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International Centre for Theoretical Physics**



2220-11

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Science: Total Energy and Force Methods**

13 - 15 January 2011

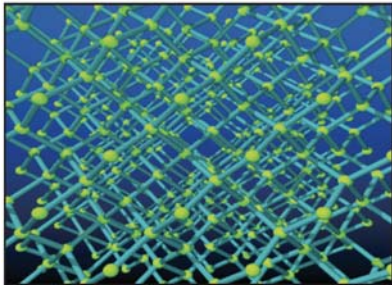
Topological insulators: overview and interface/nanostructure effects

Joel Moore

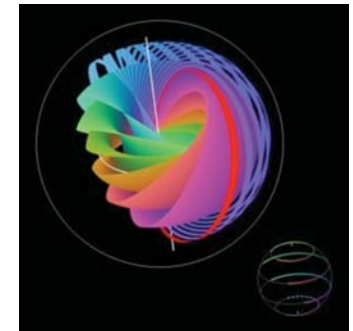
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USA*

Topological insulators: overview and interface/nanostructure effects

ICTP, 13 January 2011



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and Lawrence Berkeley National Laboratory



W/IN Western
Institute of
Nanoelectronics



Thanks

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Overview references

See articles by Hasan and Kane (RMP colloquium) and Qi and Zhang (Physics Today).

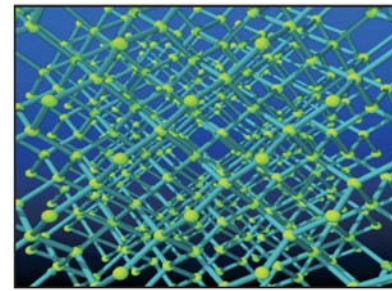
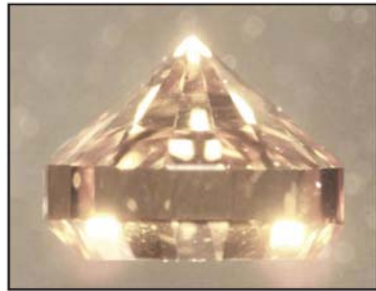
Nontechnical review: JEM, Nature **464**, 194-198 (2010) “The birth of topological insulators”

Outline

I. Motivations:

The remarkable versatility of the two-dimensional electron gas

The search for topological order



2. Are there topological phases in 3D materials and no applied field?

Yes — “topological insulators”

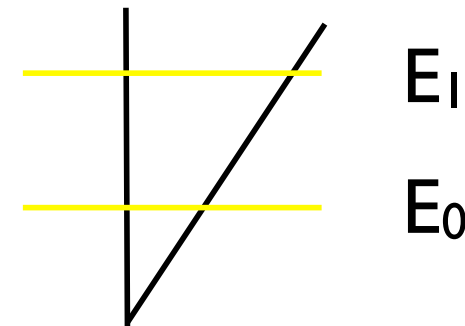
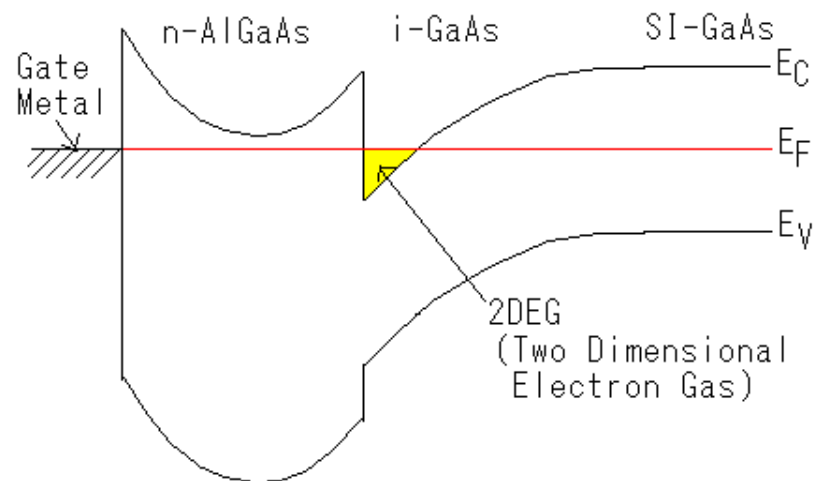
(experimental confirmation 2007 for 2D, 2008 for 3D)

3. Potential applications of the novel surface states

A brief history of low-dimensional electrons

At a planar heterojunction between two different semiconductors, electrons are trapped by a confining potential in the third direction.

2DEG = “two-dimensional electron gas”

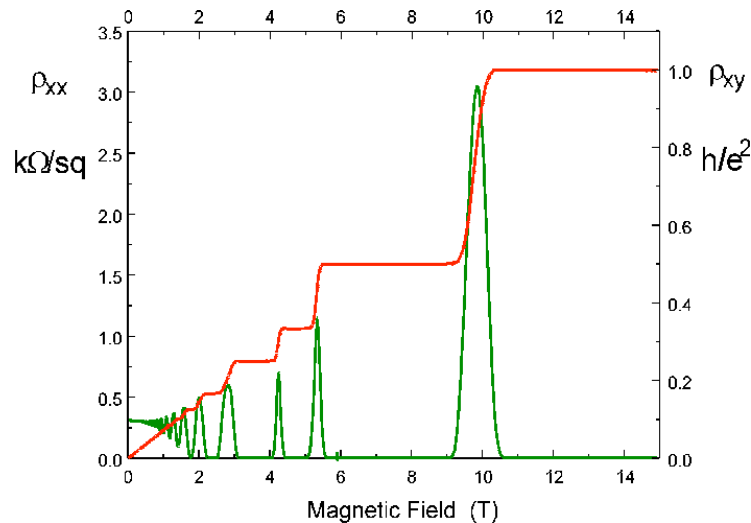


Further patterning of a 2DEG can make a 1D quantum wire with quantized conductance ne^2/h (van Wees et al., 1988) or a 0D quantum dot (“artificial atom”)

Another approach: carbon-based materials
0D fullerenes, 1D nanotubes and 2D graphene

The (integer) quantum Hall effect

A 2DEG in a strong magnetic field can show a quantized transverse conductance:

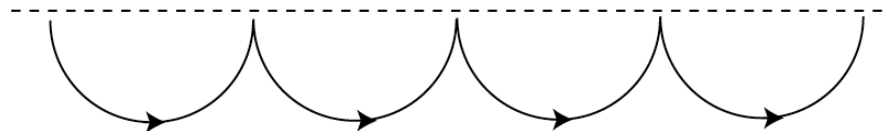


$$\sigma_{xy} = n \frac{e^2}{h}$$

to 1 part in 10^9

A semiclassical picture is that 2D electrons make circular orbits in the magnetic field. At the sample boundary, these orbits are interrupted and “skip” along the boundary, leading to a perfectly conducting *one-way quantum wire at the sample edge*.

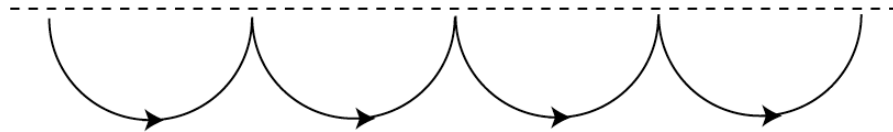
$B_z \odot$



Topological Insulators from Spin-orbit Coupling

Semiclassical picture

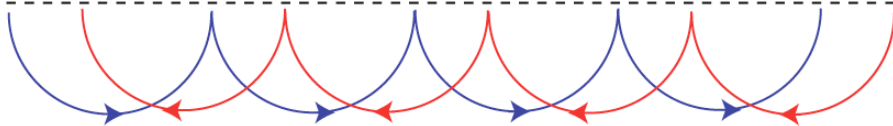
$B_z \odot$



1D edge of Quantum Hall Effect

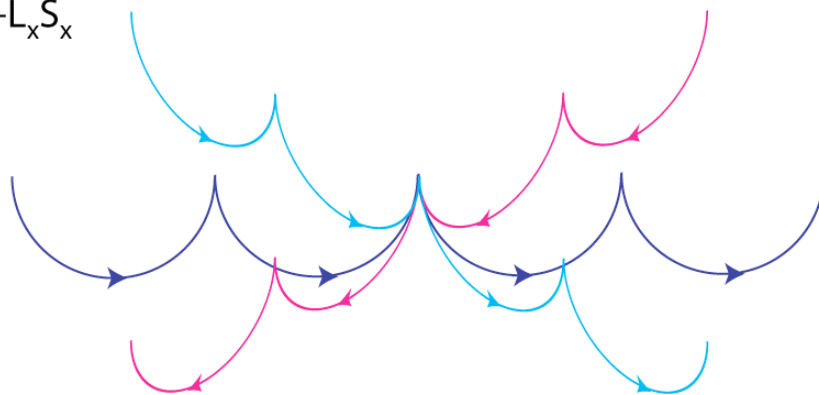
$L_z S_z$

spin up
spin down



1D edge of “Quantum Spin Hall Effect” (discovered 2007)

$L_z S_z + L_x S_x$



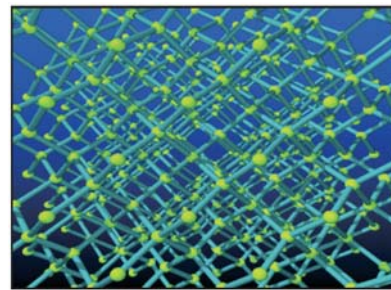
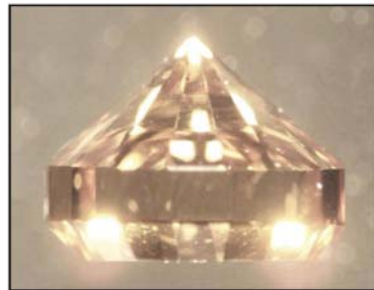
2D surface of 3D Topological Insulator (discovered 2008)

3D topological insulators have a special metallic 2DEG at any surface...

