Abelian and non-Abelian gauge fields in the Brillouin zone for insulators and metals

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Outline

0. Warm-up: Berry phases, Chern number, and topological insulators

1. Magnetoelectric response in all insulators and the non-Abelian Berry gauge field in the Brillouin zone
(thanks to A. Essin, A. Turner, D. Vanderbilt)

2. Approaching metallic transport in 2D by statistical topology
Trying to develop a topological theory of the anomalous Hall effect
(J. Dahlhaus, R. Ilan, and JEM, unpublished; JEM and J. Orenstein, PRL 2010)

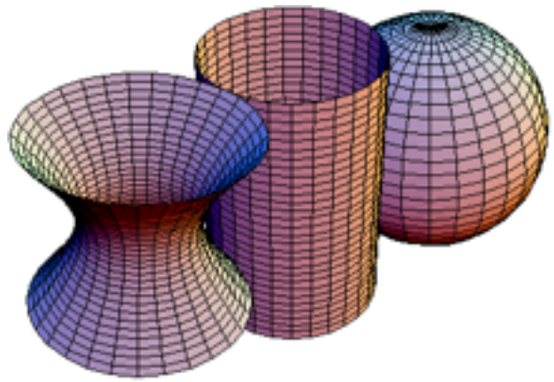
Assume noninteracting electrons unless otherwise stated.

Topological invariants

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

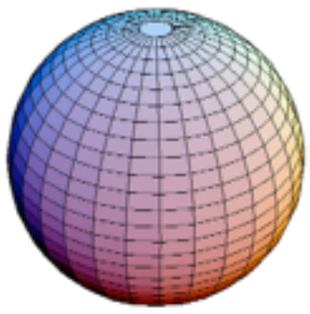
Consider a two-dimensional surface.

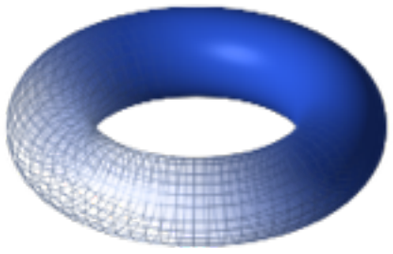
At any point on the surface, there are two radii of curvature.
We define the signed "Gaussian curvature" $\kappa = (r_1 r_2)^{-1}$



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).

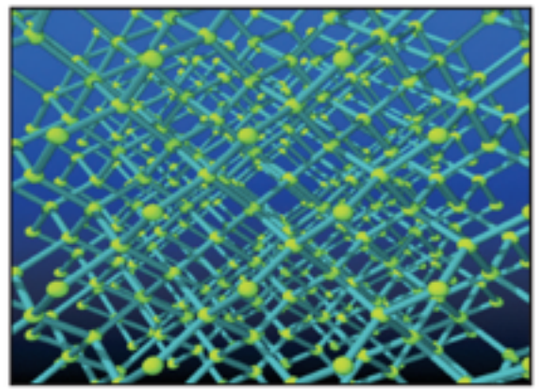
$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2 - 2g)$$

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:

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

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

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

Michael Berry

just like the vector potential in electrodynamics.

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

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

Berry phase in solids

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

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

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

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

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

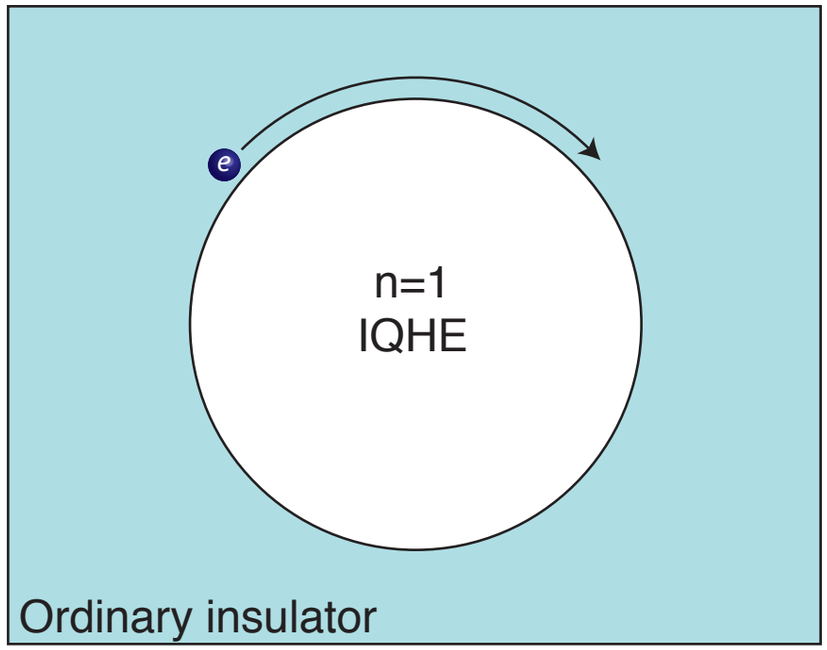
But wait a moment...

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.

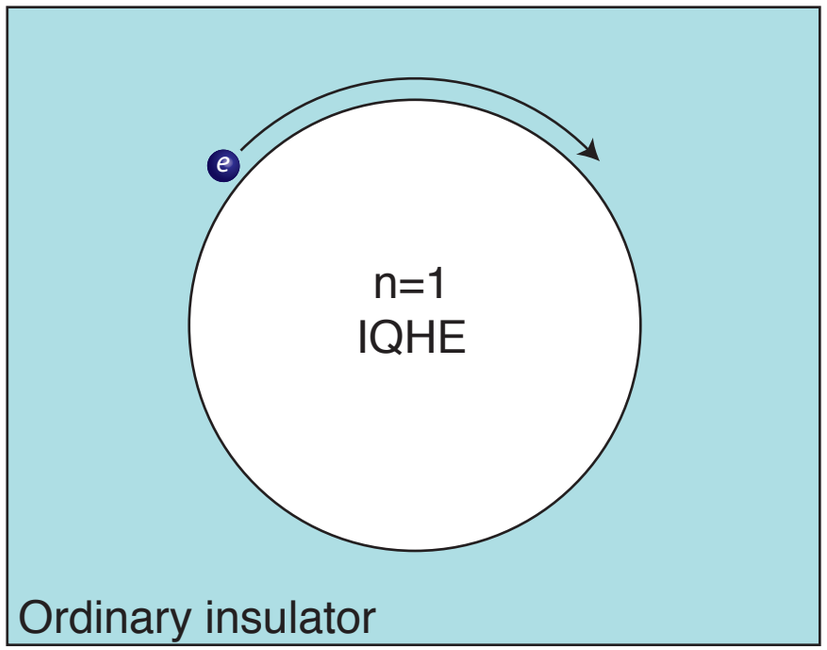
How does the bulk topological invariant "force" an edge mode?

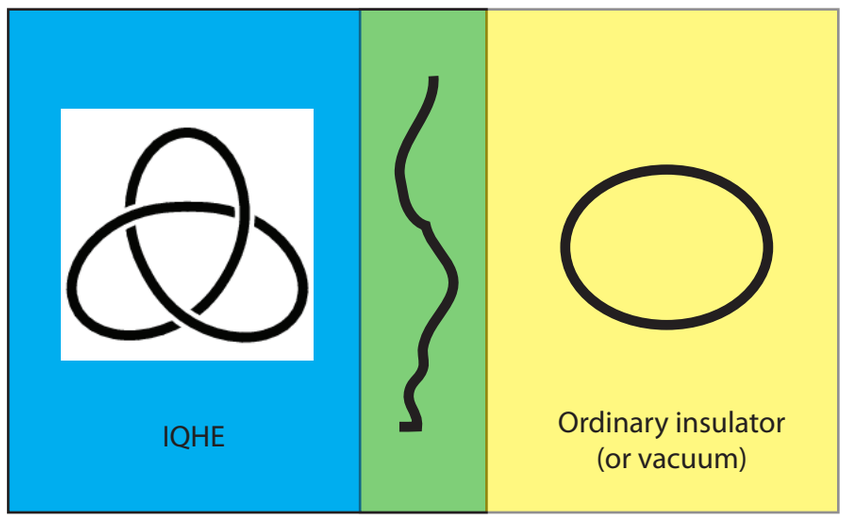
Answer:

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.





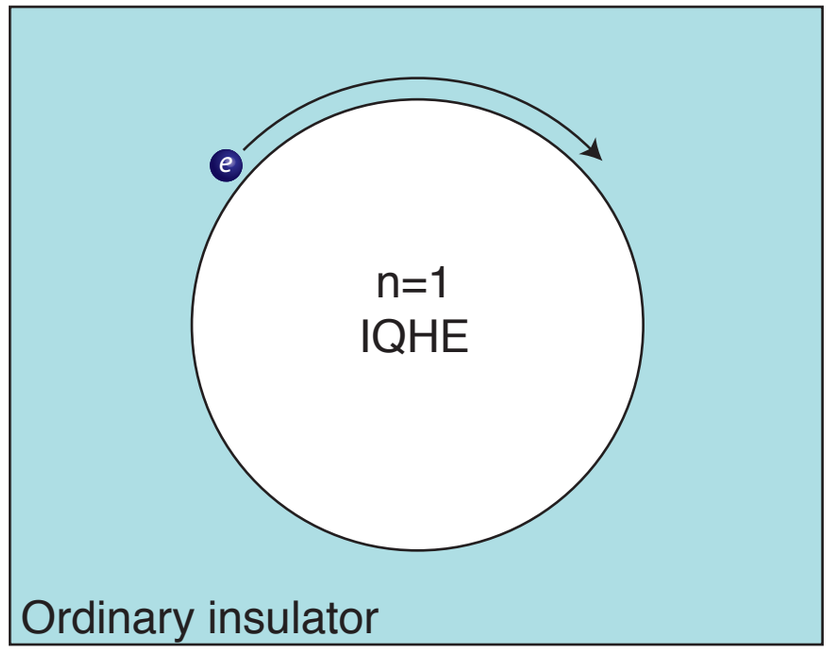
(What is "knotted" are the electron wavefunctions)

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

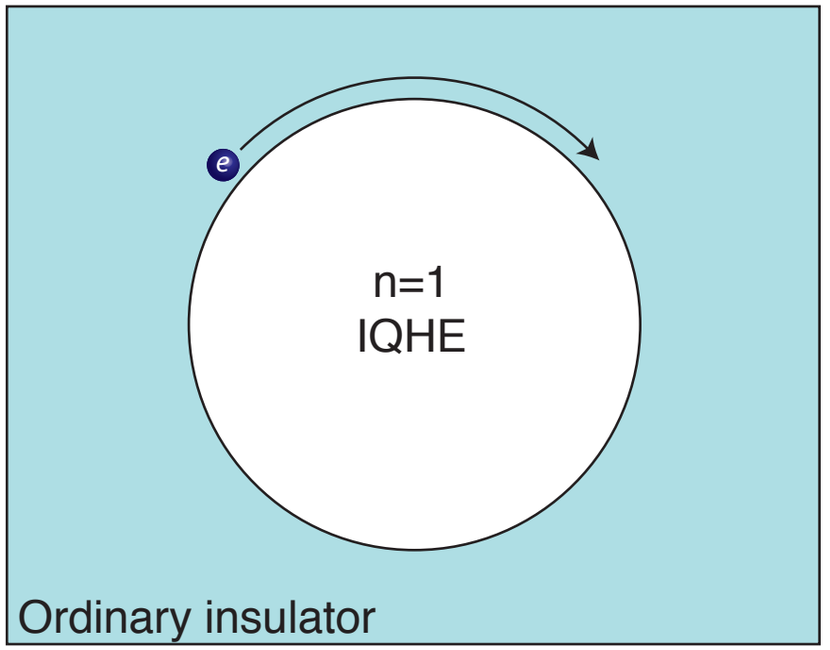
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

