Electromagnetic response of insulators and semimetals from geometry and topology

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Especially for insulators, see Les Houches lecture notes (2014).

Recent work with Fernando de Juan, Adolfo Grushin, Roni Ilan, Shudan Zhong, Takahiro Morimoto, Joe Orenstein, Dan Parker, Ivo Souza

Outline (version 0)

Lecture I: Basic ideas of topology and topological phases. Robustness to interactions/disorder.

Lecture II: Electromagnetic response of insulators

Lecture III: Electromagnetic response of metals

Main new material:

We now know that there are quantum-geometric effects in the basic theory of metals. Can measurable metallic effects be fully "topological" in the same sense as topological insulating phases?

Some lecture notes for a longer course are available
http://cmt.berkeley.edu/p250
or possibly http://cmt-old.berkeley.edu/p250

Outline

I. Intro: Emergent gauge fields and geometry of electrons in solids
An approach using Berry phases that includes one class of topological phases *and also many important non-quantized properties of solids*.

Warmup: basic idea of Berry's phase;
examples of (free-electron) topological states of matter
IQHE, topological insulators

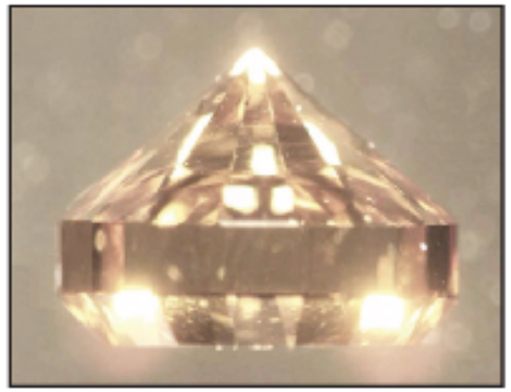
II: Electromagnetic responses (IQHE, axion electrodynamics, …)

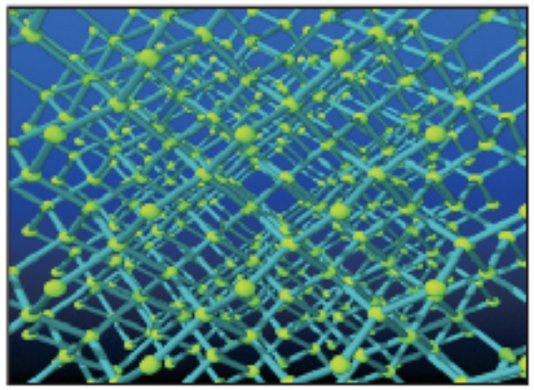
III. Recent work in *semimetals*: what are consequences in responses of Weyl/Dirac semimetals? Puzzling optical effects from low symmetry.

Also motivated by proposals of "chiral magnetic effect" and "chiral anomaly" in Weyl (and other) semimetals

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":

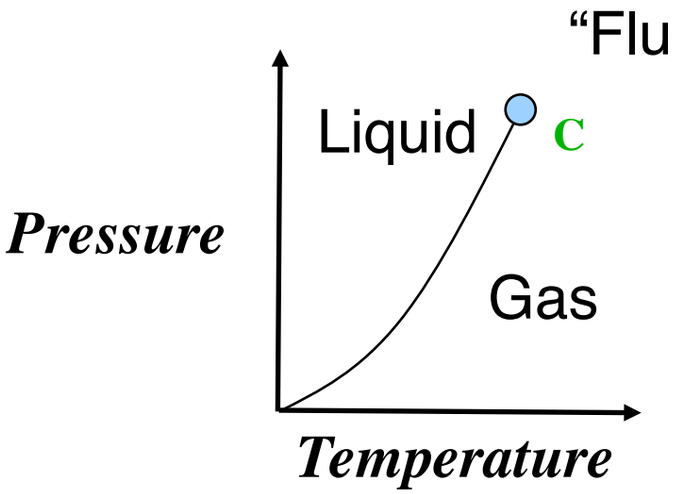
an ordered state appears at low temperature when the system spontaneously loses one of the symmetries present at high temperature.

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

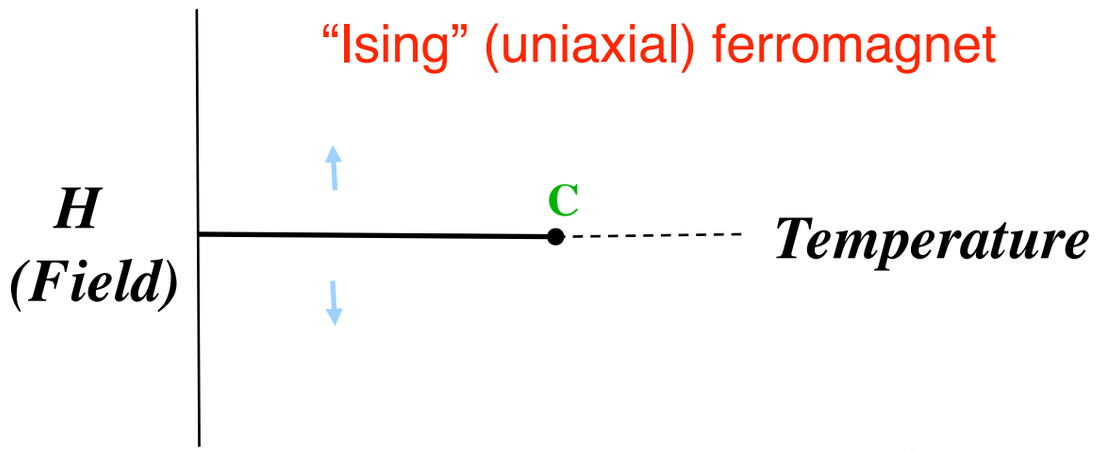
At high temperature, entropy dominates and leads to a disordered state.
At low temperature, energy dominates and leads to an ordered state.

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.

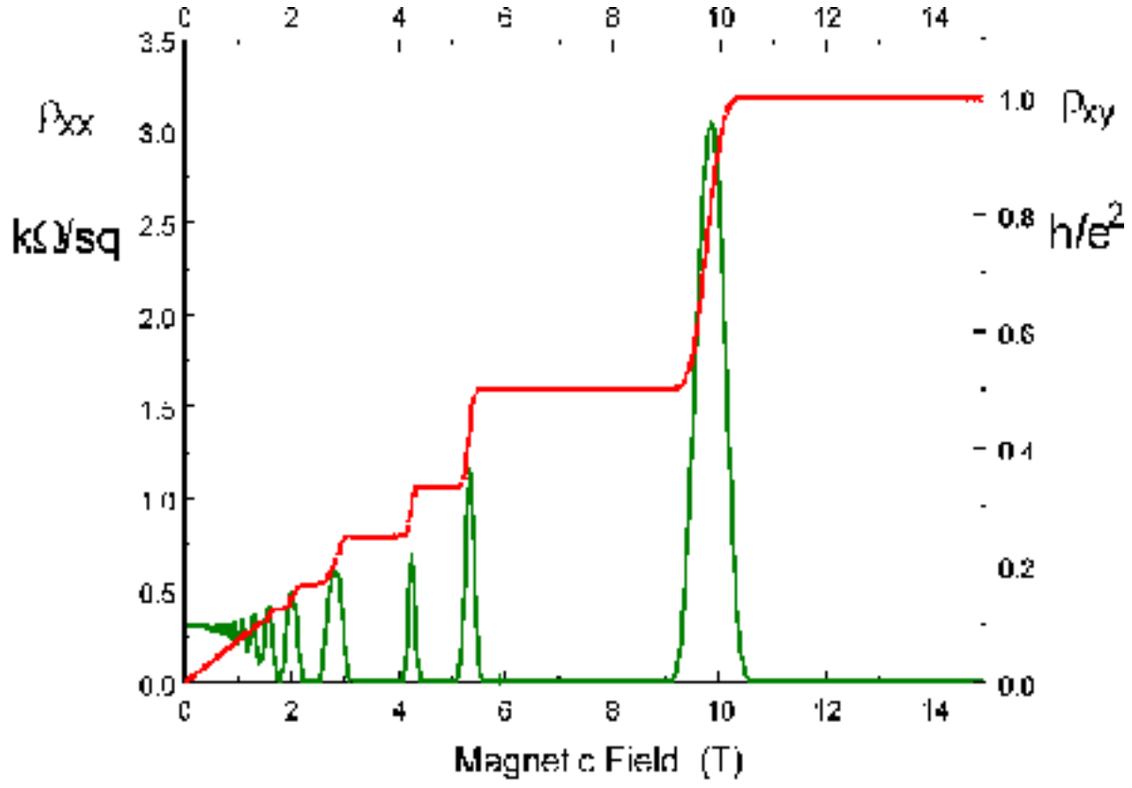
Electrons confined to a plane and in a strong magnetic field show, at low enough temperature, plateaus in the "Hall conductance":