But what is “topological” about some edge/surface states?

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

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”:

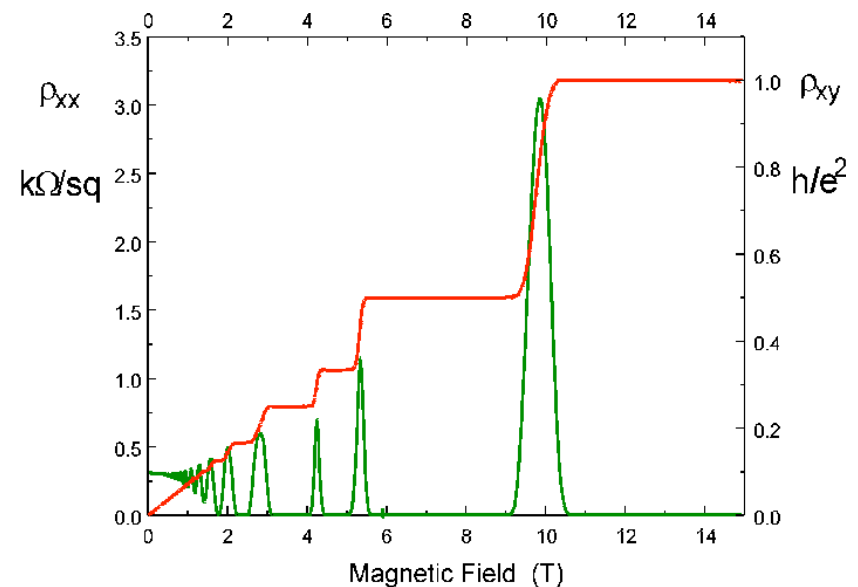
force I along x and measure V along y

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 in good (modulation-doped) samples.

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?

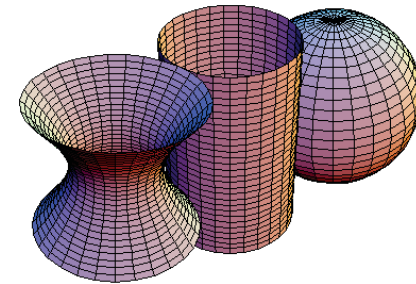
“Topological invariant” = quantity that does not change under continuous deformation

Topological invariants

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

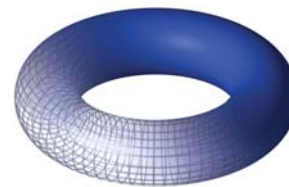
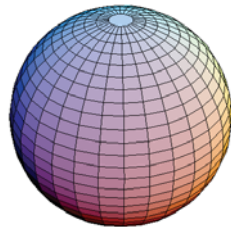
Consider a two-dimensional surface.

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”.

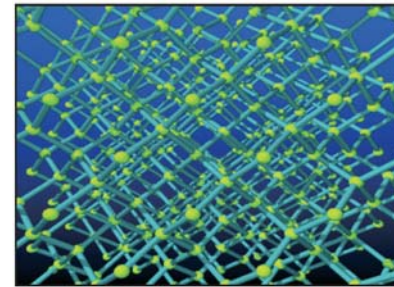
Topological invariants

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” \mathcal{A} changes by a gradient,

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

just like the vector potential in electrodynamics.

So loop integrals of \mathcal{A} will be gauge-invariant,
as will the *curl* of \mathcal{A} , which we call the “Berry curvature”.

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

Berry phases 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:

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

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

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 \mathcal{F} (like Gauss-Bonnet!). Explicitly,

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

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

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?

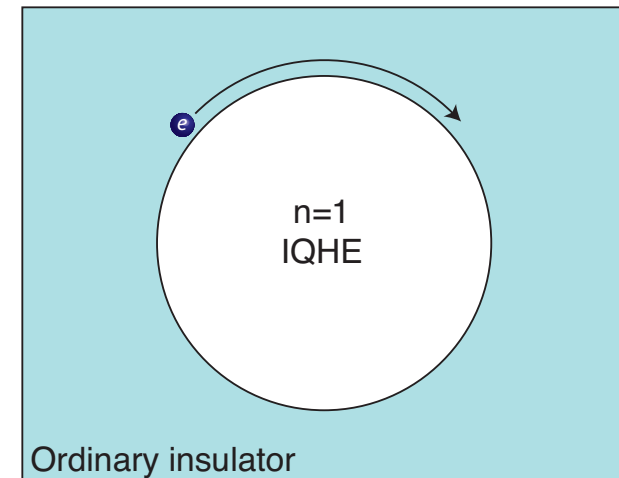
Answer: (Laughlin; Halperin)

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).

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?



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

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.

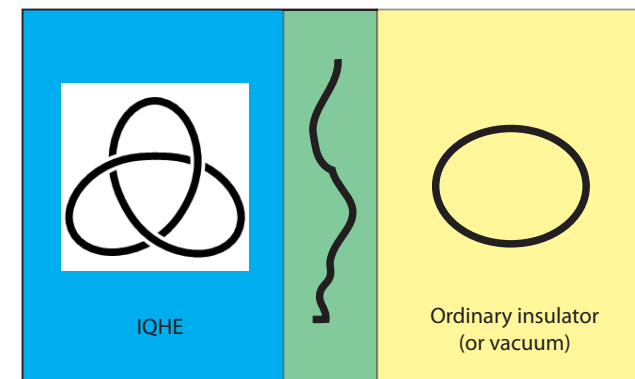
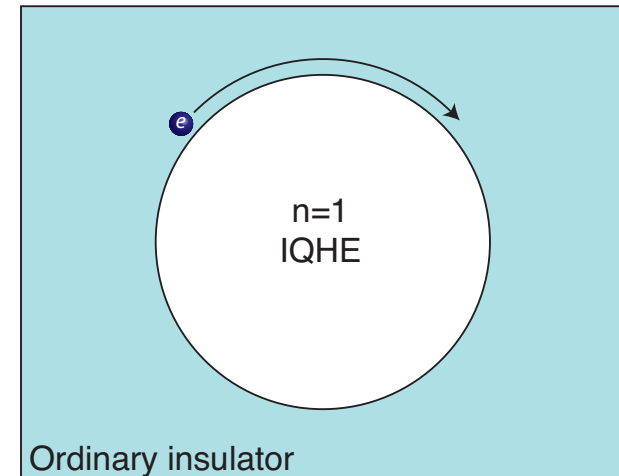
How does the bulk topological invariant “force” an edge mode?

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 applies in the new topological phases discovered recently:

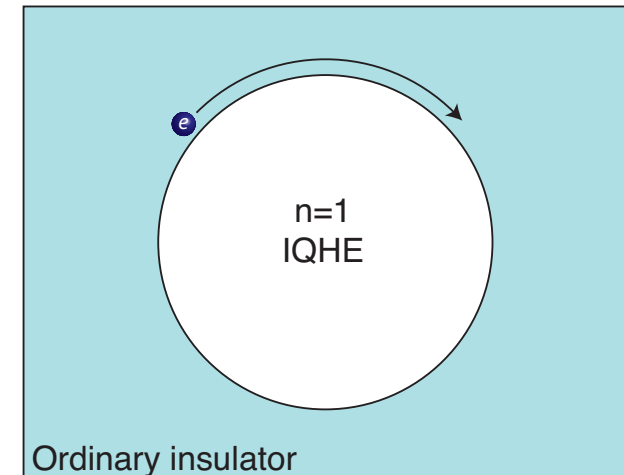
a “topological invariant”, based on the Berry phase, leads to a nontrivial edge or surface state at any boundary to an ordinary insulator or vacuum.

However, the

physical origin (spin-orbit rather than B field),

dimensionality (2 or 3 rather than 2),

and experiments are all different.



The “quantum spin Hall effect”

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

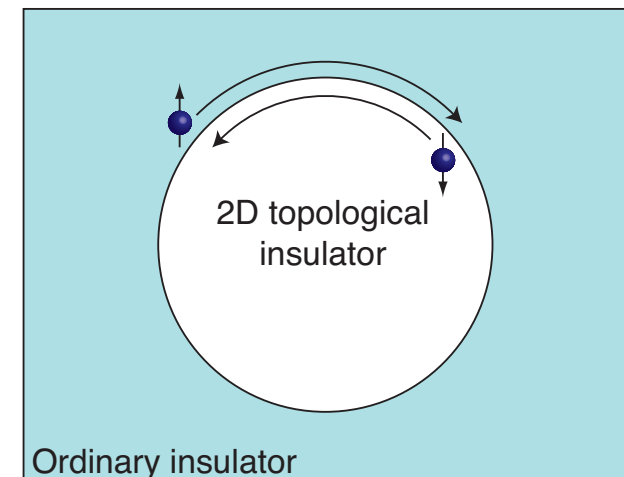
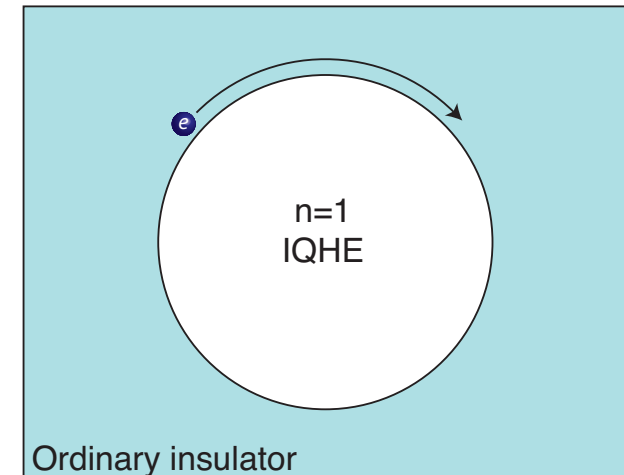
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

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”.



