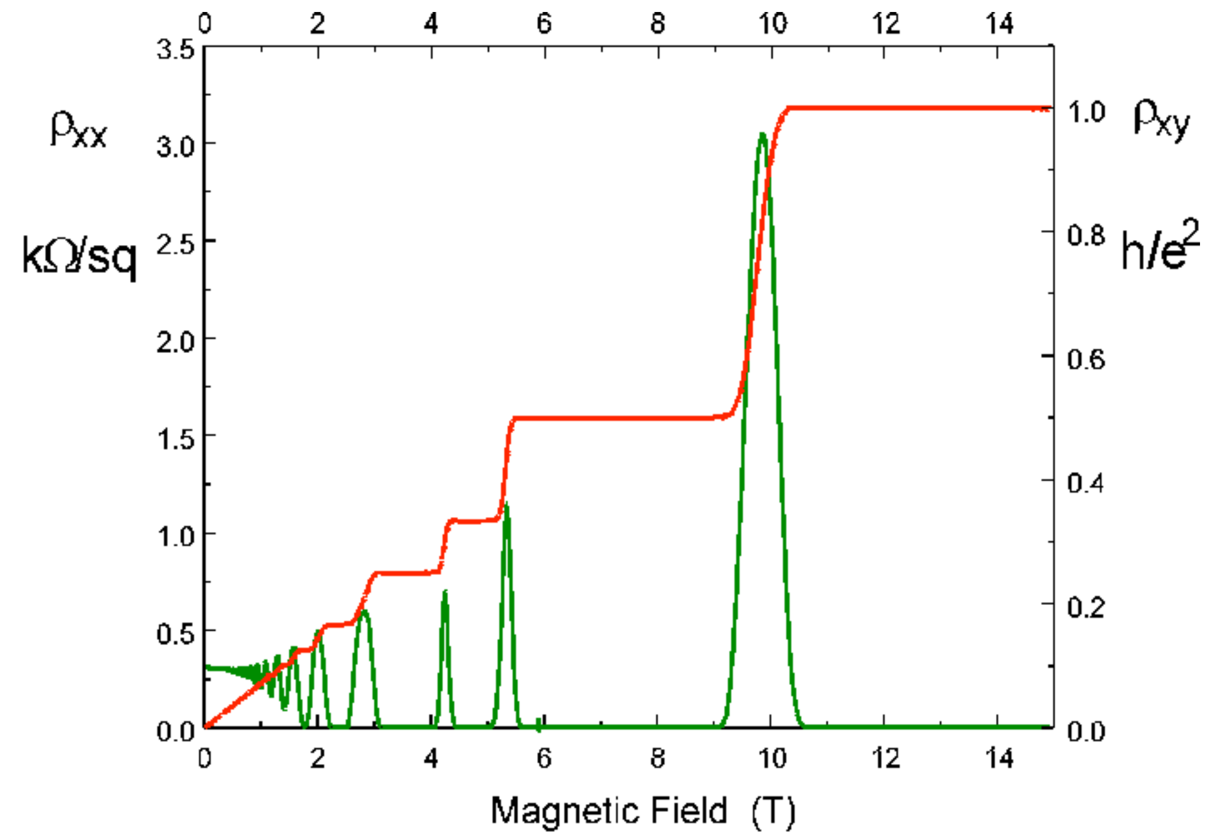
Electrons confined to a plane and in a strong magnetic field show, at low enough temperature, plateaus in the "Hall conductance":

force *I* along *x* and measure *V* along *y*

on a plateau, get

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

at least within 1 in 10^9 or so.



What type of order causes this precise quantization?

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 (lecture 2)

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 $$\frac{n}{2\pi\ell^2} = neB/hc.$$

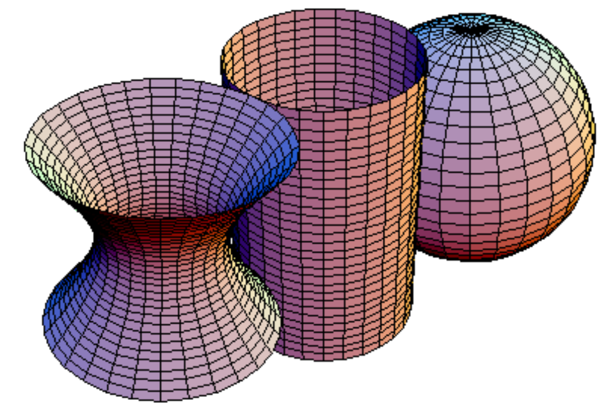
This is exactly the density of "Landau levels", the discrete spectrum of eigenstates of a 2D particle in an orbital magnetic field, spaced by the cyclotron energy. The only "surprise" is how precise the quantization is...

Topological invariants

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

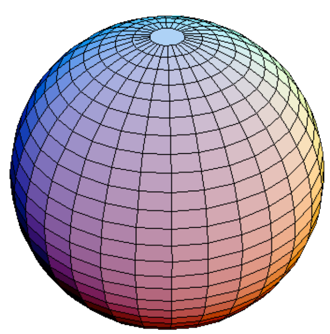
Consider a two-dimensional surface.

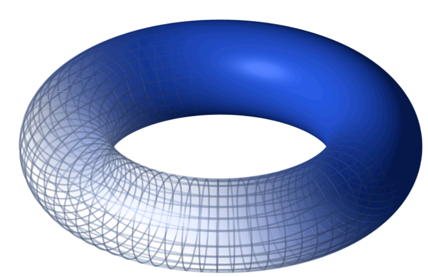
At any point on the surface, there are two radii of curvature.
We define the signed "Gaussian curvature" $\kappa = (r_1 r_2)^{-1}$



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, 1 for torus, n for "n-holed torus".

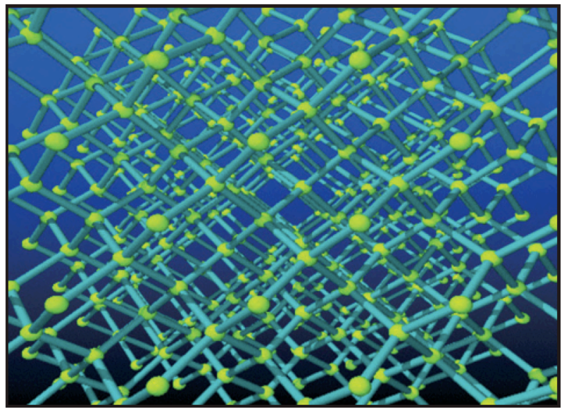
Topological invariants

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*

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

relative to the initial state.

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

Michael Berry

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:

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

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

$$\mathcal{A} \rightarrow \mathcal{A} + \nabla_k \chi$$

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:

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

$$\mathcal{A} = \langle u_{\mathbf{k}} | -i\nabla_k | u_{\mathbf{k}} \rangle \qquad \mathcal{F} = \nabla \times \mathcal{A}$$

S. S. Chern

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,

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

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

TKNN, 1982 "first Chern number"

The importance of the edge

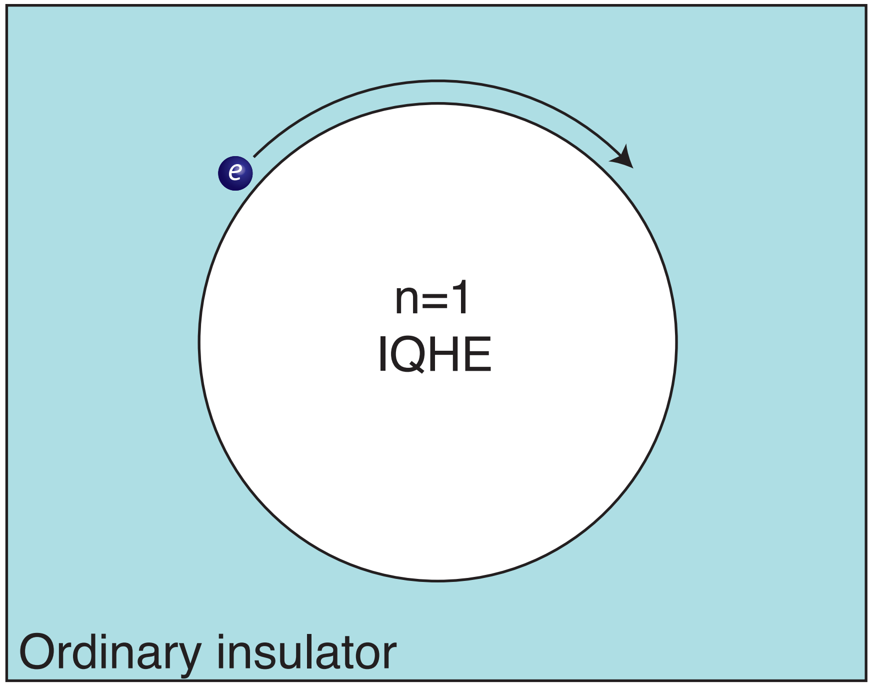
But wait a moment...

