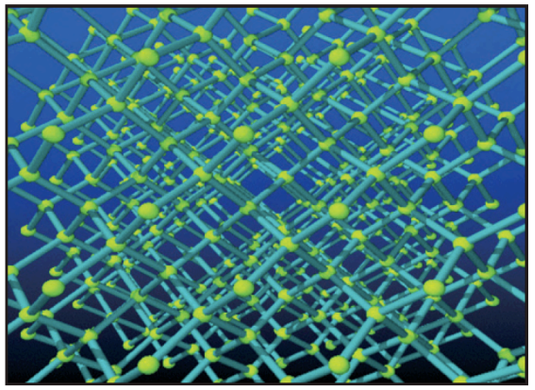
Introduction to topological phases

NORDITA school, 10-11 January 2011



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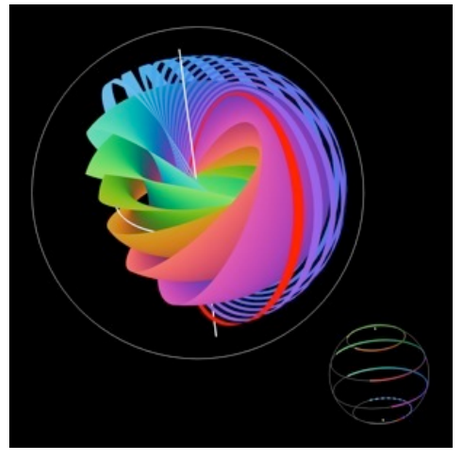

Thanks

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References

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J. E. Moore, Nature **460**, 1090 (2009)
"An insulator's metallic side"
J. E. Moore, Physics **2**, 82 (2009)
"Quasiparticles do the twist"

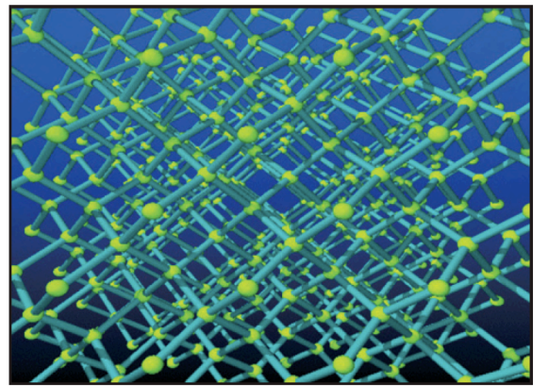
Disclaimer

These slides were used as part of a 4-lecture NORDITA minicourse for beginning condensed matter theory graduate students.

Please keep in mind that they were supplemented by considerable blackboard teaching, especially on the quantum Hall effect, topological field theories, and spin liquids. Even for topics covered in the slides, some details and references that were provided in verbal comments or blackboard notes are not evident in the slides.

The author is grateful to Prof. E. Ardonne for the opportunity to give this course.

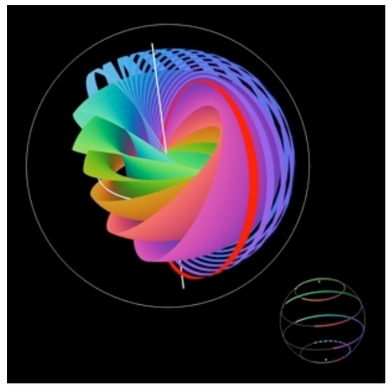
Outline of lectures



1. Overview of experimental background and idea of "topological order". Basic notions of topology relevant to condensed matter.

2. Integer quantum Hall physics. Berry phases in metals and insulators. Thouless-type order.

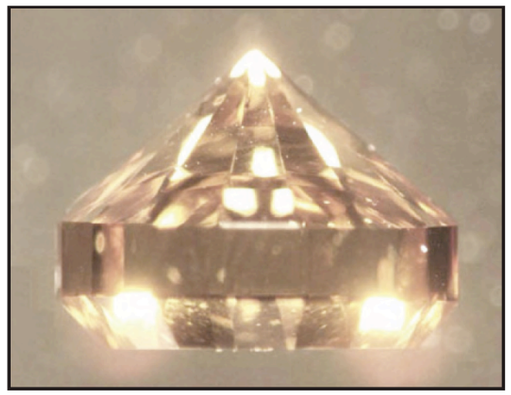
3. Fractional quantum Hall physics. Composite fermions. Wen-type order.

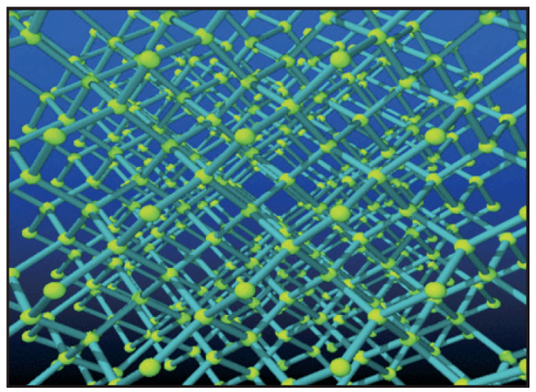


4. Some current directions:
A. Topological spin liquids.
B. Entanglement entropy and topology.
C. Topological field theories.

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":

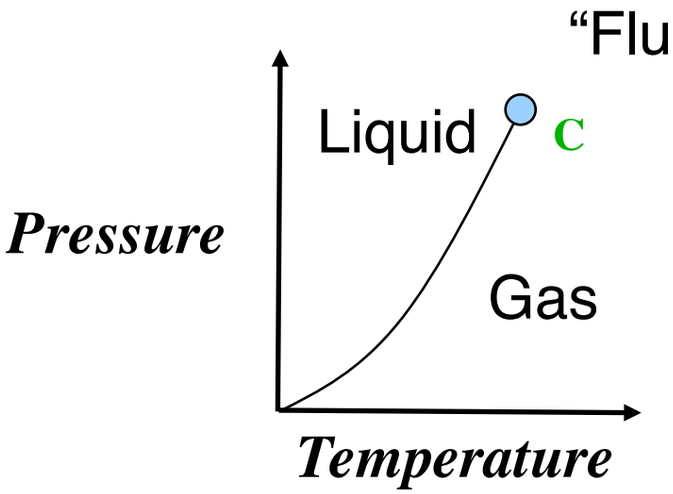
an ordered state appears at low temperature when the system spontaneously loses one of the symmetries present at high temperature.

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

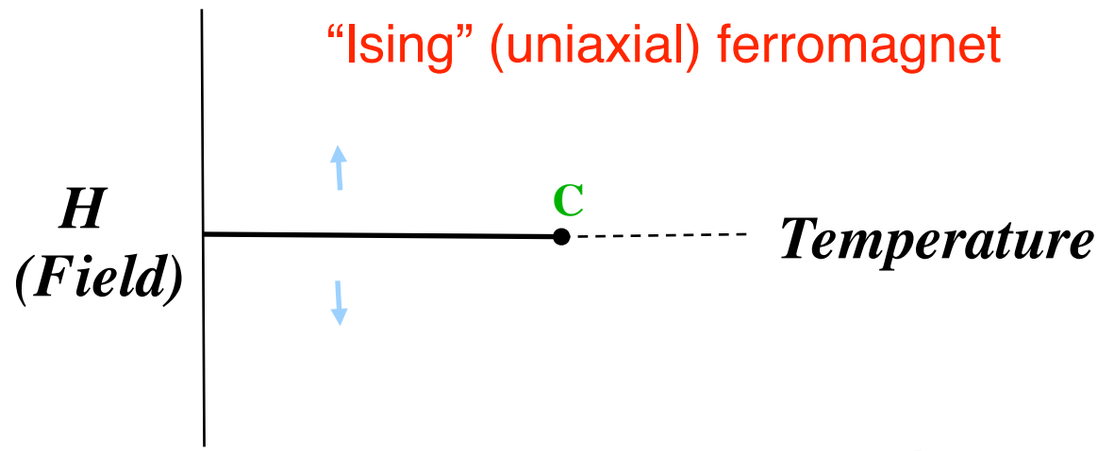
At high temperature, entropy dominates and leads to a disordered state.
At low temperature, energy dominates and leads to an ordered state.

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



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

"Ising" (uniaxial) ferromagnet



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

$$\text{Experiment}: \quad \beta = 0.322 \pm 0.005$$
$$\text{Theory}: \quad \beta = 0.325 \pm 0.002$$

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

Types of order

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

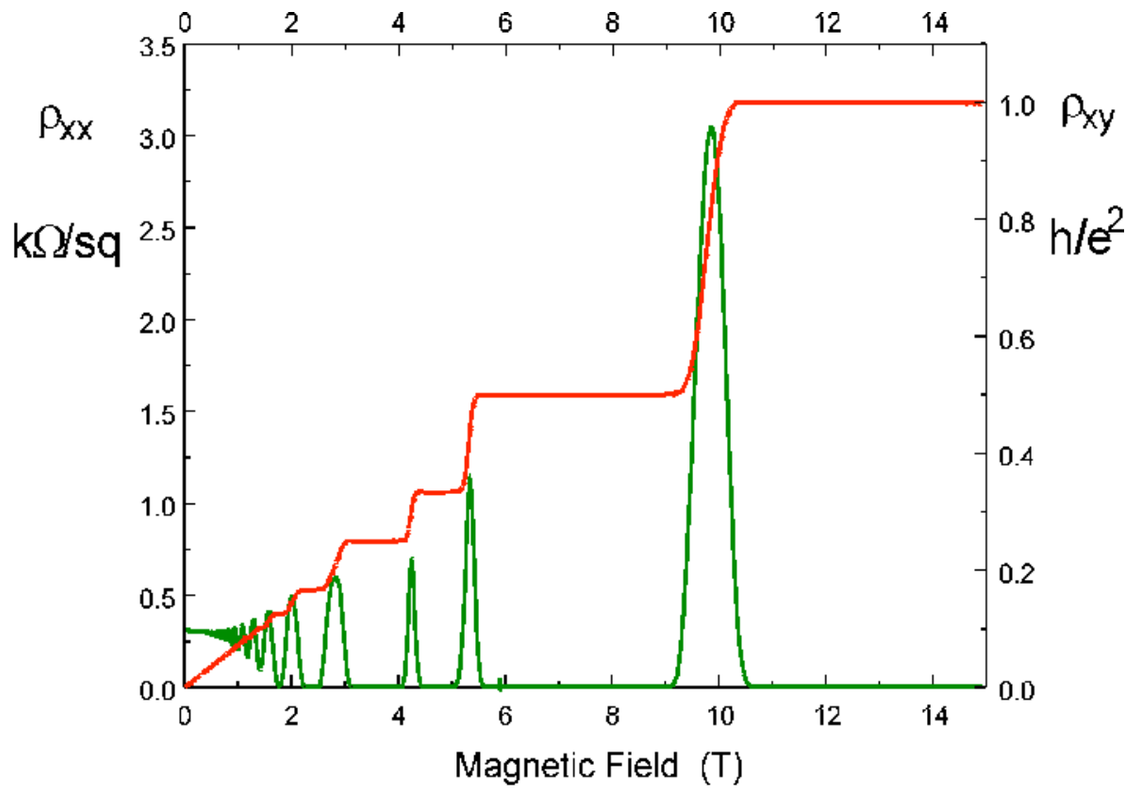
Electrons confined to a plane and in a strong magnetic field show, at low enough temperature, plateaus in the "Hall conductance":

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

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.

Traditional picture: Landau levels and edge states

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

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

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

Note: for a relativistic fermion, as in graphene, n 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".

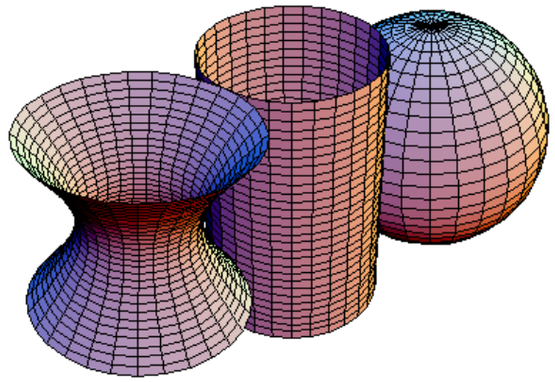
Blackboard interlude: What happens with disorder?
Where is the topology? (Laughlin argument and edge vs. bulk transport)

Topological invariants

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

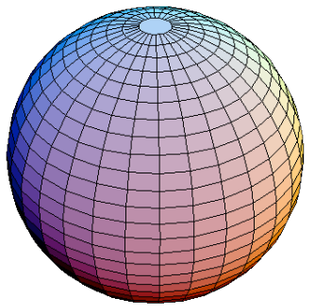
Consider a two-dimensional surface.

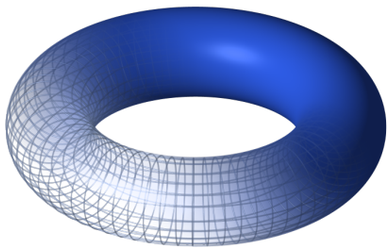
At any point on the surface, there are two radii of curvature.
We define the signed "Gaussian curvature" $\kappa = (r_1 r_2)^{-1}$



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).

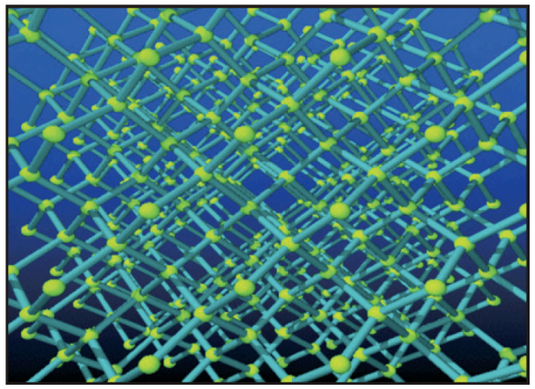
$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2 - 2g)$$

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.

Michael Berry

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

Berry phase

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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:

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

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

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

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:

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

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

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

S. S. Chern

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

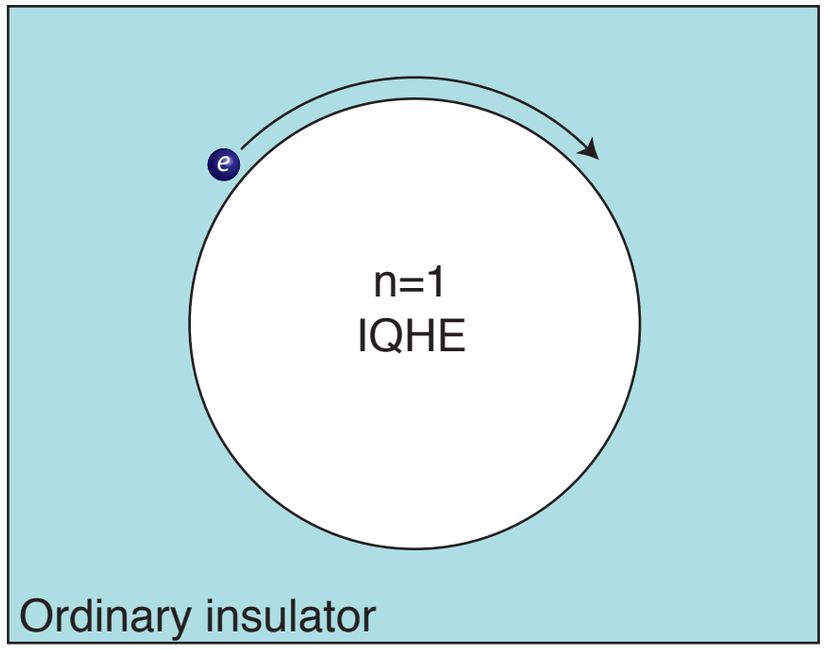
But wait a moment...

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.

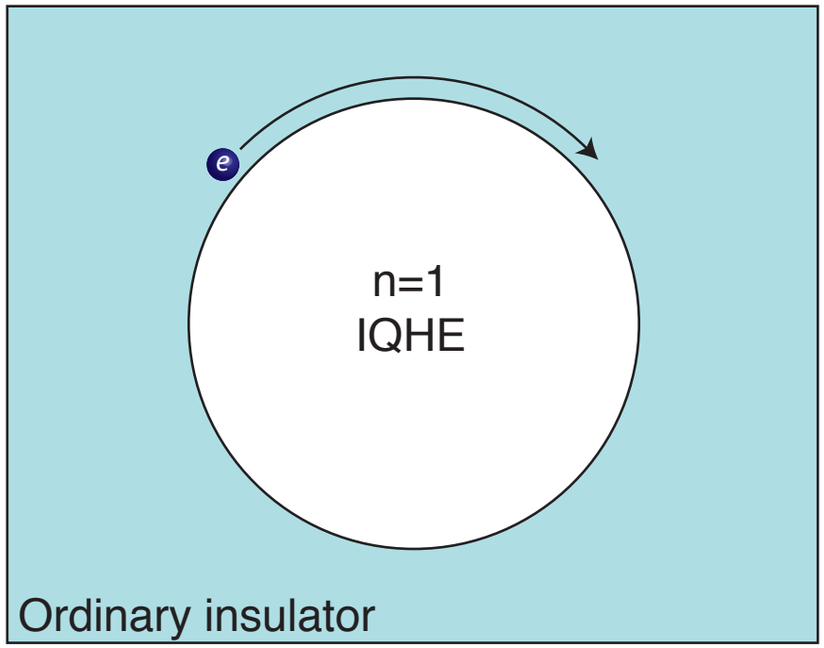
How does the bulk topological invariant "force" an edge mode?