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.



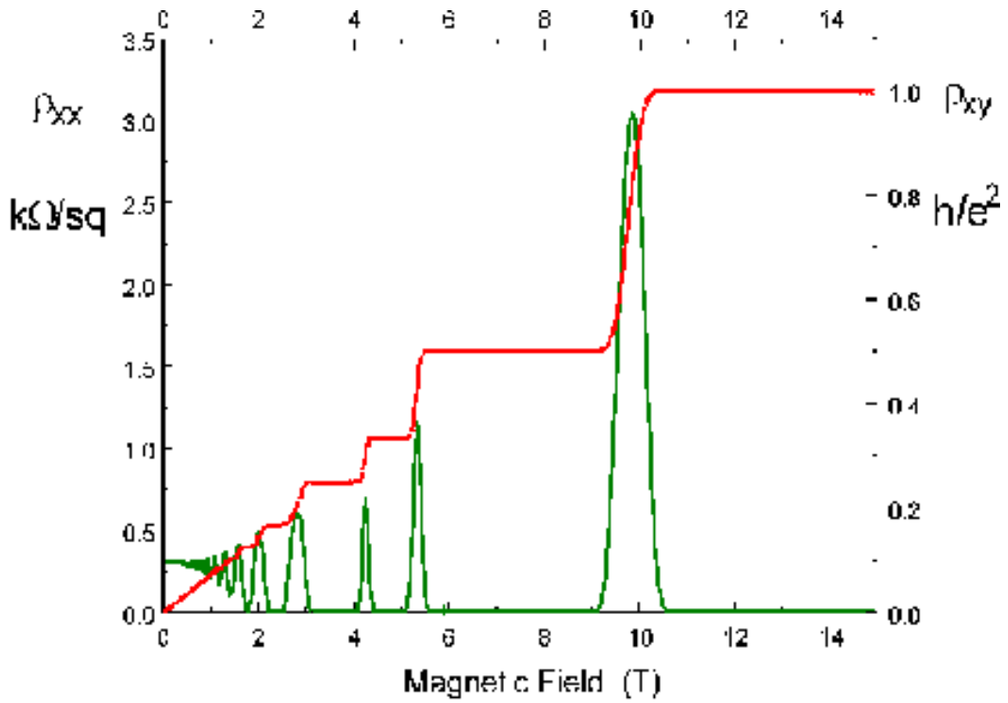
What type of order causes this precise quantization?

Note I: the AC Josephson effect between superconductors similarly allows determination of *e*/*h*.

Note II: there are also *fractional* plateaus in good (modulation-doped) samples.

The (integer) quantum Hall effect

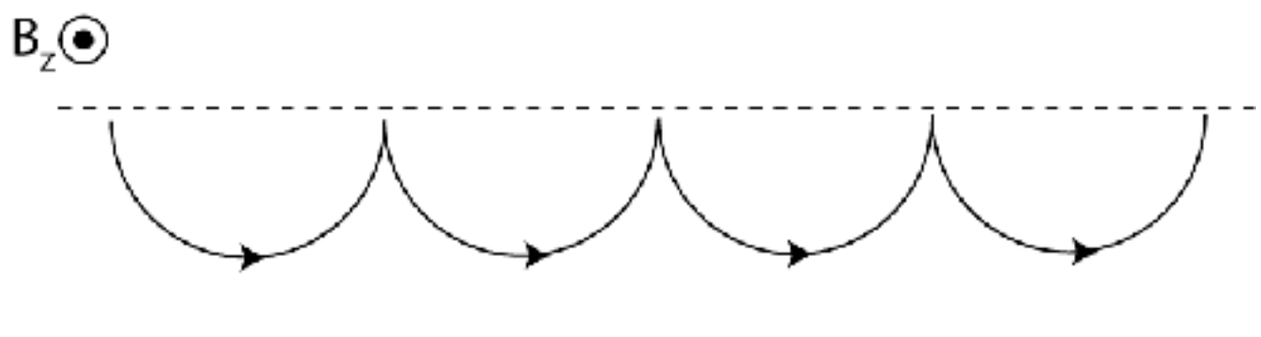
A 2DEG in a strong magnetic field can show a quantized transverse conductance:



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

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*.



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

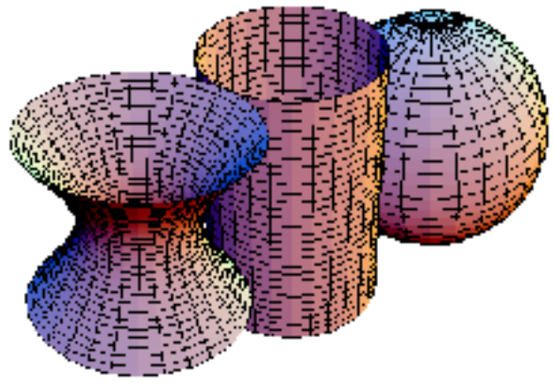
This is exactly the density of "Landau levels", the discrete spectrum of eigenstates of a 2D particle in an orbital magnetic field, spaced by the cyclotron energy. The only "surprise" is how precise the quantization is.

Topological invariants

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

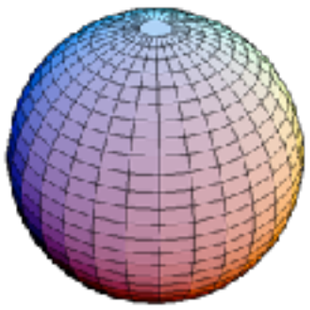
Consider a two-dimensional surface.

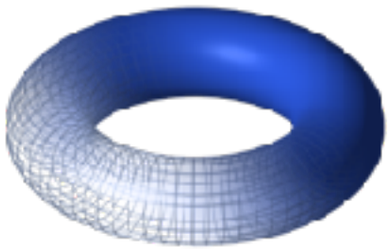
At any point on the surface, there are two radii of curvature.
We define the signed "Gaussian curvature" $\kappa = (r_1 r_2)^{-1}$



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).