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).

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

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.

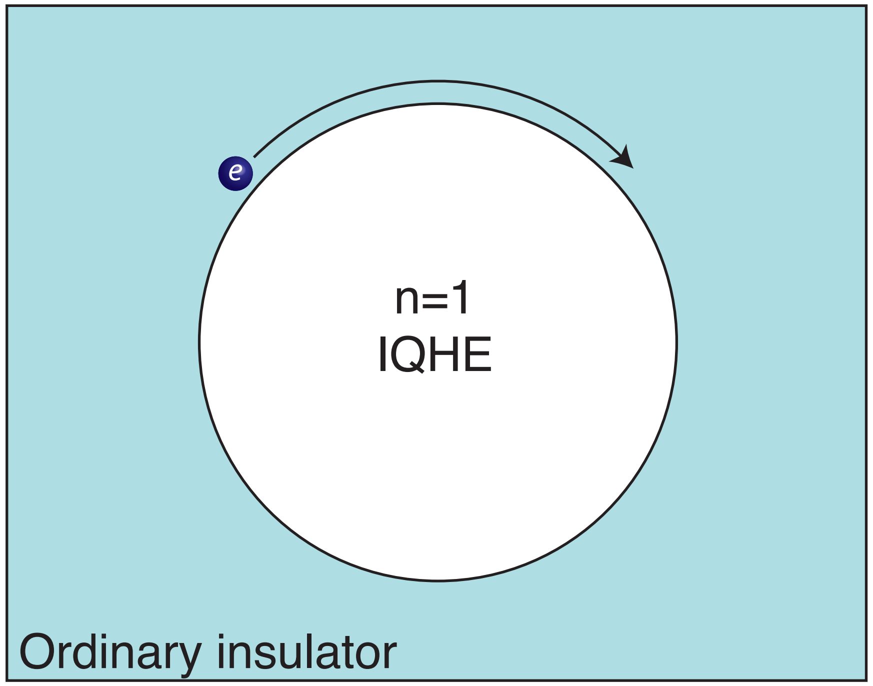
How does the bulk topological invariant "force" an edge mode?

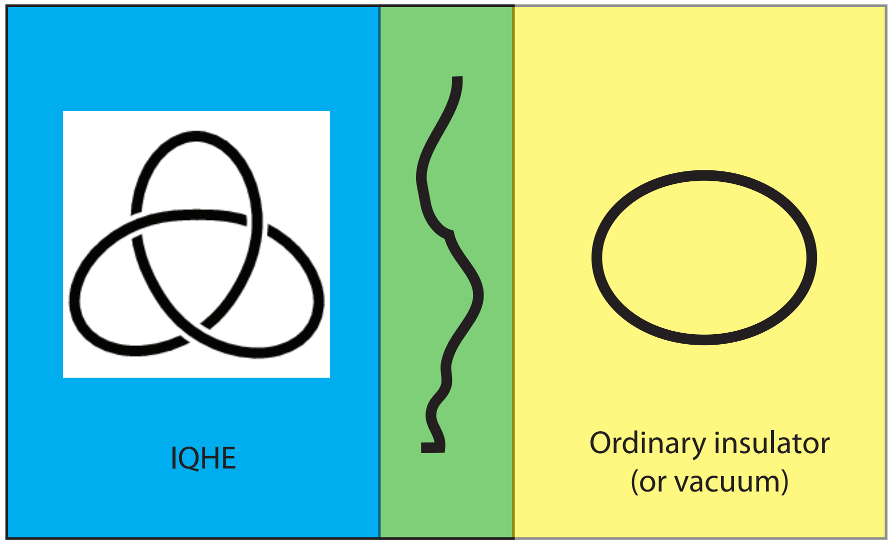
Answer:

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.

∴ the system must not remain insulating.





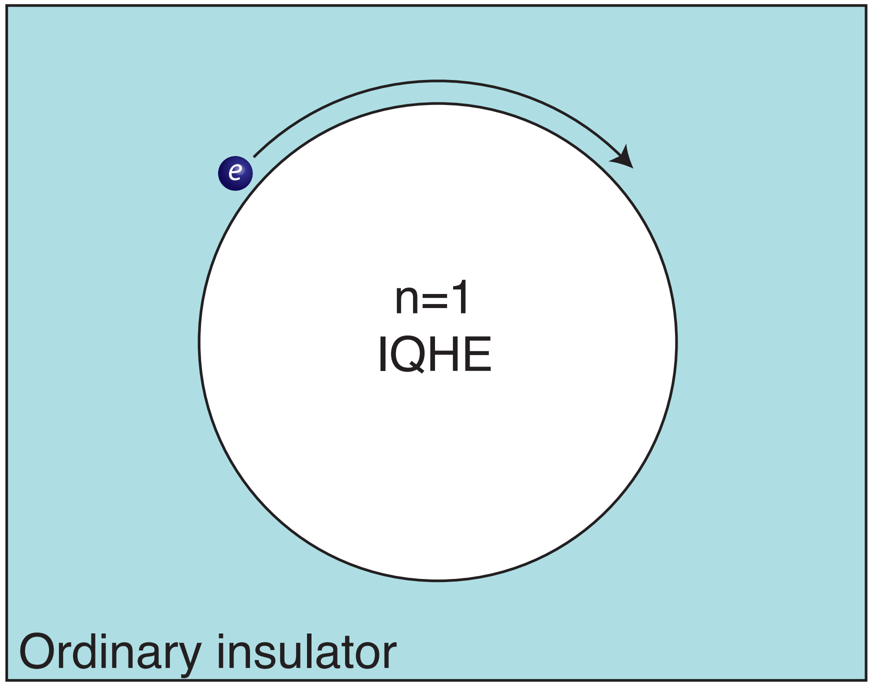
(What is "knotted" are the electron wavefunctions)

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

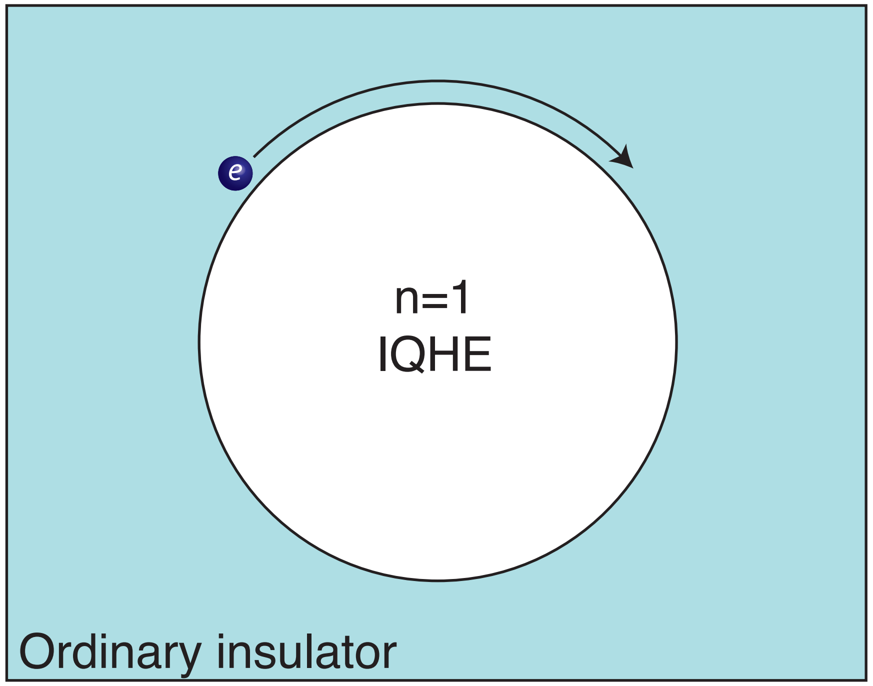
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