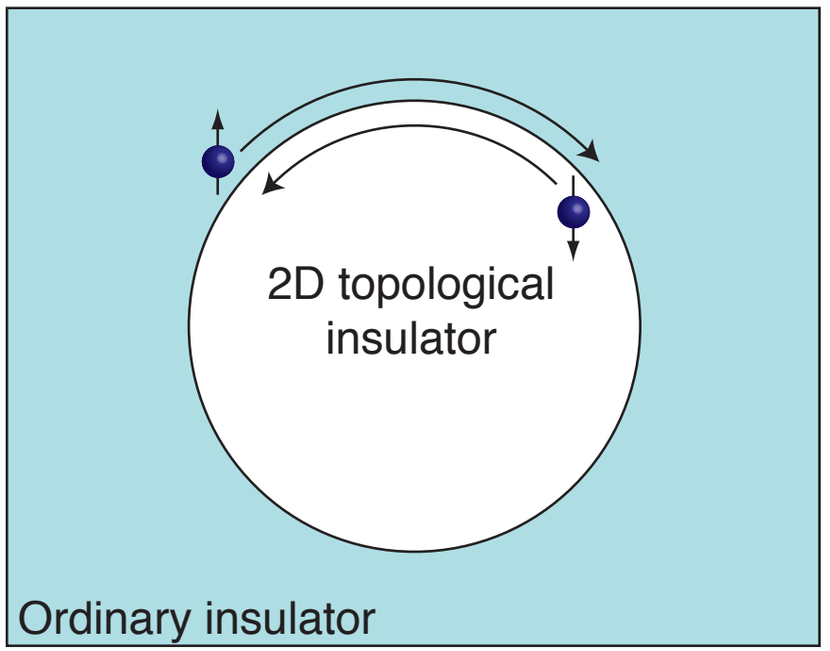
For a given spin, this term leads to a momentum-dependent force on the electron, somewhat like a magnetic field.

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".



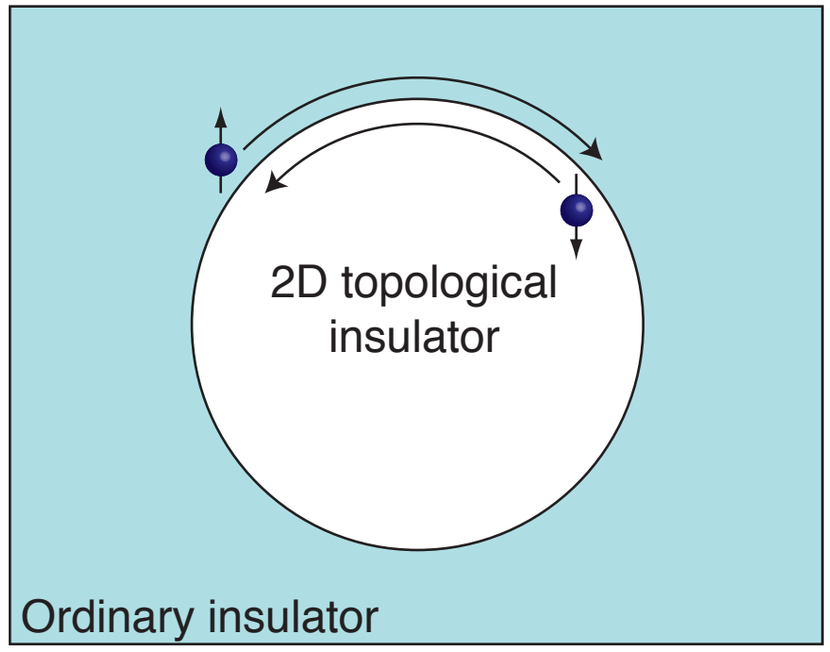


The "quantum spin Hall effect"

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.

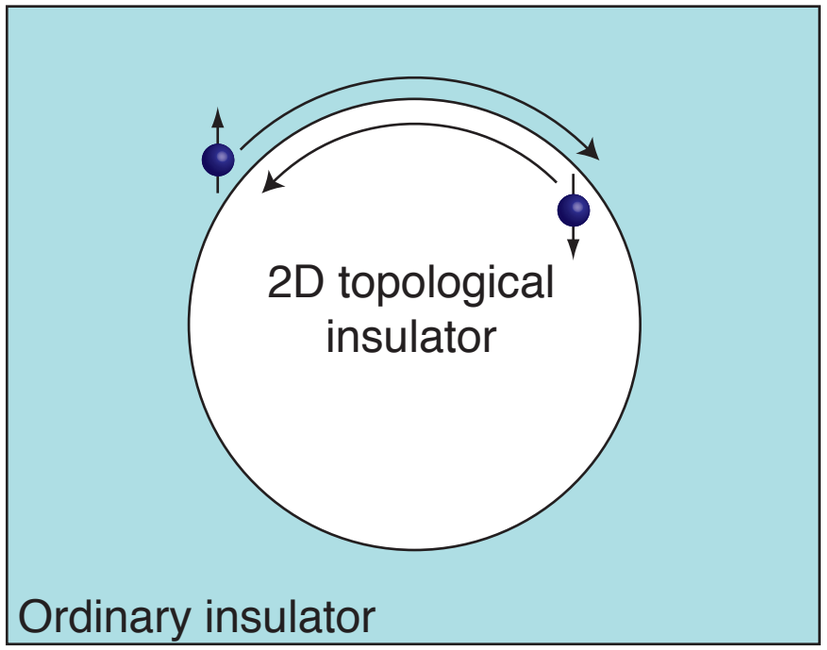
The 2D topological insulator

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?

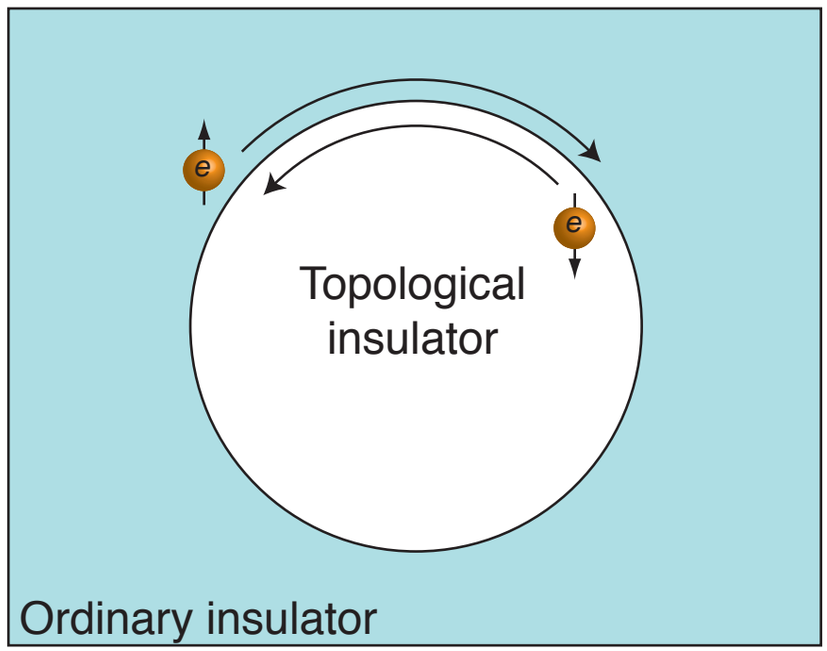
The "Chern insulator" and QSHE

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)

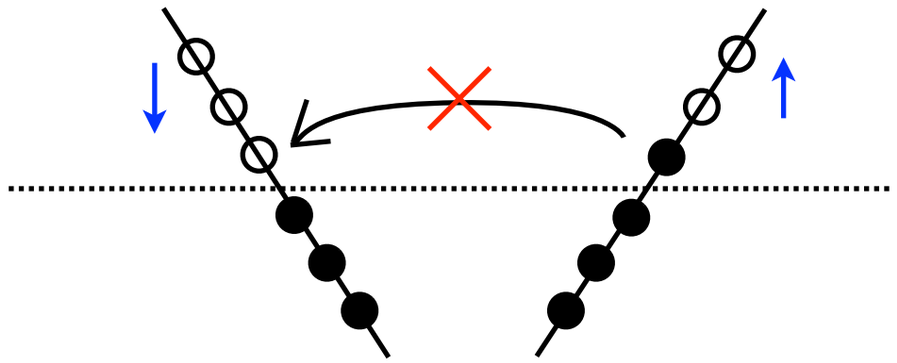


The 2D topological insulator

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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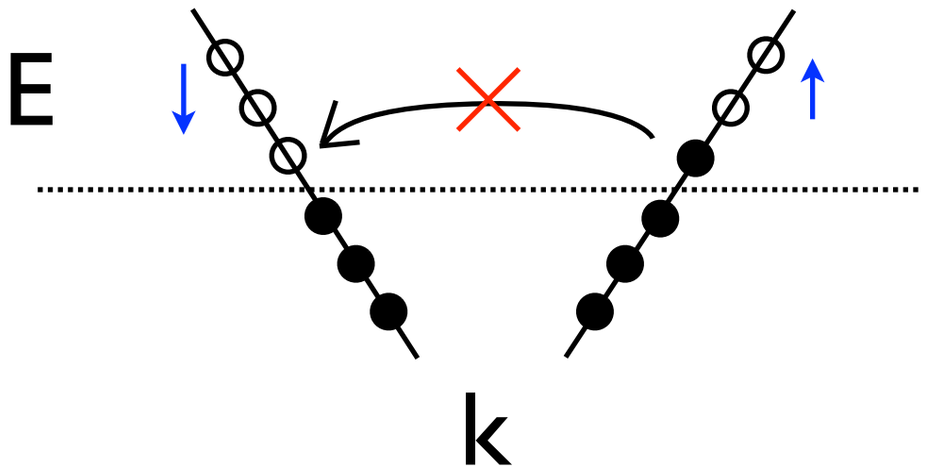
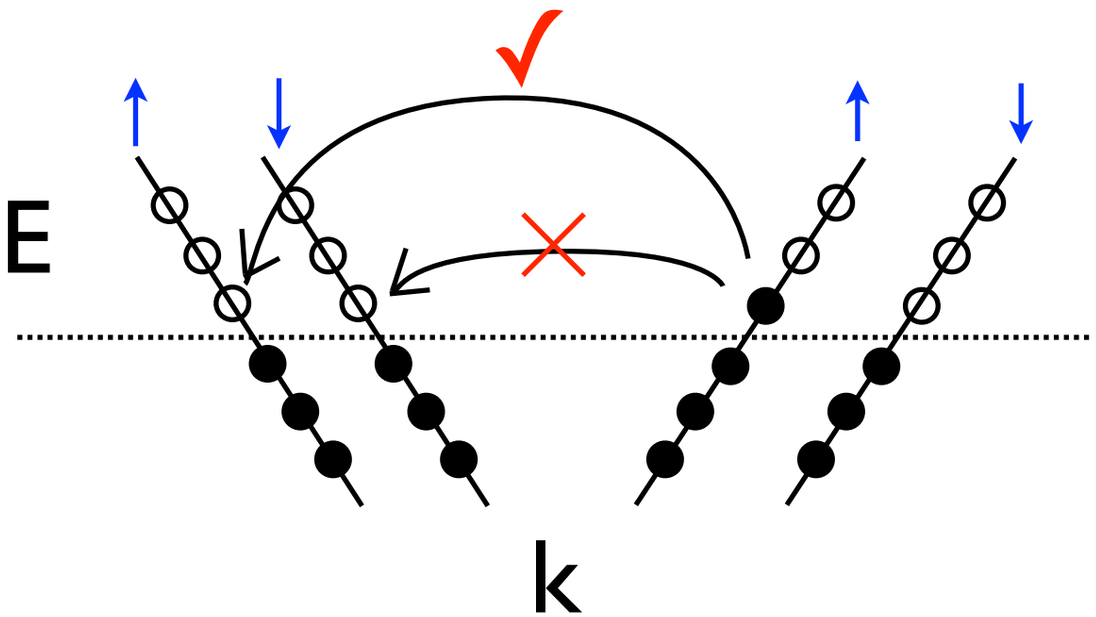