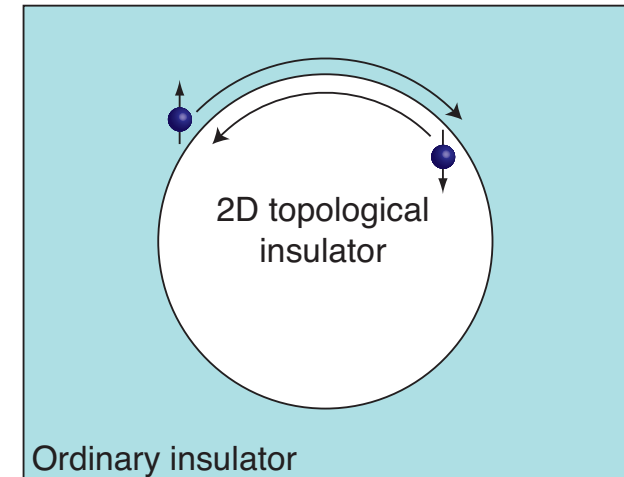
The 2D topological insulator

People were somewhat skeptical until 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 “ \mathbb{Z}_2 invariant”.



Systems in the “odd” class are “2D topological insulators”

1. Where does this “odd-even” effect come from?
2. How can this edge be seen?

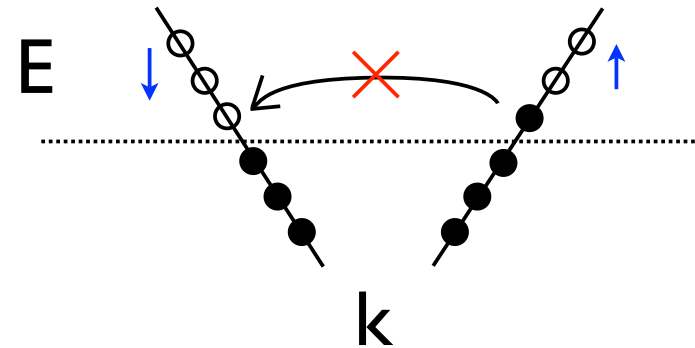
The 2D topological insulator

I. Where does this “odd-even” effect come from?

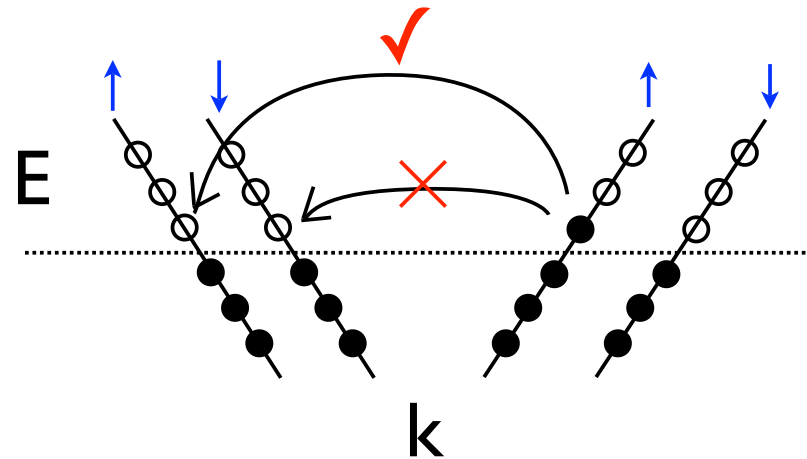
In a time-reversal-invariant system of electrons, all energy eigenstates come in degenerate pairs.

The two states in a pair cannot be mixed by any 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).



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

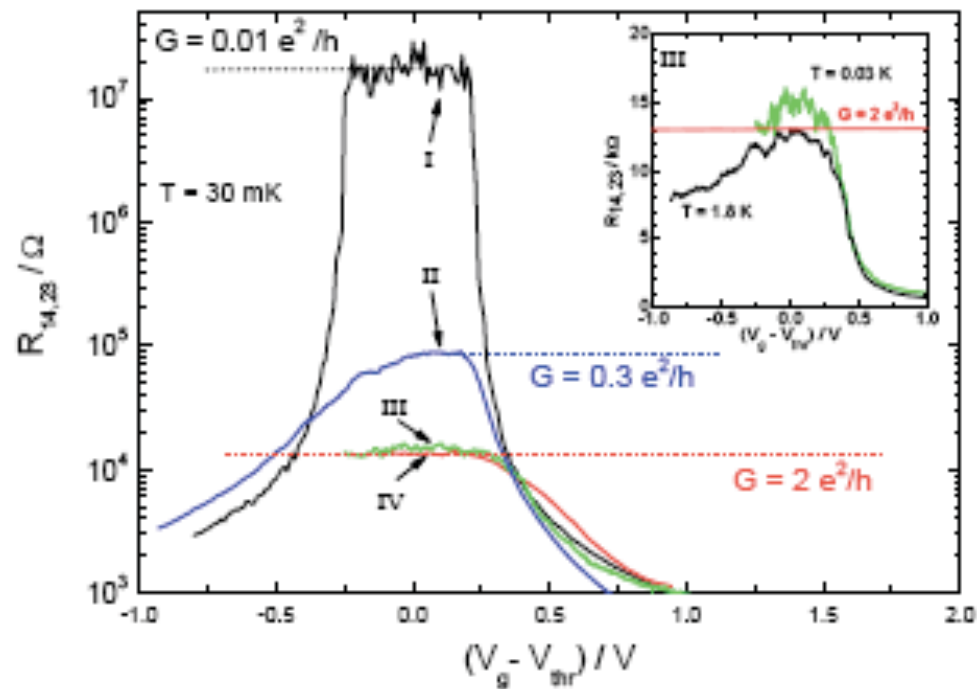
2. Key: the topological invariant predicts the “number of quantum wires”.

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 Z_2 invariants, but there is a fourth Z_2 invariant as well.

Hence there are $2^4 = 16$ different classes of “topological 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.

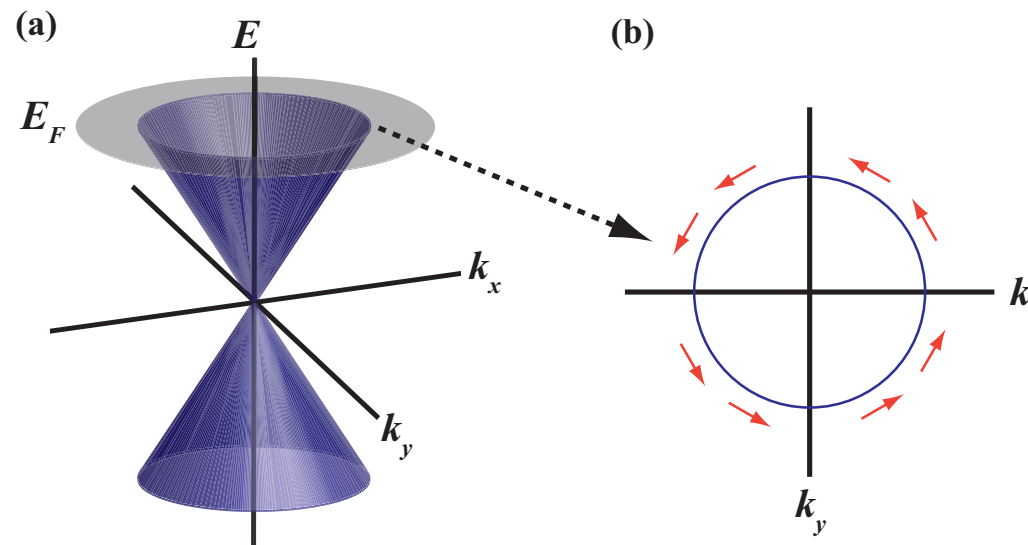
In 2D, we could use up-spin and down-spin copies to make the topological case.

There is a (technical) procedure to compute the fourth invariant for any band structure. With inversion symmetry, this procedure is considerably simplified (Fu and Kane, 2007). A topological insulator is reached from an ordinary one by an odd number of “band inversions”.