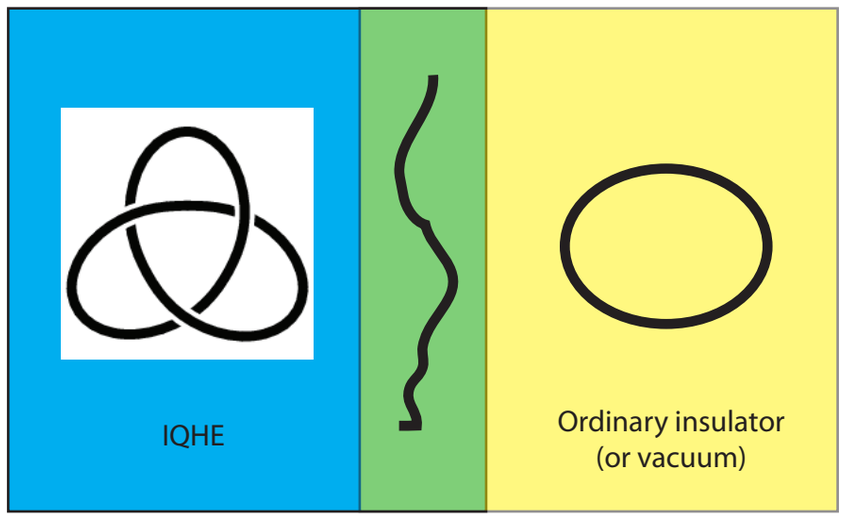
Answer:

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.

$\therefore$ the system must not remain insulating.





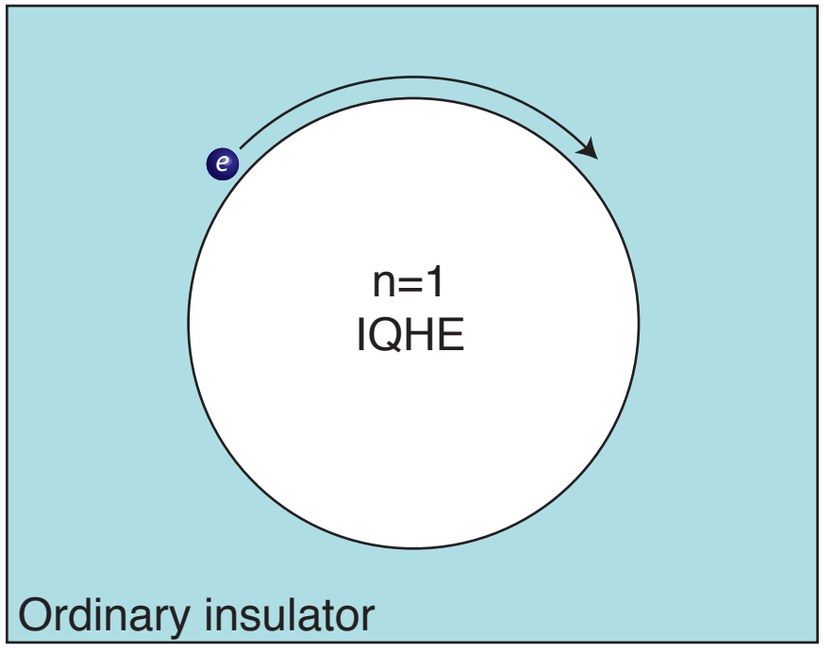
(What is "knotted" are the electron wavefunctions)

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

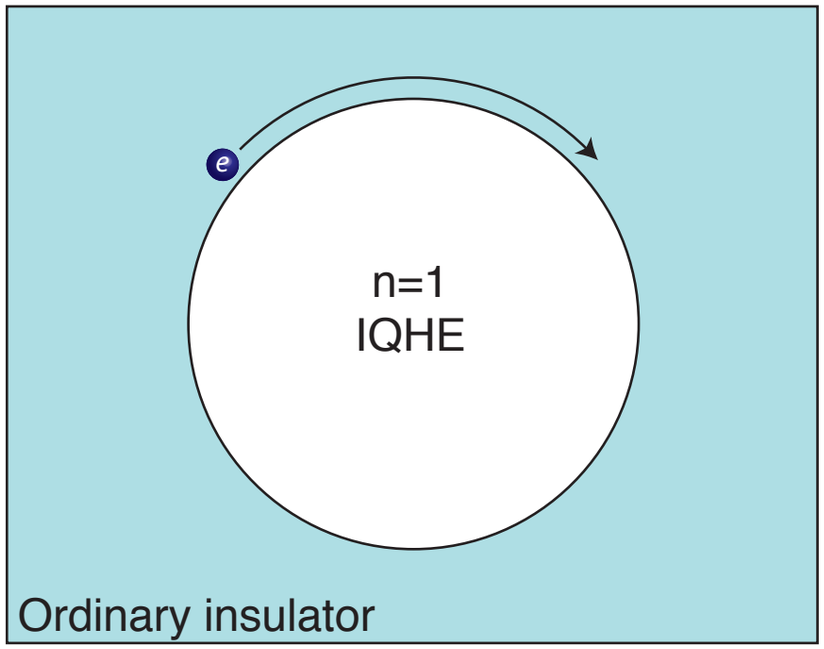
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

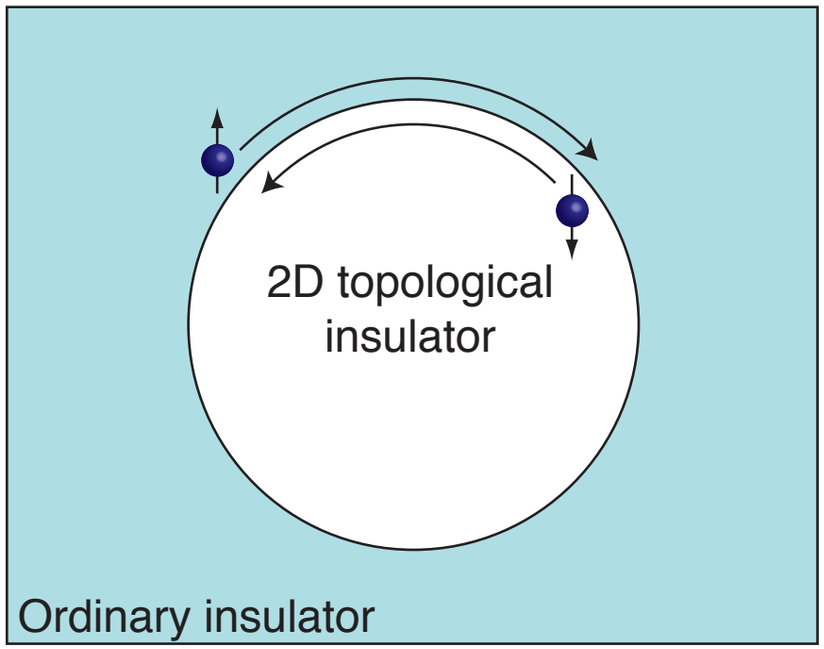
For a given spin, this term leads to a momentum-dependent force on the electron, somewhat like a magnetic field.

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".



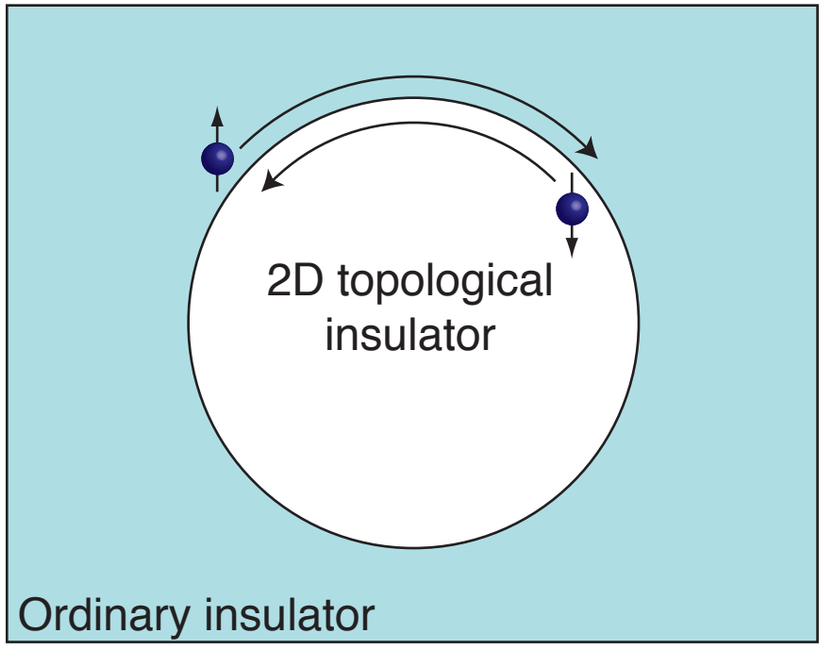


The "quantum spin Hall effect"

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.

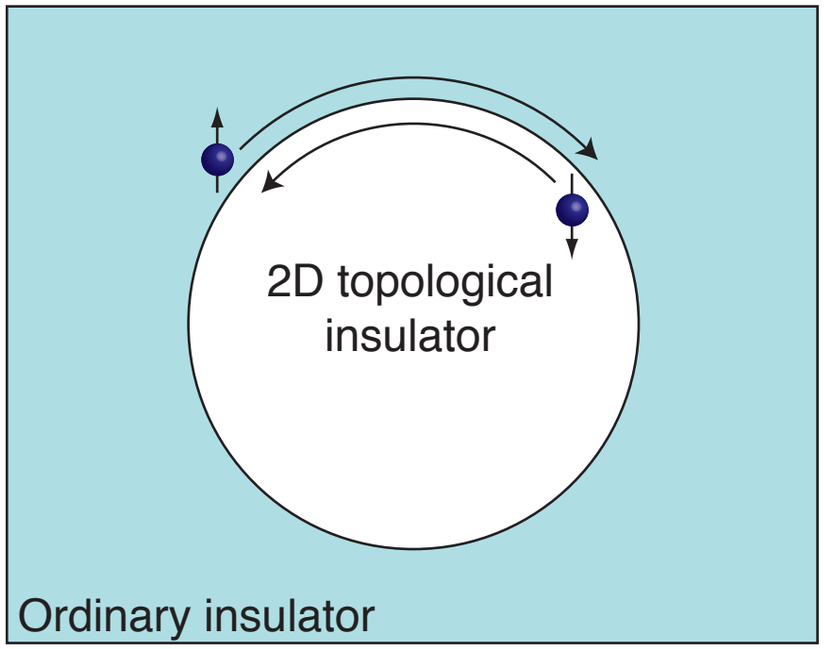
The 2D topological insulator

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?

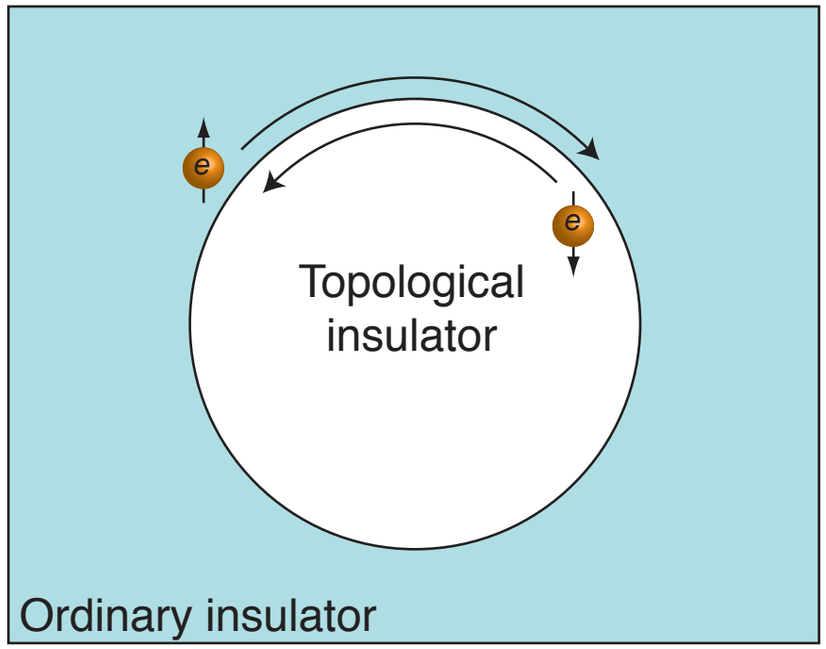
The "Chern insulator" and QSHE

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

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.

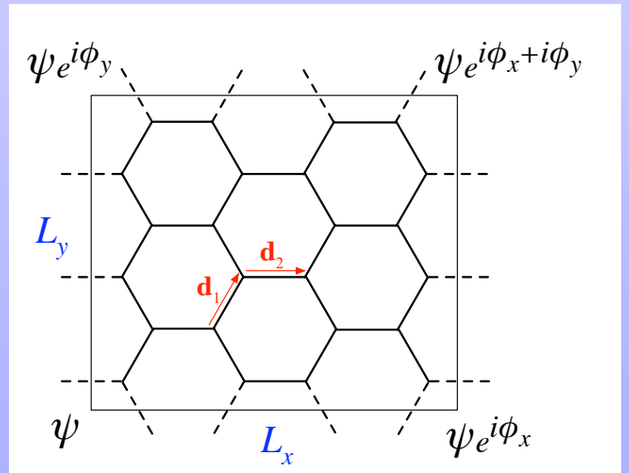
Then *SU(2)* (spin rotation symmetry) is broken, but time-reversal symmetry is not:

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



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

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

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.

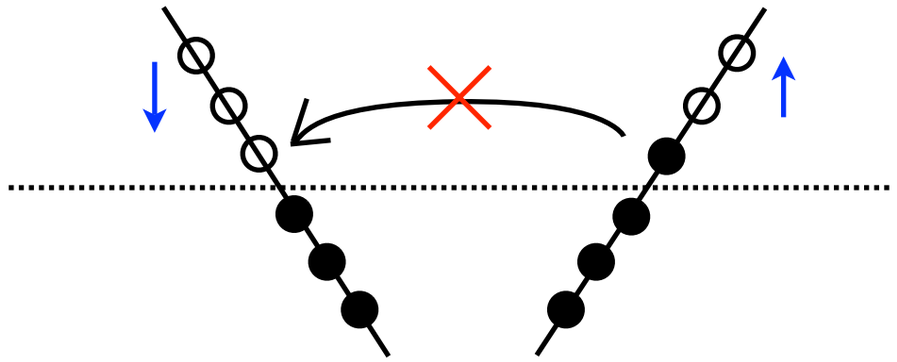
Instead, a fairly technical analysis shows

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

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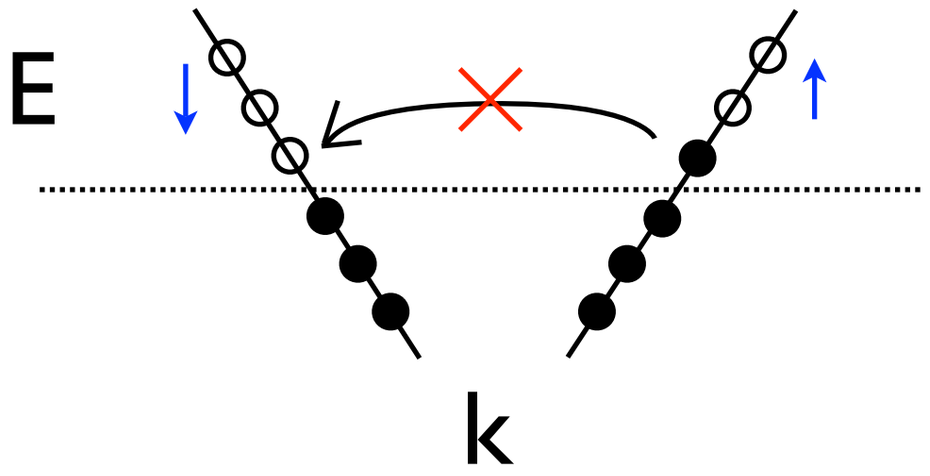
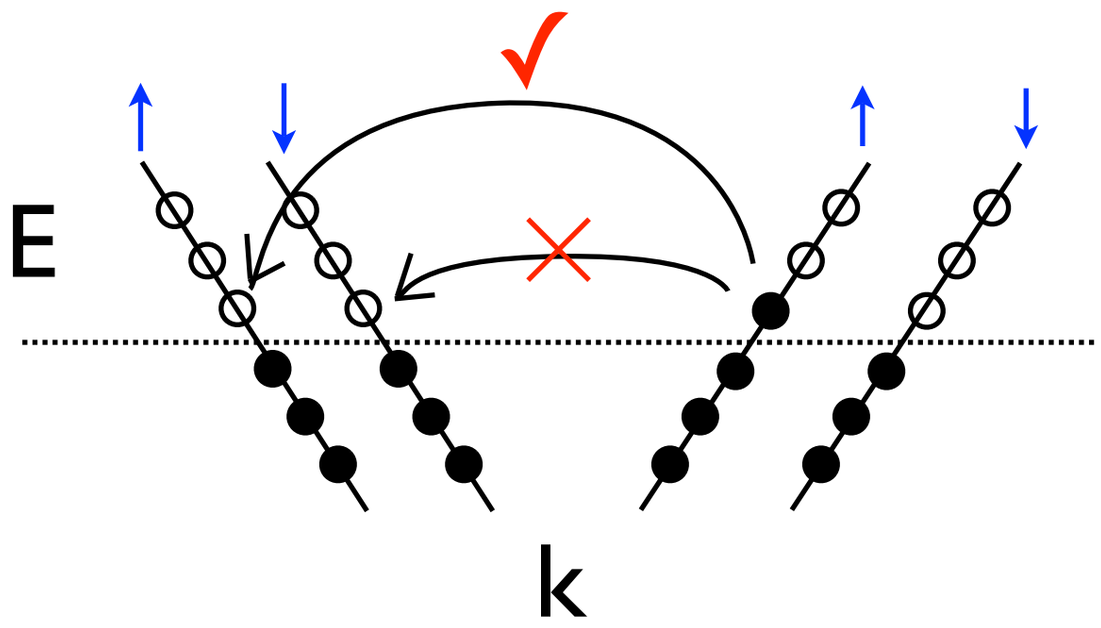