But this rule does not protect an ordinary quantum wire with 2 Kramers pairs:



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

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

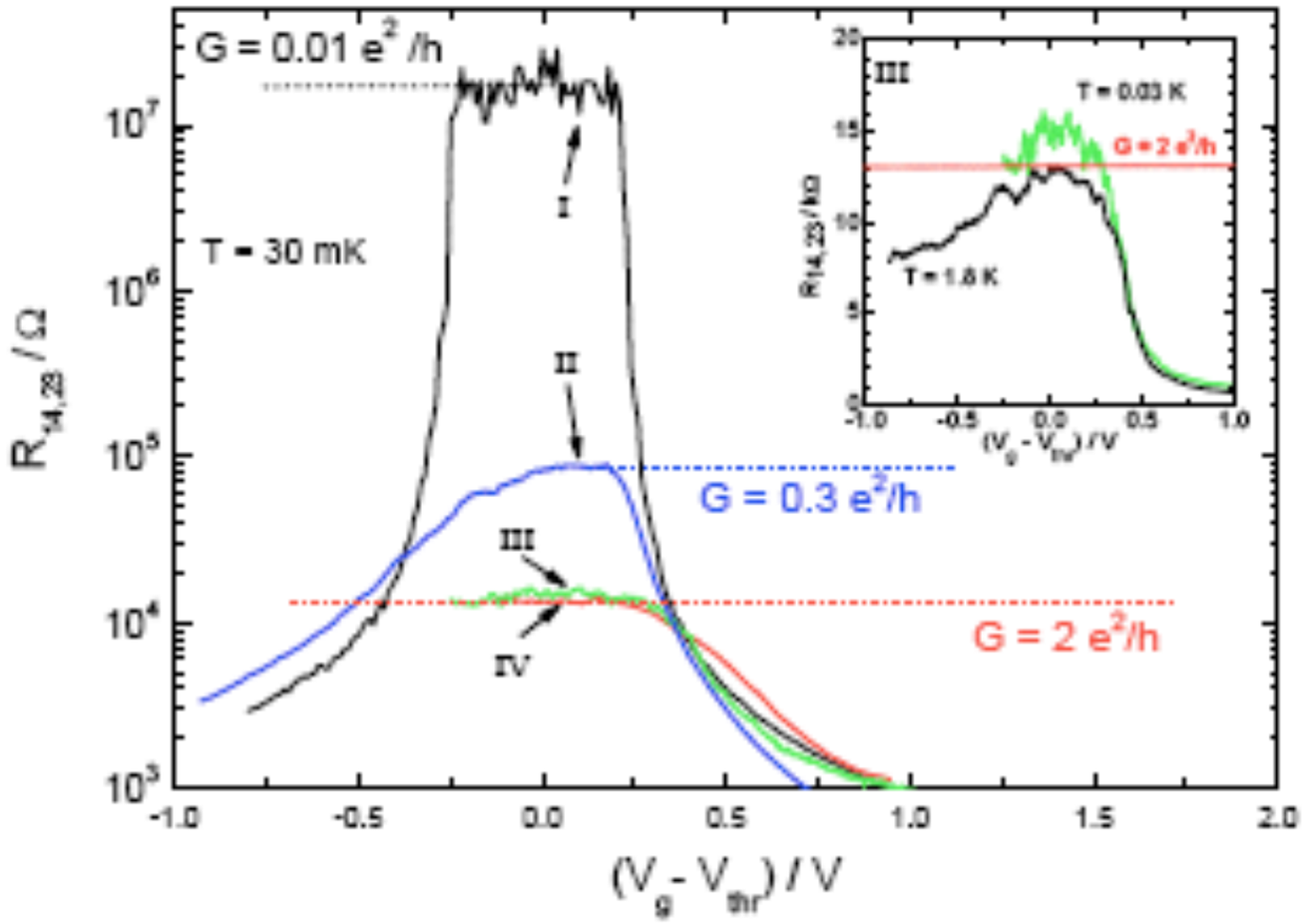
Key: the topological invariant predicts the "number of quantum wires".

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.

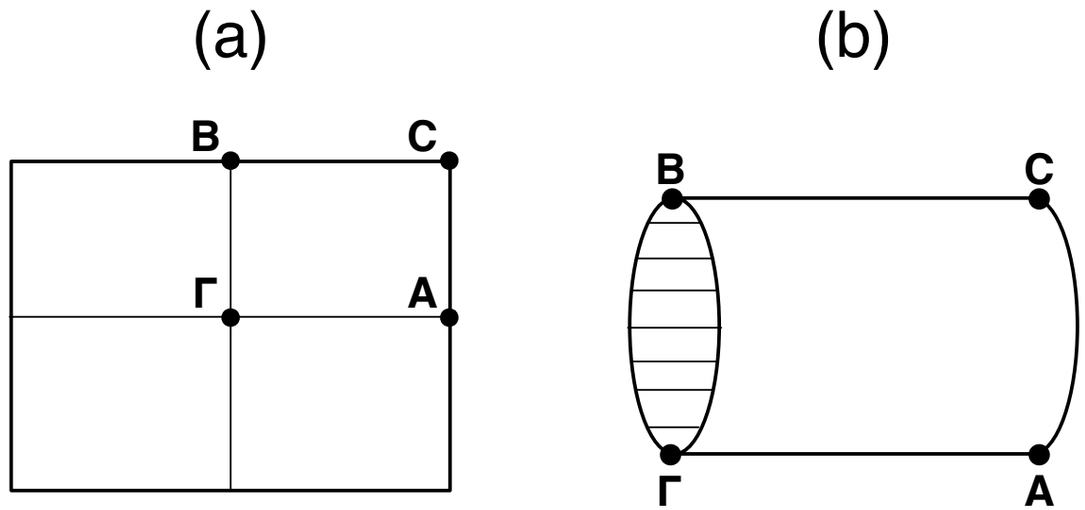
However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

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, PRB 2009.

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:

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

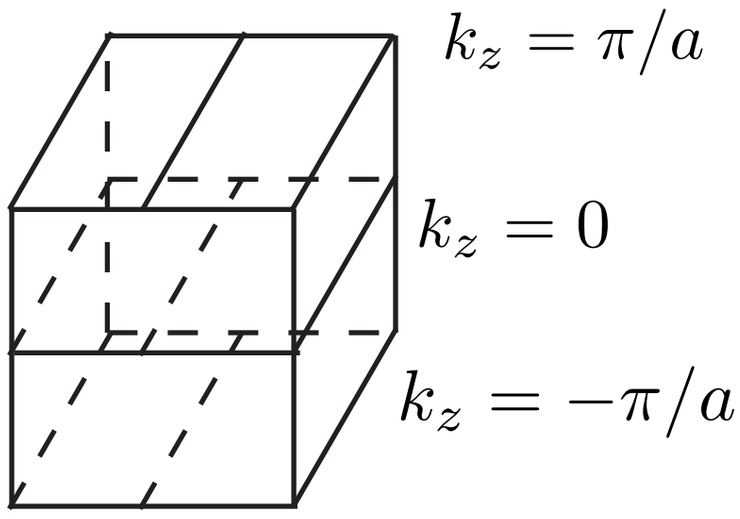


"effective BZ"

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

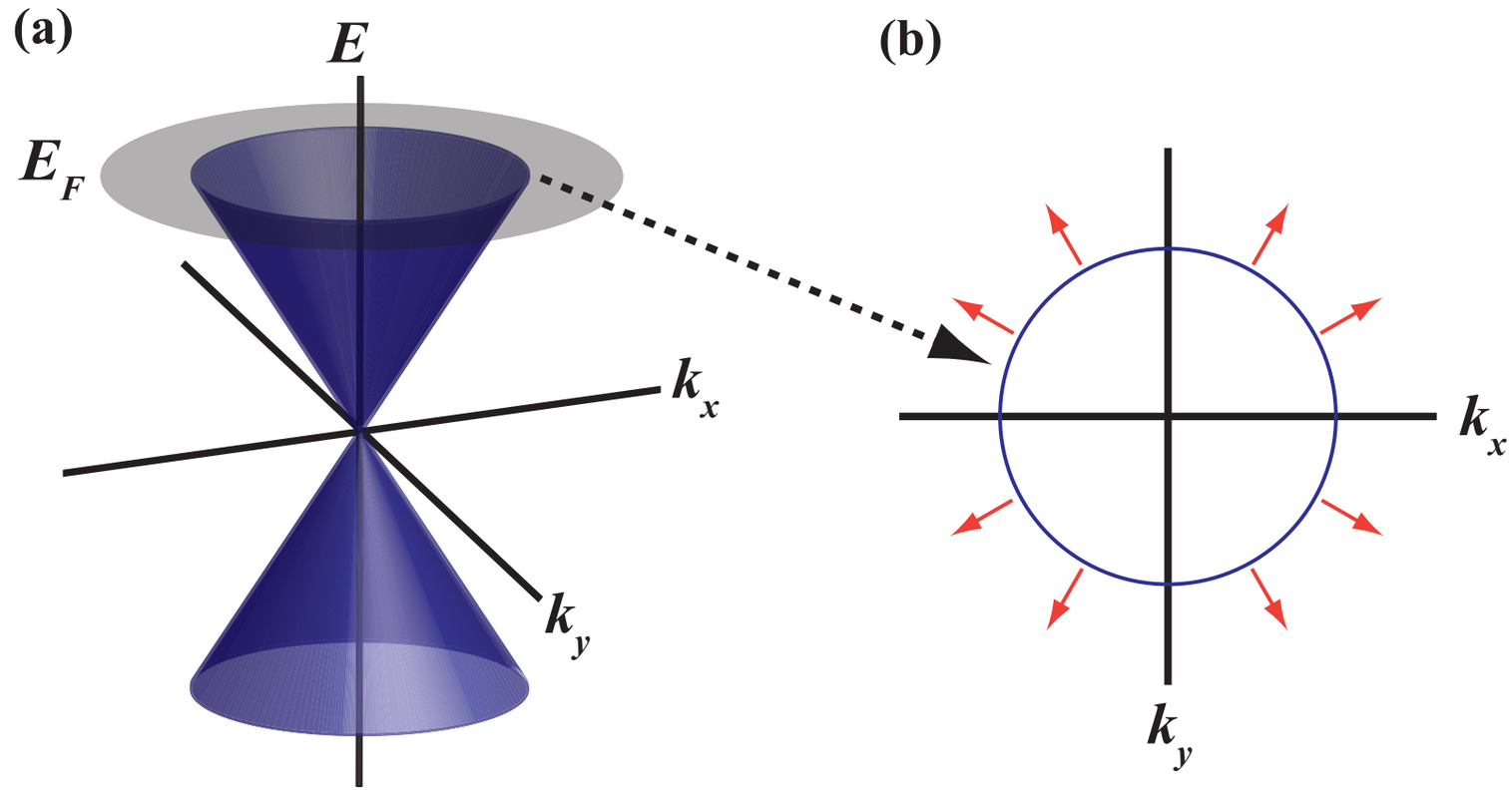


3D "strong topological insulators" go from an 2D *ordinary* insulator to a 2D *topological* insulator (or vice versa) in going from k_z=0 to k_z=±π/a.