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 phase whose metallic surface state in the simplest case is a single massless “Dirac fermion” (Fu-Kane-Mele, 2007)



Surface state = “1/4 of graphene”: no spin or valley degeneracy

2. Some fairly standard 3D materials turn out to be topological insulators!

Claim:

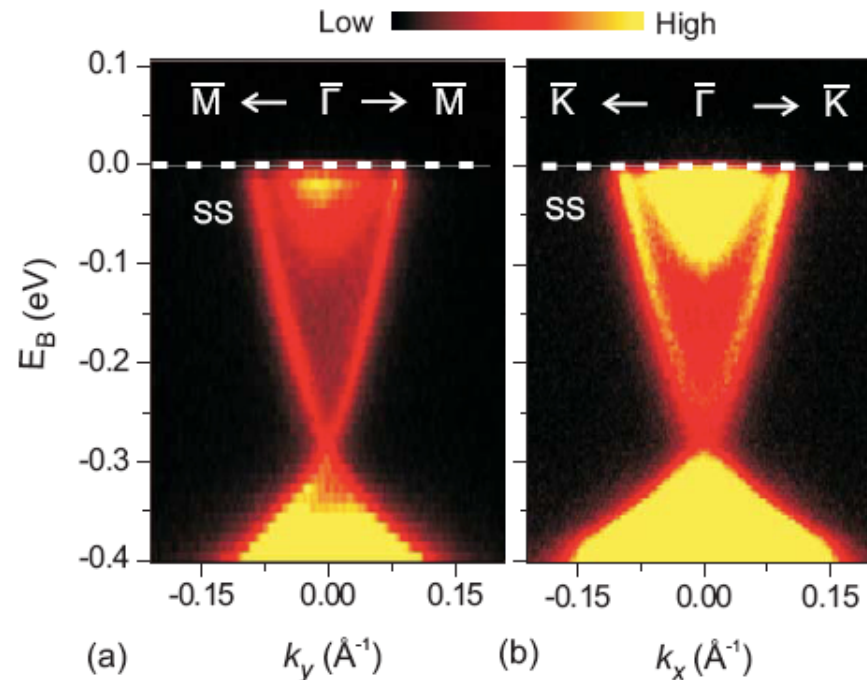
Certain insulators will *always* have metallic surfaces with strongly spin-dependent structure

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

ARPES of topological insulators

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.

Summary of basics

1. There are now at least 3 strong topological insulators that have been seen experimentally ($\text{Bi}_x\text{Sb}_{1-x}$, Bi_2Se_3 , Bi_2Te_3), and many more predicted theoretically.
2. Their metallic surfaces exist in zero field and have the predicted form. Similar surface states should exist in B phase of ^3He .
3. The temperature over which topological behavior is observed can extend up to room temperature or so ($0.3 \text{ eV} = 3600 \text{ K}$).

Last part

What are important consequences of these surface states?

Thermoelectricity

Unusual Berry phases in transport

Spintronics

Future needs and a puzzle

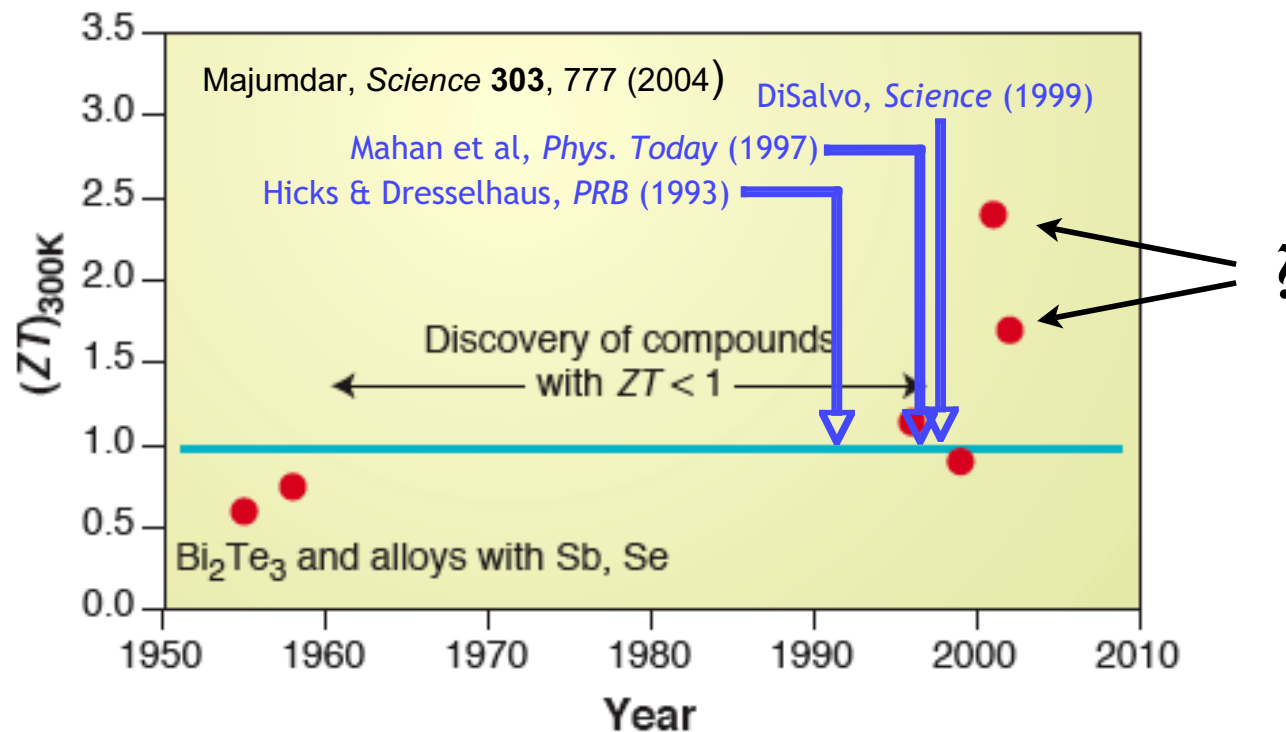
Topological insulators and energy

Topological insulators already have one application: thermoelectricity

“(Gordon) Moore’s Law”: (1965-present)

The number of transistors on an IC doubles every 2 years

“Moore’s Law” of thermoelectrics: the figure of merit doubles every 50 years



Our proposal for how to use TI behavior in thin thermoelectric films: [Ghaemi, Mong, JEM, PRL 2010](#)

A. Balandin’s group (Riverside) has recently created monolayers by exfoliation ([APL 2010](#))

Topological insulators and energy

Big question:

Does knowing that Bi_2Te_3 has these unusual surface states help with thermoelectric applications?

Yes, at least for low temperature (10K - 77K), where $ZT=1$ is not currently possible. We hope to double achievable ZT in this regime.

(P. Ghaemi, R. Mong, JEM, PRL, 2010)

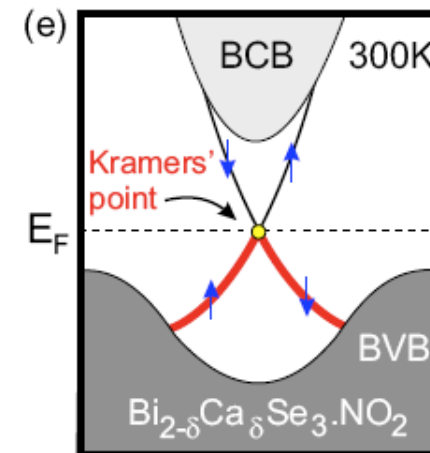
Thermoelectrics work best when the band gap is about 5 times kT .

Gap of $\text{Bi}_2\text{Te}_3 = 1800 \text{ K} = 0.15 \text{ eV}$.

Idea: *in a thin film*, the top and bottom surfaces of a topological insulator “talk” to each other, and a *controllable* thickness-dependent gap opens.

Key: good thickness and Fermi-level control

Recent development: exfoliated thin films
(Balandin et al., UC Riverside, APL)



Fermi-level control
in crystals (Hsieh et al., 2009)

Berry phases in transport

For observation of the above in existing TIs, reduction of bulk residual conductivity is important and seems to be underway.

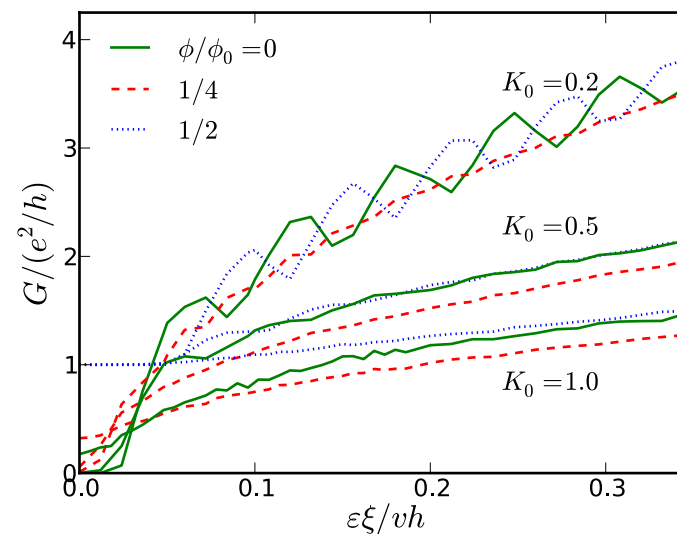
Magnetic field experiments can isolate 2D surface state features.

Puzzle 1: Stanford nanowire experiment (Yi Cui et al., Nature Materials)

sees Aharonov-Bohm (h/e) oscillations, as expected for a clean system, rather than Sharvin & Sharvin ($h/2e$), as expected for a

The *sign* is also not what is expected in the strong-disorder limit: the Berry phase protects a mode at π flux, rather than 0 flux as in a nanotube.

(Bardarson, Brouwer, JEM, PRL 2010;
Zhang and Vishwanath, arXiv 1005.3042).



Puzzle 2: Where is the Zeeman effect in surface-state magnetoconductance?

Key difference between TIs and either graphene or a 2DEG.