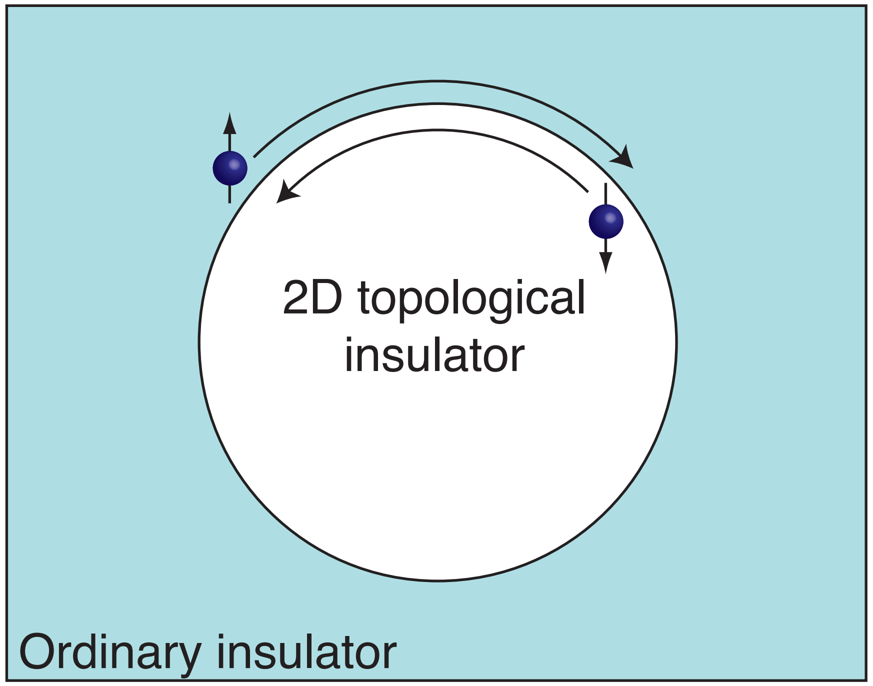
For a given spin, this term leads to a momentum-dependent force on the electron, somewhat like a magnetic field.

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".



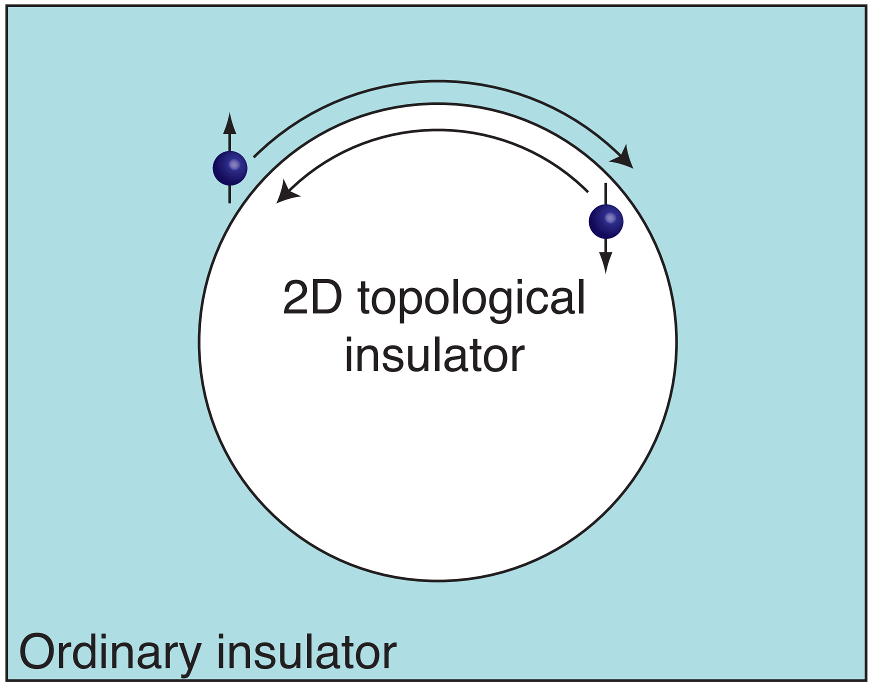


The "quantum spin Hall effect"

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!



$$\mathcal{J}_j^i = \sigma_H^s \epsilon_{ijk} E_k$$

However...

1. 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.

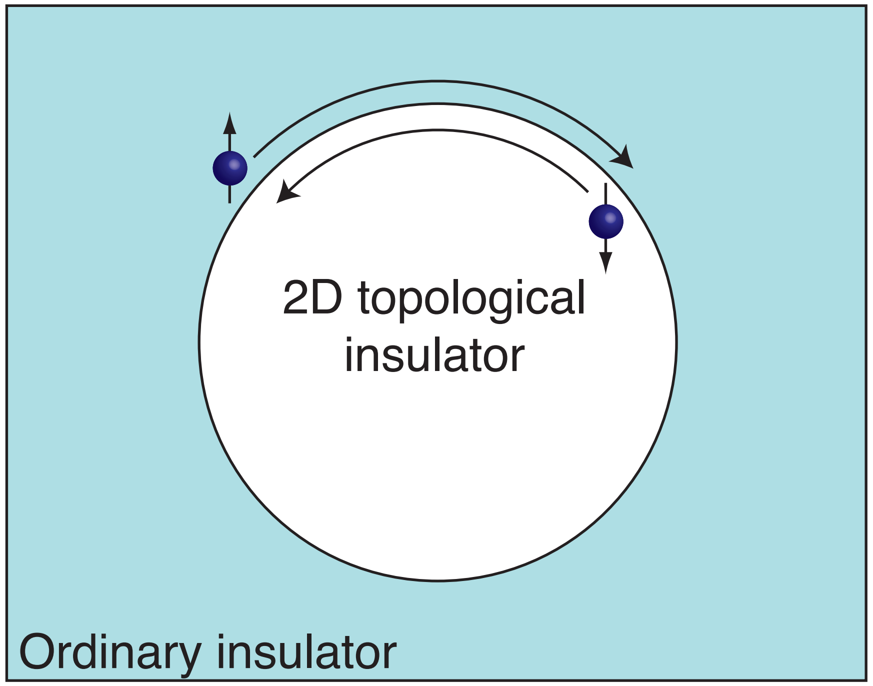
The 2D topological insulator

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".



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

1. 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?

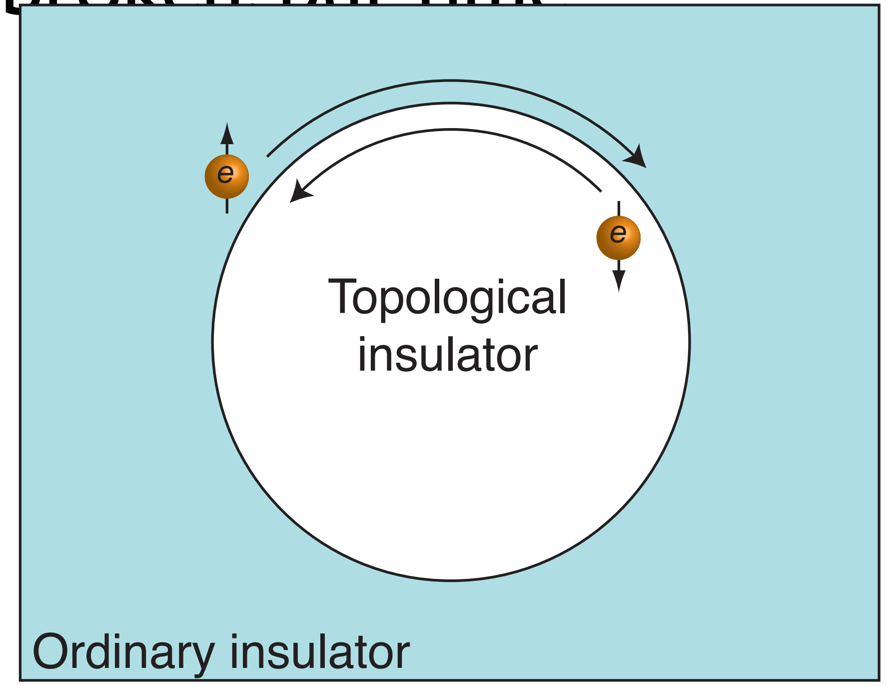
The "Chern insulator" and QSHE

Haldane showed that although *broken time-reversal* is necessary for the QHE, it is not necessary to have a net magnetic flux.
("Chern insulator"=lattice QHE)

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.