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)



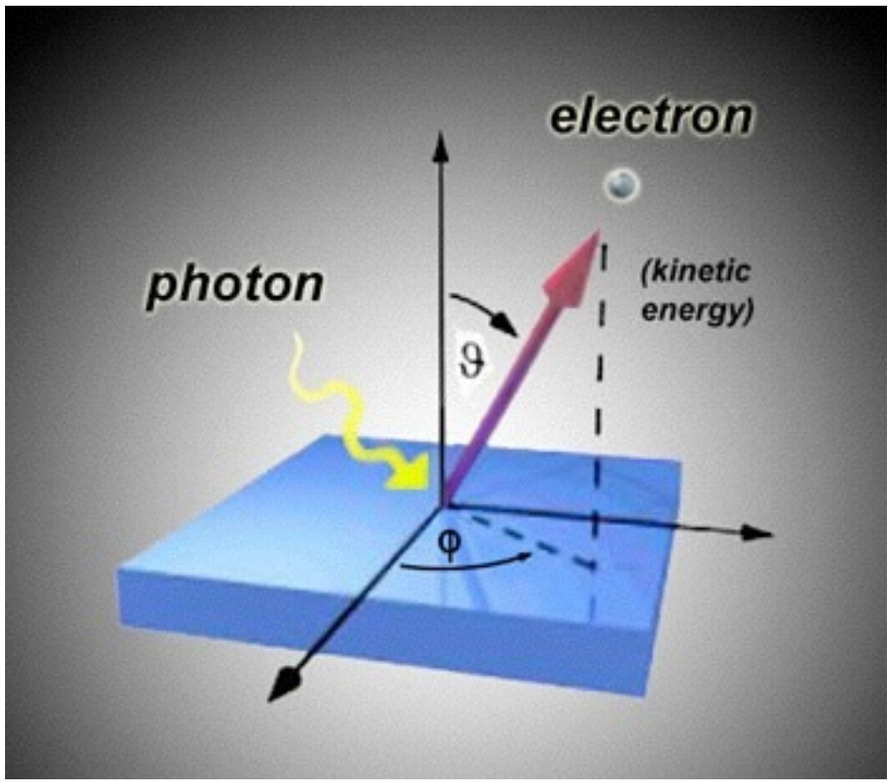
2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

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.



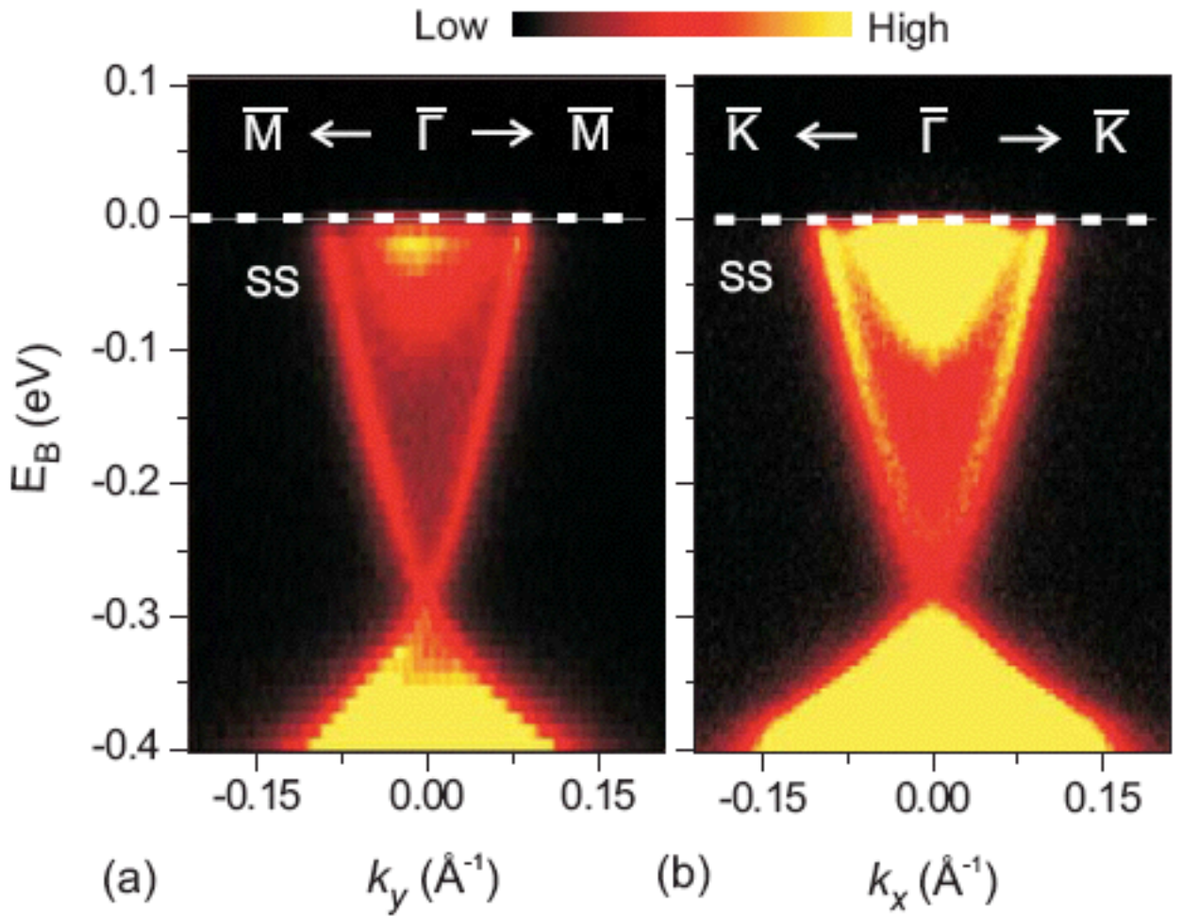
Measure as many properties as possible of the outgoing electron
to deduce the momentum, energy, and spin it had while still in the solid.

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.

Periodic table of one-fermion TIs

In every dimension, of the 10 Altland-Zirnbauer symmetry classes, there are 3 with integer invariants and 2 with Z2 invariants. But different symmetry classes are topological in different dimensions. (Schnyder et al.; Kitaev)

In the table below, A = unitary class (no symmetry).
AII = symplectic class (time-reversal symmetry that squares to -1)

TABLE II. Topological insulators (superconductors) with an integer ($\mathbb{Z}$) classification, (a) in the complex symmetry classes, predicted from the chiral U(1) anomaly, and (b) in the real symmetry classes, predicted from the gravitational anomaly (red), the chiral anomaly in the presence of background gravity (blue), and the chiral anomaly in the presence of both background gravity and U(1) gauge field (green).

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	⋯
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	⋯
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	⋯
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	⋯
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	⋯
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	⋯
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	⋯
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	⋯
CII	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	⋯
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	⋯
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	⋯

Recall ordinary electrical polarization

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.

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*.

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

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.

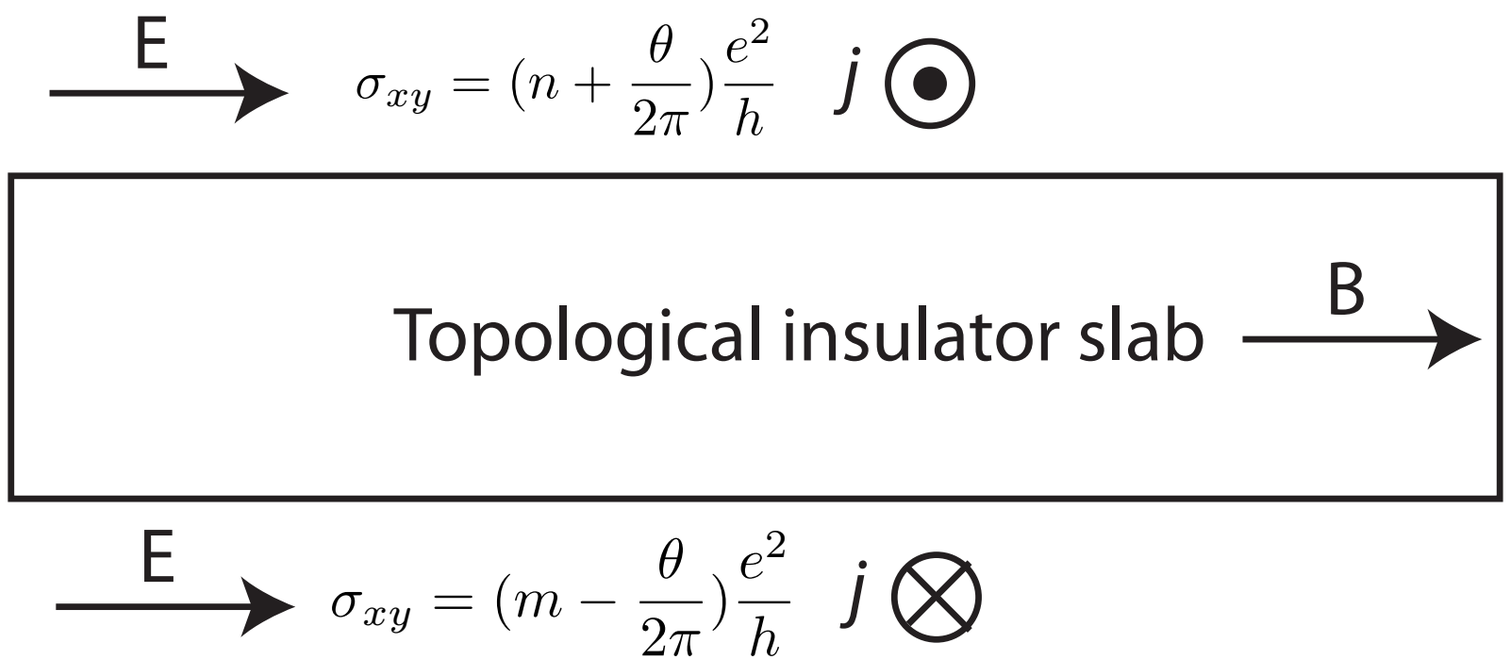
A T-invariant insulator can have *two* possible values: 0 or π.