An alternate mechanism to E-dependent velocity

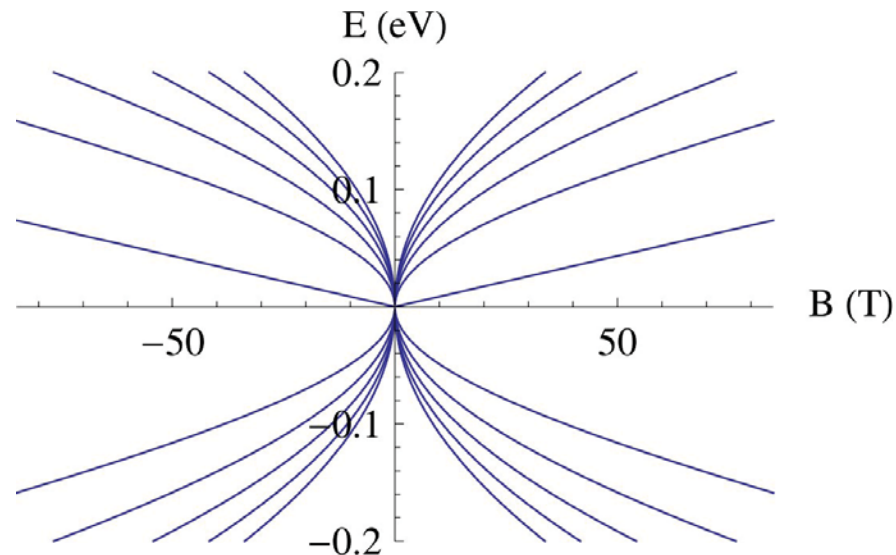
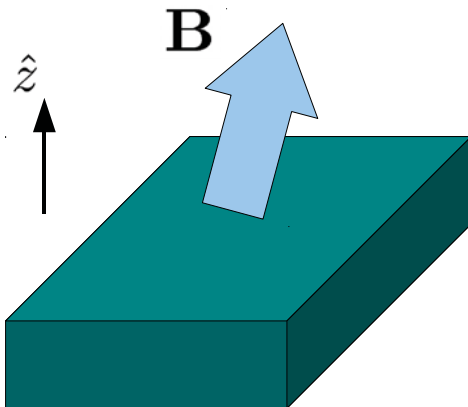
Landau Levels with Zeeman Coupling

Surface effective Hamiltonian

$$H = v(\sigma^x \pi_y - \sigma^y \pi_x) - \frac{g\mu_B}{2} \mathbf{B} \cdot \boldsymbol{\sigma} \quad (\pi = \mathbf{p} + e\mathbf{A})$$

Landau Levels

$$E_{\pm n} = \begin{cases} \frac{g\mu_B}{2} |B_z| & n = 0 \\ \pm \sqrt{2n\hbar v^2 e |B_z| + \left(\frac{g\mu_B}{2} |B_z|\right)^2} & n > 0 \end{cases}$$



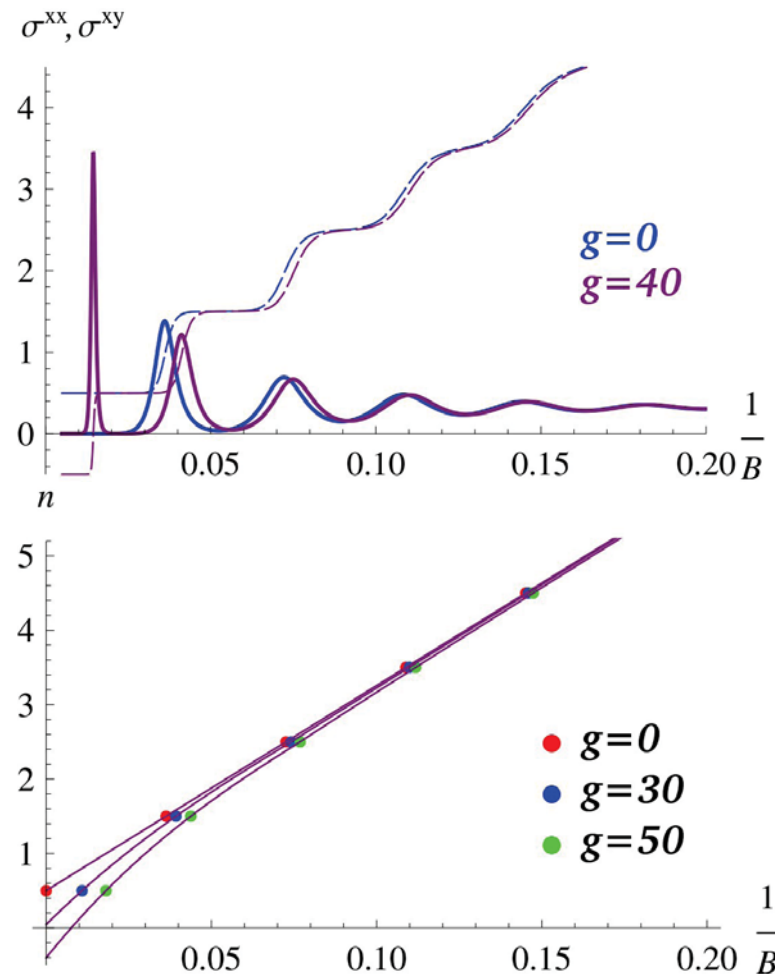
Quantum Oscillations and Landau Indexing

The chemical potential may be computed by examining the spacing between Landau transitions.

The g-factor may be measured by the last peak in the signal:

$$E_0 = \frac{g\mu_B}{2} |B_z|$$

The vertical intercept is less than 1/2 due to Zeeman coupling.



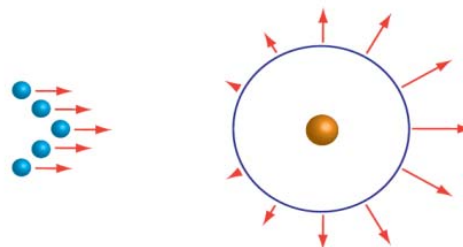
Goals with current materials

- Observation of giant spin-charge coupling

Spin-charge coupling

Charge current = spin density
About 100 times larger than QWs

Align 10 spins/micron² \Rightarrow 1 microamp



The locking of spin and momentum at a TI surface means that a charge *current* at one surface generates a spin *density*.

Similarly a charge *density* is associated with a spin *current*.

While these effects could cancel out between the top and bottom surfaces of an unbiased thin film, any asymmetry (such as electrical bias or substrate effects) leads to a net spin-charge coupling.

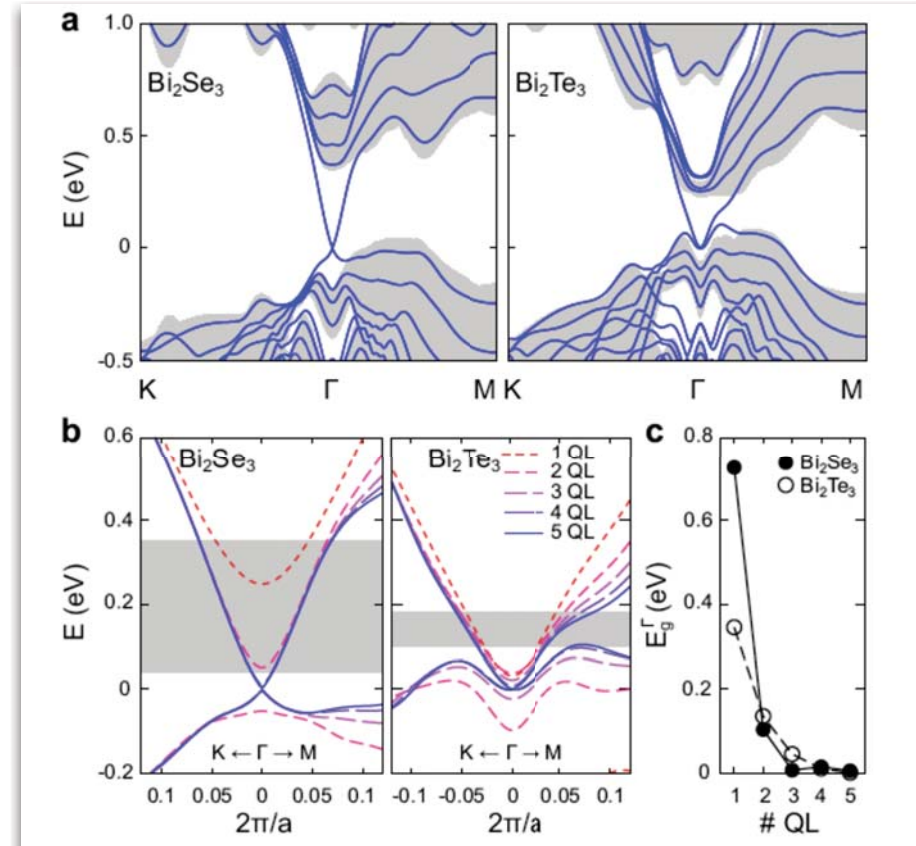
(O. Yazyev, JEM, S. Louie, PRL 2011)



Goals with current materials

- Observation of giant spin-charge coupling

First-principles calculations of surface states, including reduced spin polarization (O. Yazyev, JEM, S. Louie, PRL 2011)



1. Gives numerical strength of spin-charge coupling, e.g., in “inverse spin-galvanic effect’ (Garate and Franz): use TI surface current to switch an adsorbed magnetic film
2. Can bias electrically so that *combination of* surfaces has net spin-charge coupling

A puzzle. Future directions.

The Hall effect is quantized in the IQHE.

What is quantized in topological insulators?

Hint: There is something special about the diagonal part of dP/dB .

The “polarization quantum” of one charge per unit cell area at the surface (King-Smith and Vanderbilt) combines nicely with the flux quantum:

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

see Malashevich, Souza, Coh, Vanderbilt, NJP 2010; Essin, Turner, Moore, Vanderbilt, PRB 2010

Future insights that could come from electronic structure theory:

1. Better understanding of interfaces between TIs and magnetic/superconducting materials.
2. Multifunctional TI materials (combinations with antiferromagnetism, superconductivity, ...)
3. Are there plausible realizations of “fractional” topological insulators?