But this rule does not protect an ordinary quantum wire with 2 Kramers pairs:



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

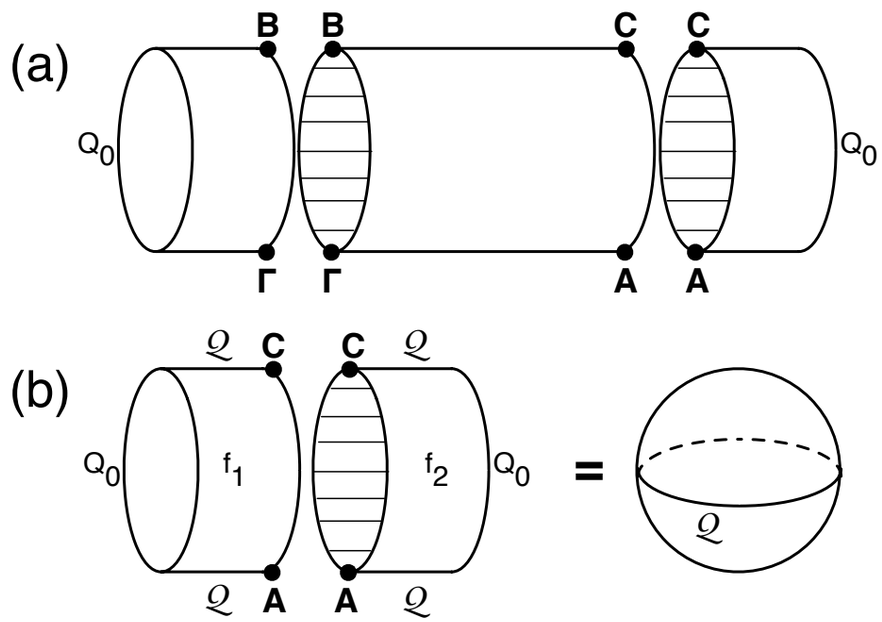
The 2D topological insulator

2. What is the Berry phase expression of the invariant?

It is an integral over *half* the Brillouin zone,

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

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 ~ 0.3 G_0)*

The 2D topological insulator

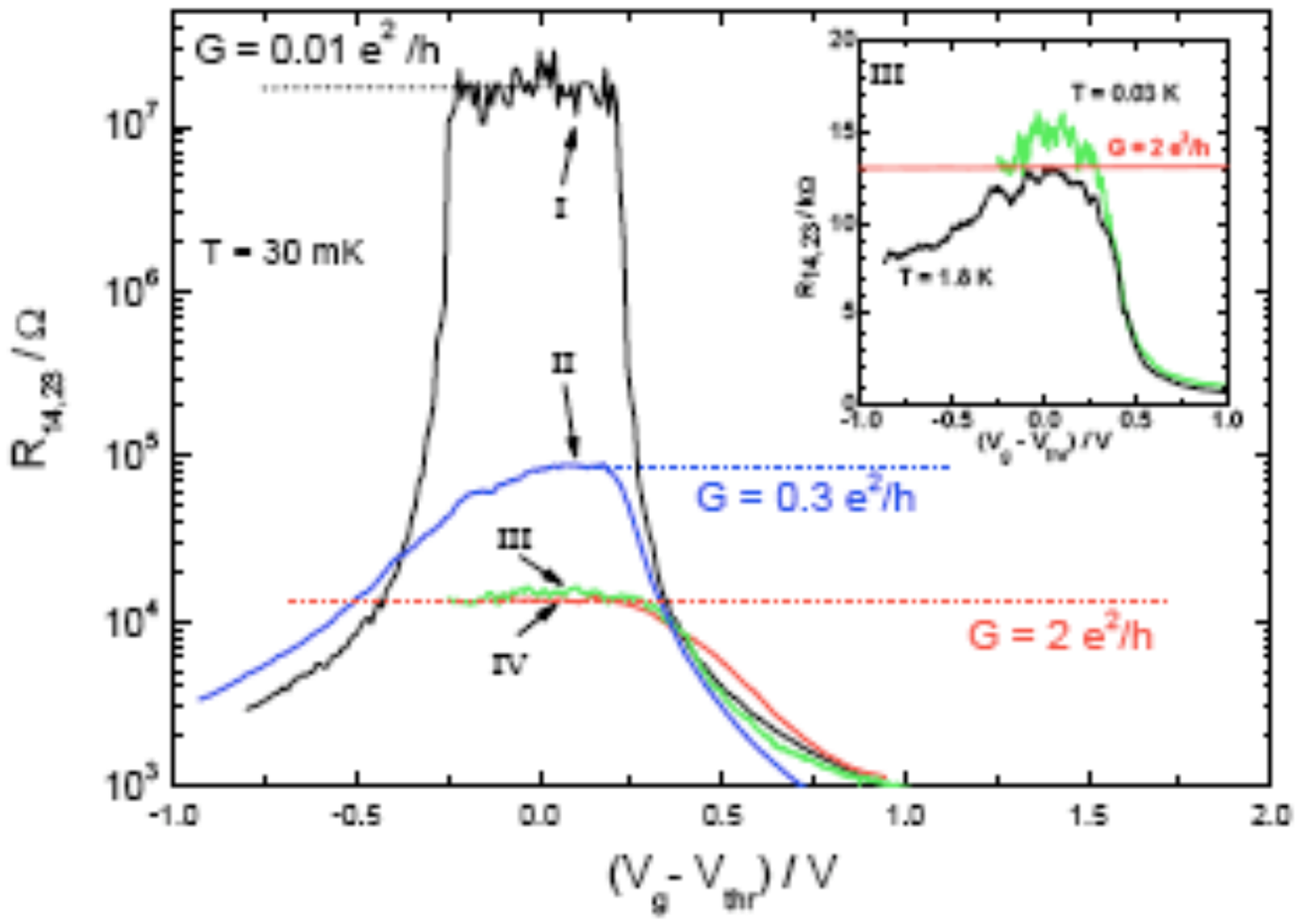
Key: the topological invariant predicts the "number of quantum wires".

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.*

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.

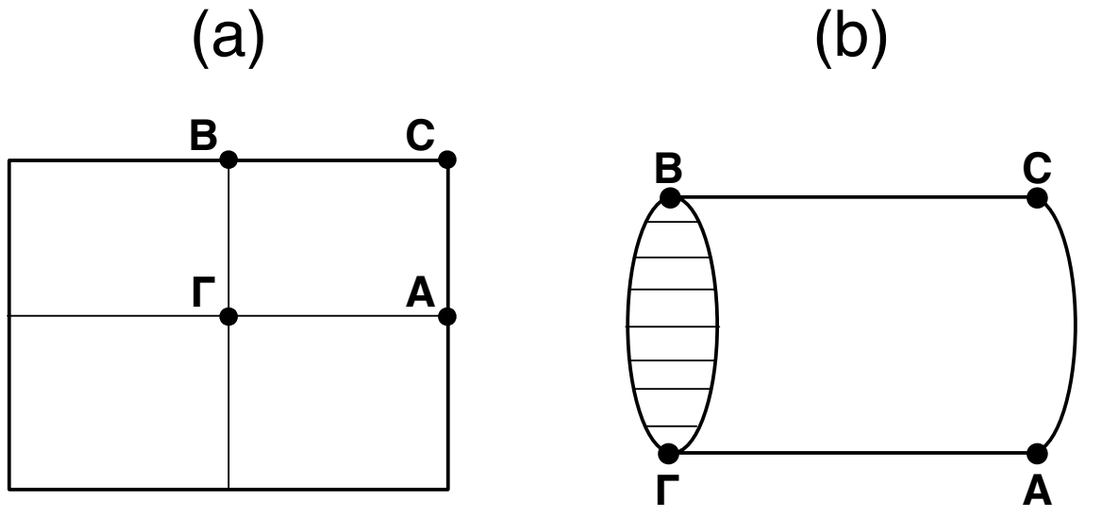
However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

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:

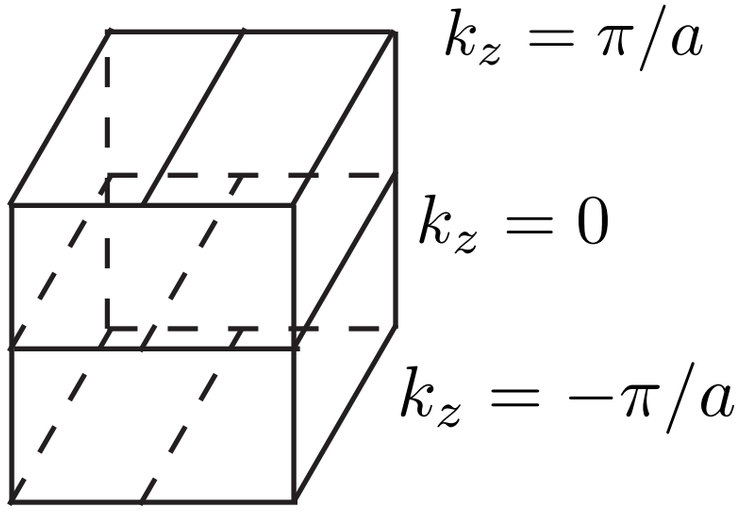
$$H(-k) = TH(k)T^{-1}$$



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

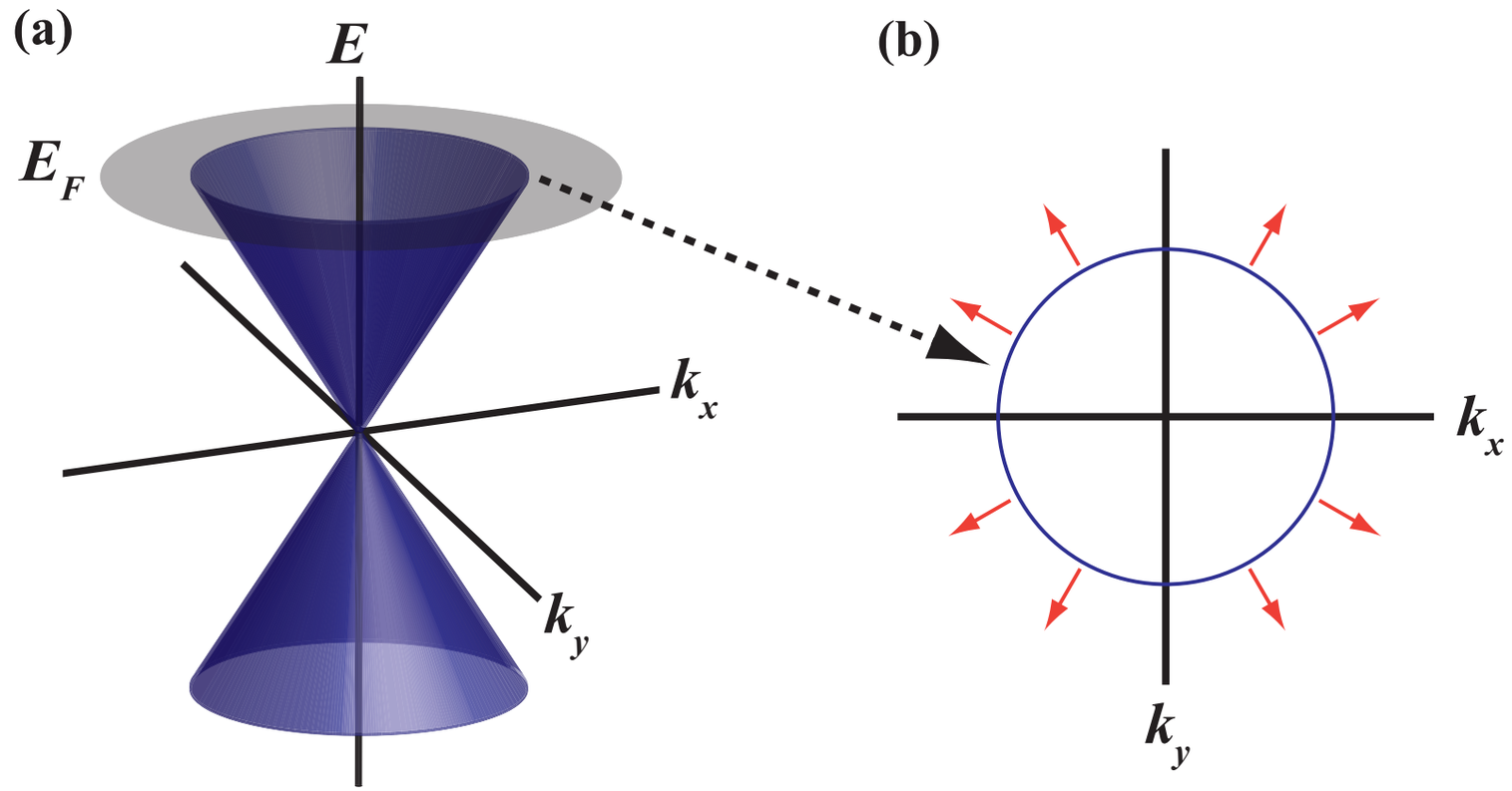


3D "strong topological insulators" go from an 2D *ordinary* insulator to a 2D *topological* insulator (or vice versa) in going from k_z=0 to k_z=±π/a.

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

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)



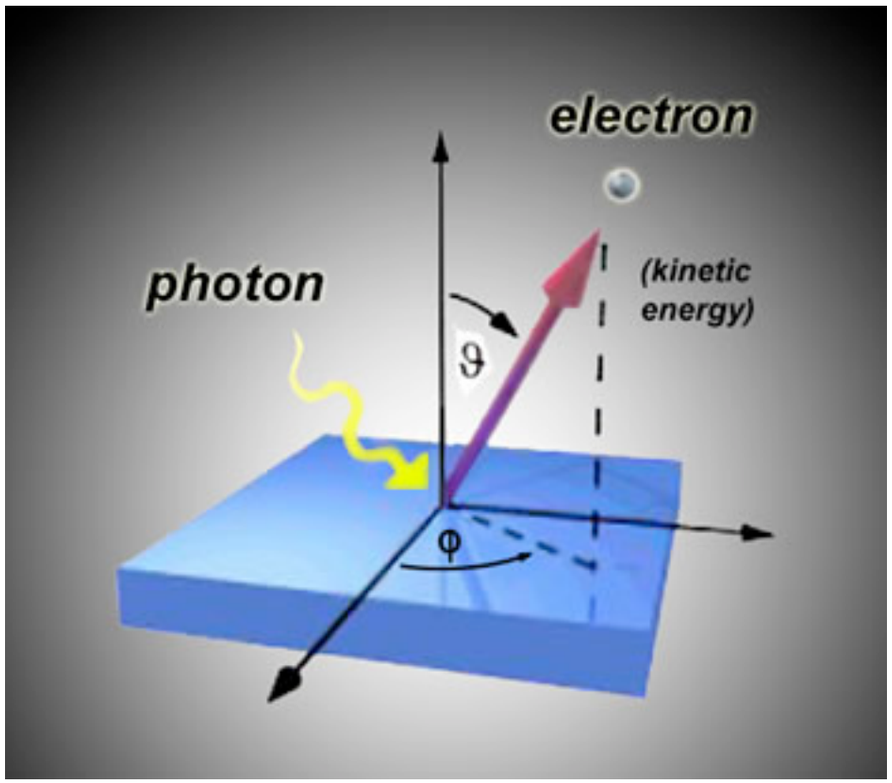
2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

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.