Axion E&M

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

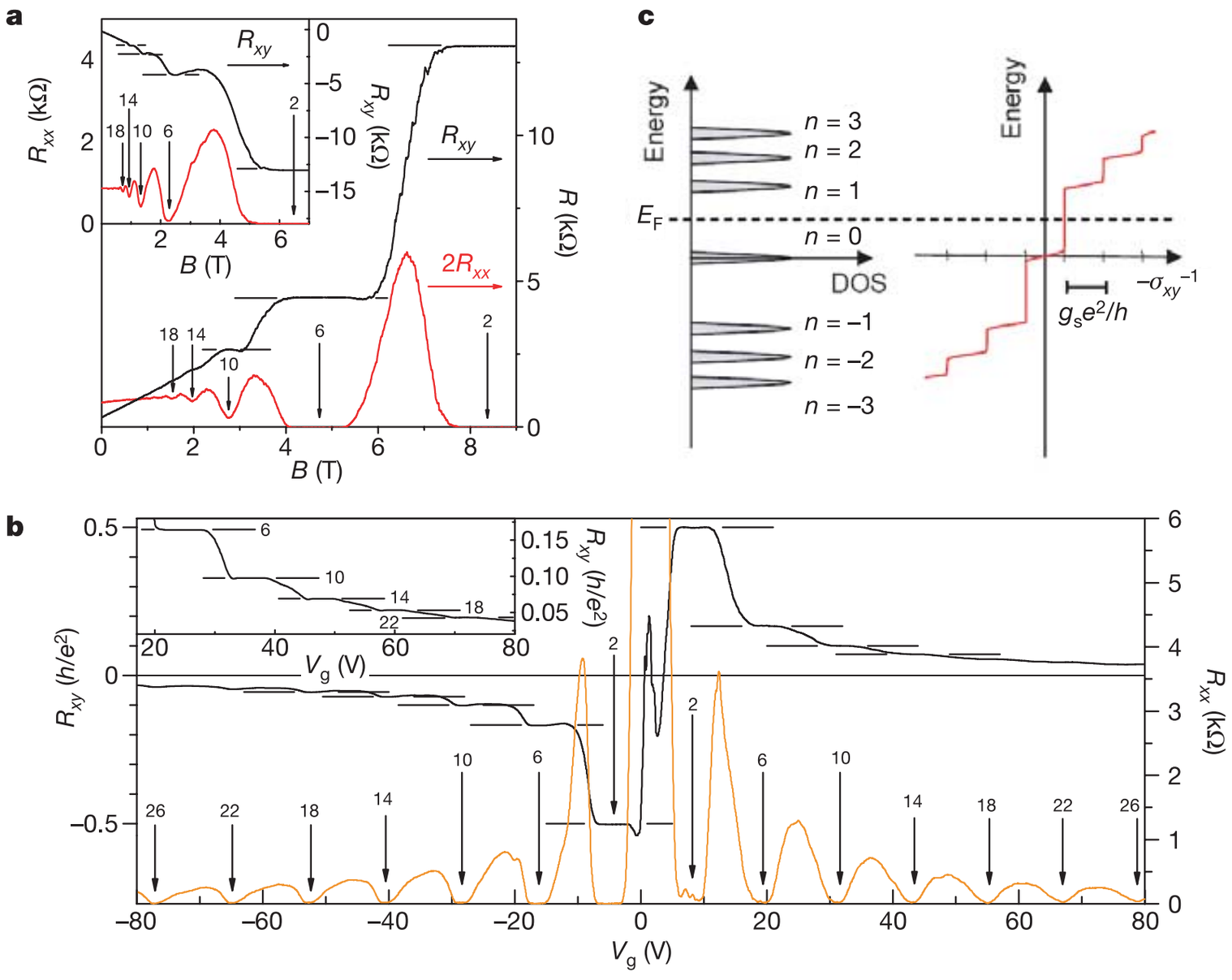
This explains a number of properties of the 3D topological insulator when its surfaces become gapped by breaking T-invariance:

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



Graphene QHE

The connection is that a single Dirac fermion contributes a *half-integer QHE*: this is seen directly in graphene if we recall the extra fourfold degeneracy. (Columbia data shown below)



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.

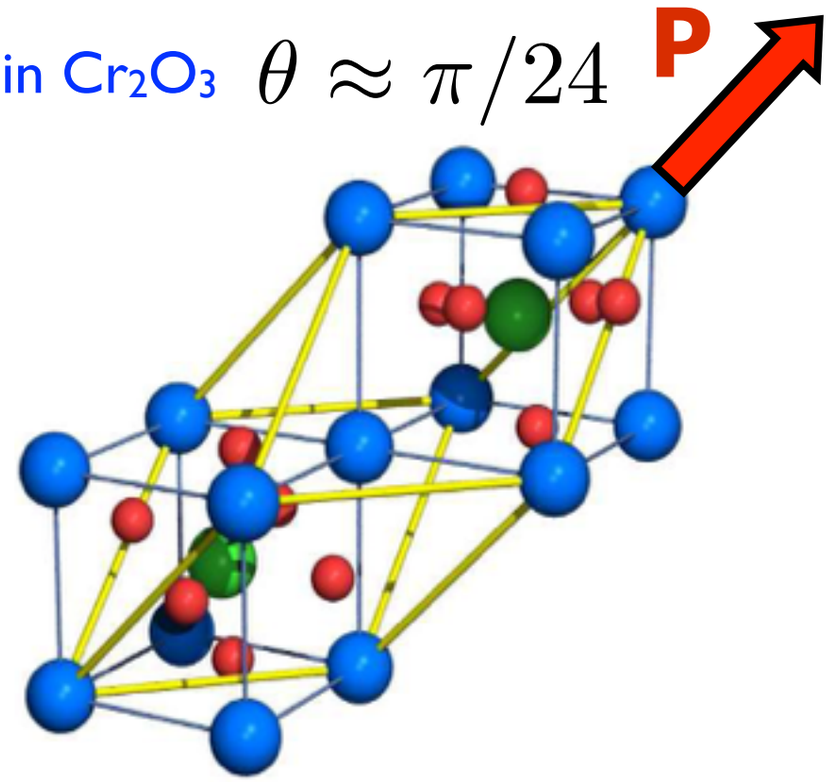
Magnetoelectric theory: a spinoff of TIs

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.

But what does *F* do in metals?

It is useful to get some intuition about what the Berry F means:

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; wait one moment…

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

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

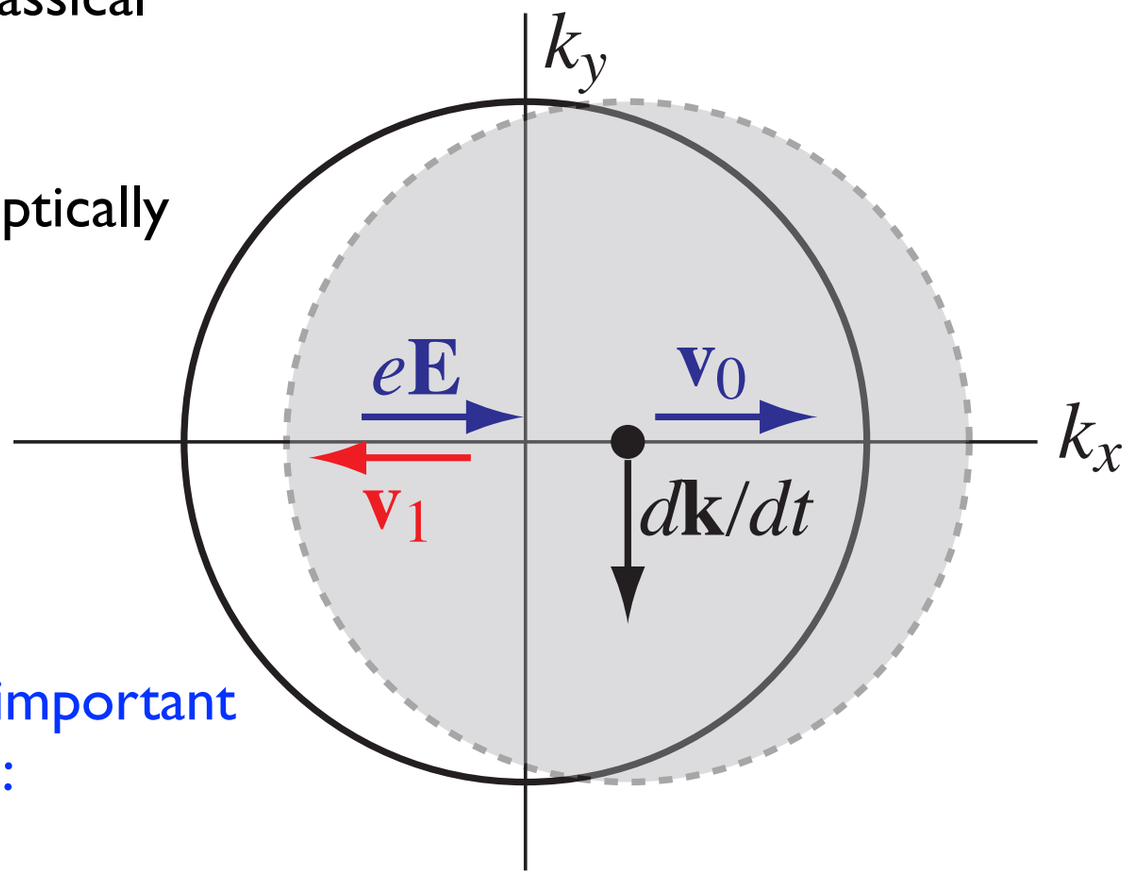
Smit's objection: in steady state the electron distribution is stationary; why should the anomalous velocity contribute at all?

(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, PRL 2010). See also 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.