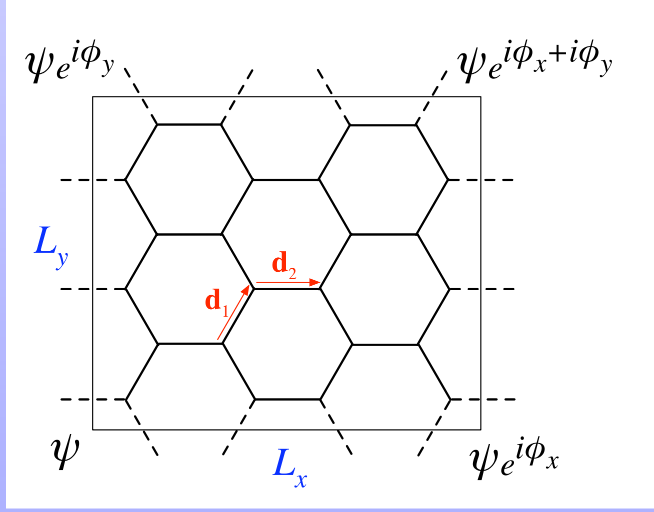
Then *SU(2)* (spin rotation symmetry) is broken, but time-reversal symmetry is not:

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)



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



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

$$\xi_i = \begin{cases} 1 & \text{if i in } A \text{ sublattice} \\ -1 & \text{if i in } B \text{ sublattice} \end{cases}$$

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

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

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

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.

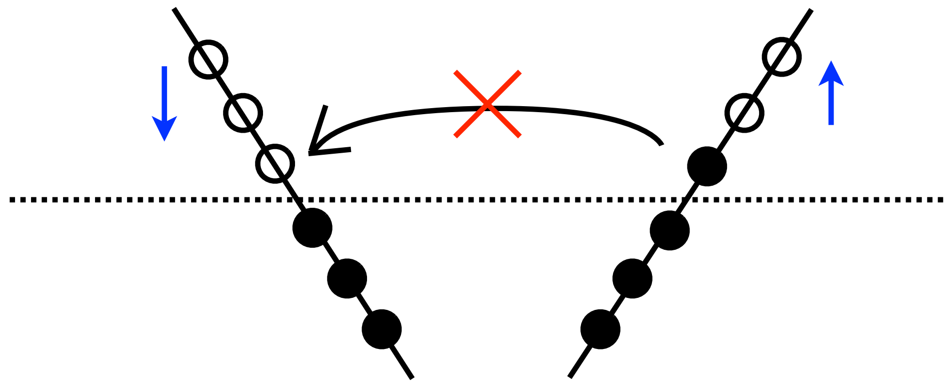
Instead, a fairly technical analysis shows

1. 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

The 2D topological insulator

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



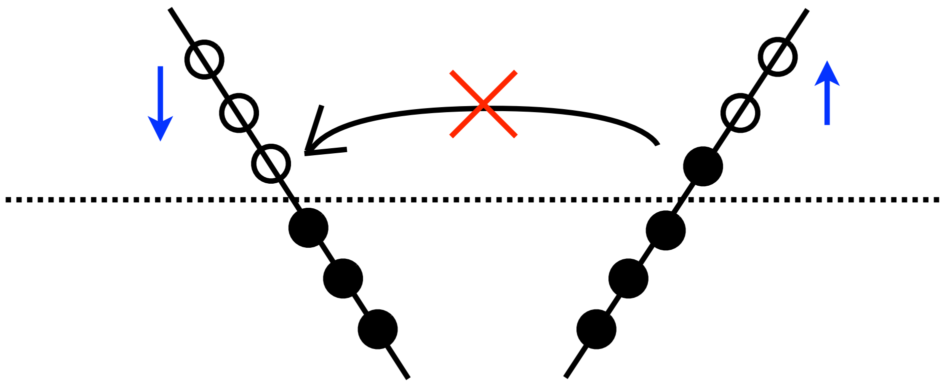
In a time-reversal-invariant system of electrons, all energy eigenstates come in degenerate pairs.

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

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

The 2D topological insulator

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



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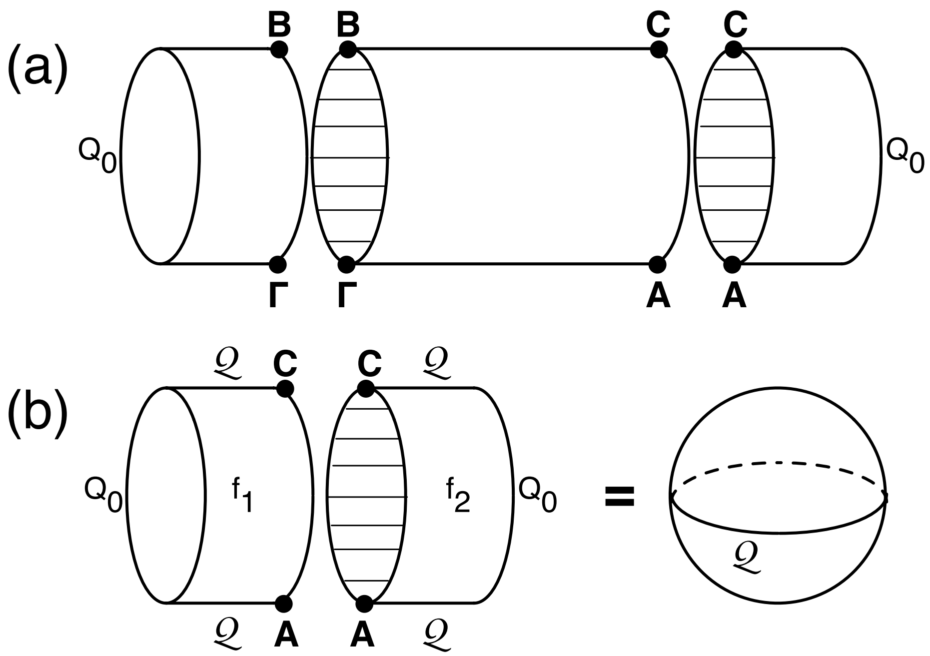
The two states in a pair cannot be mixed by any T-invariant perturbation. (disorder)

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

2. What is the Berry phase expression of the invariant?
It is an integral over *half* the Brillouin zone,

(1)

$$D = \frac{1}{2\pi}\left[\oint_{\partial(EBZ)} d\mathbf{k}\cdot\mathcal{A} - \int_{EBZ} d^2\mathbf{k}\,\mathcal{F}\right] \bmod 2$$



3. How can this edge be seen?

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 1D 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, but $G \sim 0.3\ G_0$)*

Ultracold atoms?

What we've just said is that there are 2D non-interacting lattice models of s=1/2 fermions that can show topological phases.

Before going on to the condensed matter experiments that saw these, we can consider trying to realize the IQHE in a optical lattice by an artificial gauge field (Spielman talk).

We could also try to realize the 2D topological insulator using spin-dependent Hamiltonians (DeMarco talk).

Challenges:
1) Strong enough fields (getting into the topological phase; was difficult in rotated Bose condensates for FQHE).

2) Detection of the phase--surface currents?