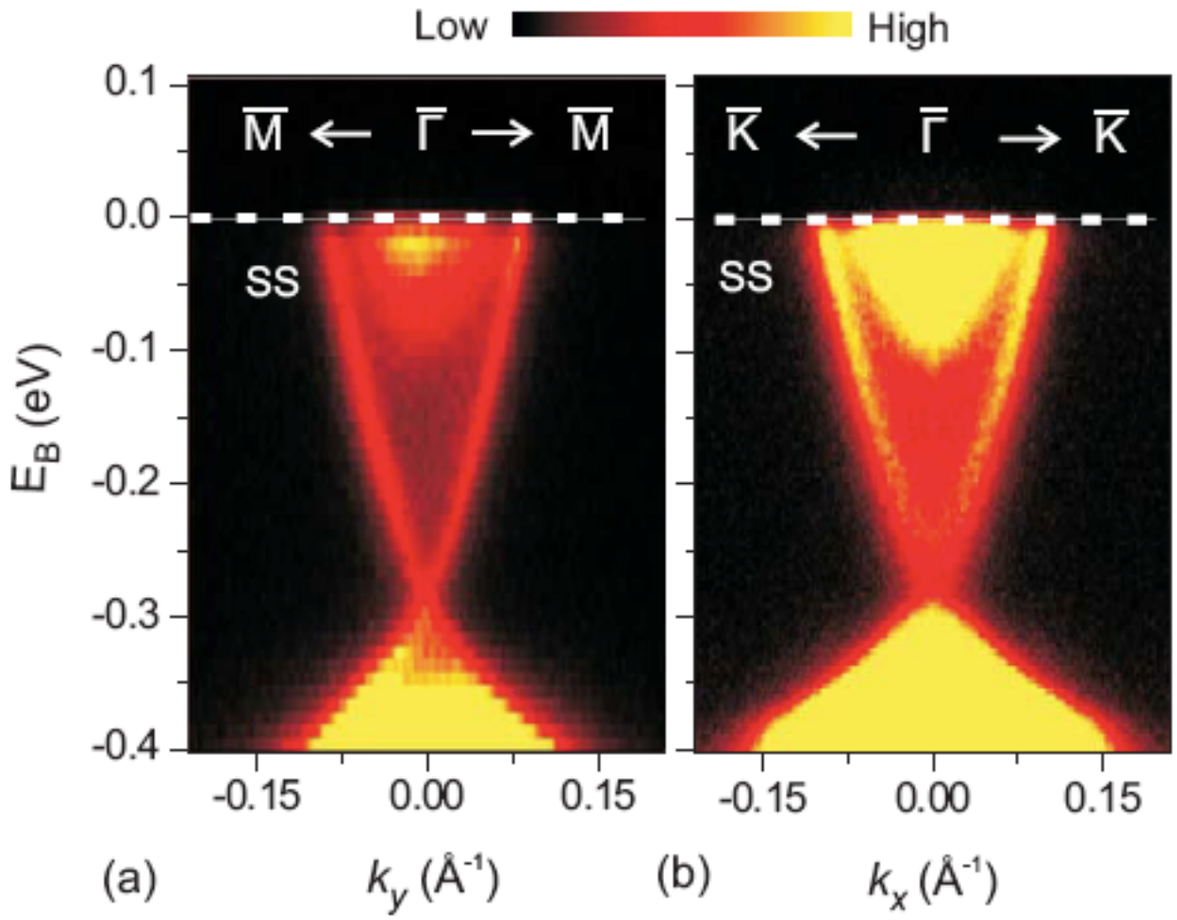
Measure as many properties as possible of the outgoing electron
to deduce the momentum, energy, and spin it had while still in the solid.

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:

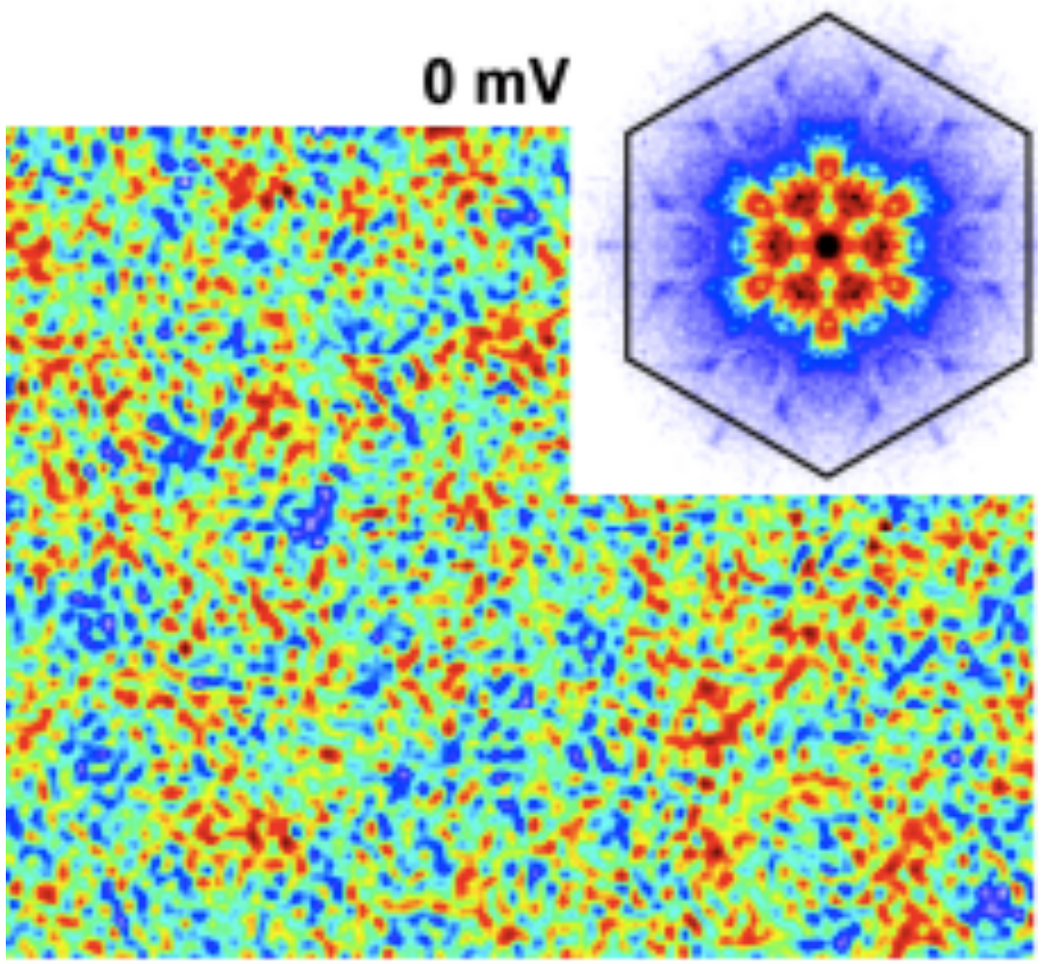


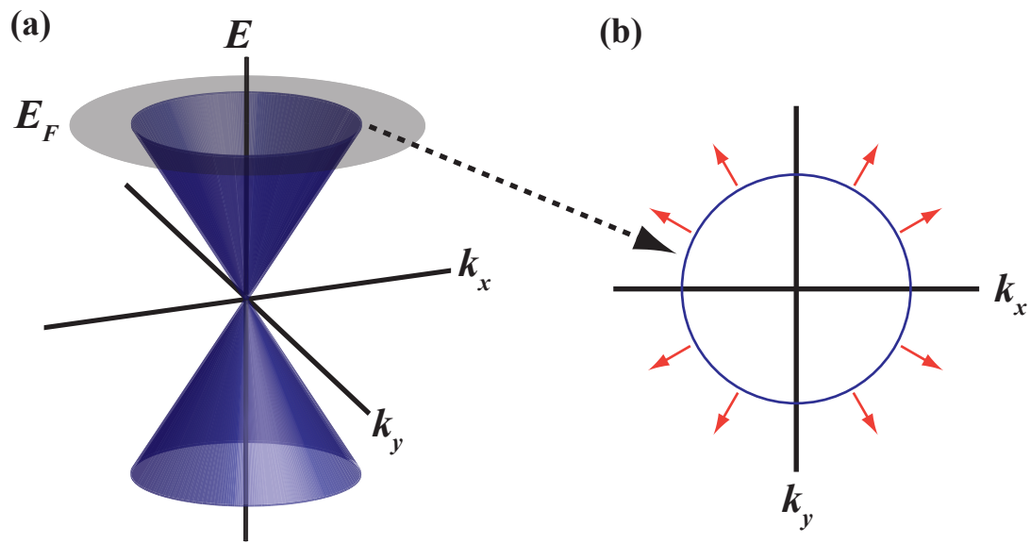
The states shown are in the "energy gap" of the bulk material--in general no states would be expected, and especially not the Dirac-conical shape.

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)

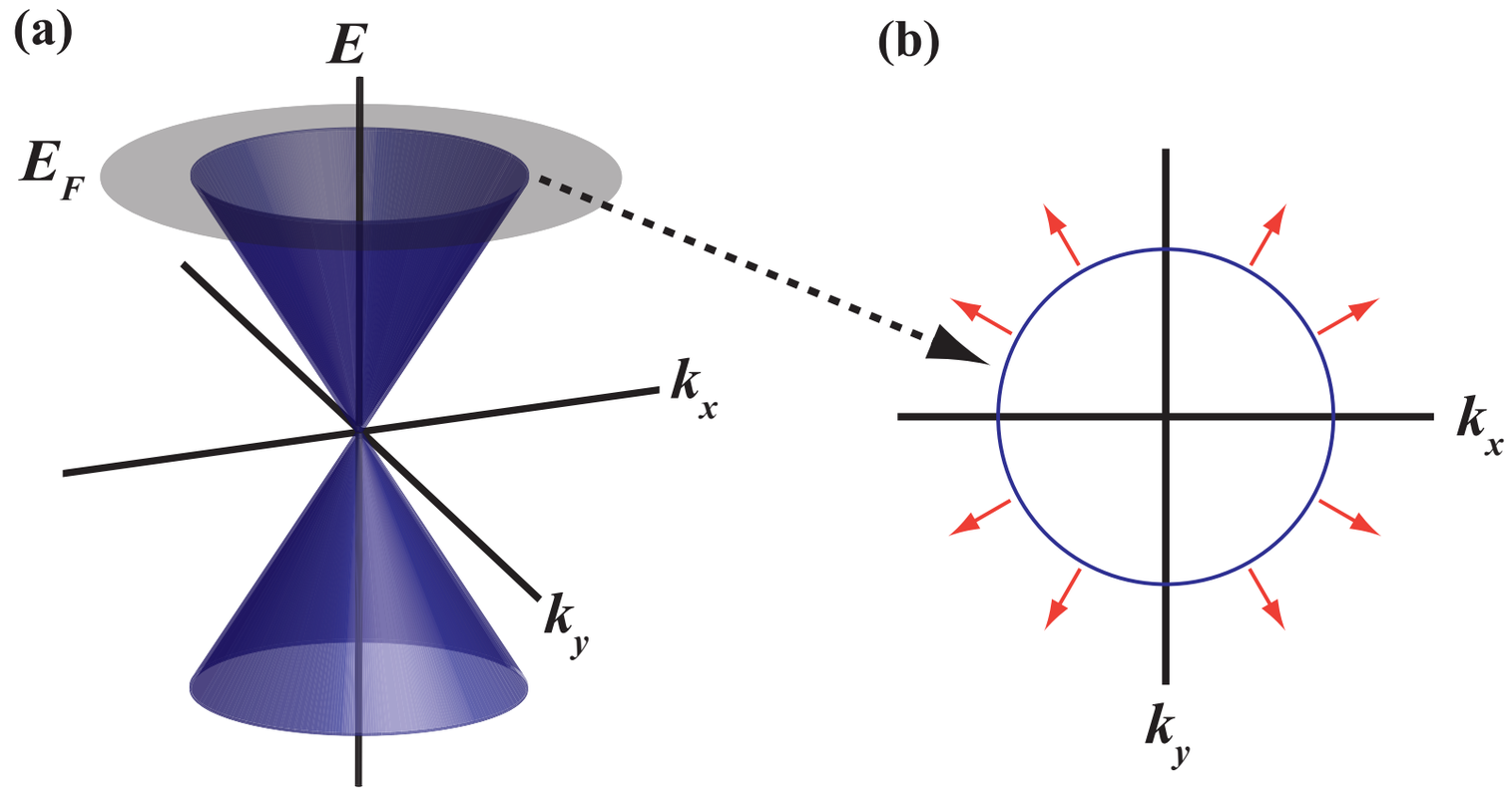




STM can see the absence of scattering within a Kramers pair (cf. analysis of superconductors using quasiparticle interference, D.-H. Lee and S. Davis).

Spintronic applications of 3D TIs

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



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 1D. In 1D, 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 SQHE? 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,

$$n = \int_0^{2\pi} \int_0^{2\pi} d\theta \, d\varphi \, \frac{1}{2\pi i} \left| \left\langle \frac{\partial \phi_0}{\partial \varphi} \middle| \frac{\partial \phi_0}{\partial \theta} \right\rangle - \left\langle \frac{\partial \phi_0}{\partial \theta} \middle| \frac{\partial \phi_0}{\partial \varphi} \right\rangle \right|$$

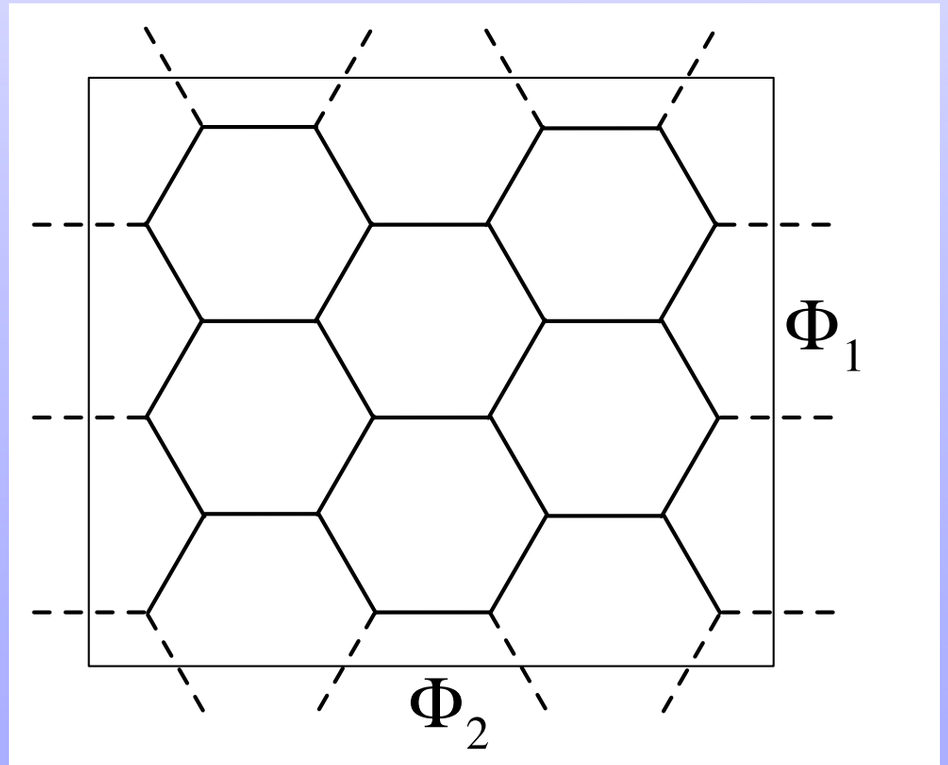
This quantity is an integer.
For T-invariant systems, all ordinary Chern numbers are zero.

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.

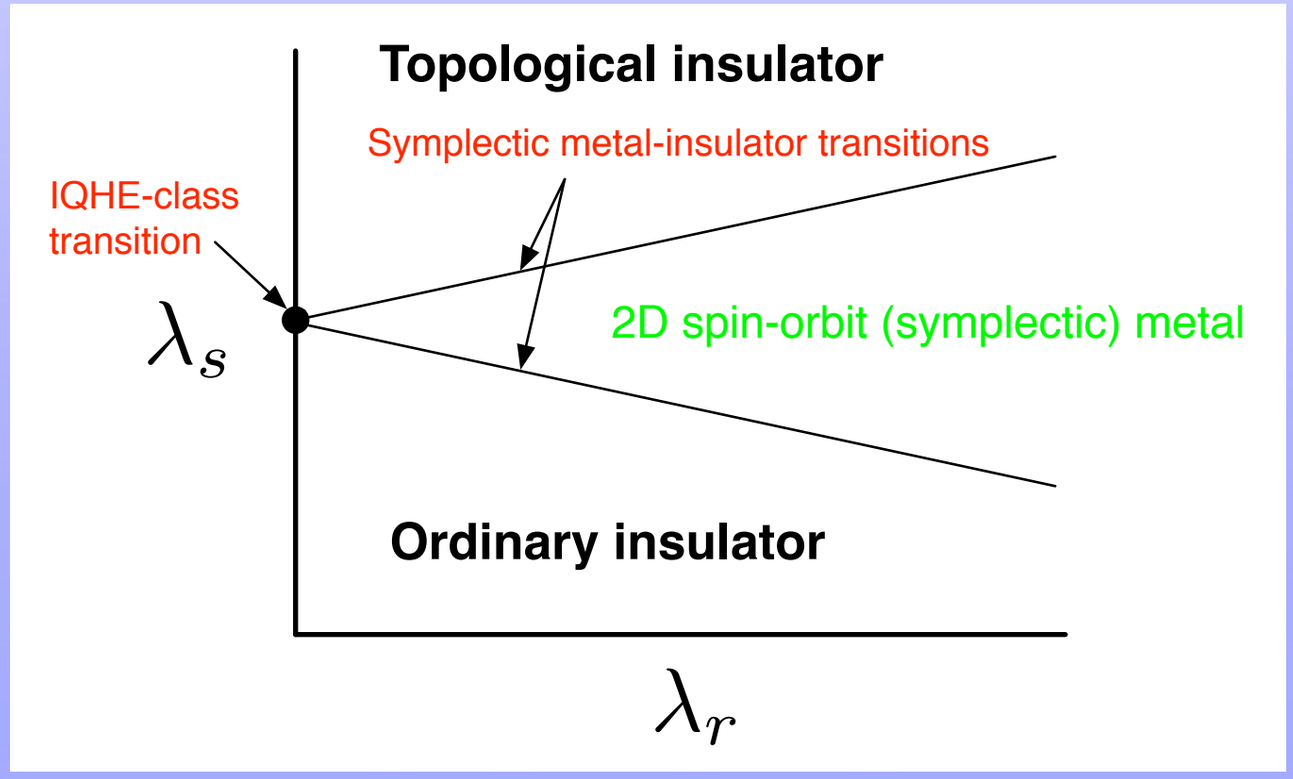
Effect of boundary phase is to shift *k*: alternate picture of topological invariant is in terms of half the (Φ_1,Φ_2) torus.