What about other symmetries?

It turns out that interesting things happen when we think about breaking some of the symmetries of the original topological insulators.

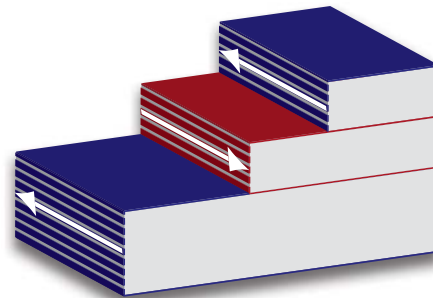
1. We can add a weak magnetic field, or surface magnetic impurities, which leads to a half-integer quantum Hall effect at each surface.

(One Dirac fermion contributes a *half-integer* times e^2/h , as observed in graphene.)

2. We can consider the interaction between topological insulators and superconductivity, which breaks a $U(1)$ symmetry.

(3. We can consider materials that support antiferromagnetism and TI behavior:)

“antiferromagnetic topological insulators”
(Mong, Essin, JEM, 2010)
possibly GdPtBi?



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.

The angle θ is periodic “as a bulk property” and odd under T.

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

These correspond to “positive” and “negative” Dirac mass for the electron (Jackiw-Rebbi, Callan-Harvey, ...)

Axion E&M, then and now

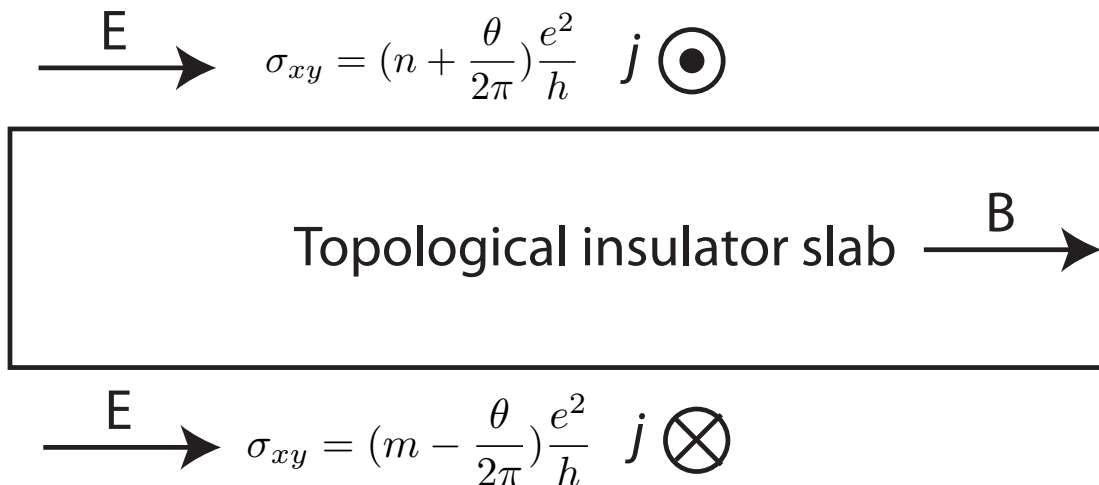
$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h} \mathbf{E} \cdot \mathbf{B} = \frac{\theta e^2}{16\pi h} \epsilon^{\alpha\beta\gamma\delta} F_{\alpha\beta} F_{\gamma\delta}.$$

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

Quantized magnetoelectric effect: (Qi et al., 2008; ...)

applying **B** generates polarization **P**, applying **E** generates magnetization **M**

Quantized coefficient in Gaussian units is essentially the fine structure constant



Orbital magnetoelectric polarizability

One mysterious fact about the previous result:

We reproduced the “Chern-Simons term” of Qi et al. from a semiclassical approach.

But in our 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

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

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., PRB 2010)

For dM/dE approach and numerical tests, see Malashevich, Souza, Coh, Vanderbilt, NJP 2010.

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

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).

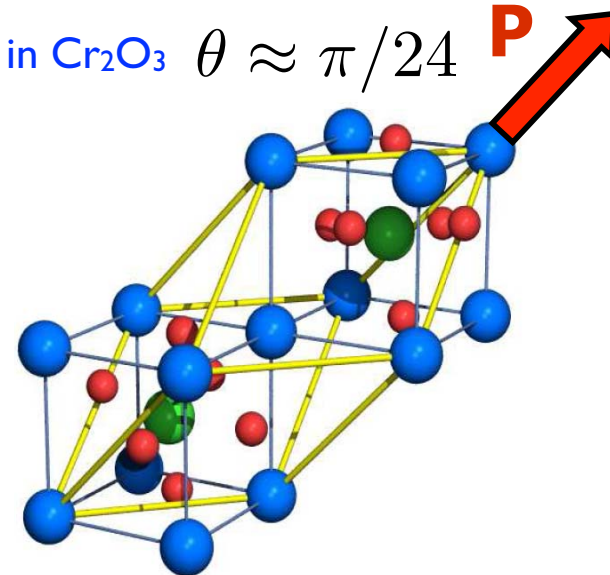
It is not a pure Berry phase in general, but *it is in topological insulators*.

Such magnetoelectric responses have been measured, e.g., in Cr_2O_3 $\theta \approx \pi/24$ **P**
(Obukhov, Hehl, et al.).

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.

Application I of topological insulators:

The hunt for new particles

We all know that “quarks” have fractional electric charge and are not seen in isolation.

Condensed matter systems sometimes generate “emergent” quasiparticles with different quantum numbers than the original nuclei and electrons.
A familiar example is the “Cooper pairs” in a superconductor.

Another example:

Fractional plateaus in the quantum Hall effect are seen experimentally (1983).
Eventually many fractions are seen, all with odd denominators. The strongest is often at $1/3$ filled Landau level.

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 ($1/3$ in simplest case) and *fractional* “anyonic” statistics

What other particles remain to be found?

The hunt for the Majorana fermion

Prehistory:

We can imagine splitting one ordinary spinless fermion (a “Dirac fermion”) into two Majorana fermions as

$$\gamma_1 = \frac{c + c^\dagger}{\sqrt{2}}, \gamma_2 = i \frac{c^\dagger - c}{\sqrt{2}}$$

Then these “Majorana fermions” are their own antiparticles.

We can always rewrite Dirac fermions in this form, but when is it physically meaningful? When are there isolated Majorana fermions?



Majorana fermions as fundamental particles

Neutrinoless double beta decay:

If the neutrino is a Majorana fermion, the neutrino and antineutrino are the same particle.

Then the two (anti-)neutrinos produced in a double beta decay of an element such as U-238 can annihilate as particle and antiparticle.

There is at least one claim from 2001 that neutrinoless double beta decay has actually been observed; future experiments are a high priority.



Gran Sasso

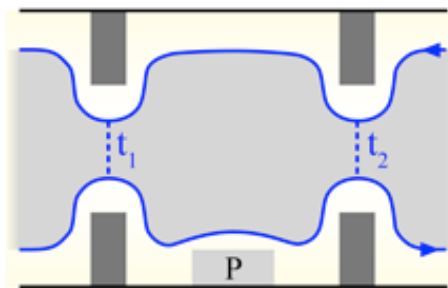
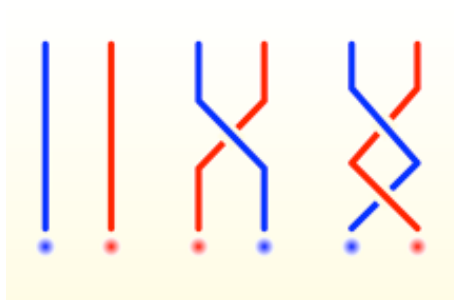


Majorana fermions as emergent particles

Several condensed matter systems are believed to support Majorana fermion excitations.

The first was an unusual fractional quantum Hall state at $5/2$ filled Landau levels, first observed around 1990. In the most popular theoretical model for this state, there are Majorana fermion quasiparticles.

A 2009 experiment (R. L. Willett et al., PNAS) constructing an interferometer to “braid” one Majorana fermion around another supports this theoretical model, but is rather indirect.



Majorana fermions from SC/TI junctions

It turns out that the core of a magnetic vortex in a two-dimensional “ $p+ip$ ” superconductor should have a Majorana fermion. (But we haven’t found one yet.)

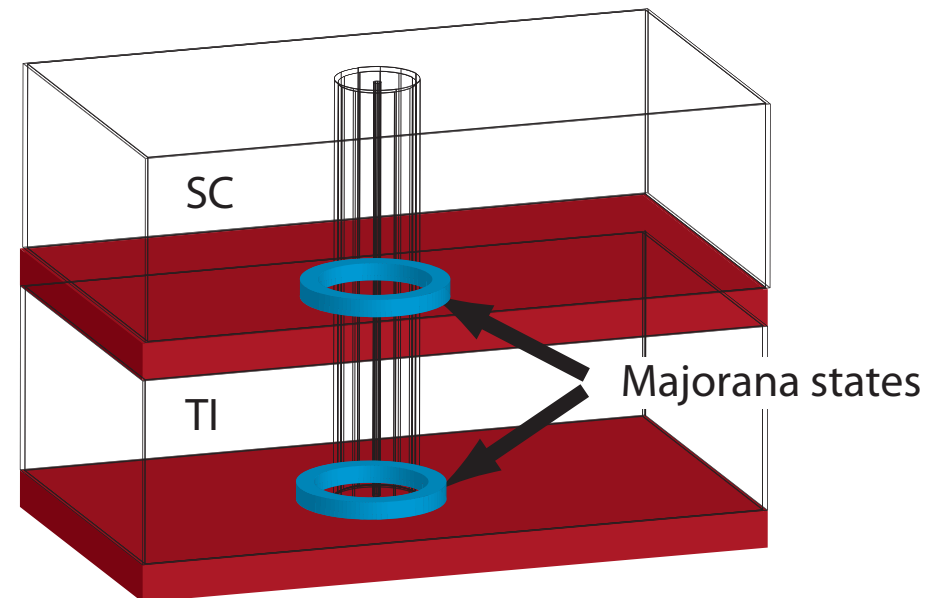
However, a superconducting layer with similar properties exists at the boundary between a 3D topological insulator and an ordinary 3D superconductor (Fu and Kane, 2007).