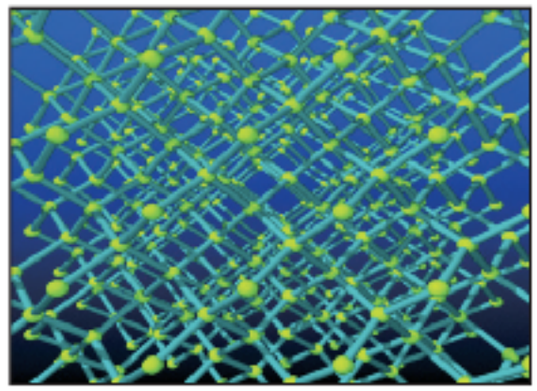
$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2 - 2g)$$

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,

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

just like the vector potential in electrodynamics.

Note: If more than 1 degenerate state, the connection is *non-Abelian*:

$$\mathcal{A}^{\alpha\beta} = \langle \psi_k^\alpha | -i\nabla_k | \psi_k^\beta \rangle$$

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

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

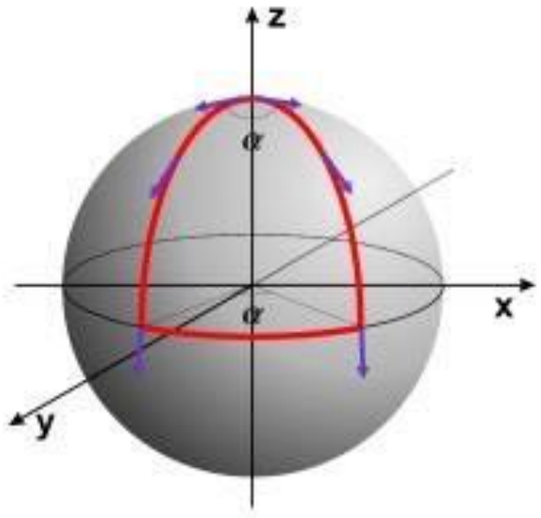
Berry phase: an example

Consider the Zeeman Hamiltonian for a spin-half moving in a magnetic field whose direction varies in time,

$$H = -\frac{g_s \mu B_0}{\hbar} \hat{\mathbf{n}}(t) \cdot \mathbf{S}$$

The resulting Berry phase around a closed path on the Bloch sphere is proportional to the (signed) area enclosed.

One can view this as the Aharonov-Bohm phase from the flux of a magnetic monopole located at the center of the Bloch sphere.



A sign of topology: when such a magnetic monopole has nonzero flux, there is no globally well-defined gauge for A (the gauge singular at the north pole has a "Dirac string" coming in that pole, e.g.).

Consequently, there is no globally well-defined smooth choice of wave functions for the Bloch sphere, as having such a smooth choice would lead to a smooth 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"

Mathematical sidebar

What is this integrand? Chern is a "cohomology class".

There are many flavors of algebraic topology. Two that appear frequently in this field are *homotopy* and *cohomology*.

Homotopy = generalization of "winding number"
Cohomology = generalization of "almost path-independent integral"

An example of how these are connected: suppose we went back to the simple spin-half Hamiltonian

$$H = -\frac{g_s \mu B_0}{\hbar} \hat{\mathbf{n}}(t) \cdot \mathbf{S}$$

and now let **n** be a function of (kx,ky) to make a simple band structure. Strictly speaking **n** need not be a unit vector as long as it never vanishes.

Some facts: **n** cannot wind nontrivially around the non contractible circles, since $\pi_1(S^2)$ is 0 (trivial).

Computing the Chern number for the lower (upper) band of this two band Hamiltonian gives k (-k), where k is the integer-valued "winding number" of the map from T^2 to S^2. Nonzero Chern number is an *obstruction* to global definition of *A*.

The importance of the edge

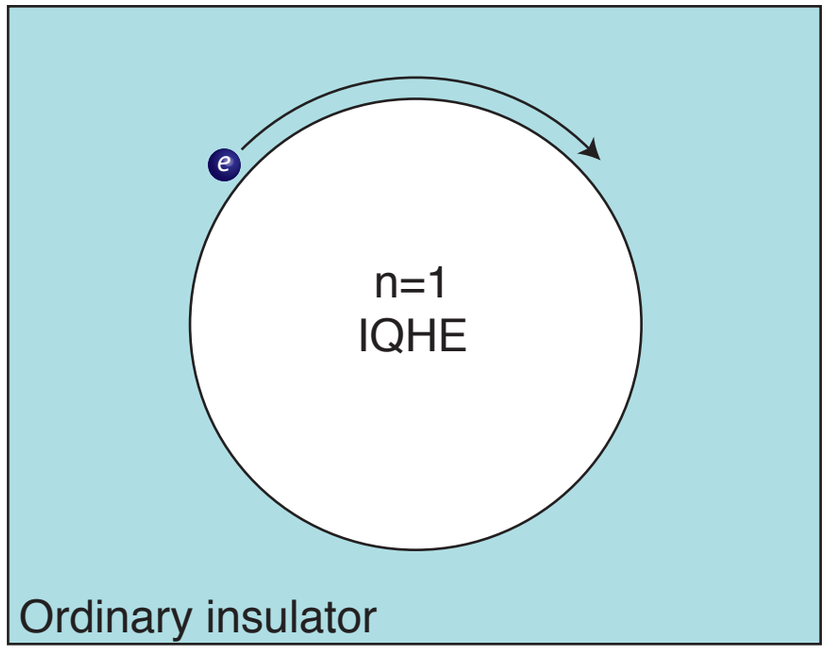
But wait a moment...

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.

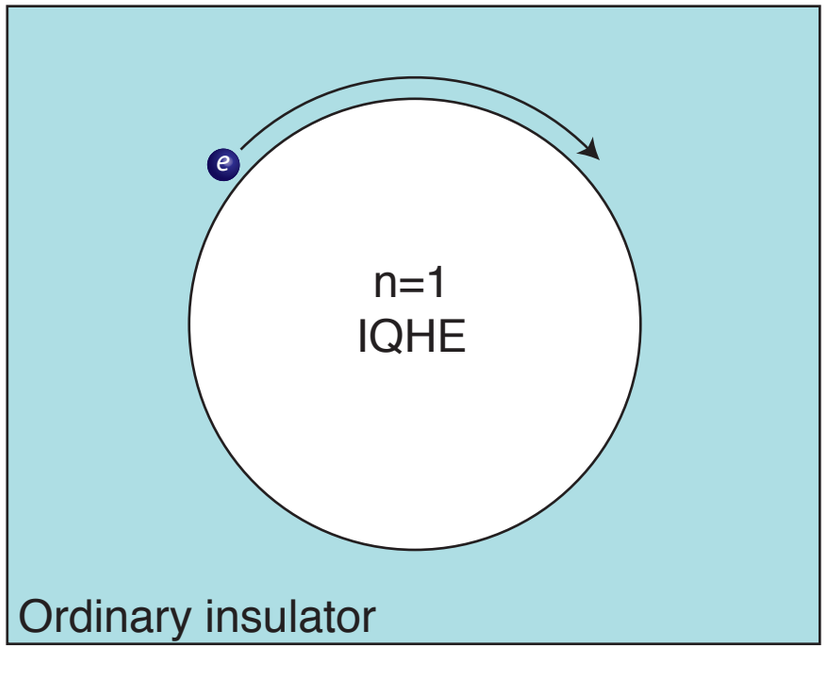
How does the bulk topological invariant "force" an edge mode?