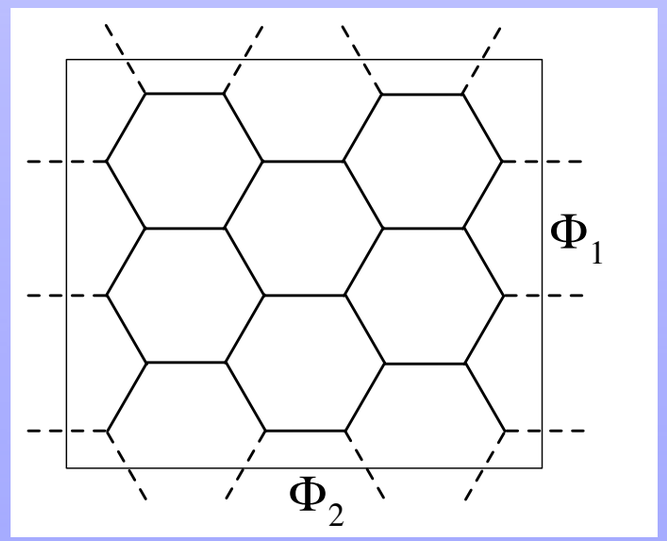


Can define Chern parities by pumping, analogous to Chern numbers, and study phase diagram w/disorder

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.





We compute this numerically using Fukui-Hatsugai algorithm (PRB 2007) to compute invariants in terms of *boundary phases* (A. Essin and JEM, PRB 2007). See also Obuse et al., Onoda et al. for other approaches with higher accuracy->scaling exponents for transitions; Ryu et al. for theory.

Summary of recent experiments

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?)

Are there more profound consequences of geometry and topologiy?
Lecture 2: Many basic phenomena in matter
Lecture 3: New types of particles, with new types of statistics
Lecture 4:The future

But first we need a few basic notions from topology.

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

What are they good for?

What's left

1. Berry phases--what do they mean?

2. Are there other ways to tell if a material is a topological insulator?

3. What's quantized in a topological insulator?

4. What do we learn about general "multiferroic" materials?

(materials that break inversion *and* time-reversal symmetries)

Outline of lecture 2

1. Intuitive picture of the Berry phase. What does it control in *insulators* and *metals*?

Insulators: Polarization, IQHE, "topological insulators", ...

Metals: New semiclassical term for electron motion.

2, How do we define Berry phases in a disordered system?

3. What is the physical effect or response that defines a topological insulator beyond single electrons? *Quantized magnetoelectric effect*

4. What do we learn about magnetoelectric effects more generally? ("multiferroic" materials)

5. Experimental probes

Berry phase review

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:

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

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

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

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".

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

How can we picture *A*?

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

To get a physical interpretation of what *A* means, note that
if we consider a plane wave exp(*i k r*), then the vector potential just gives the position **r**.

Now in a periodic crystal, the position can't be uniquely defined, but we nevertheless expect that *A* might reflect something to do with the position of the wavefunction *within the unit cell.*

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

What about non-magnetic insulators?

Electrical polarization: another simple Berry phase in solids
(Will eventually give another picture of topological insulators)

Sum the integral of *A* over bands: in one spatial dimension,

$$P = \sum_v e \int \frac{dq}{2\pi} \langle u_v(q)| - i\partial_q |u_v(q)\rangle$$

Intuitive idea: think about the momentum-position commutation relation,

$$A = \langle u_k| - i\nabla_k |u_k\rangle \approx \langle r \rangle$$

There is an ambiguity of e per transverse unit cell, the "polarization quantum."

Note: just as dA=F is a "closed form" and very useful to define Chern number, in 4 dimensions there is a "second Chern form"

Fact from cohomology:
Odd dimensions have Chern-Simons forms that have a "quantum" ambiguity;
Even dimensions have Chern forms that are quantized.

But what does *F* do?

It is useful to get some intuition about what the Berry F means in simpler physical systems first.

Its simplest consequence is that it modifies the semiclassical equations of motion of a Bloch wavepacket:

$$\frac{dx^a}{dt} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k})\frac{dk_b}{dt}.$$

a "magnetic field" in momentum space.

The anomalous velocity results from changes in the electron distribution *within the unit cell*: the Berry phase is connected to *the electron spatial location.*

Example I: the intrinsic anomalous Hall effect in itinerant magnets
still no universal agreement on its existence

Example II: helicity-dependent photocurrents in optically active materials
(Berry phases in nonlinear transport)

But what does *F* do?

Example I: the anomalous Hall effect in itinerant magnets

An electrical field **E** induces a transverse current through the anomalous velocity if *F* is nonzero averaged over the ground state.

$$\frac{dx^a}{dt} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k})\frac{dk_b}{dt}.$$

A nonzero Hall current requires T breaking; microscopically this follows since time-reversal symmetry implies

$$\mathcal{F}^{ab}(\mathbf{k}) = -\mathcal{F}^{ab}(-\mathbf{k}).$$

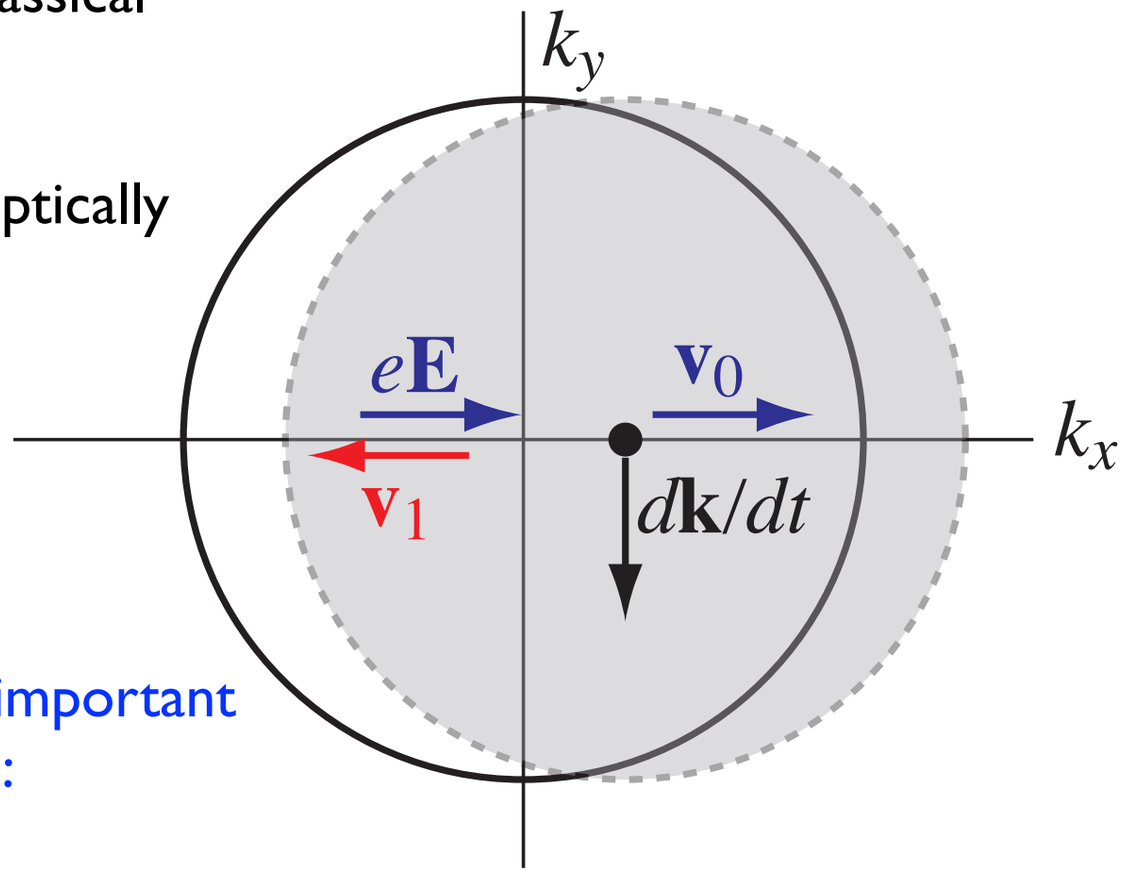
Smit's objection: in steady state the electron distribution is stationary; why should the anomalous velocity contribute at all?

(In a quantum treatment, the answer is as if *dk*/*dt* resulted only from the macroscopic applied field, which is mostly consistent with experiment)

But what does *F* do?

To try to resolve the question of what the semiclassical equation means:

Example II: helicity-dependent photocurrents in optically active materials
(Berry phases in nonlinear transport)



In a T-symmetric material, the Berry phase is still important at finite frequency. Consider circular polarization:

The small deviation in the electron distribution generated by the electrical field gives an anomalous velocity contribution that need not average to zero over the wave.

Smit vs. Luttinger

The resulting formula has 3 terms, of which one is "Smit-type" (i.e., nonzero even with the full **E**) and two are "Luttinger-type".

$$\begin{aligned}
\beta &= \frac{\partial F}{\partial k_x} \\
\mathbf{j}_{dc} &= \frac{\beta n e^3}{2\hbar^2} \frac{1}{1/\tau^2+\omega^2} \Big[i\omega (E_x E_y^* - E_y E_x^*)\hat{\mathbf{x}} \\
&\quad + 1/\tau (E_x E_y^* + E_y E_x^*)\hat{\mathbf{x}} + |E_x|^2 \hat{\mathbf{y}} \Big].
\end{aligned}$$

(JEM and J. Orenstein, 2009). The full semiclassical transport theory of this effect was given by Deyo, Golub, Ivchenko, and Spivak (arXiv, 2009).

We believe that the circularly switched term actually explains a decade of experiments on helicity-dependent photocurrents in GaAs quantum wells.

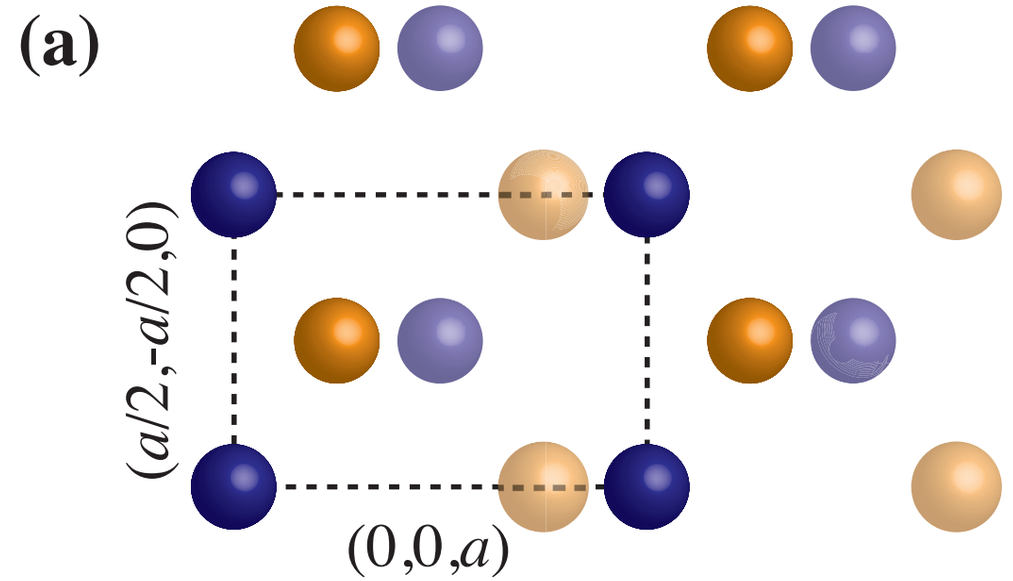
Bulk GaAs has too much symmetry to allow the effect; these quantum wells show the effect because the well confinement breaks the symmetry ("confinement-induced Berry phase").

Confinement-induced Berry phases

Bulk GaAs has too much symmetry to allow the effect; these quantum wells show the effect because the well confinement breaks the symmetry ("confinement-induced Berry phase").

Our numerics and envelope approximation suggest a magnitude of 1 nA for incident power 1W in a (110) well, which is consistent with experiments by S. D. Ganichev et al. (Regensburg).

Only one parameter of GaAs is needed to describe **F** at the Brillouin zone origin: symmetries force



$$\mathcal{F} = \lambda \left(k_x(k_y^2 - k_z^2), k_y(k_z^2 - k_x^2), k_z(k_x^2 - k_y^2) \right), \lambda \approx 410 \mathring{A}^3$$

Electrodynamics in insulators

We know that the constants ε and μ in Maxwell's equations can be modified inside an ordinary insulator.

Particle physicists in the 1980s considered what happens if a 3D insulator creates a new term ("axion electrodynamics", Wilczek 1987)

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

This term is a total derivative, unlike other magnetoelectric couplings.
It is also "topological" by power-counting.

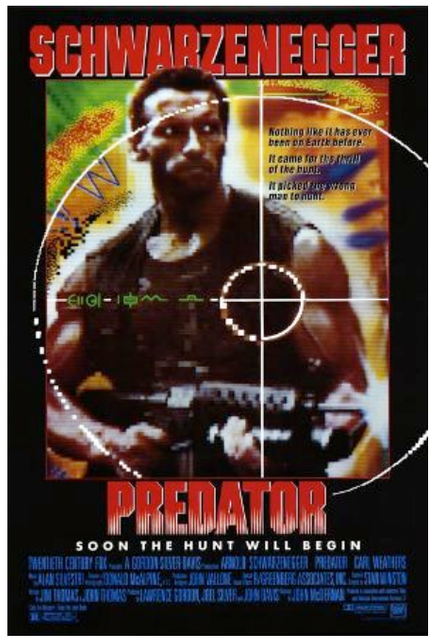
The angle θ is periodic and odd under T.

A T-invariant insulator can have *two* possible values: 0 or π.

Axion E&M, then and now

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

1987



2007

A T-invariant insulator can have *two* possible values: 0 or π.

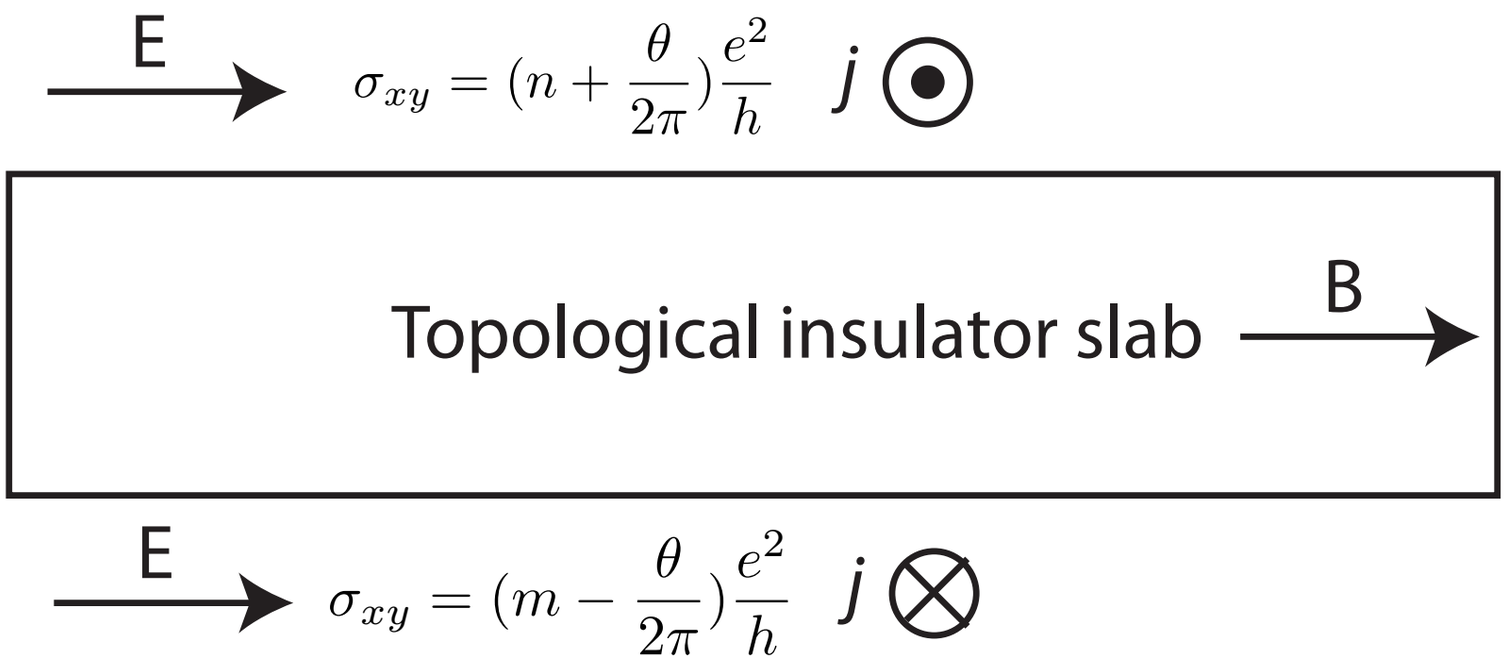
These two values correspond to ordinary and topological 3D insulators.
(Qi, Hughes, and Zhang, 2008)

Axion E&M, then and now

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

This explains a number of properties of the 3D topological insulator when its surfaces become gapped by breaking T-invariance:

Magnetoelectric effect:
applying B generates polarization P, applying E generates magnetization M)



Topological response

Idea of "axion electrodynamics in insulators"

there is a "topological" part of the magnetoelectric term

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

that is measured by the orbital magnetoelectric polarizability

$$\theta\frac{e^2}{2\pi h} = \frac{\partial M}{\partial E} = \frac{\partial}{\partial E}\frac{\partial}{\partial B}H = \frac{\partial P}{\partial B}$$

and computed by integrating the "Chern-Simons form" of the Berry phase

$$\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\ \epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k] \qquad (2)$$

(Qi, Hughes, Zhang, 2008; Essin, JEM, Vanderbilt 2009)

This integral is quantized only in T-invariant insulators, but contributes in all insulators.