3) For T-invariant systems: T-invariance is artificial if "spin states" are not intrinsically T conjugates

The 2D topological insulator

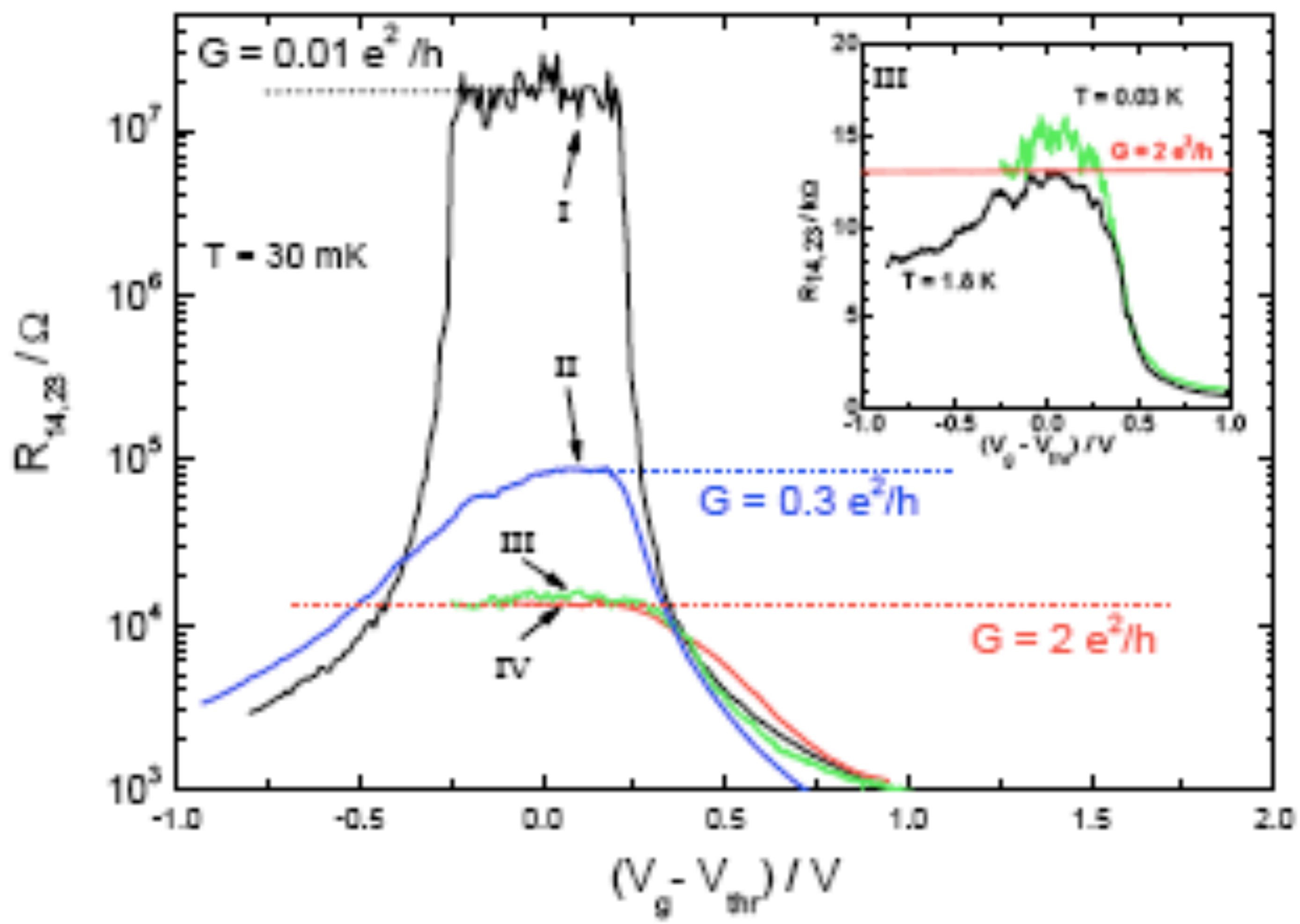
Key: the topological invariant predicts the "number of quantum wires".

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:

$$G = \frac{2e^2}{h}$$

König et al., *Science* (2007)



Laurens Molenkamp

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

What about 3D?

There is no truly 3D quantum Hall effect. There are only layered versions of 2D.
(There are 3 "topological invariants", from *xy*, *yz*, and *xz* planes.)

Trying to find Kane-Mele-like invariants in 3D leads to a surprise: (JEM and Balents, 2007)

1. There are still 3 layered Z2 invariants, but there is a fourth Z2 invariant as well.

Hence there are $2^4 = 16$ different classes of band insulators in 3D.

2. The nontrivial case of the fourth invariant is fully 3D and cannot be realized in any model that doesn't mix up and down spin.

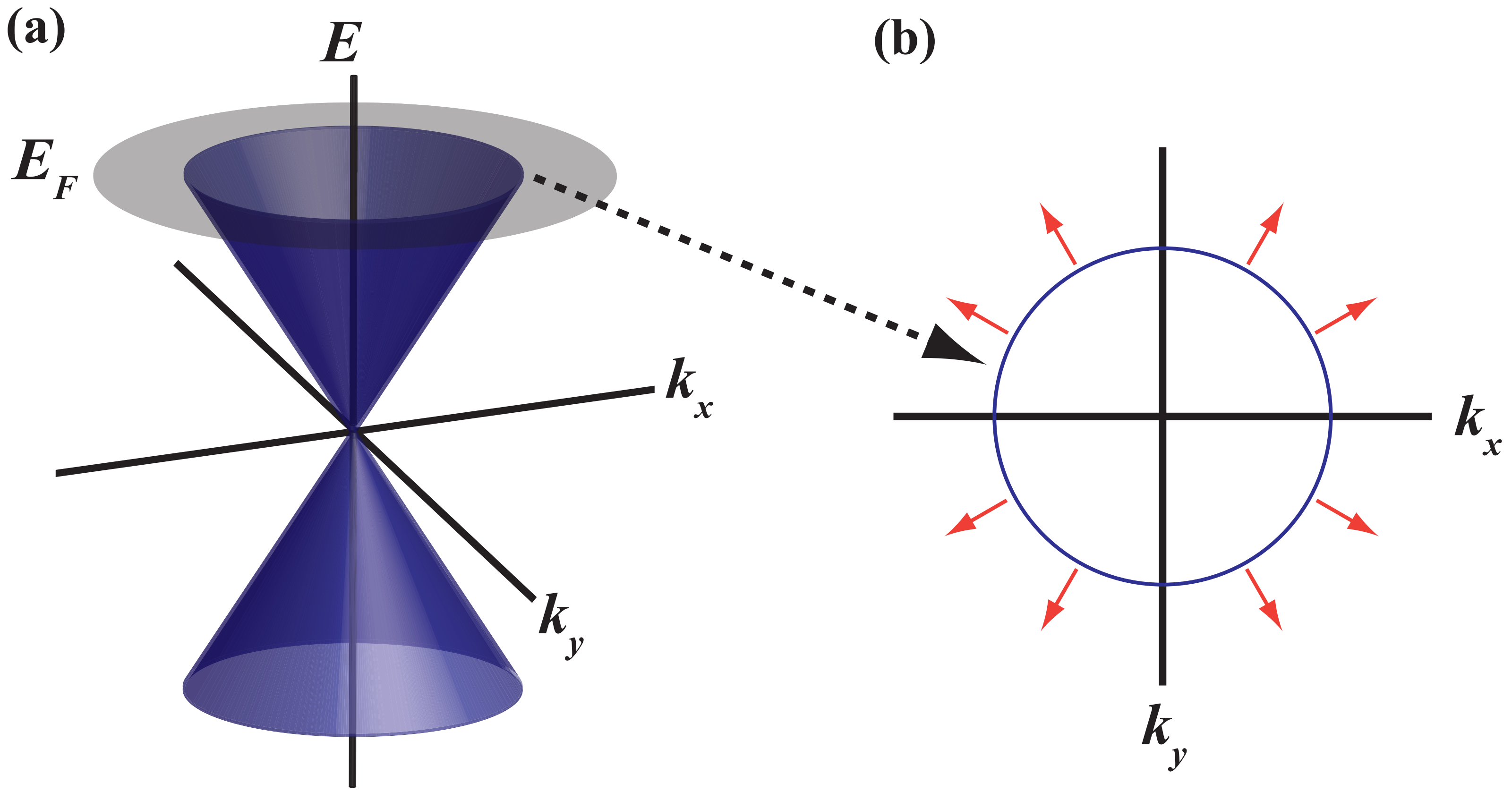
In 2D, we could use up-spin and down-spin copies to make the topological case.

There is a (technical) procedure to compute the fourth invariant for any band structure.