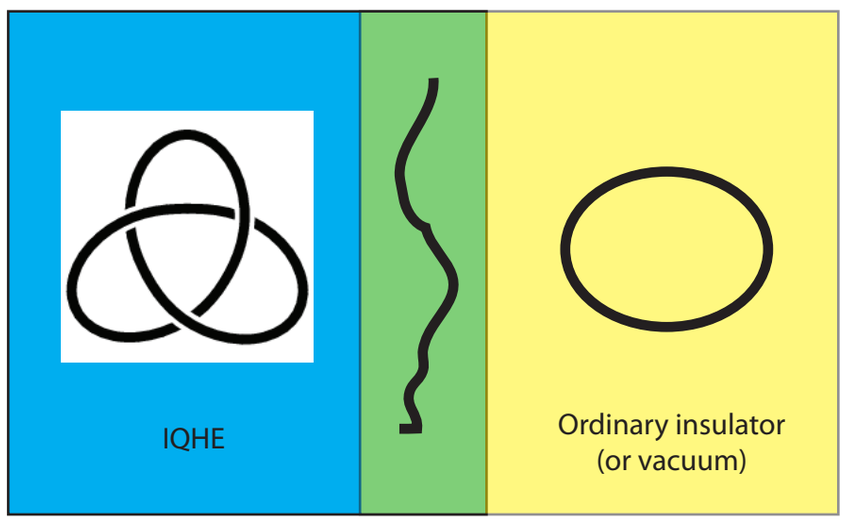
Answer:

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)

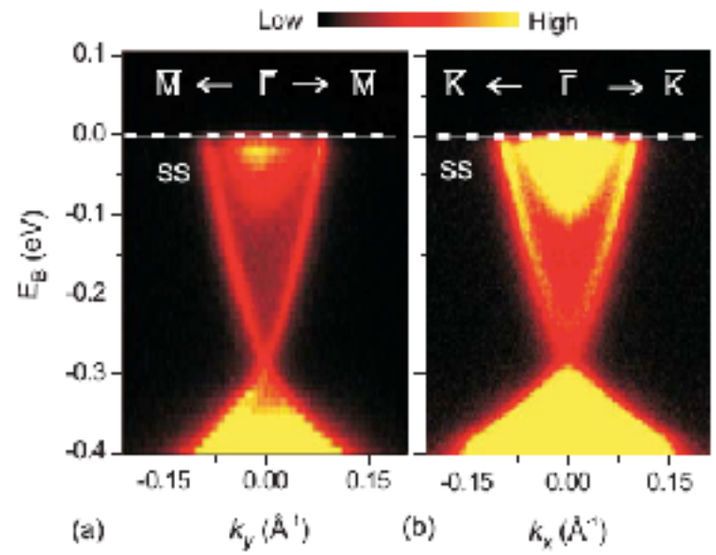
Berry phase in solids

Every simple gauge-invariant object made from A and F seems to mean something physically. We can identify several types of Berry-phase phenomena of nearly free electrons:

Insulators:

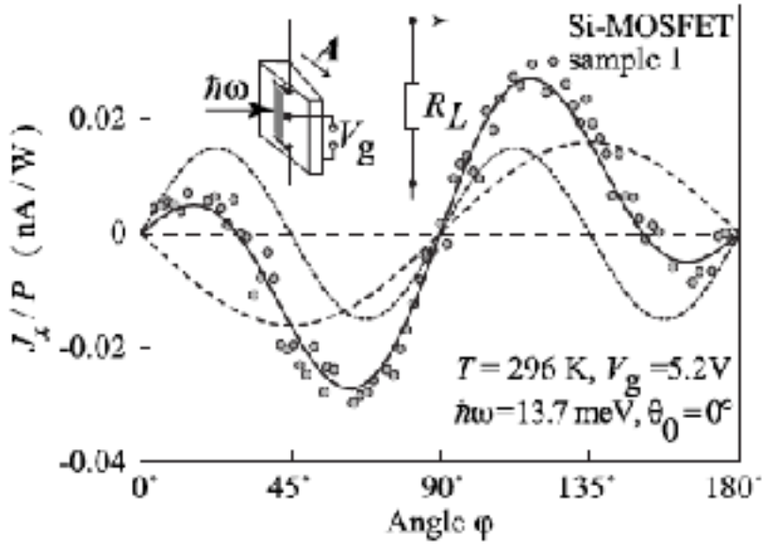
Topological phases independent of symmetry:
Examples: 2D and 4D QHE (1982,1988)

Topological phases dependent on symmetry
Examples: 2D and 3D Z2 topological insulators (2005,2007)



The Berry-phase approach to understanding these leads to expressions that are physically meaningful without symmetries:

Examples: electrical polarization (1987-1990); magnetoelectric effect (2009-2010)



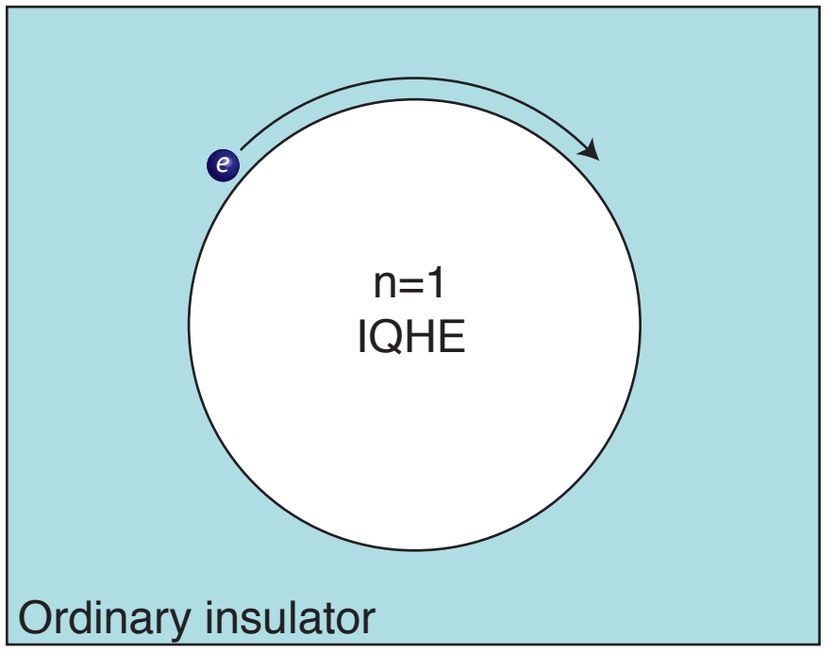
Metals: Several long-observed phenomena in metals are now believed to be Berry-phase effects. I will give a quick descriptio of 3 (1999,2010,2012).

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.