Topological response

Many-body definition: the Chern-Simons or second Chern formula does not directly generalize. However, the quantity dP/dB *does* generalize:
a clue is that the "polarization quantum" combines nicely with the flux quantum.

$$\frac{\Delta P}{B_0} = \frac{e/\Omega}{h/e\Omega} = e^2/h.$$

So dP/dB gives a *bulk*, *many-body* test for a topological insulator.

(Essin, JEM, Vanderbilt 2009)

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

= contact resistance in 0D or 1D
= Hall conductance quantum in 2D
= magnetoelectric polarizability in 3D

Orbital magnetoelectric polarizability

One mysterious fact about the previous result:

We indeed found the "Chern-Simons term" from the semiclassical approach.

But in that approach, it is not at all clear why this should be the only magnetoelectric term from orbital motion of electrons.

More precisely: on general symmetry grounds, it is natural to decompose the tensor into *trace* and *traceless* parts

$$\frac{\partial P^i}{\partial B^j} = \frac{\partial M_j}{\partial E_i} = \alpha^i_j = \tilde{\alpha}^i_j + \alpha_\theta \delta^i_j.$$

The traceless part can be further decomposed into symmetric and antisymmetric parts.
(The antisymmetric part is related to the "toroidal moment" in multiferroics;
cf. M. Fiebig and N. Spaldin)

But consideration of simple "molecular" models shows that even the trace part is not always equal to the Chern-Simons formula...

Orbital magnetoelectric polarizability

Computing orbital dP/dB in a fully quantum treatment reveals that there are additional terms in general. (Essin et al., 1002.0290)

For dM/dE approach and numerical tests, see Malashevich, Souza, Coh, Vanderbilt, 1002.0300.

$$
\begin{aligned}
\alpha_j^i &= (\alpha_I)_j^i + \alpha_{CS}\delta_j^i \\
(\alpha_I)_j^i &= \sum_{\substack{n\,\mathrm{occ} \\ m\,\mathrm{unocc}}} \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \mathrm{Re}\left\{ \frac{\langle u_{n\mathbf{k}}|e\,r_{\mathbf{k}}^i|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|e(\mathbf{v}_{\mathbf{k}}\times r_{\mathbf{k}})_j - e(r_{\mathbf{k}}\times\mathbf{v}_{\mathbf{k}})_j - 2i\partial H'_{\mathbf{k}}/\partial B^j|u_{n\mathbf{k}}\rangle}{E_{n\mathbf{k}} - E_{m\mathbf{k}}} \right\} \\
\alpha_{CS} &= -\frac{e^2}{2\hbar}\epsilon_{abc}\int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\,\mathrm{tr}\left[\mathcal{A}^a\partial^b\mathcal{A}^c - \frac{2i}{3}\mathcal{A}^a\mathcal{A}^b\mathcal{A}^c\right].
\end{aligned}
$$

The "ordinary part" indeed looks like a Kubo formula of electric and magnetic dipoles.

Not inconsistent with previous results:
in topological insulators, time-reversal means that only the Berry phase term survives.

There is an "ordinary part" and a "topological part", which is scalar but is the only nonzero part in TIs. But the two are not physically separable in general.
Both parts are nonzero in multiferroic materials.

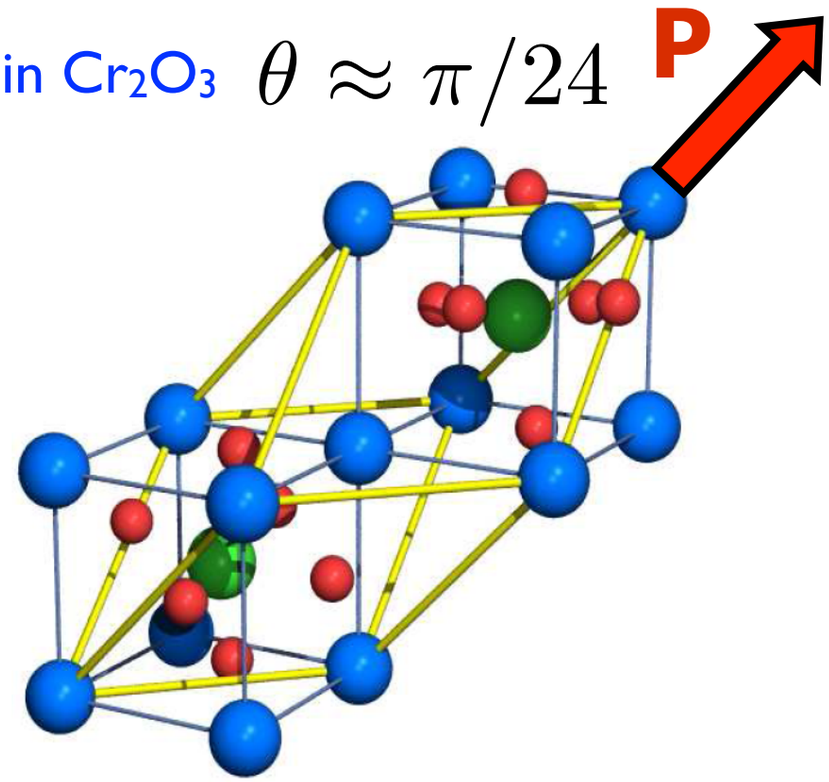
Magnetoelectric theory: a spinoff of TIs

This leads to a general theory for the orbital magnetoelectric response tensor in a crystal, including contributions of all symmetries (Essin, Turner, Vanderbilt, JEM, 2010).

It is not a pure Berry phase in general, but *it is in topological insulators*.

Such magnetoelectric responses have been measured, e.g., in Cr_2O_3 (Obukhov, Hehl, et al.).

$\theta \approx \pi/24$



Example of the ionic "competition": $BiFeO_3$

Can make a 2x2 table of "magnetoelectric mechanisms": (ignore nuclear magnetism)

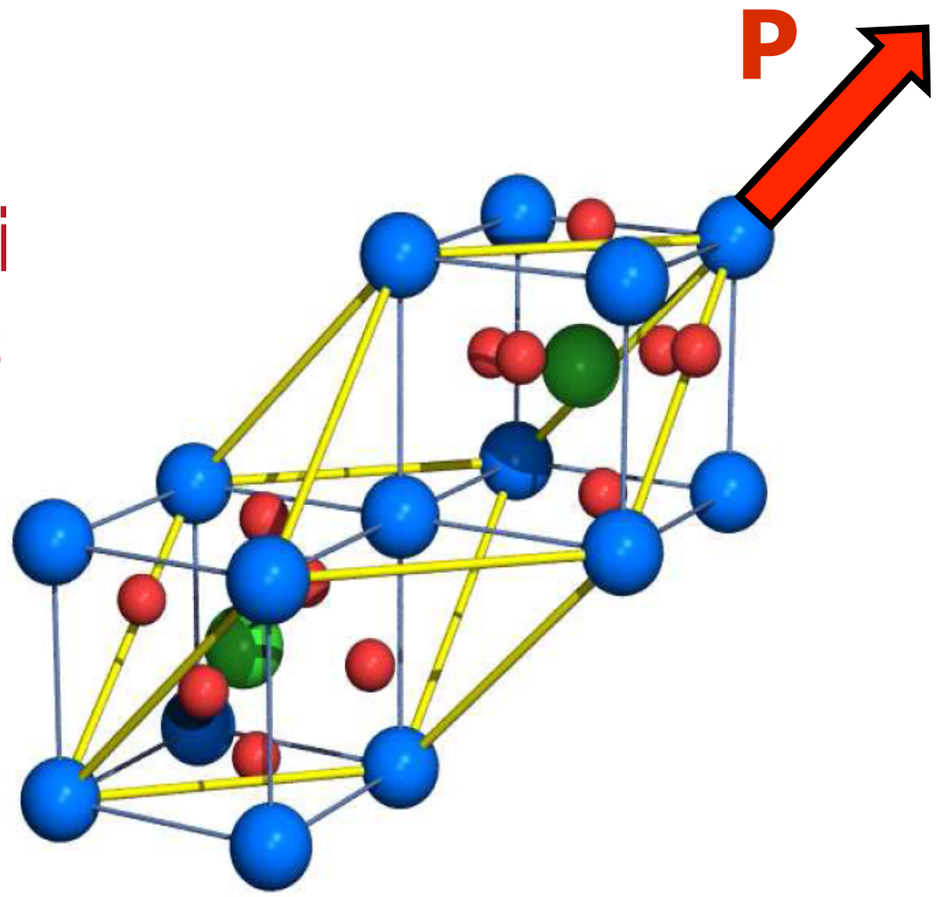
electronic P, orbital M	ionic P orbital M
electronic P, spin M	ionic P spin M

electronic P effects (left column) should be faster and less fatiguing than magnetoelectric effects requiring ionic motion.

The competition:
$BiFeO_3$, a high-T multiferroic
Coupled polar (P), antiferromagneti (L), and ferromagnetic (M) orders

$BiFeO_3$ BULK

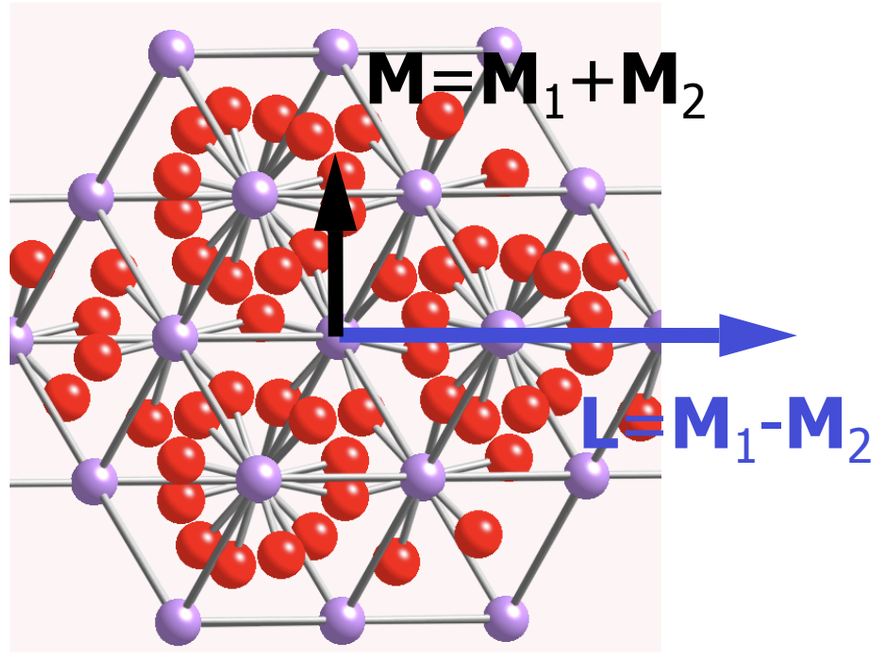
- **Rhombohedral R3c: a=3.96Å, α=89.46º**
- **No inversion symmetry, but "close"**
- **T_N~ 650K; T_C ~ 1120K**
- **Spiral, canted AFM order**
- **P ~ 6 $\mu C/cm^2$**



Figs. courtesy R. Ramesh

$BiFeO_3$ FILM on (100) $SrTiO_3$

- **Tetragonal distortion a=3.91Å, c=4.06Å**
- **Homogeneous, canted AFM order**
- **Giant ME effect: P ~ 90 $\mu C/cm^2$**



Electrical coupling to fast (AF) spin waves

(R. de Sousa and JEM, PRB 08, PRL 09)

Picturing a topological insulator

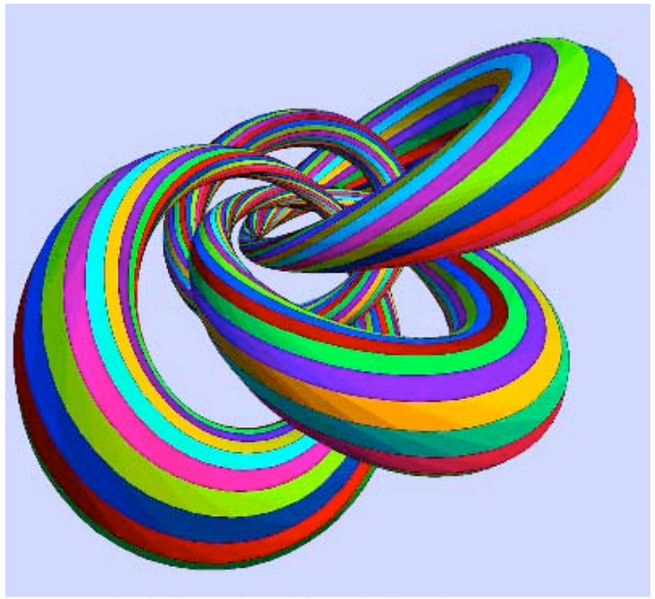
A question: why don't you just draw a topological band structure?

$$\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\ \epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k]$$

The "simplest" topological insulator where this Chern-Simons type of integral is nonzero breaks time-reversal and has only one occupied band.

It comes from making a band structure based on the "Hopf map" from the unit sphere in 4d to the unit sphere in 3d. (JEM, Ran, Wen 08)

$$\begin{aligned} S^3 &\rightarrow S^2 \\ \mathbf{z}^\dagger\sigma_i\mathbf{z} &= n_i \\ |\mathbf{z}|^2 &= 1 \rightarrow \mathbf{n}^2 = 1 \end{aligned}$$



"Hopf Fibered Linked Tori," by The 3DXM Consortium

The "real" T-invariant topological insulator has ≥2 occupied bands; harder to draw.

Outline of lecture III

Interactions and new particles

Topological mechanism for emergence of new particles

Alternative to standard mechanisms, e.g., establish an order parameter and "Goldstone bosons" (e.g., phonon)

1. Anyonic (fractional statistics) quasiparticles in the FQHE

2. Majorana fermions in non-Abelian FQHE and p+ip superconductor

INTERLUDE

3. New states/materials with interactions

Application I:

"Advanced" topological order and quantum computing

A history of theoretical efforts to understand quantum Hall physics:

1. Integer plateaus are seen experimentally (1980).

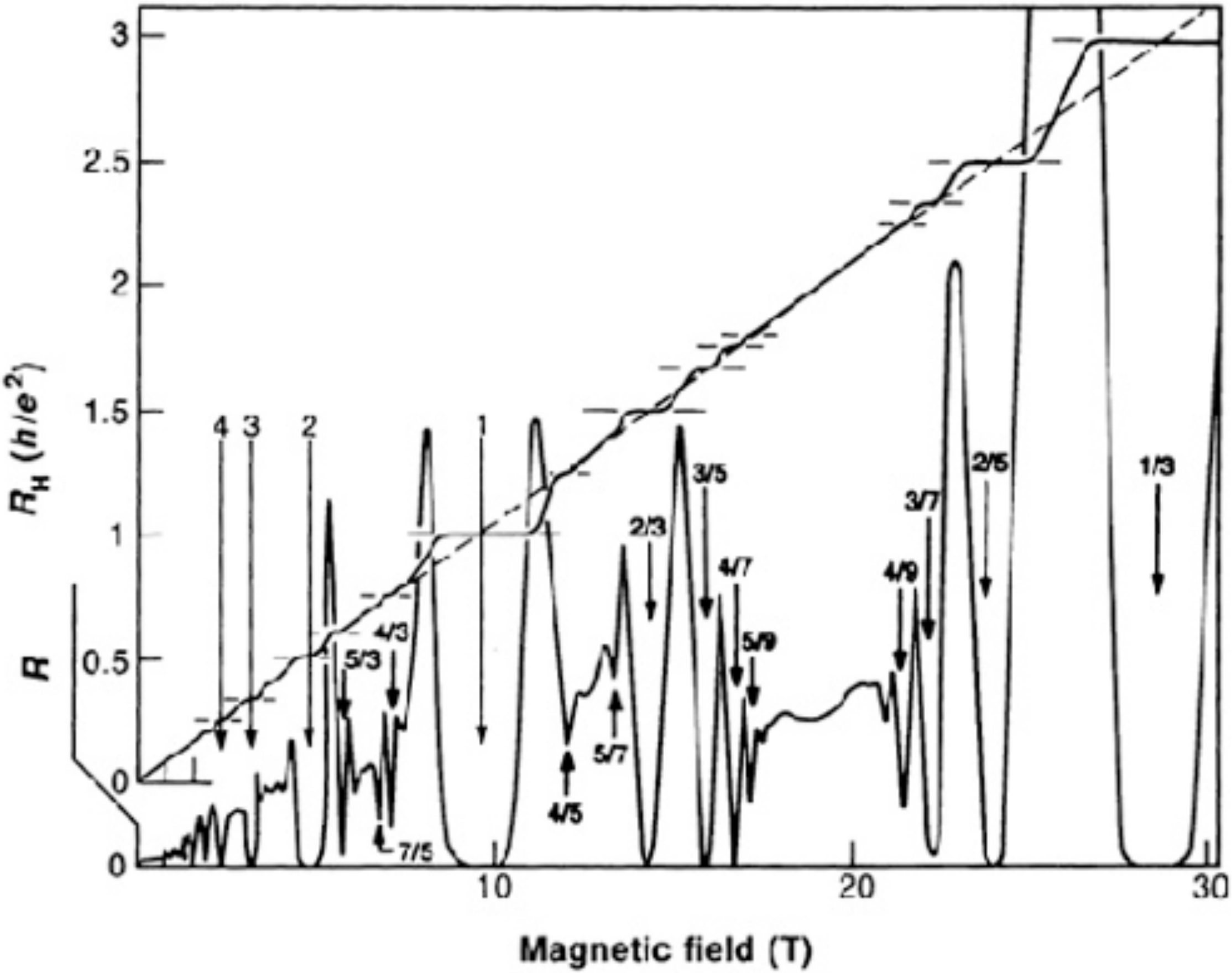
Theorists find profound explanation why integers will always be seen.
Their picture involves nearly free electrons with ordinary fermionic statistics.