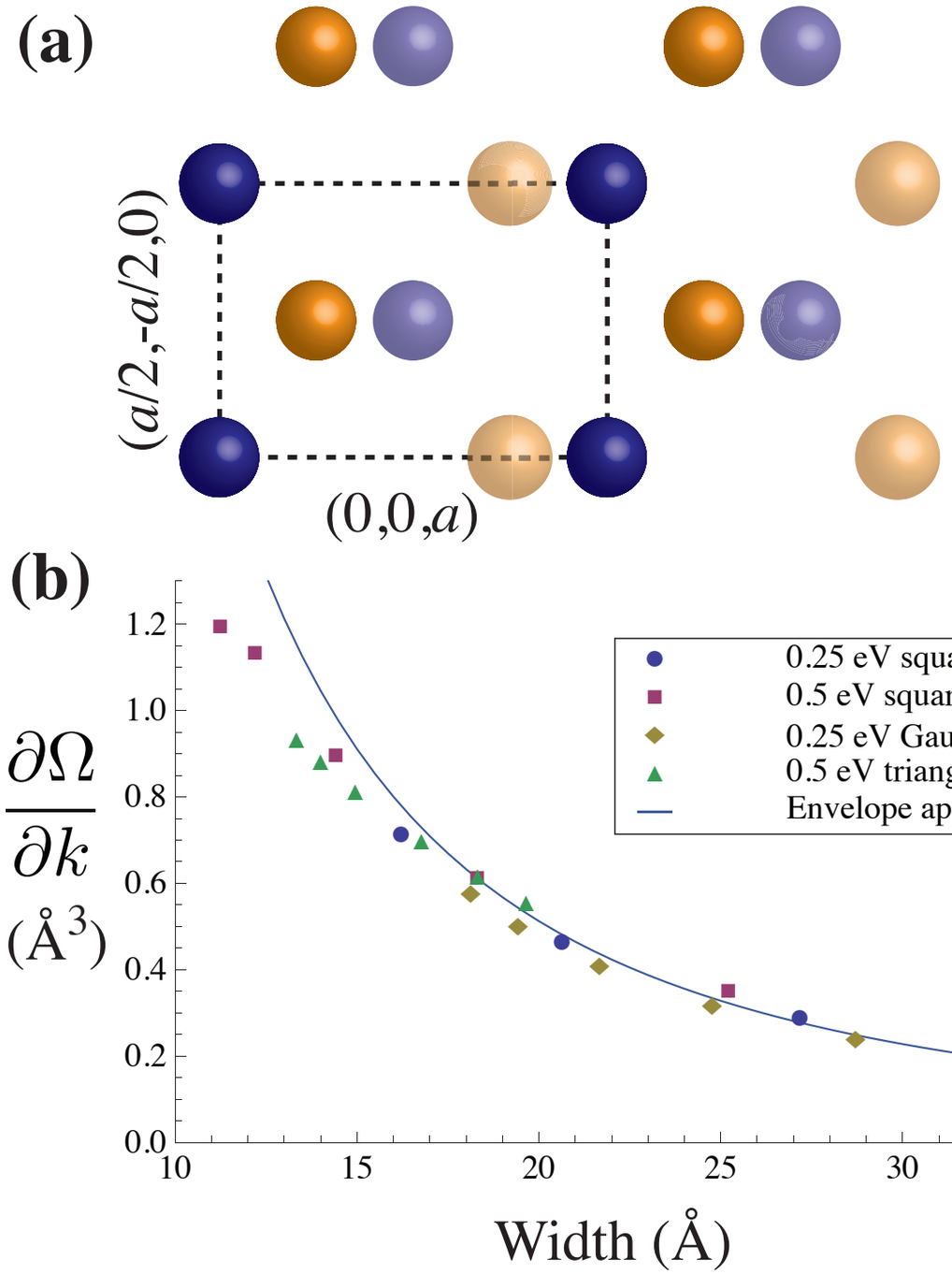
Bulk GaAs has too much symmetry to allow the effect; these quantum wells show the effect because the well confinement breaks the symmetry ("confinement-induced Berry phase").

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



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

Anomalous Hall effect from topology

Problem with semiclassical (and other) approaches:

Focus on 2D systems to make the problem especially clear. Without disorder, there are "Bloch oscillations" and transport samples all states, not just initially occupied states.

With disorder, there is no true metal at T=0 without interactions in 2D with broken time-reversal symmetry.

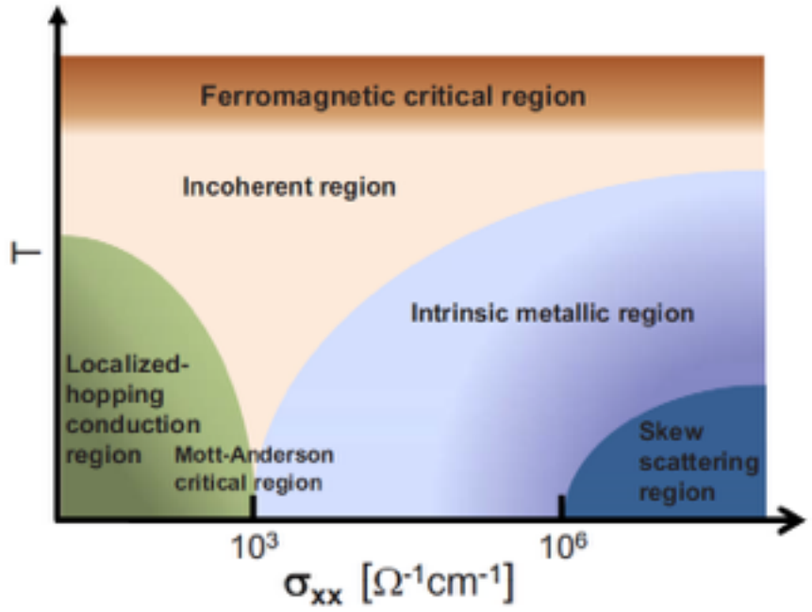


FIG. 47. (Color online) A speculative and schematic phase diagram for the anomalous Hall effect in the plane of the diagonal conductivity σ_{xx} and the temperature T.

From Nagaosa et al., RMP 2011

T=0 approach to disorder-averaged Hall conductivity

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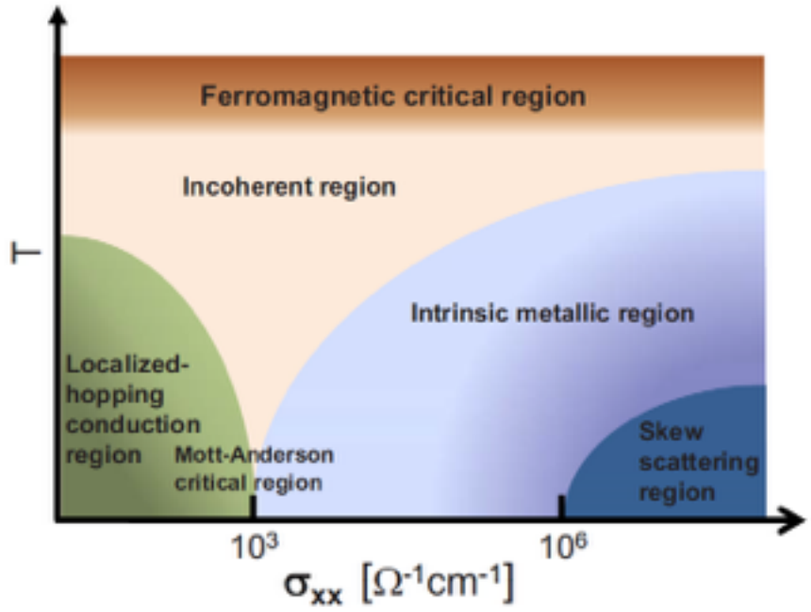
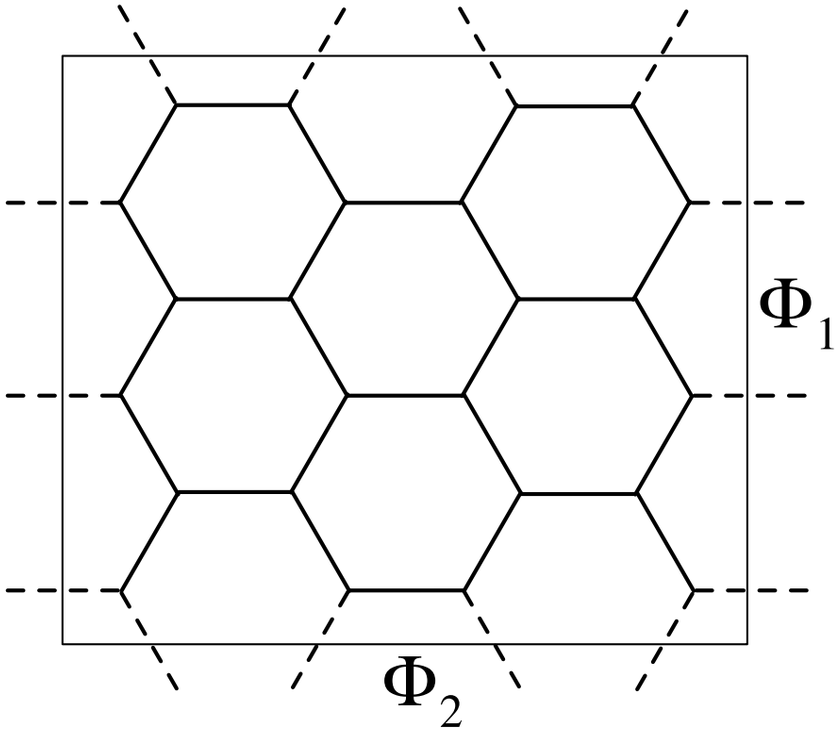


FIG. 47. (Color online) A speculative and schematic phase diagram for the anomalous Hall effect in the plane of the diagonal conductivity σ_{xx} and the temperature T.

From Nagaosa et al., RMP 2011

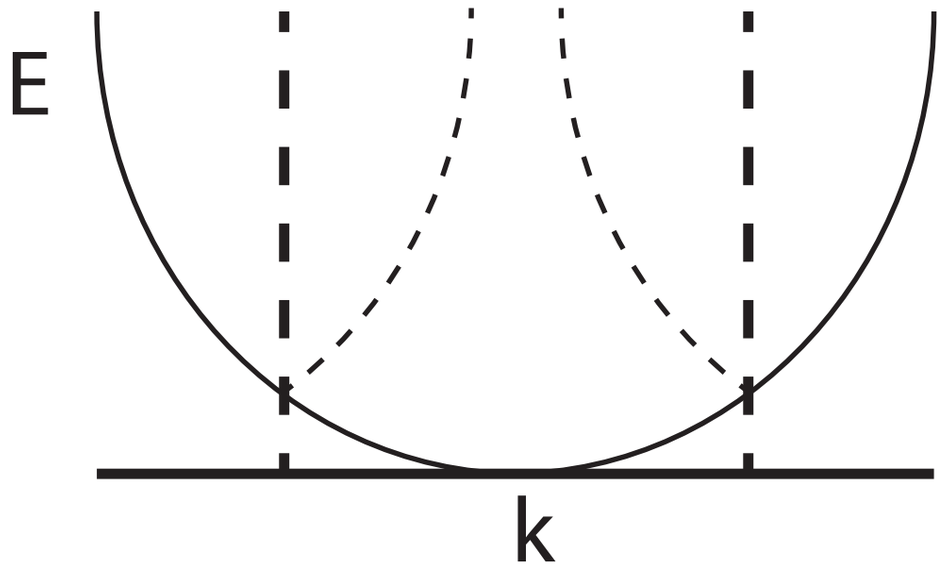
Take a "supercell" of many unit cells



Phase boundary conditions = momentum in band structure

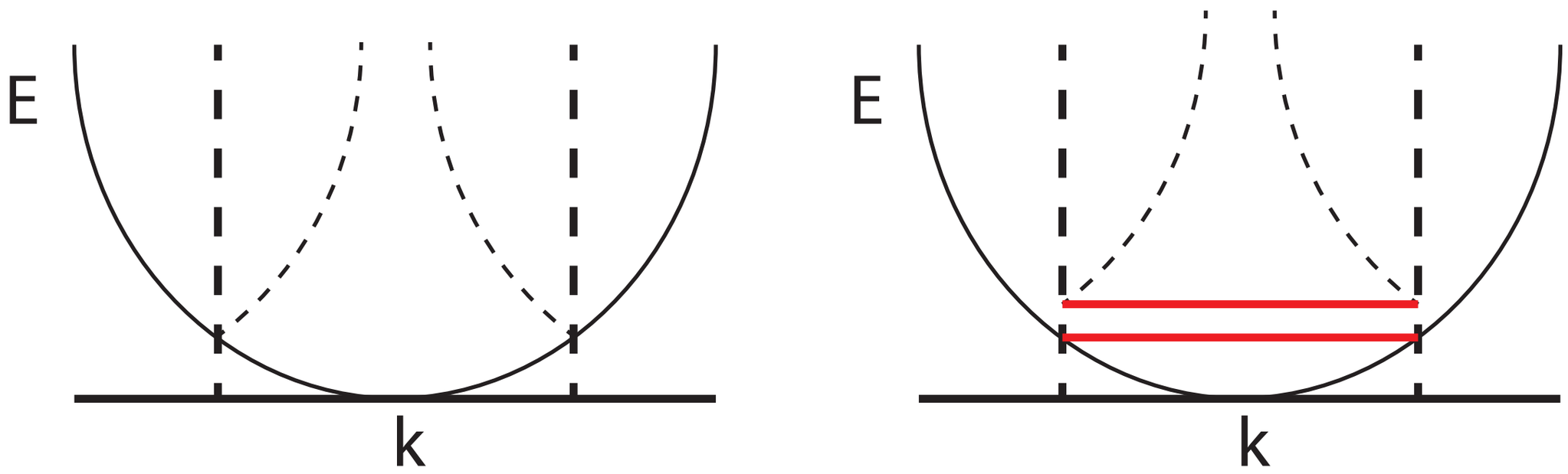
Larger real-space unit cell = smaller momentum-space "Brillouin zone"

Bands touch at zone boundaries since they came from 1 band in the original (small) unit cell



Supercell Chern number

When bands touch, only the total Chern number is well-defined.