Lecture II

1. Time-reversal symmetry: quantum spin Hall effect and 3D topological insulator

2. How topology can still be defined with disorder and interactions

3. Electromagnetic response in insulators: polarization and magnetoelectric effect

The "quantum spin Hall effect"

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

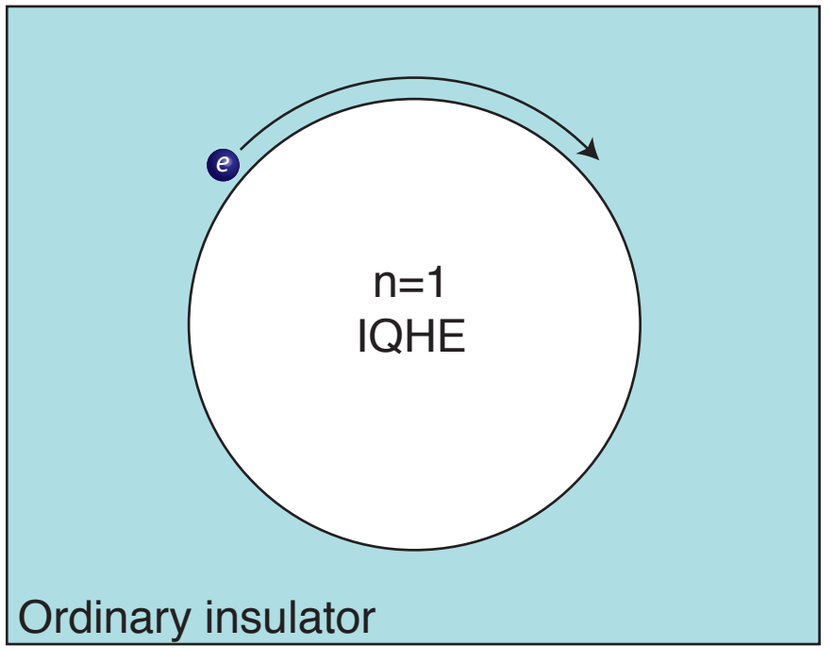
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

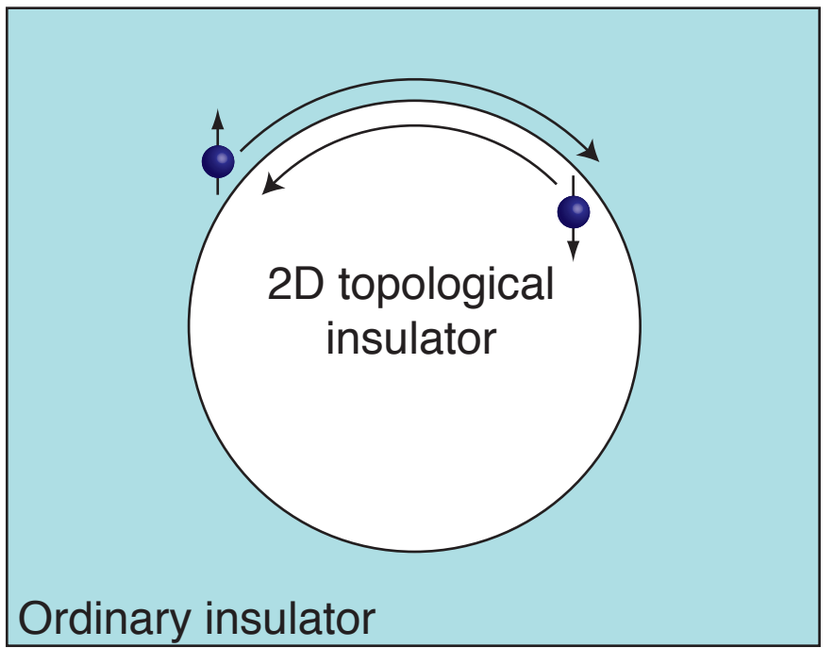
For a given spin, this term leads to a momentum-dependent force on the electron, somewhat like a magnetic field.

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".



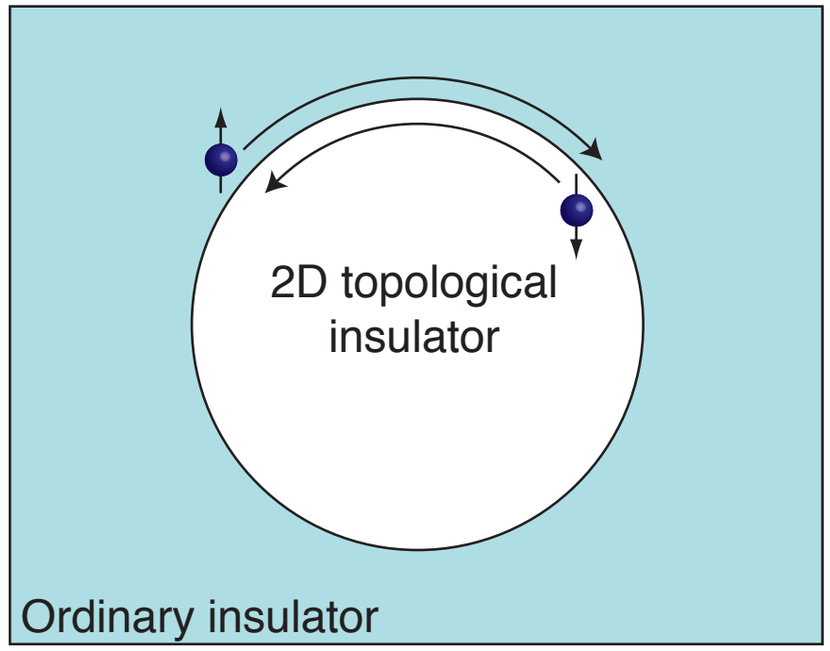


The "quantum spin Hall effect"

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.

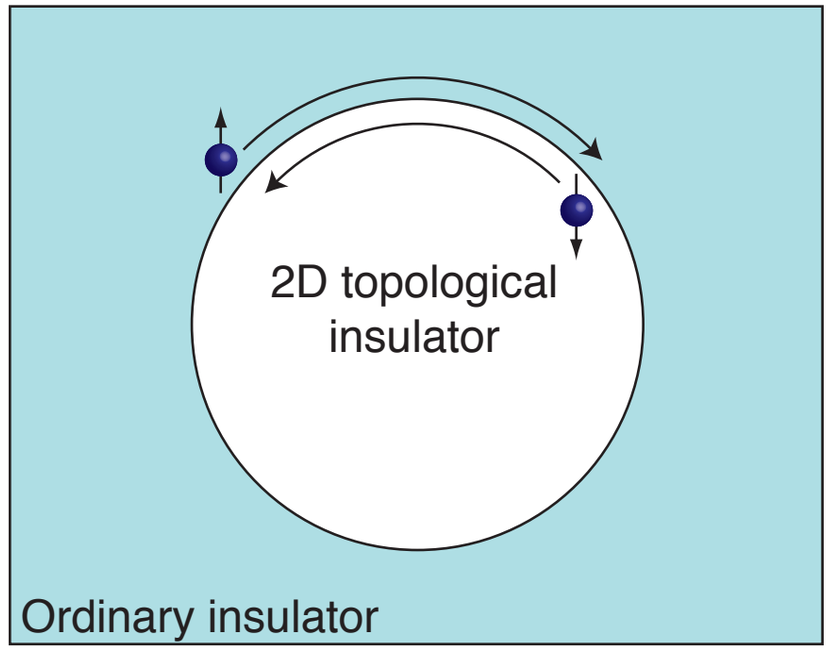
The 2D topological insulator

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?