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?


R_H (h/e^2)
R
3
2.5
2
1.5
1
0.5
0
0
4
3
2
1
5/3
4/3
7/5
4/5
5/7
2/3
3/5
4/7
5/9
3/7
4/9
2/5
1/3
10
20
30
Magnetic field (T)

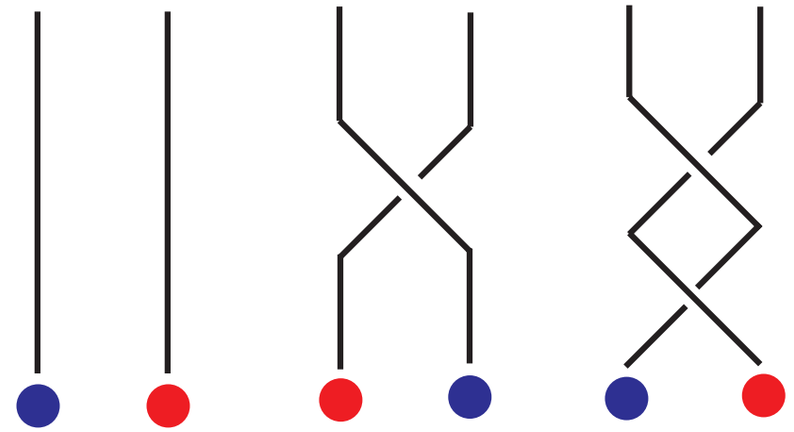
Statistics in 2D

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.



$$e^{i\theta}$$

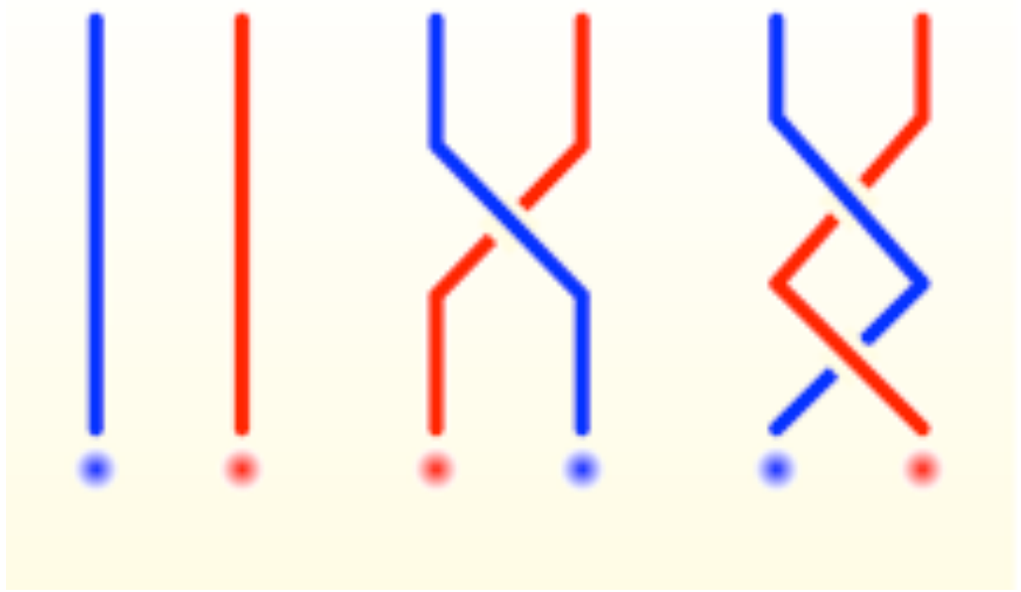
Most fractional quantum Hall states, such as the Laughlin state, host "quasiparticles" with anyonic statistics.

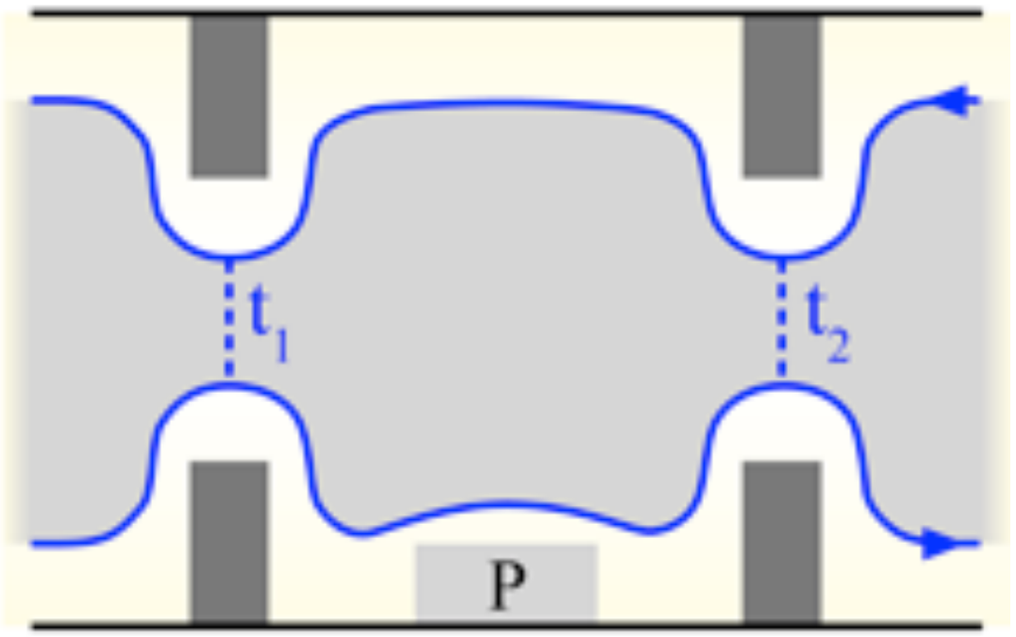
Degenerate ground states

A beautiful wavefunction is likely to describe the ground state at filling 5/2.
(Greg) Moore and Read, 1990.

The 5/2 state becomes degenerate when quasiparticles are added. Braiding quasiparticles can act as a *matrix on the space of ground states*.

Mathematically, the braid group with more than 3 particles is "non-Abelian": different exchanges can be described by non-commuting matrices.





The non-Abelian statistics at 5/2 may have been seen experimentally earlier this year.
(Willett et al., 2009)

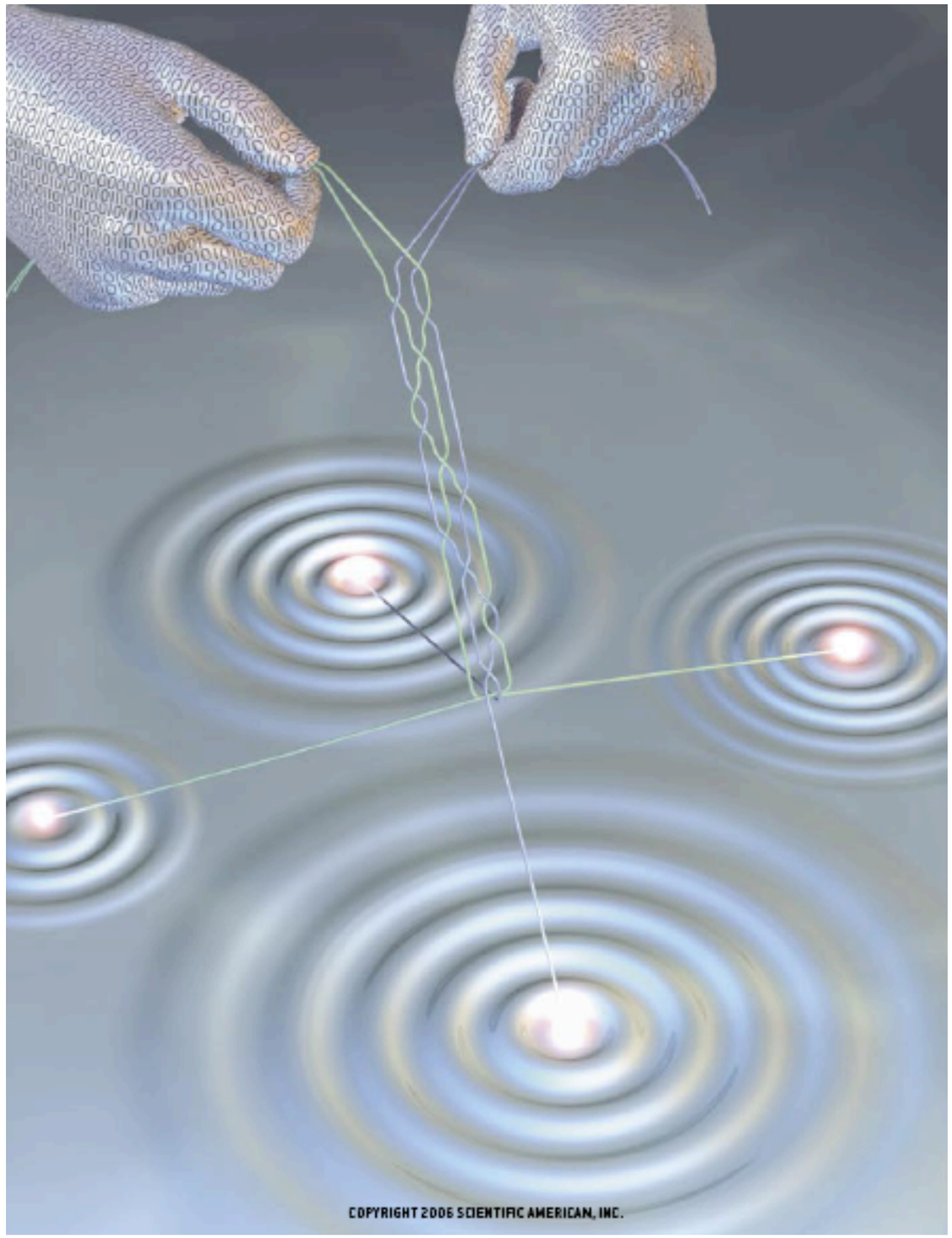
Topological quantum computing

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.

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



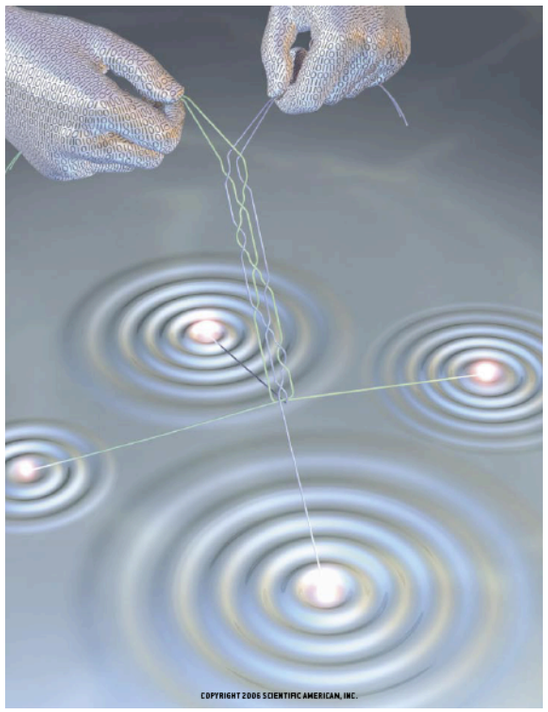
Quantum computing and memory

Majoranas for memory: 1 spinless Dirac fermion = one "qubit":
there are two states, occupied and empty

$$\gamma_1 = (c^\dagger + c), \quad \gamma_2 = i(c^\dagger - c)$$

Majoranas alone might not be quite good enough for a universal "quantum computer"--not enough operations in the braid group?

Can either try to fix this or try to find more complex states with a "universal" representation of the braid group (12/5, 4/7)



New particles from interactions using topological insulators

I. Correlation and new particles:
There are two ways to make "Majorana fermions" from topological insulators:

Method I: start from a different "universality class", a topological *superconductor* driven by interactions (3He is an example)

Method II: build the Majorana fermions using "ordinary" topological insulators and "normal" superconductors

2. Can make a new type of vortex just by biasing a thin film of topological insulator.

Proximity effect and quantum computing

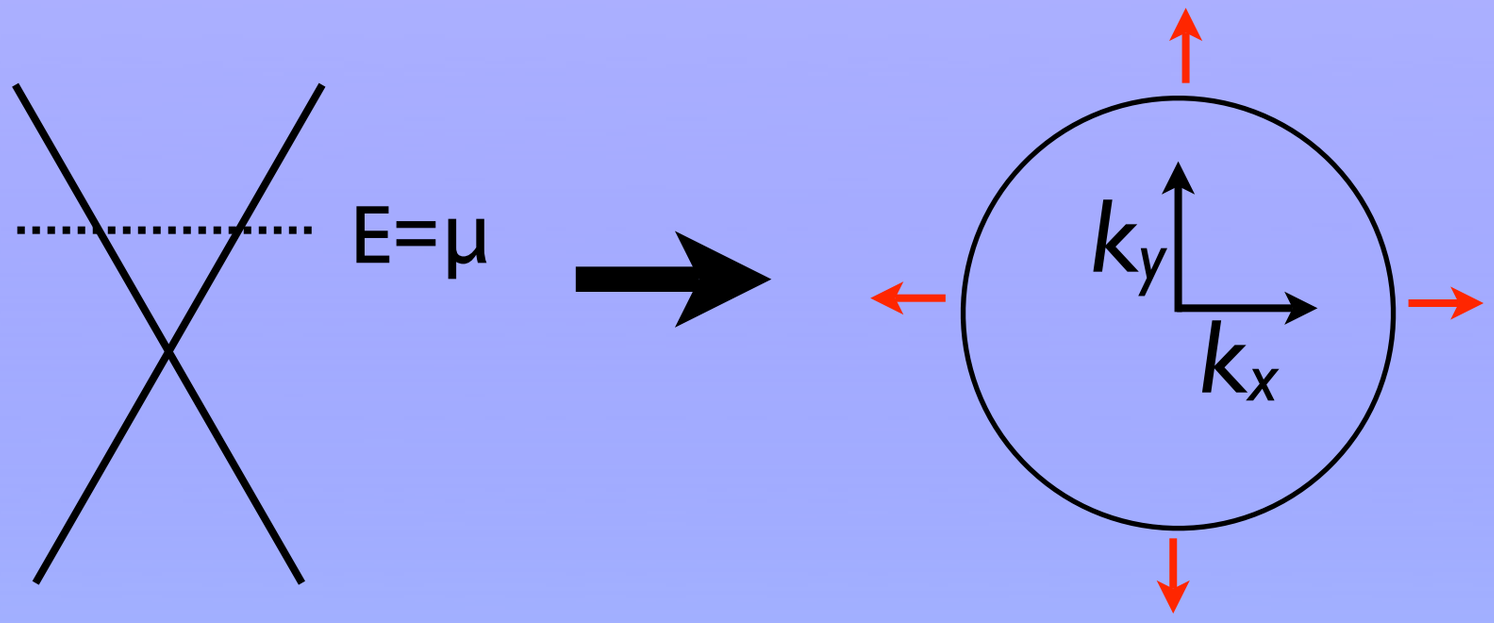
A natural question is whether the surface of a Z2 topological insulator is stable beyond single-particle models.

Time-reversal-breaking perturbations (coupling to a magnetic material or magnetic field) certainly can gap the surface modes.

What about coupling to a superconductor?