Idea: the proximity effect

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

couples to the “time-reversal-symmetric half-metal” at the TI surface

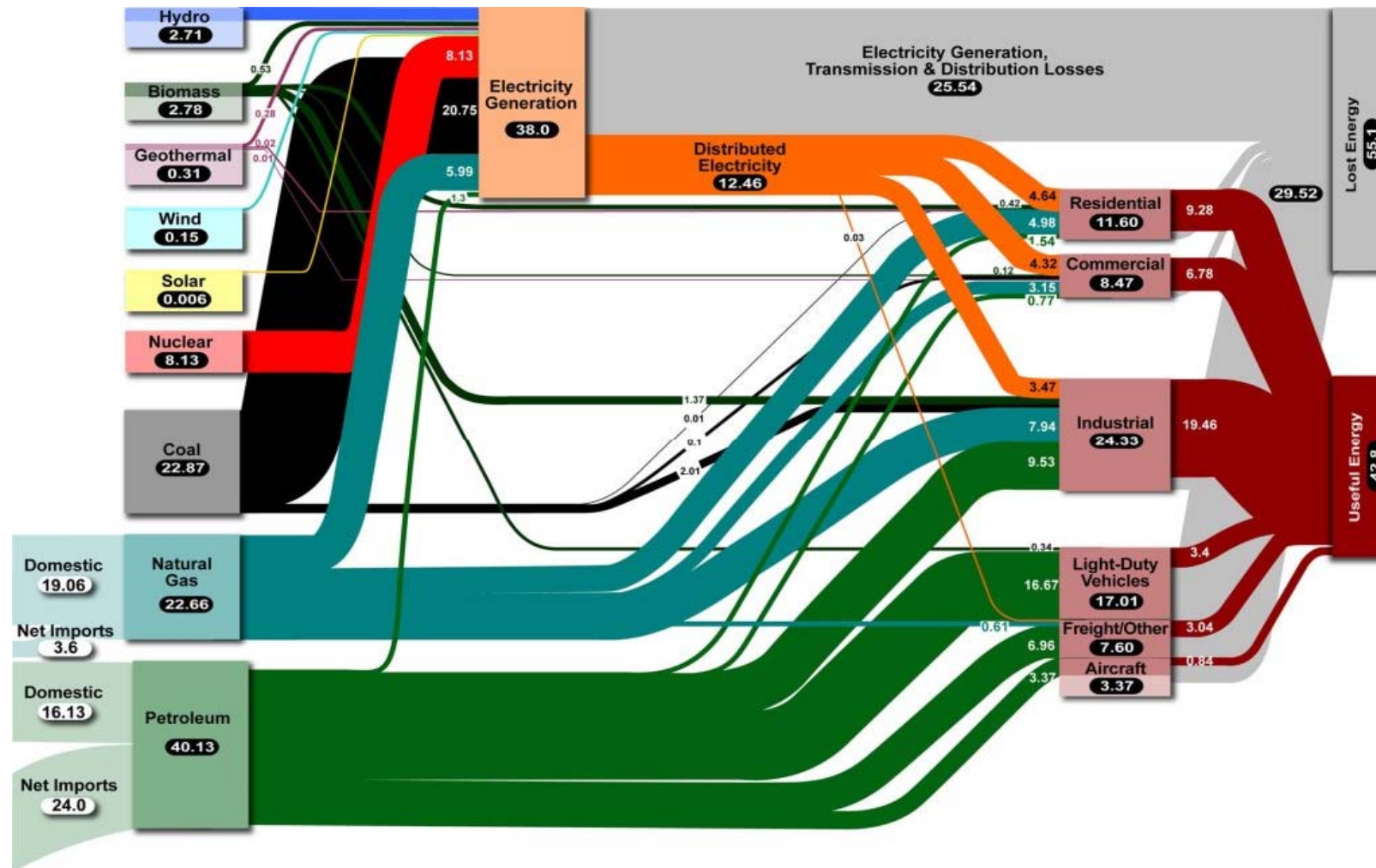
to create a superconductor with *half* as many degrees of freedom as a normal s-wave superconductor.



Can store one “qubit” in two spatially separated Majorana fermions--protected quantum memory.

Can we find topological superconductors that host Majoranas by themselves?

An existing application of TIs: Energy



Thermoelectric materials can convert waste heat to electrical energy.
The 3D topological insulators discovered so far are all useful thermoelectric materials.

Topological insulators and energy

Thermoelectric cooling: refrigeration with no moving parts.

Some consumer thermoelectrics use Bi_2Te_3 , a topological insulator.

Cuisinart CWC-600 6-Bottle Private Reserve Wine Cellar

6 Bottle Wine Cooler:

FRYS.com #: 5049475

Protect the integrity of your favorite wines with the Cuisinart Private Reserve Wine Cellar. This elegant countertop cellar chills wines using thermoelectric cooling technology, which eliminates noise and vibration. Eight temperature presets for a variety of reds and whites keep up to 6 bottles of wine at the perfect serving temperature. Designed in the style of full-size cellars, with a stainless steel door and interior light, the Cuisinart Private Reserve is a beautiful way to display wines and champagnes.

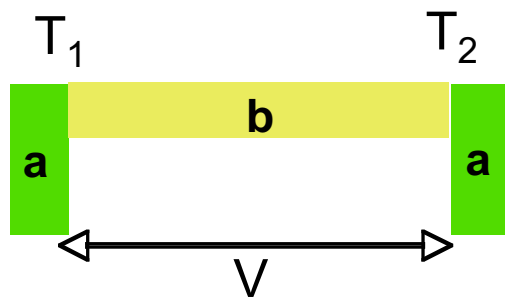


Topological insulators and energy

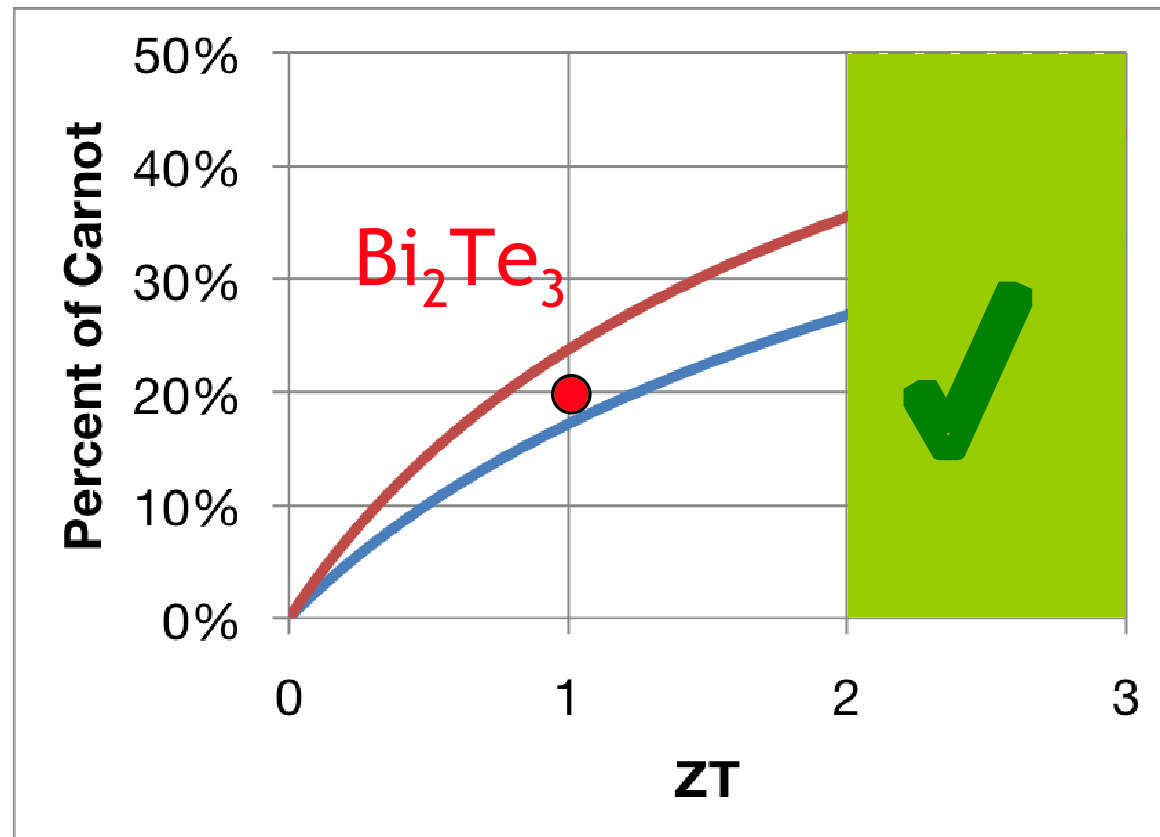
What makes a material a good thermoelectric?