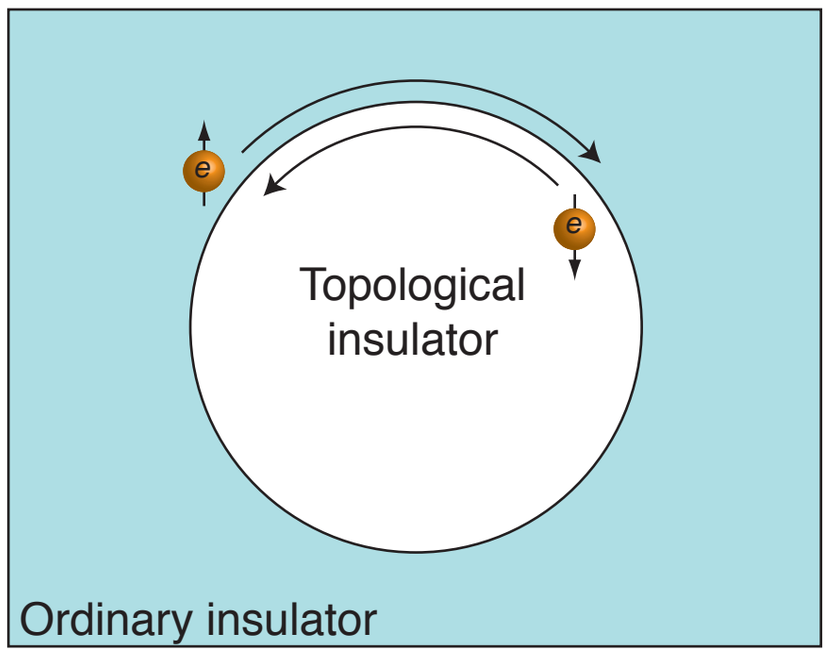
The "Chern insulator" and QSHE

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.

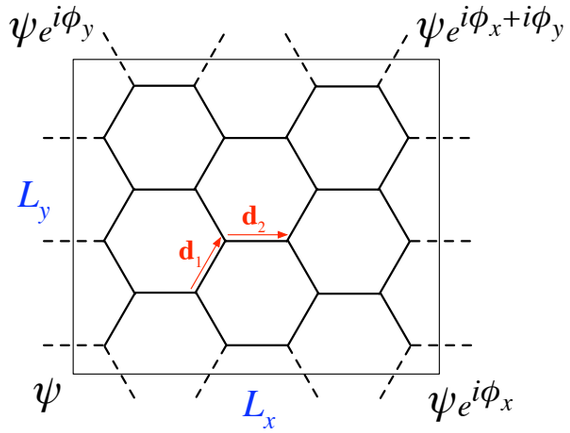
Then *SU(2)* (spin rotation symmetry) is broken, but time-reversal symmetry is not:

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:

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

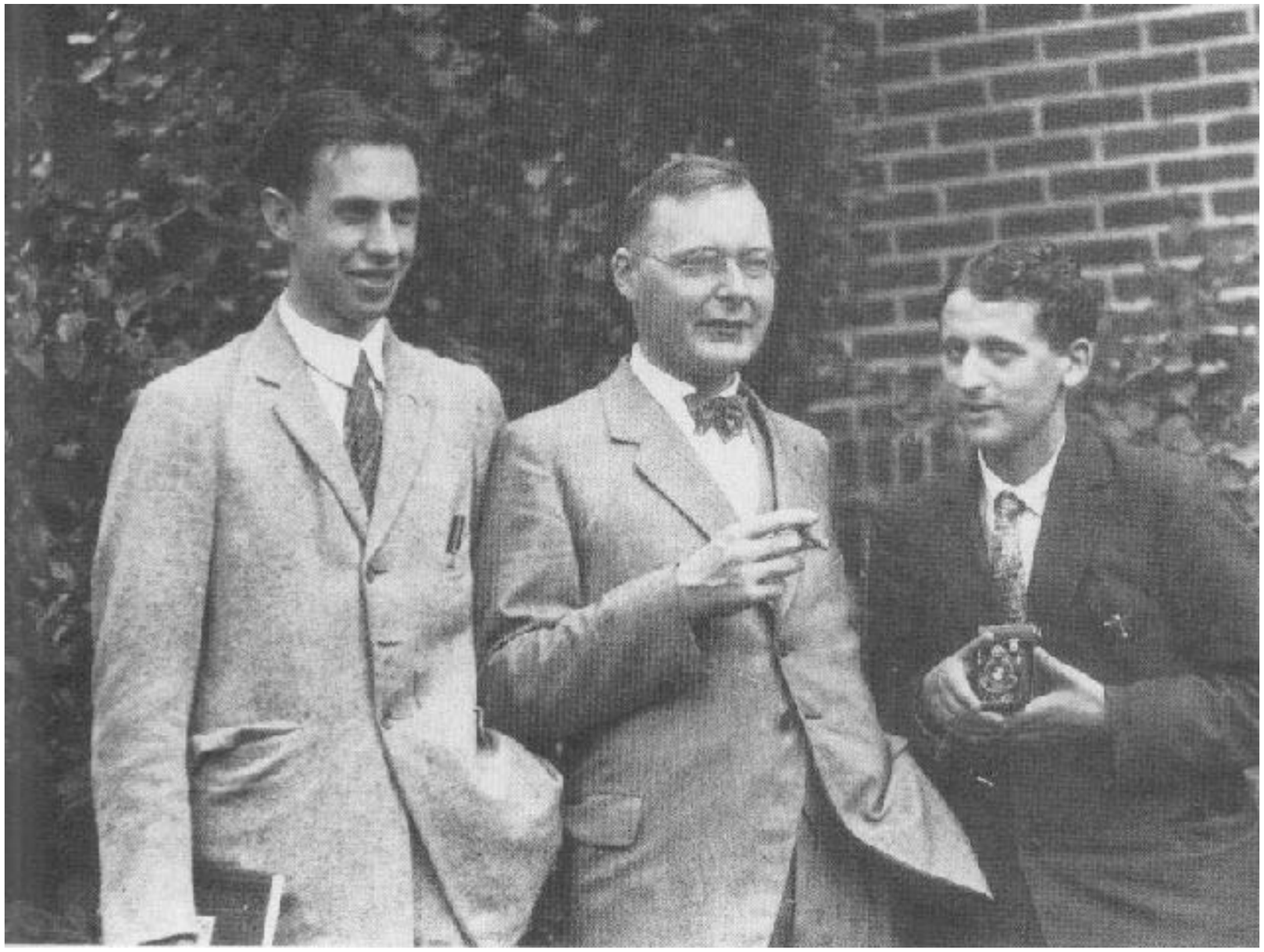
For general spin-orbit coupling, there is no conserved quantity that can be used to classify bands in this way, and no integer topological invariant.

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

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



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

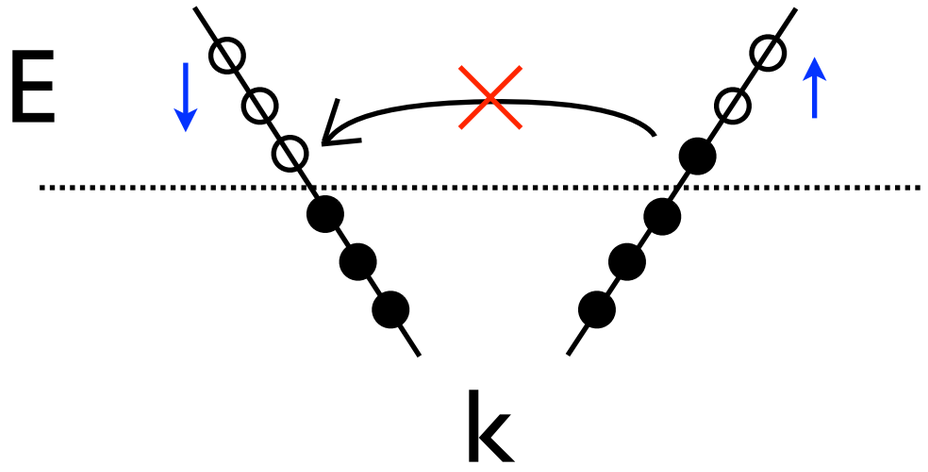
The 2D topological insulator

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).