Idea: an s-wave proximity effect term $H = \sum_{\mathbf{k}} (\Delta c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + h.c.)$

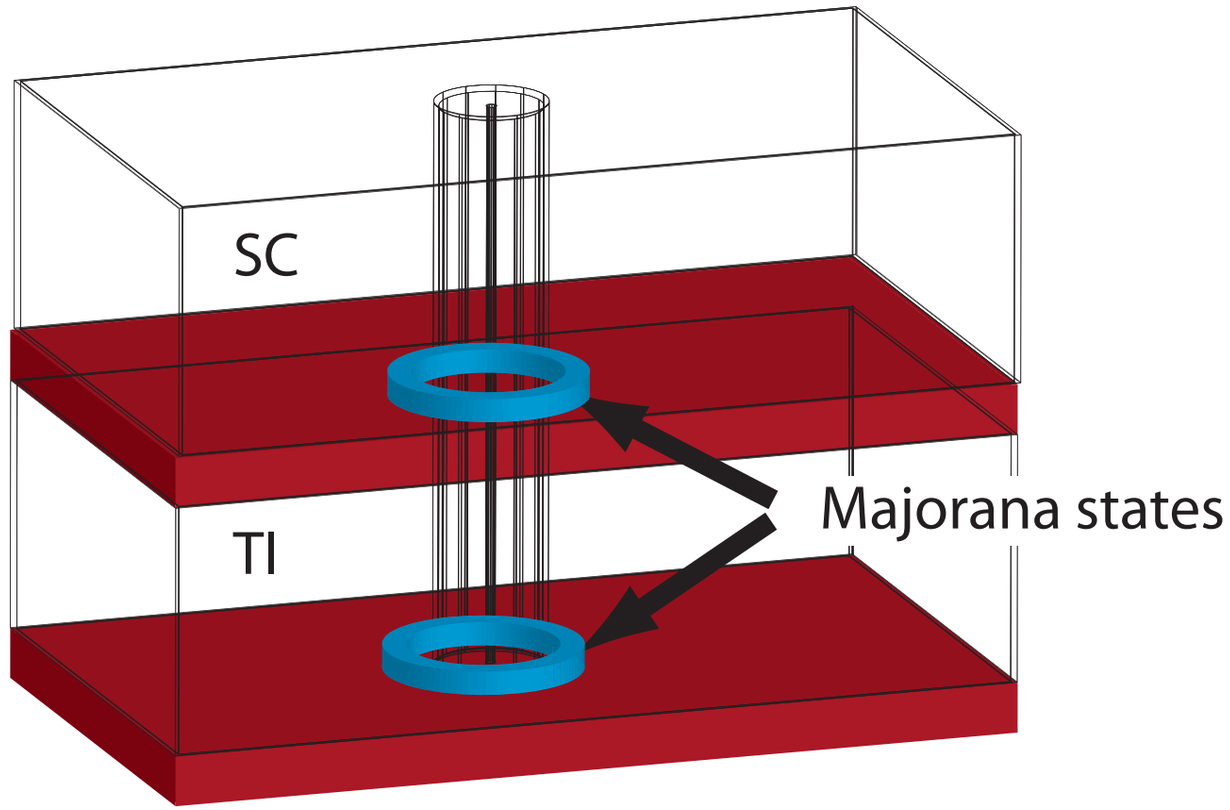
couples within the low-energy chiral fermion, and hence gives a "spinless" p-wave superconductor (Fu and Kane, PRL 2007).



Topological quantum computing

It turns out 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.)

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).



(Recent theoretical work by Sau et al. (Das Sarma) suggests that one doesn't even need a topological insulator. Another piece of breaking news: FQHE observed in graphene.)

“Interacting” topological insulators

There may be many topological insulators in correlated materials classes:

Topological superconductor? (Cu-doped Bi2Se3)

“Topological antiferromagnets”: GdPtBi? (Mong, Essin, JEM)

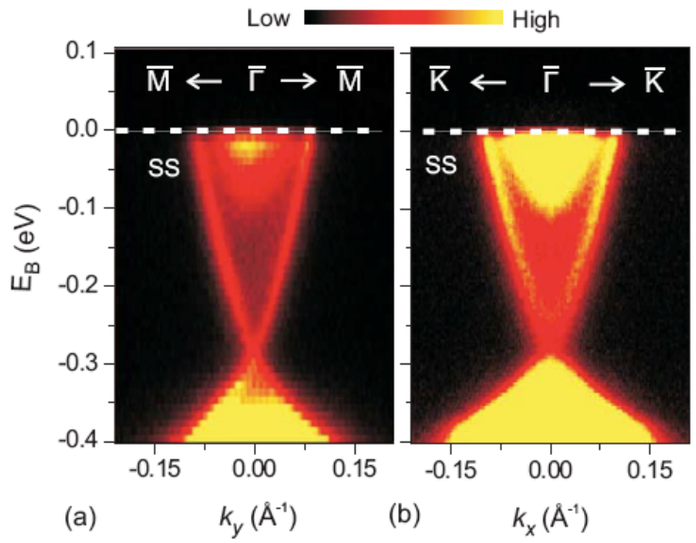
Topological Kondo insulators (Coleman et al.)

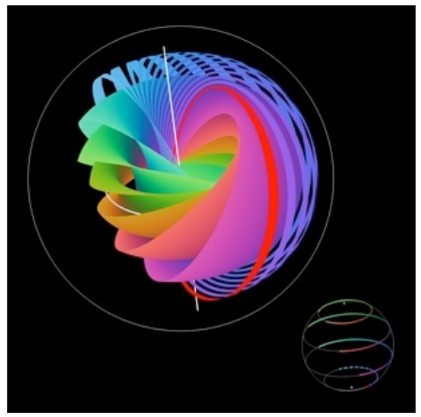
Topological Mott insulator (TI of spinons) (Pesin and Balents in 3D; Raghu et al. in 2D)

What about interactions in existing materials?

The future

1. "Topological insulators" exist in two and three dimensions in zero magnetic field.





In the 2D case, they have surface Dirac fermions with an unusual spin structure.

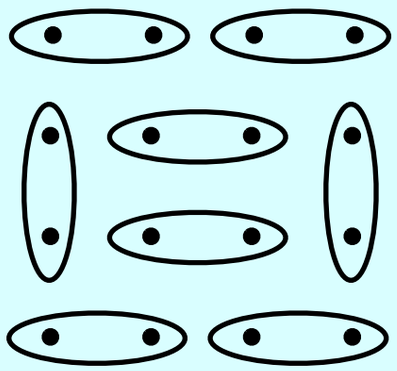
Are there correlated topological insulators and superconductors?
Are there "fractional" topological insulators?

Can we use these materials to create new particles?

Topological spin liquids: quantum Dimer model

$$|\psi_0\rangle = \frac{1}{\sqrt{Z_c}} \int (d\phi)\, e^{-S(\{\phi\})/2} |\{\phi\}\rangle.$$

An example of such a quantum critical point:
the "Rokhsar-Kivelson" point of the square lattice quantum dimer model



Hilbert space basis =
dimer coverings

Some uses of RK points and quantum dimer models:
1. Solvable z=2 quantum critical points in 2D
2. Quantum spin liquid on triangular lattice (Moessner & Sondhi), from quantum Monte Carlo numerics. Four-fold topological ground state degeneracy.

$$H = -t(\text{flip plaquettes with parallel dimers}) + V(\text{count flippable plaquettes})$$

$$H = -t \sum \left(|\square\rangle\langle| \;\; || + || \;\; |\rangle\langle\square| \right) + V \sum \left(|\square\rangle\langle\square| + || \;\; |\rangle\langle| \;\; || \right)$$

Conformal quantum critical points

$$|\psi_0\rangle = \frac{1}{\sqrt{Z_c}} \int (d\phi)\, e^{-S(\{\phi\})/2} |\{\phi\}\rangle.$$

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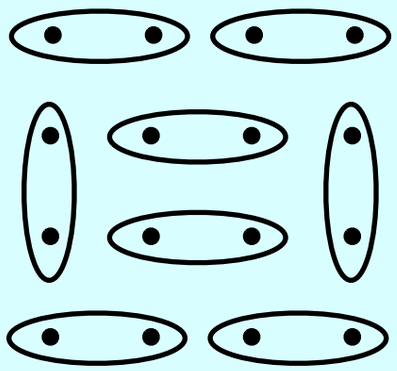

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2D conformal quantum critical points

Example: critical point of quantum dimer model
Hilbert space basis: classical dimer coverings of square lattice

$$H = -t(\text{flip plaquettes with parallel dimers}) + V(\text{count flippable plaquettes})$$

$$H = -t \sum \left(|\square\rangle\langle| \; || + || \; |\rangle\langle\square| \right) + V \sum \left(|\square\rangle\langle\square| + || \; |\rangle\langle| \; || \right)$$

$$H = \begin{pmatrix} n_1 V & -t & 0 & 0 & -t & \dots \\ -t & n_2 V & -t & 0 & 0 & \dots \\ 0 & -t & n_3 V & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

2D conformal quantum critical points

Resulting form of Hamiltonian matrix:

$$H = \begin{pmatrix} n_1 V & -t & 0 & 0 & -t & \dots \\ -t & n_2 V & -t & 0 & 0 & \dots \\ 0 & -t & n_3 V & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Here the diagonal terms counts the number of flippable plaquettes, which is also the number of nonzero off-diagonal elements

At *t*=*V*, equal-weight superposition is an exact E=0 eigenstate: quantum critical wavefunction with correlations given by classical critical model (dimer packings).

Continuum wavefunction: one free boson (c=1 CFT)

$$|\psi\rangle = e^{-S_E(\{\phi\})/2} |\{\phi\}\rangle$$

Outline of entanglement topics

0. What is entanglement entropy? Why compute it?

an "entangled" state $|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_A\rangle \otimes |\downarrow_B\rangle - |\downarrow_A\rangle \otimes |\uparrow_B\rangle\right)$

1. What does it reveal about topological phases?

2. What about d=2 critical points? Is the "area law" the whole story? Is there anything topological?

Is there any universal behavior in entanglement?
Are interacting theories different from free ones?

Quantum entanglement

Sometimes a pure quantum state of a bipartite system *AB* is also a pure state of each subsystem separately:

Example: S_z=1 state of two s=1/2 spins, A and B

$$|\Psi_{AB}\rangle = |\uparrow_A\rangle \otimes |\uparrow_B\rangle$$

a “product” state

Sometimes a pure quantum state of a bipartite system *AB* is **not** a pure state of each subsystem separately:

Example: singlet state of two s=1/2 spins

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_A\rangle \otimes |\downarrow_B\rangle - |\downarrow_A\rangle \otimes |\uparrow_B\rangle\right)$$

an “entangled” state

Entanglement entropy

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_A\rangle \otimes |\downarrow_B\rangle - |\downarrow_A\rangle \otimes |\uparrow_B\rangle\right)$$

an “entangled” state

In an entangled state, the state of subsystem A or B is not a pure quantum state, but rather a **density matrix**

For the singlet

$$\rho_A = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} = \rho_B$$

A classical uncertainty or **entropy** has been created by the operation of looking at only part of the system.

Entanglement entropy

Definition: the entanglement entropy of a pure state,
with respect to a given partition into A and B,
is the von Neumann entropy of the partial density matrices

$$\langle\phi_1|\rho_A|\phi_2\rangle = \sum_j (\langle\phi_1| \times \langle\psi_j|)|\psi\rangle\langle\psi|(|\phi_2\rangle \times |\psi_j\rangle)$$

$$S(\rho) = -\mathrm{Tr}\rho_A \log_2 \rho_A = -\mathrm{Tr}\rho_B \log_2 \rho_B$$

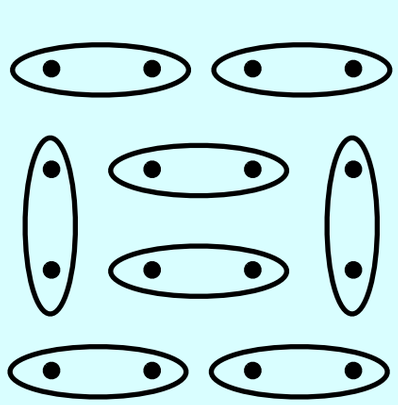
The singlet generates one bit of classical entropy when the two spins are separated

Note that the partial density matrix for subsystem A gives the results of *all* experiments limited to A

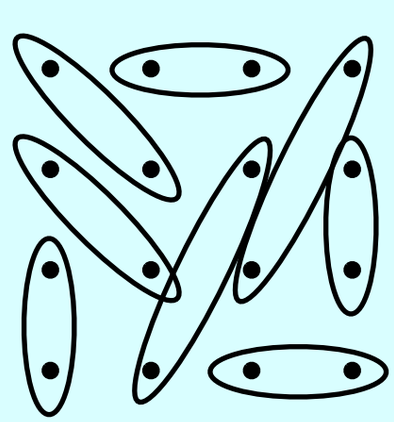
How much entanglement entropy occurs in ground states of local Hamiltonians?

To get some intuition for how entanglement behaves in statistical physics, consider "valence bond states" of $s=1/2$ systems:

Rule: every spin forms a singlet with some other spin



Short-ranged VBS
(= "dimer covering")



Long-ranged VBS

In these states, entanglement entropy S just counts singlets:
S = 1 bit for each singlet crossing the AB boundary.

How much entanglement entropy occurs in ground states of local Hamiltonians?

Consider partitions of a *d*-dimensional infinite system *AB* into a subregion *A* of linear size *L* and an infinite subregion *B*.

How should entanglement entropy scale with *L*?

If we can ignore entanglement between points farther apart than some length scale ξ, then entanglement entropy should be determined by a shell of thickness ~ ξ around the *AB* boundary:

$$S \sim L^{d-1}\xi \Rightarrow S \sim L^{d-1} \text{as } L \to \infty \text{ with system parameters fixed}$$

the "area law"

If there is no notion of locality, any site in *A* is as likely to be entangled with a site in *B* as with another site in *A*, and $S \sim L^d$

Critical points in two dimensions

We will show that for a class of quantum critical points in two dimensions, there are *universal divergent corrections* to the area law that depend on the critical point and on the topology of the partition.

Outline: at "conformal quantum critical points" where the wavefunction of a 2D quantum critical point is determined by a 2D conformal field theory,

$$|\psi_0\rangle = \frac{1}{\sqrt{Z_c}} \int (d\phi)\, e^{-S(\{\phi\})/2} |\{\phi\}\rangle.$$

the entanglement behaves as

$$S = \beta(L/a) + \alpha c \log(L/a) + O(\log\log(L/a))$$

Here c is the central charge of the CFT and α is a function of the partition topology. β gives the expected nonuniversal area law.

2D conformal quantum critical points

Step I: the universal part of von Neumann entropy of such a wavefunction under a partition into A and B is determined by free energy in the CFT:

$$S = F_A + F_B - F_{A\cup B}$$

Here the first two terms are with Dirichlet boundary conditions at the AB boundary.

Start from "replica trick" for entanglement:

$$S = -\mathrm{Tr}\,\rho\log\rho = -\lim_{n\to 1}\frac{\partial}{\partial n}\mathrm{Tr}\,\rho^n.$$

Since the trace of a density matrix is 1, we can write this as

$$S = -\lim_{n\to 1}\frac{\partial}{\partial n}\frac{\mathrm{Tr}\,\rho^n}{(\mathrm{Tr}\,\rho)^n}.$$

2D conformal quantum critical points

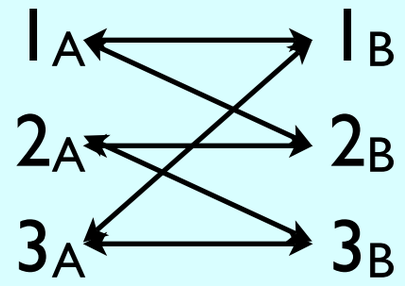
$$S = -\lim_{n\to 1} \frac{\partial}{\partial n} \frac{\mathrm{Tr}\,\rho^n}{(\mathrm{Tr}\,\rho)^n}.$$

Write the density matrix in terms of A and B parts, with a coupling on the boundary:

$$\begin{aligned}
\langle\{\phi_1^A\}|\rho_A|\{\phi_2^A\}\rangle &= \mathrm{Tr}_{\phi^B}\left(\langle\{\phi_1^A\}|\otimes\langle\{\phi^B\}|\psi_0\rangle\langle\psi_0(|\{\phi_2^A\}\rangle\otimes|\{\phi^B\}\rangle\right.\\
&= \frac{1}{Z_c}\int(d\phi^B)e^{-(S^A(\phi_1^A)/2+S^A(\phi_2^A)/2+S^\partial(\phi_1^A,\phi^B)/2+S^\partial(\phi_2^A,\phi^B)/2+S^B(\phi^B))}
\end{aligned}$$

At a critical point, the boundary coupling enforces continuity.

In the *numerator*, each A field replica is stitched to two B field replicas at the boundary, and vice versa.



In the *denominator*, A and B fields are paired one-to-one.

2D conformal quantum critical points

The trace becomes a ratio of CFT partition functions:

$$\mathrm{Tr}\,\rho_A^n = \frac{Z(n \text{ configurations agreeing on the boundary})}{Z(n \text{ independent configurations})}.$$

Example: for any free field, *n* configurations agreeing at the boundary are equivalent to 1 free field and *n-1* Dirichlet BC's.

Then replica limit gives $S = F_A + F_B - F_{A\cup B}$

The universal part of the entanglement entropy is related to the free energy change from inducing the boundary in the CFT!

Now use spectral theory on "hearing the shape of a drum": for a 2D connected region with smooth boundary, generalized by Cardy and Peschel to a general CFT.

2D conformal quantum critical points

Example of a free field: the free energy is determined by the eigenvalues of the Laplacian with specified boundary condition. For a 2D connected region with smooth boundary,

$$F_A \sim f_0 (L/a)^2 + f_s (L/a) - \frac{c\chi}{6} \log(L/a)$$

(cf. Mark Kac lecture on "hearing the shape of a drum")

Euler characteristic

$$\chi = 2 - 2g - b$$

g=genus (# of holes), *b*=# of boundaries, *c*=central charge

(general statement for all CFT's by Cardy and Peschel)
Additional log contributions if boundary has sharp corners

2D conformal quantum critical points

$$F_A \sim f_0 (L/a)^2 + f_s (L/a) - \frac{c\chi}{6} \log(L/a)$$

Area part cancels, leaving boundary and log terms.

$$S = 2 f_s (L/a) - \frac{c(\chi_A + \chi_B - \chi_{A\cup B})}{6} \log(L/a)$$

(There are nonuniversal short-distance contributions to the boundary part as well, in general, but the logarithmic part is universal.)

Conservation of the Euler characteristic implies no log if *A* is surrounded by *B* or vice versa.

However, there are logarithmic corrections if the partition "separates" *A* and *B* or if there are sharp corners...

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