3. There should be some type of metallic surface resulting from this fourth invariant, and this is easier to picture...

Topological insulators in 3D

1. 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)



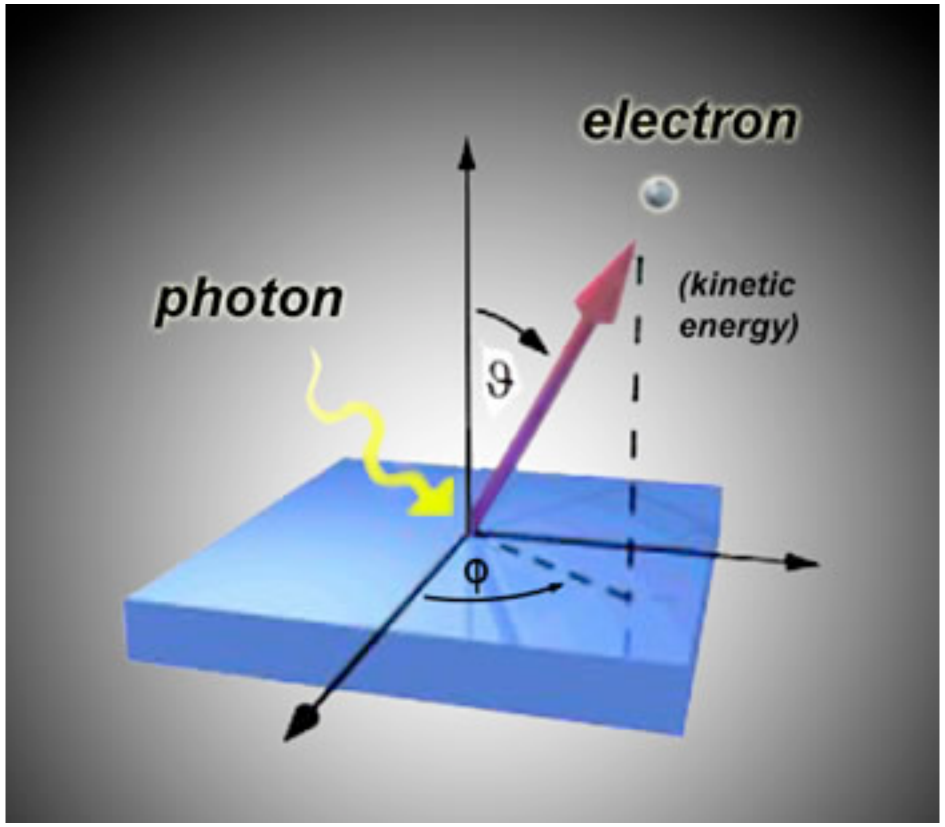
2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

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.



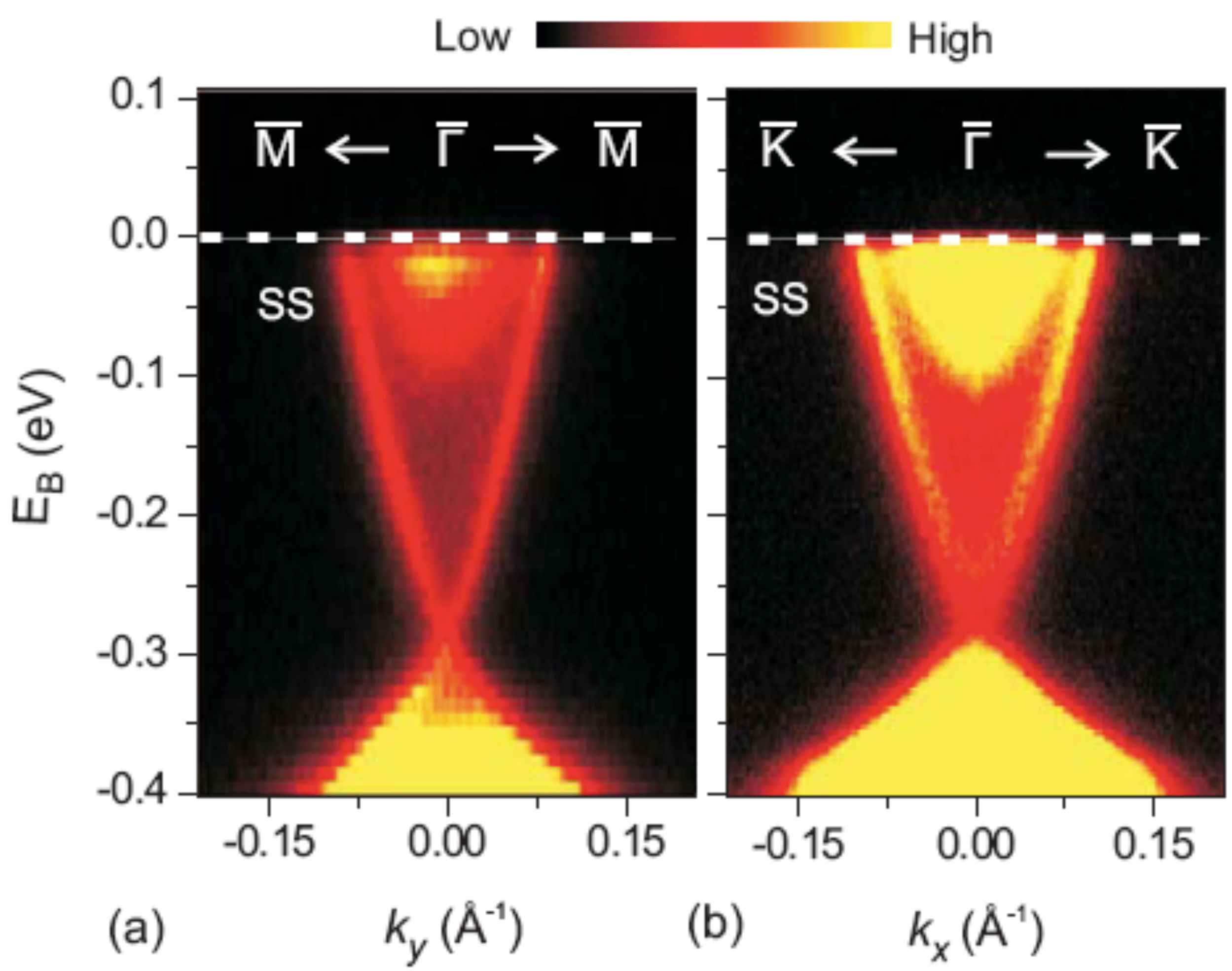
Measure as many properties as possible of the outgoing electron
to deduce the momentum, energy, and spin it had while still in the solid.

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:

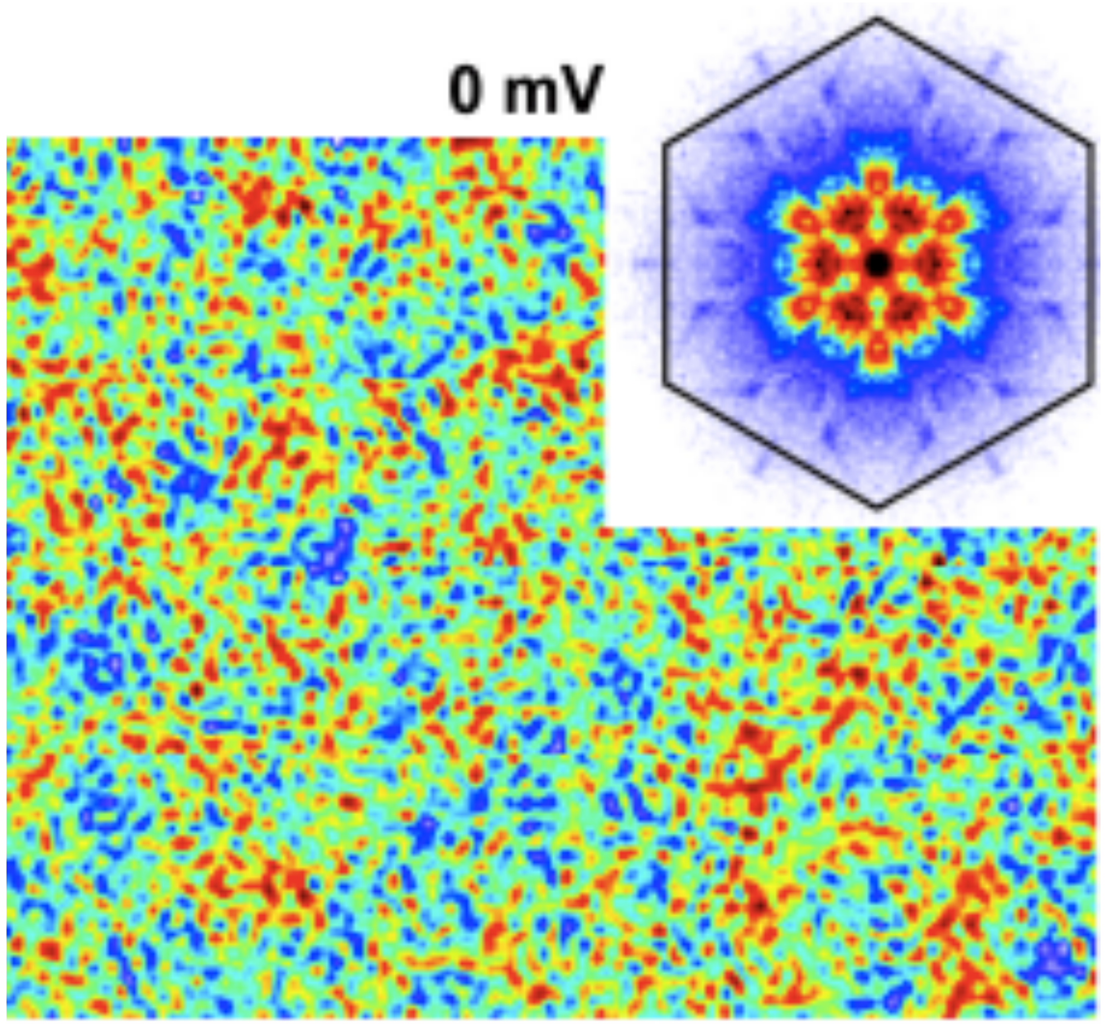


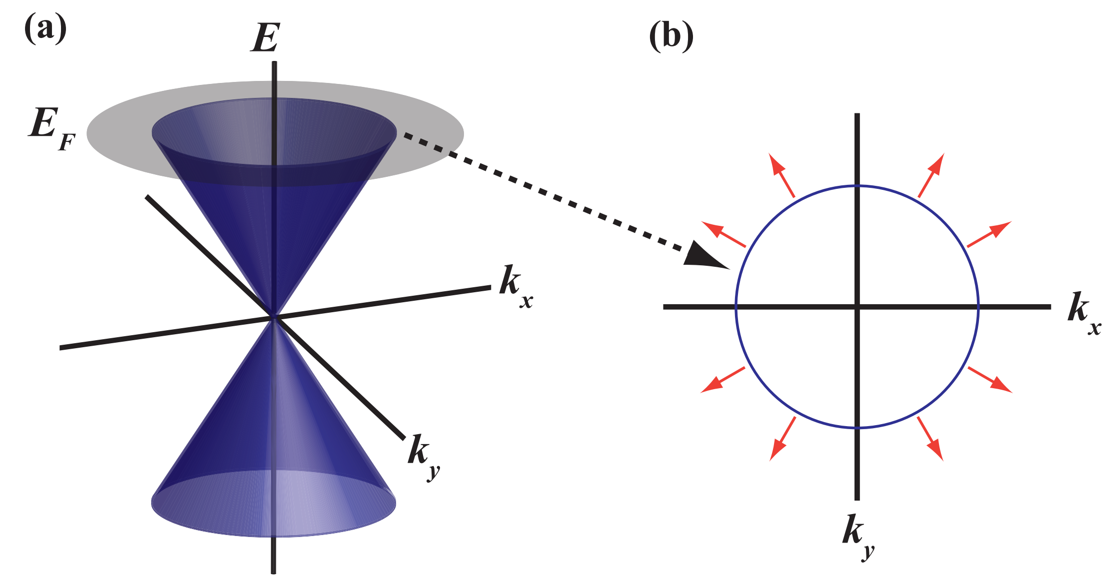
The states shown are in the "energy gap" of the bulk material--in general no states would be expected, and especially not the Dirac-conical shape.

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)





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

Quasiparticles:
“Wen-type” topological order and Majorana fermions

A history of theoretical efforts to understand quantum Hall physics:

1. Integer plateaus are seen experimentally (1980).

Theorists find profound explanation why integers will always be seen.
Their picture involves nearly free electrons with ordinary fermionic statistics.

2. Fractional plateaus are seen experimentally (1983).
Eventually many fractions are seen, all with odd denominators.

Theorists find profound explanation why odd denominators will always be seen.
The picture (Laughlin) involves an interacting electron liquid that hosts “*quasiparticles*” with *fractional* charge and *fractional* “anyonic” statistics.

3. A plateau is seen when 5/2 Landau levels are filled (1989).
Theorists find profound explanation: an interacting electron liquid that hosts “*quasiparticles*” with *non-Abelian* statistics.

What does fractional or non-Abelian statistics mean? Why is 2D special?

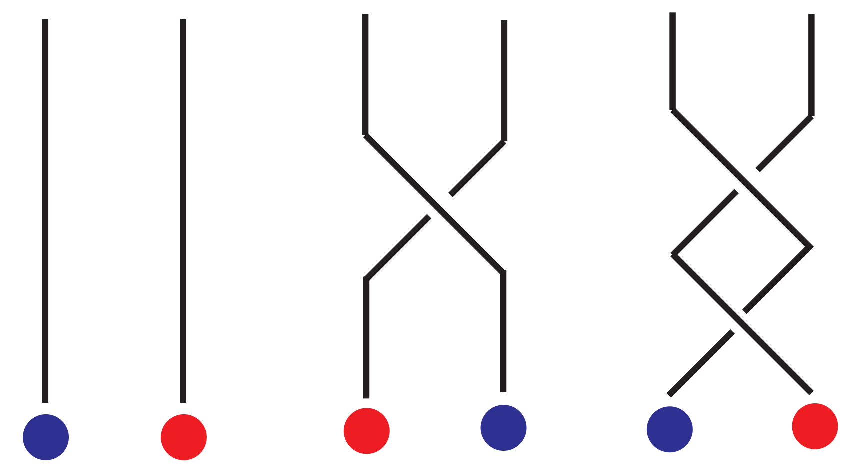
Statistics in 2D

What makes 2D special for statistics? (Leinaas and Myrheim, 1976)

Imagine looping one particle around another to detect their statistics. In 3D, all loops are equivalent.

In 2D, but not in 3D, the result can depend on the "sense" of the looping (clockwise or counterclockwise).
Exchanges are not described by the permutation group, but by the "braid group".

The effect of the exchange on the ground state need not square to 1. "Anyon" statistics: the effect of an exchange is neither +1 (bosons) or -1 (fermions), but a phase.



$$e^{i\theta}$$

Most fractional quantum Hall states, such as the Laughlin state, host "quasiparticles" with anyonic statistics.