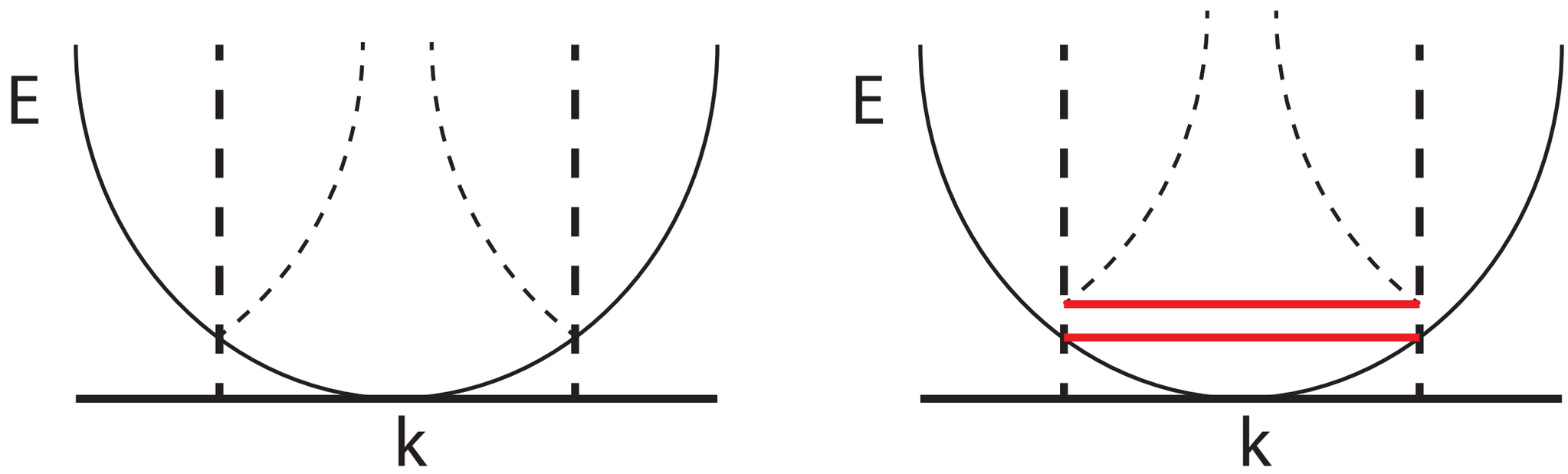


Adding disorder splits degeneracies and leads to “minibands”, each with its own Chern number. These must sum to the original Chern number of the whole band.

The precise disorder distribution determines how the Chern numbers are assigned to each miniband, consistent with this rule.

Supercell Chern number

Simplest case:



Now we can compute the Hall conductivity in each realization, as each realization is (almost) an insulator: since each miniband is very narrow in energy, almost every band is completely filled or completely empty.

In each realization, compute total Chern number of the bands occupied at each filling.

The Chern number "shell game"

Simplest case: total Chern is 1; which mini band gets it?

(This picture is not strictly correct, since there can be Chern numbers of either sign.)

There are clearly strong fluctuations in the Chern number of each mini band. But what can determine its average?

Idea: (like equipartition) at weak disorder, the resolving of anti crossings does not shift Chern weight *on average*; the average is just determined by the Chern density.

Obtaining the metal as a statistical limit of Chern insulators

$$\langle \sigma_{xy}(E_F) \rangle \equiv \frac{e^2}{h} \lim_{\substack{N\to\infty \\ n_F/N = n(E_F)}} \sum_{i=1}^{n_F} \langle C_i \rangle = \frac{e^2}{h} \int_{E(k_x,k_y)<E_F} F(k_x,k_y)\, dk_x\, dk_y$$

Here *N* is the (large) number of bands in the supercell and angle brackets mean averaging over disorder.

The metallic limit is that disorder is *weak* (it only opens the minigaps). More precisely:

In standard IQHE limit (Chalker-Coddington physics): disorder fixed as system size increases. Eventually IQHE transition becomes sharp, occurs at a fixed energy.

Here we should scale disorder to 0 as size increases.

Preliminaries: IQHE and QSHE

One prediction of the localization theory of the IQHE plateau transition is:
as the system size *L* increases at fixed disorder, the transition width in energy or density shrinks as a power law in *L*.

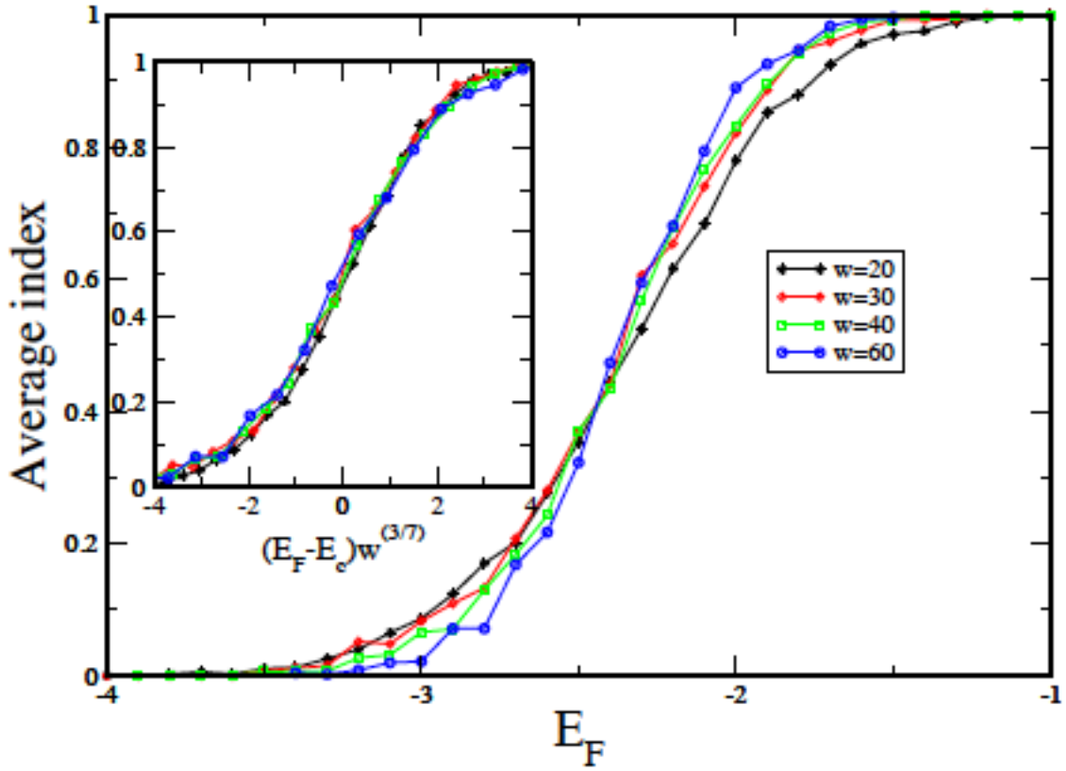
This can be measured by asking over what region of density the topological index is fluctuating for a given size.

In the QSHE, this is esp. interesting as whether or not a U(1) is preserved determines whether transition collapses or not.

Essin and Moore, PRB 2009: approached using Avron, Seiler, Simon “projection operator” method of computing Chern number, which still involves an integral over boundary fluxes.

Hastings and Loring, EPL & Ann. Phys. 2011: developed new operator algebra approach via “almost commuting matrices”.

IQHE-type width collapse



from Loring and Hastings, EPL 2011

Point of Hastings-Loring approach: computing the topological invariant for one disorder realization requires (usually) just *one* diagonalization of the Hamiltonian, not one for each point in the boundary-condition torus.

Not as robust as disorder goes to 0, but computationally very nice.

Point of Hastings-Loring approach: computing the topological invariant for one disorder realization requires (usually) just *one* diagonalization of the Hamiltonian, not one for each point in the boundary-condition torus.

The band-projected "position" operators almost commute and are almost unitary for a system with a mobility gap (satisfied?).

$$P\exp(i\Theta)P \sim \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}, \quad P\exp(i\Phi)P \sim \begin{pmatrix} 0 & 0 \\ 0 & V \end{pmatrix},$$

Can they be deformed to exactly unitary and exactly commuting?