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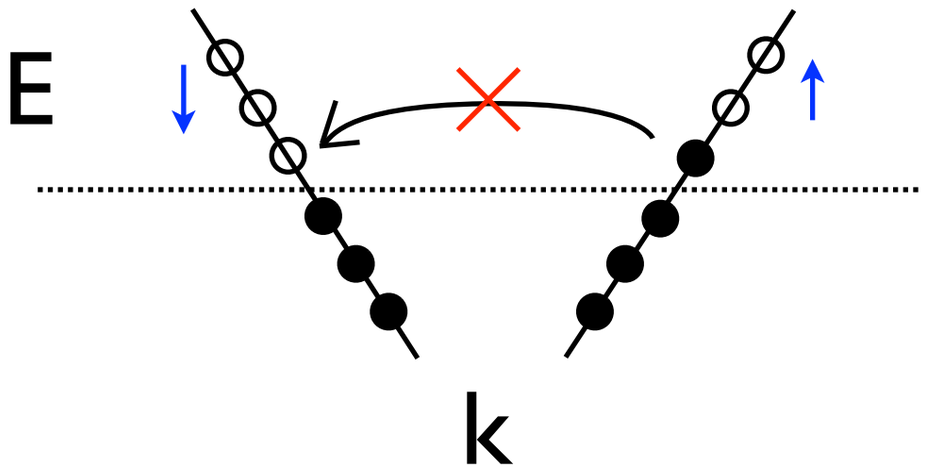
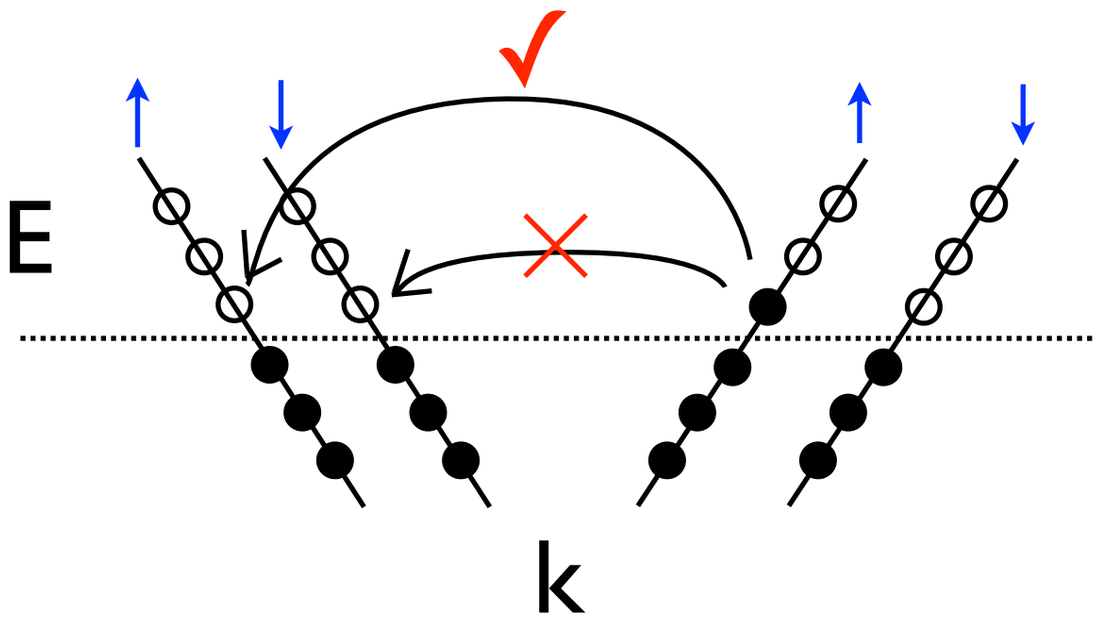


But this rule does not protect an ordinary quantum wire with 2 Kramers pairs:



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

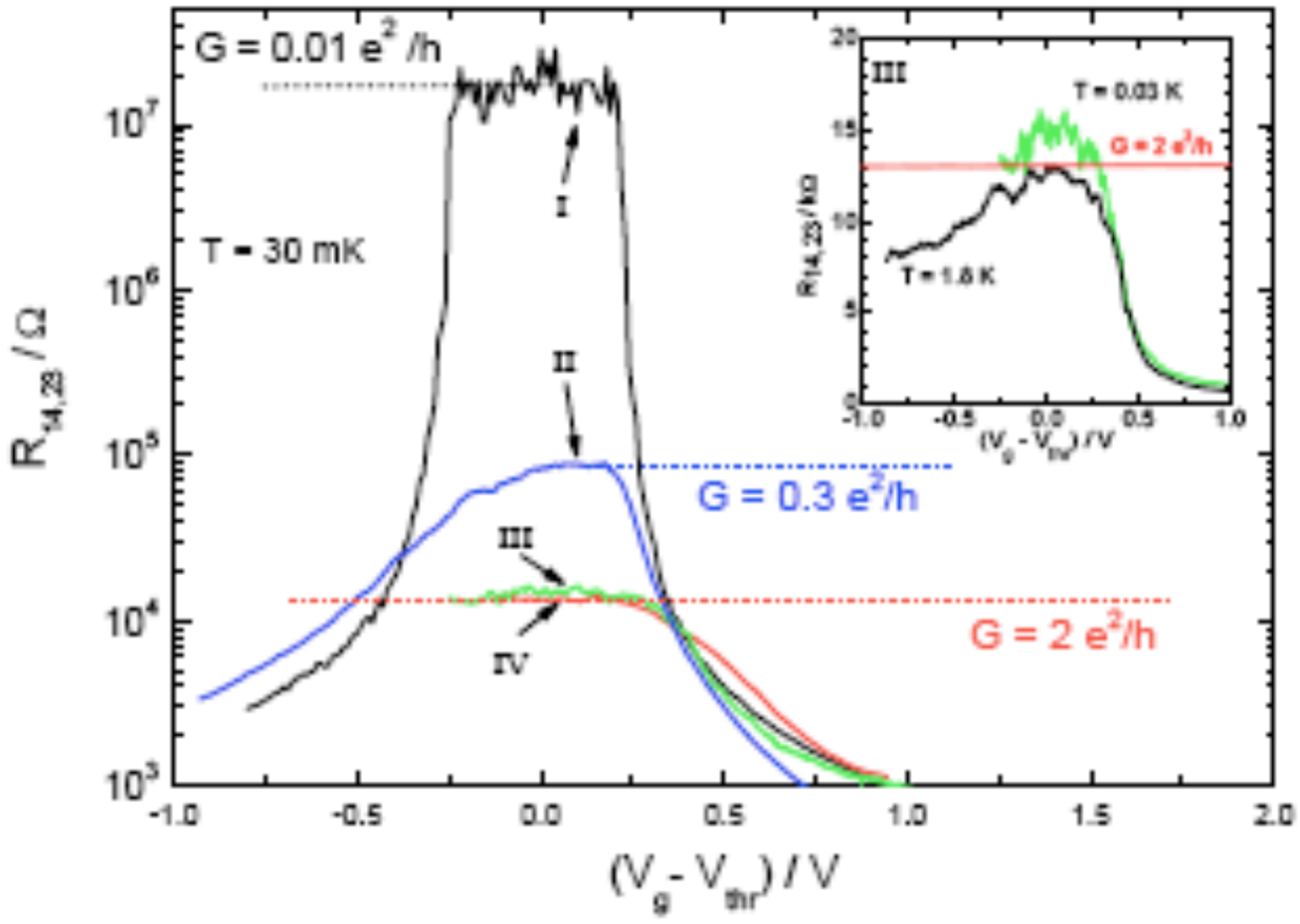
Key: the topological invariant predicts the "number of quantum wires".