The “thermoelectric figure of merit” ZT determines Carnot efficiency:

$$ZT = \frac{S^2 \sigma T}{k}$$



$S = V / \Delta T$
“Seebeck
coefficient”



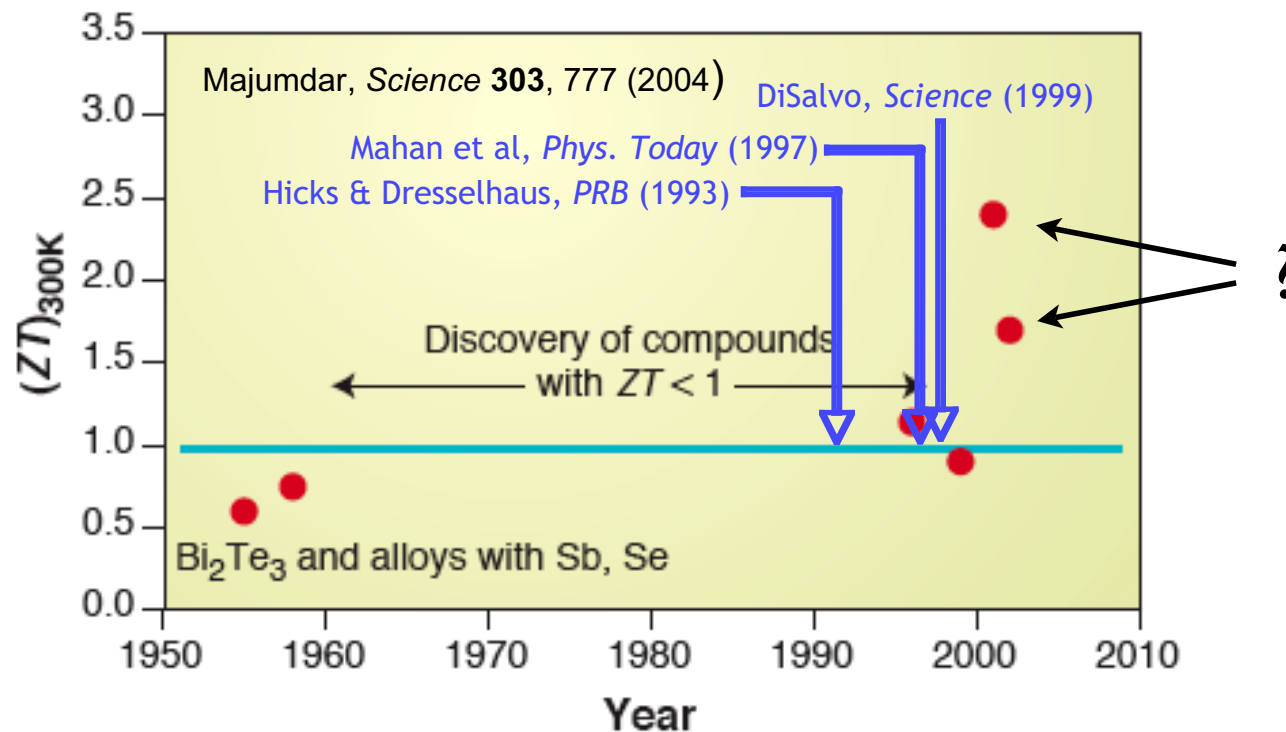
Topological insulators and energy

So why aren't thermoelectrics everywhere? Will they be soon?

“(Gordon) Moore’s Law”: (1965-present)

The number of transistors on an IC doubles every 2 years

“Moore’s Law” of thermoelectrics: the figure of merit doubles every 50 years

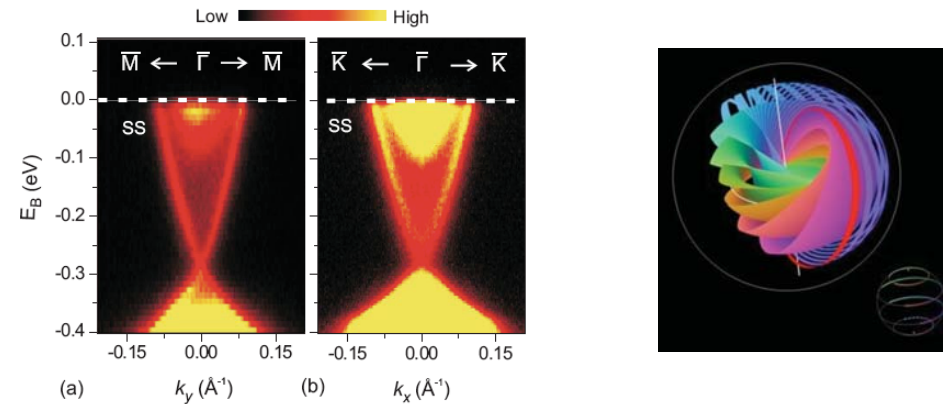


Our proposal for how to use TI behavior in thin thermoelectric films: [Ghaemi, Mong, JEM, PRL 2010](#)

[A. Balandin's group \(Riverside\) has recently created monolayers by exfoliation \(APL 2010\)](#)

Conclusions

1. “Topological insulators” exist in two and three dimensions in zero magnetic field. The 3D topological insulator has a special metallic 2DEG at any surface.



2. When the surfaces are gapped, the 3D topological insulator generates a quantized magnetoelectric coupling

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

3. These insulators might be useful to find the Majorana fermion, for spintronic devices, or for improved thermoelectrics (not so big a leap).

4. The combination of *symmetry* and *topology* probably has more surprises in store.

Advertisement: CM seminar tomorrow, 1:25 pm,
“Optical signatures of spin transport, Berry's phase, and unconventional superconductivity”

Thanks

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Selected references

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A. M. Essin, J. E. Moore, and D. Vanderbilt, PRL **102**, 146805 (2009)

B. Seradjeh, J. E. Moore, M. Franz, PRL **103**, 066402 (2009)

A. M. Essin, A. Turner, J. E. Moore, and D. Vanderbilt, 1002.0290

JEM, Nature **460**, 1090 (2009)

“An insulator’s metallic side”

JEM, Nature **464**, 194-198 (2010)

“The birth of topological insulators”

See also reviews by Hasan and Kane (RMP colloquium) and Qi and Zhang (Physics Today).

Correlated phases from TI surfaces

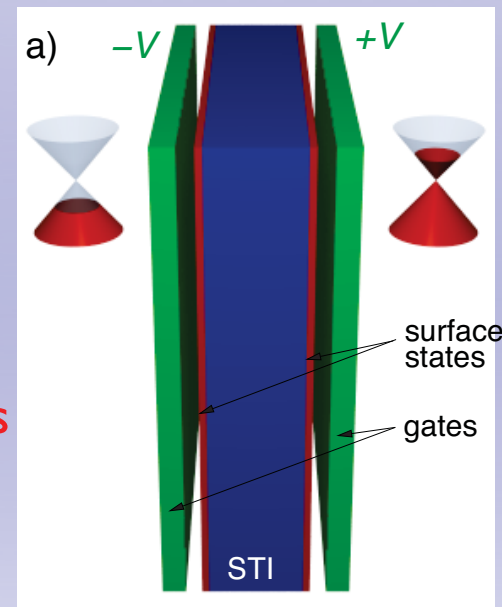
Idea of exciton condensation:

(Conventional) Superconductivity occurs when we have identical spin-up and spin-down electron Fermi surfaces and a weak attractive interaction.

Exciton condensation occurs when we have identical *electron* and *hole* Fermi surfaces and an attractive interaction between electrons and holes, i.e., Coulomb *repulsion*.

Why is this difficult? Need an applied field or some other mechanism to keep electrons and holes from recombining.

Alternately can study nonequilibrium condensation before electrons & holes recombine (Butov, Chemla et al.)



Correlated phases from TI surfaces

Formally, exciton condensation is like BCS in the “particle-hole” channel: continuously connected to BEC of excitons.

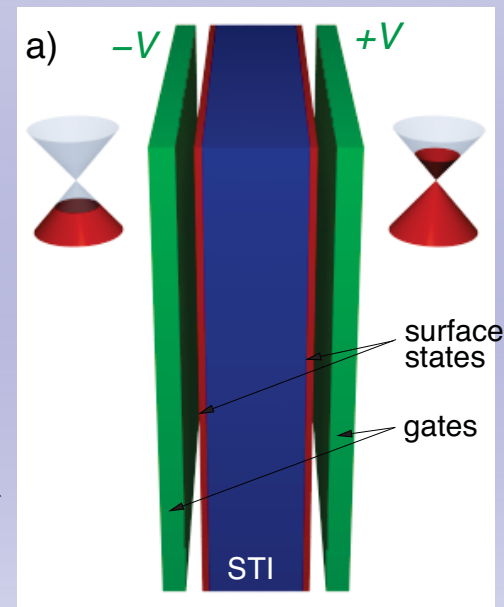
$$H_{\text{MF}} = H_0 + (\psi_1^\dagger M \psi_2 + \text{h.c.}) + \frac{1}{U} \text{Tr}(M^\dagger M),$$

Key: unscreened interlayer Coulomb repulsion, with no tunneling.

Generated gap in weak-coupling limit:

$$m \approx 2\sqrt{V}\Lambda e^{-\Lambda^2/UV}$$

Need large voltage V and coupling U , with chemical potentials symmetric around Dirac point. New materials (e.g., Ca doping) allow the Dirac point to be moved out of the bulk bandgap.



Transition temperature is of same order or higher than in graphene.
Goal: first stable exciton condensate outside quantum Hall regime.