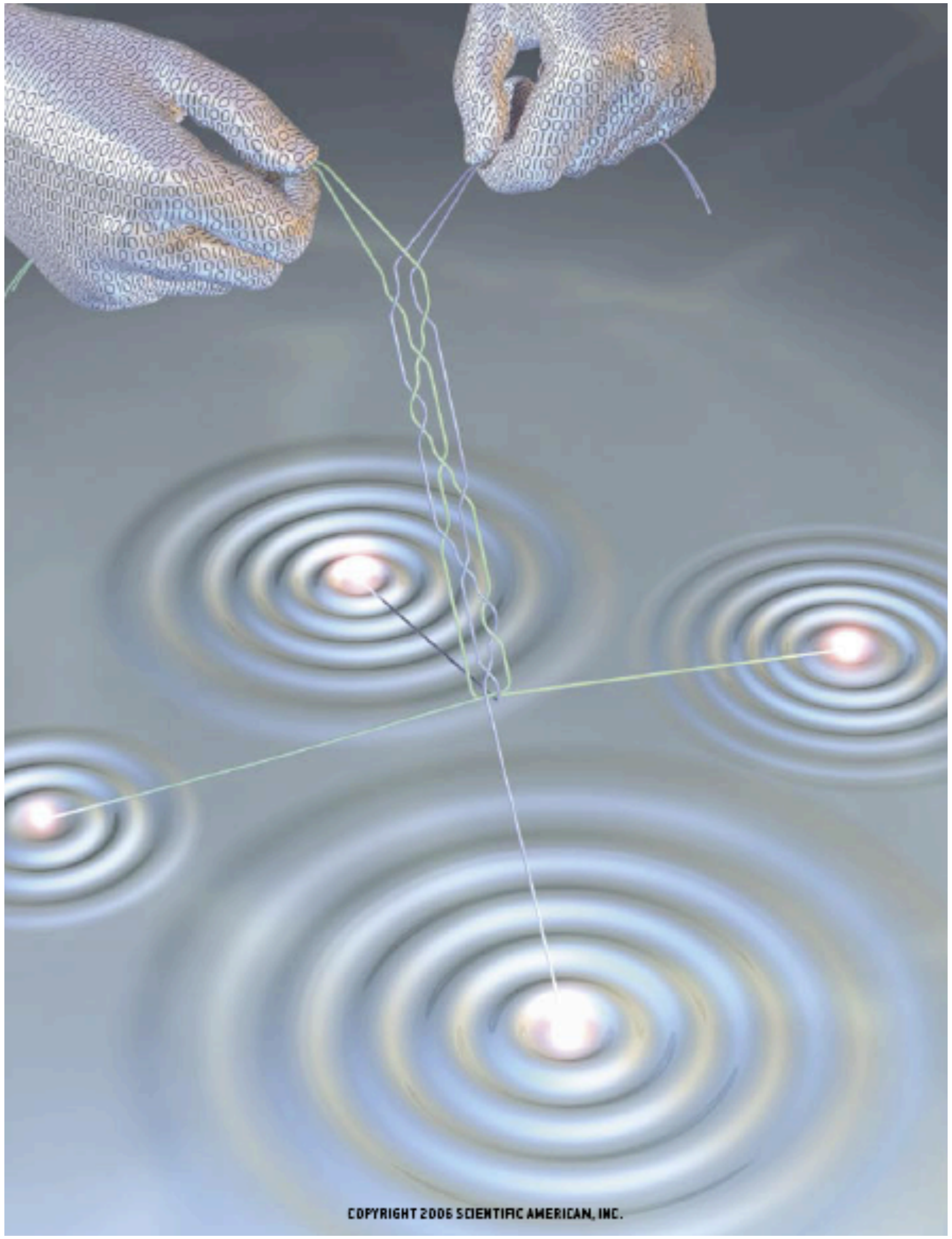
Topological quantum computing

A classical computer carries out logical operations on classical "bits".

A **quantum computer** carries out unitary transformations on "qubits" (quantum bits).

A remarkable degree of protection from errors can be obtained by implementing these via braiding of non-Abelian quasiparticles:
braiding acts as a matrix on a degenerate space of states.

The relevant quasiparticle in the Moore-Read state is a "Majorana fermion":
it is its own antiparticle
and is "half" of a normal fermion.



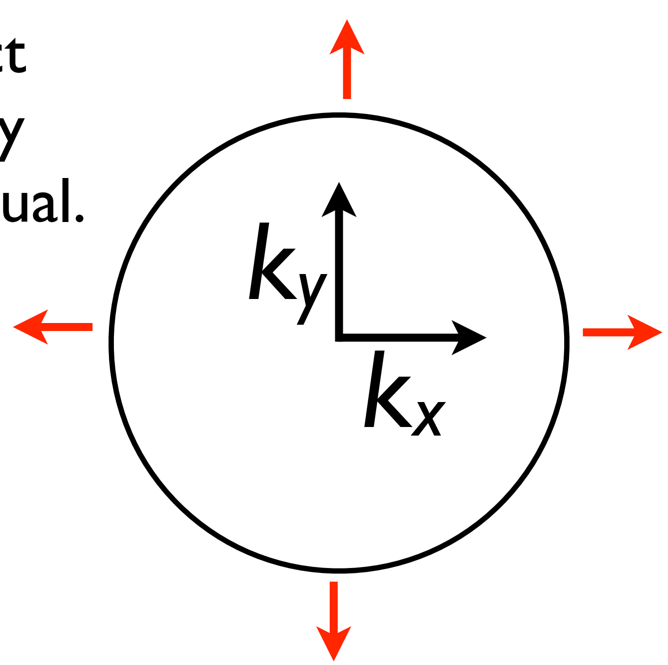
Topological insulators for topological quantum computing

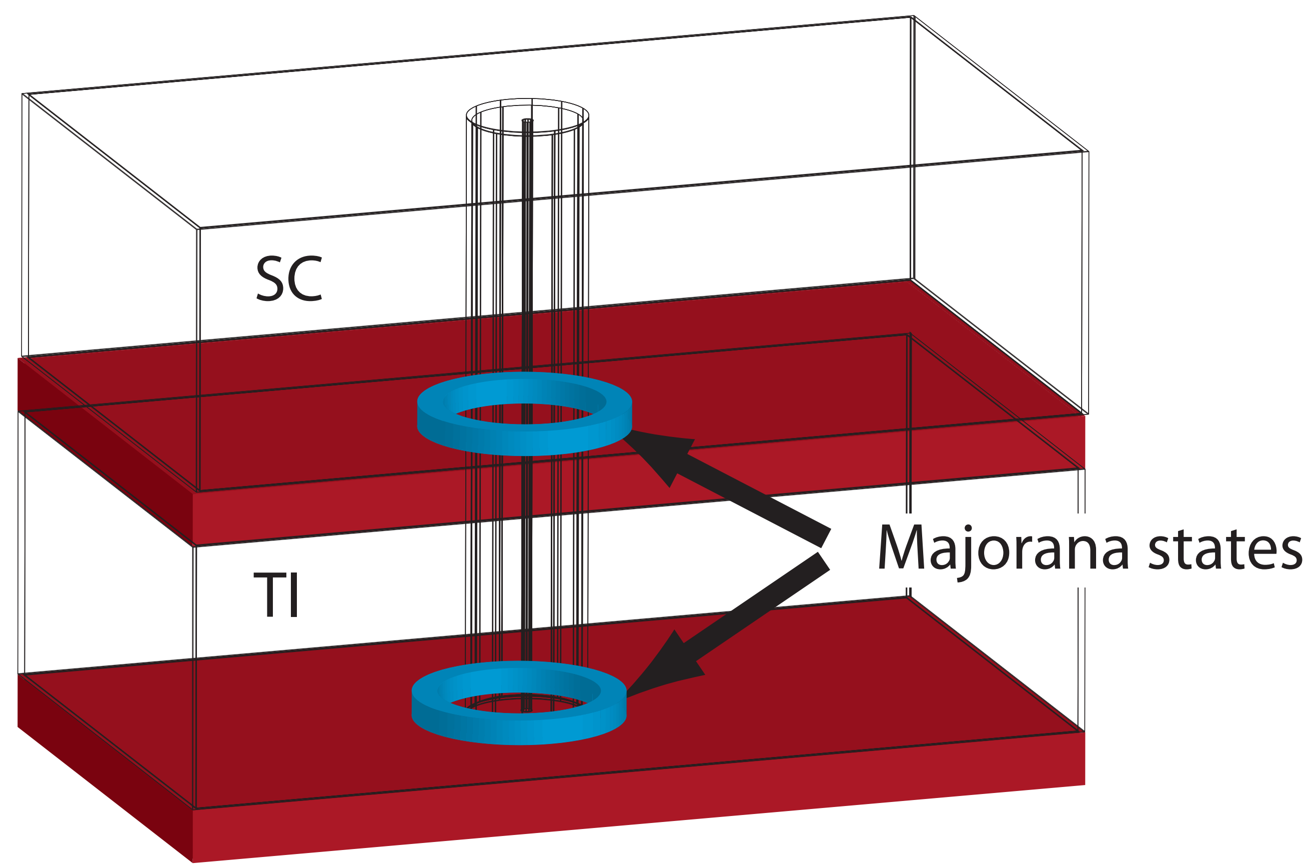
It is believed that the core of a magnetic vortex in a two-dimensional "*p*+*ip*" superconductor can have a Majorana fermion. (But we haven't found one yet.)
A Majorana fermion is its own antiparticle and is "half" of a (spinless) Dirac fermion.

However, a superconducting layer with this property exists at the boundary between a 3D topological insulator and an ordinary 3D superconductor (Fu and Kane, 2007).

$$H = \sum_{\mathbf{k}} (\Delta c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + h.c.)$$

This proximity effect involves *half* as many electronic states as usual.





Transport in topological insulators

As we will discuss in Lecture II, transport reveals some interesting properties of Dirac electrons in a disorder potential.

But the situation is far from clear: one experiment (Yi Cui's group, Stanford) shows unambiguous evidence of transport from surface states.

Method: Aharonov-Bohm oscillations in conductance of a "nanoribbon"

Strong periodic part in flux indicates transport by surface

Summary so far

1. There are now at least 3 strong topological insulators that have been seen experimentally (Bi_xSb_{1-x}, Bi_2Se_3, Bi_2Te_3).

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

3. These are fairly common bulk 3D materials (and also ^{3}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?