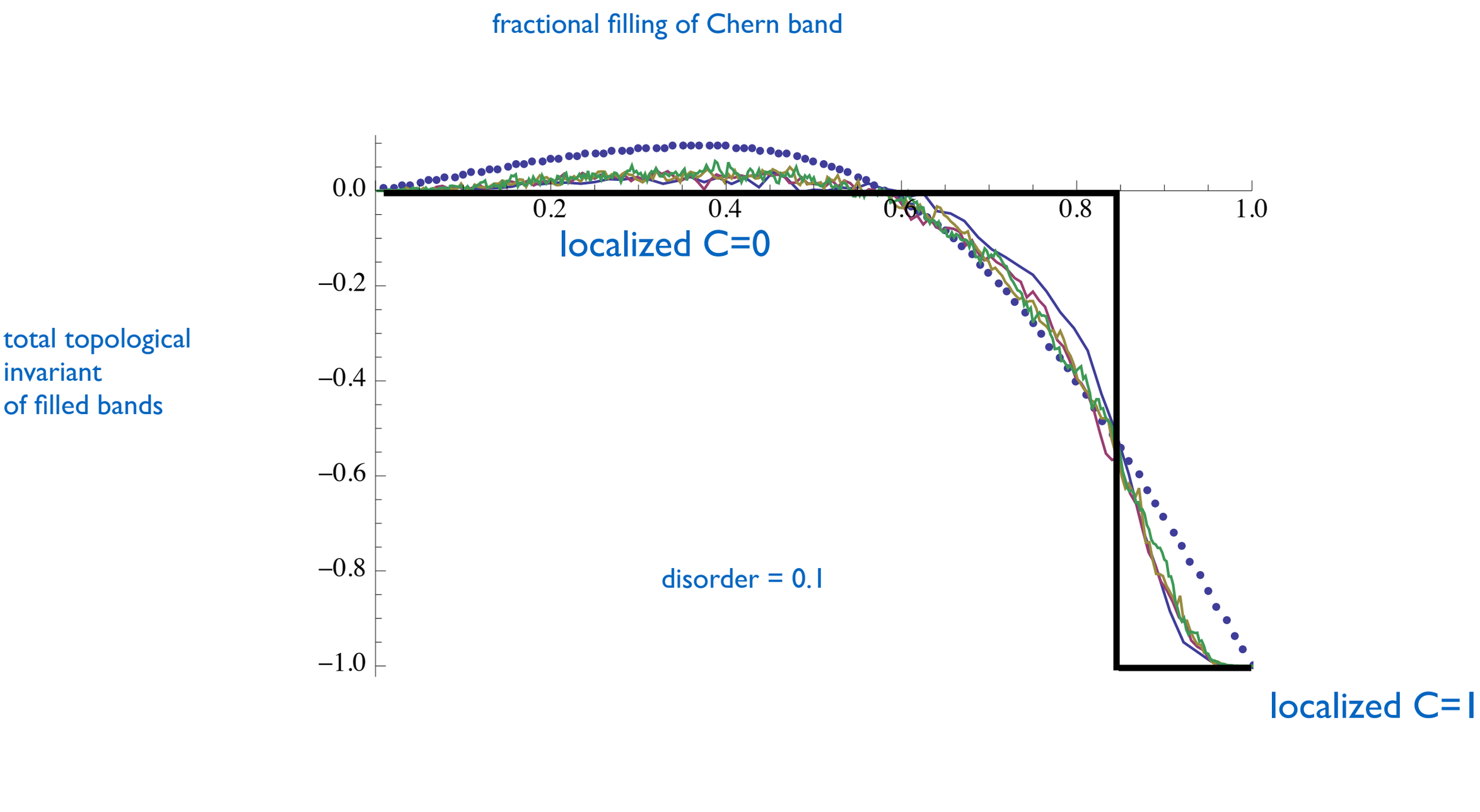
$$\det(VUV^\dagger U^\dagger) = \exp(2\pi i m + r), \quad m \in \mathbb{Z}$$

Clearly not robust as disorder goes to 0 since then individual-band Chern number m isn't even defined, but algorithm forced to return an integer.

from Loring and Hastings, EPL 2011

Metallic limit of topology

Our claim is that there is also an interesting limit different from the scaling collapse: suppose we let the effect of disorder get *weaker*.



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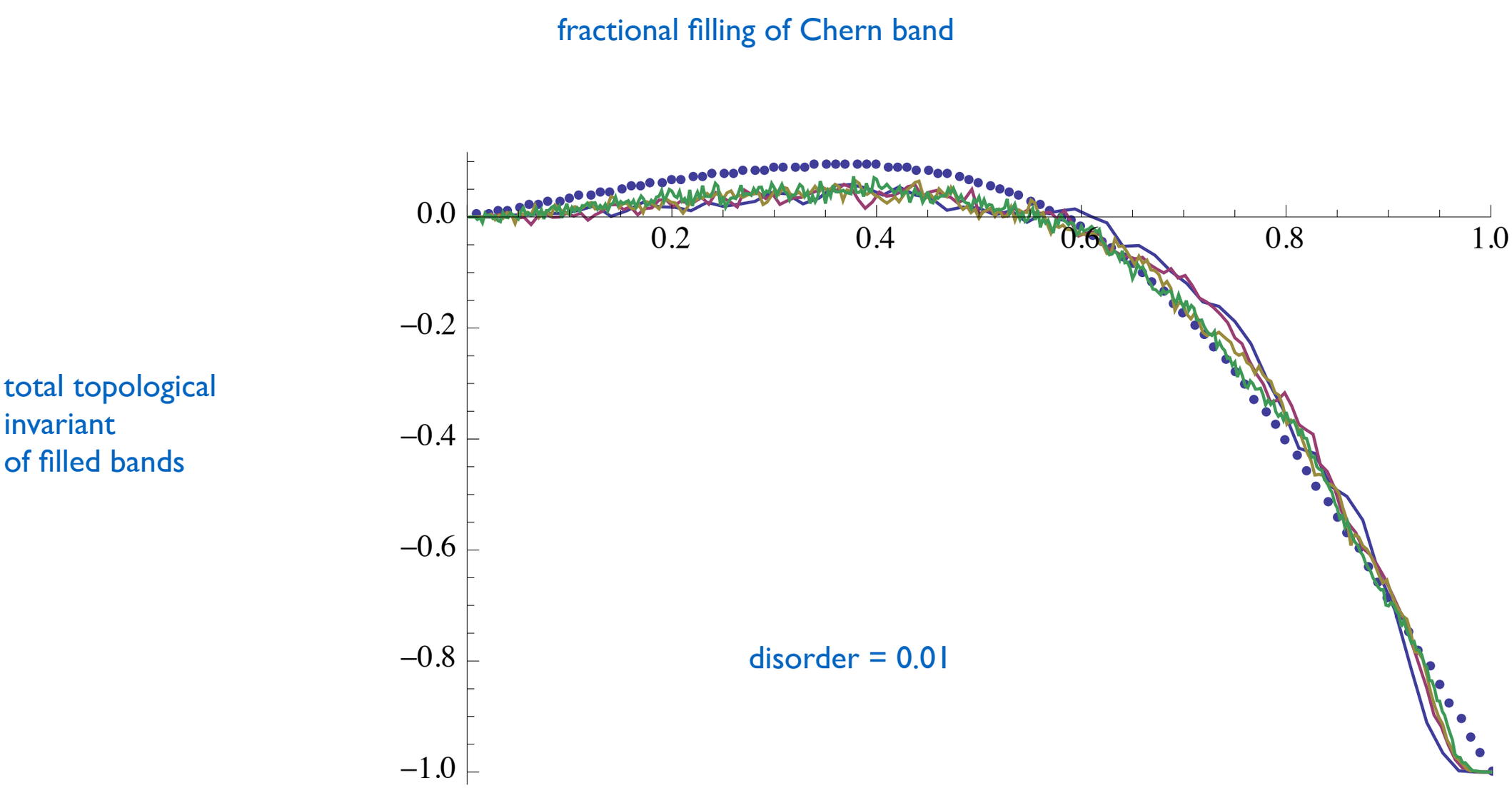

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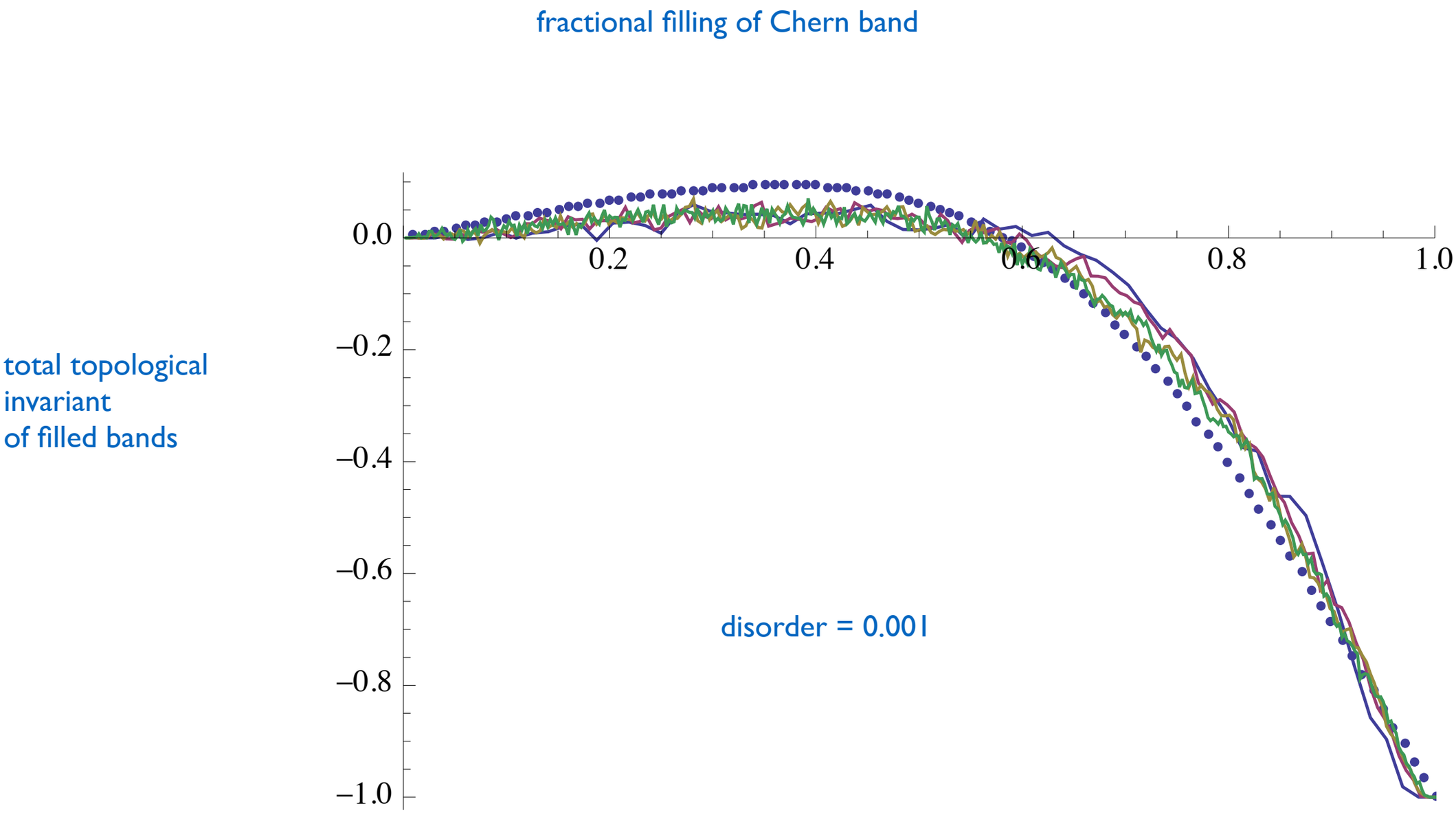

Metallic limit of topology

So, even when the topological invariants of a system are strongly fluctuating, the average has meaningful information.

We believe this is the correct route to a precise theory of the anomalous Hall effect in ordinary *metals*, and that this concept might be generalized to a few other symmetry classes.

$$\langle \sigma_{xy}(E_F) \rangle \equiv \frac{e^2}{h} \lim_{\substack{N\to\infty \\ n_F/N = n(E_F)}} \sum_{i=1}^{n_F} \langle C_i \rangle = \frac{e^2}{h} \int_{E(k_x,k_y)<E_F} F(k_x,k_y)\, dk_x\, dk_y$$

Conclusion: even when the topological invariants of a system are strongly fluctuating, the average has meaningful information.

We believe this is the correct route to a precise theory of the anomalous Hall effect in ordinary *metals*, and that this concept might be generalized to a few other symmetry classes.

Conclusions

1. Beyond topological invariants in insulators

For symmetry-protected phases, it appears that if we can find the right way to write the topological invariant, it remains physical (though not quantized) even without the symmetry.

2. Metals

If there is a limit where the “intrinsic AHE” formula is exact, it may be the disorder-averaged pumping conductance. This is an adiabatic process so the diagonal conductivity is effectively 0. The intrinsic AHE describes the mean Chern numbers in a weak-disorder regime where the Chern numbers fluctuate strongly between realizations.