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 topological 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.

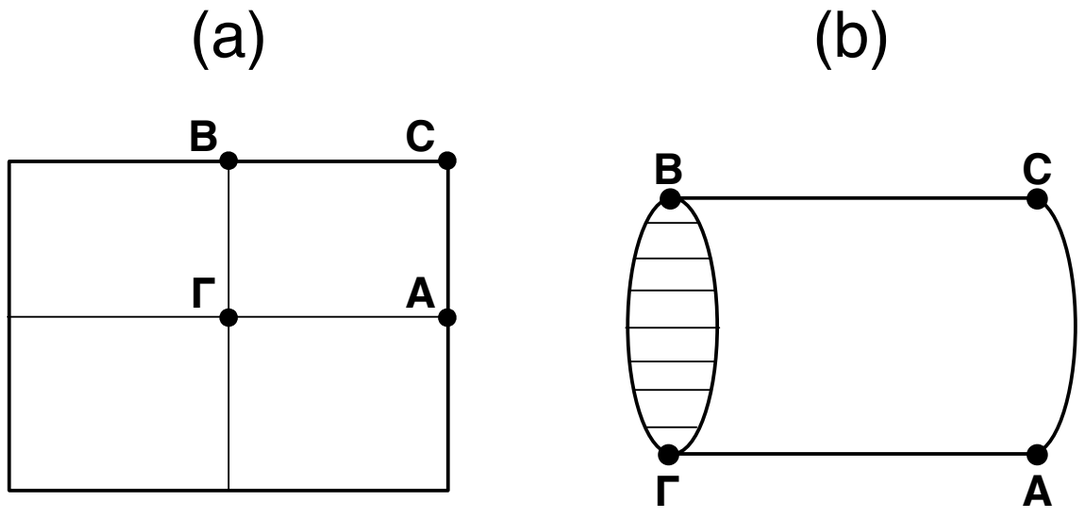
However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

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:

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

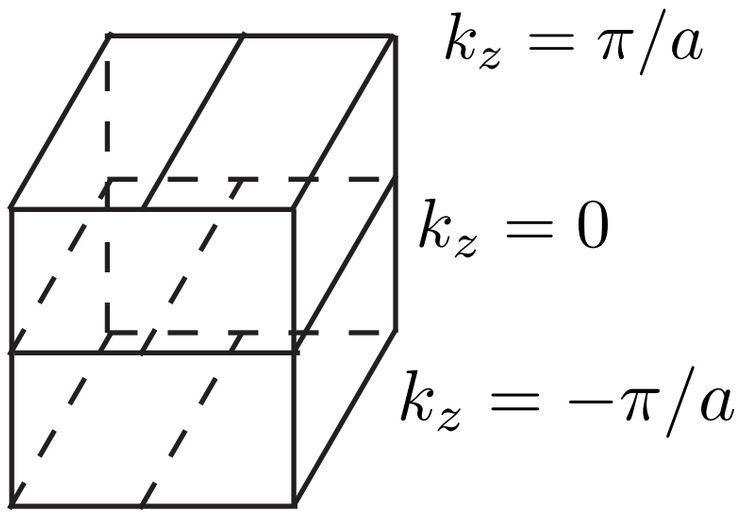


"effective BZ"

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

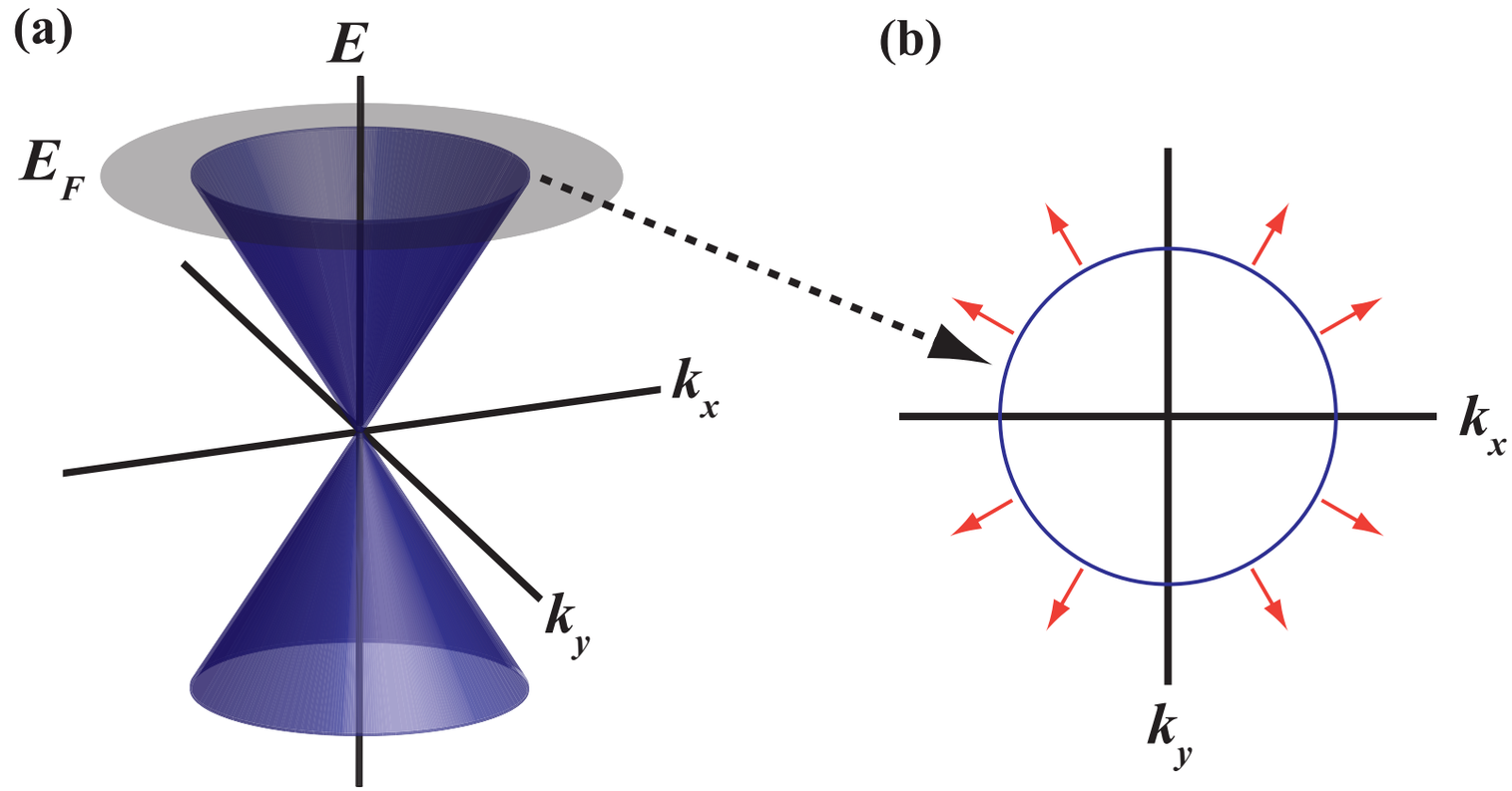


3D "strong topological insulators" go from an 2D *ordinary* insulator to a 2D *topological* insulator (or vice versa) in going from k_z=0 to k_z=±π/a.

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"



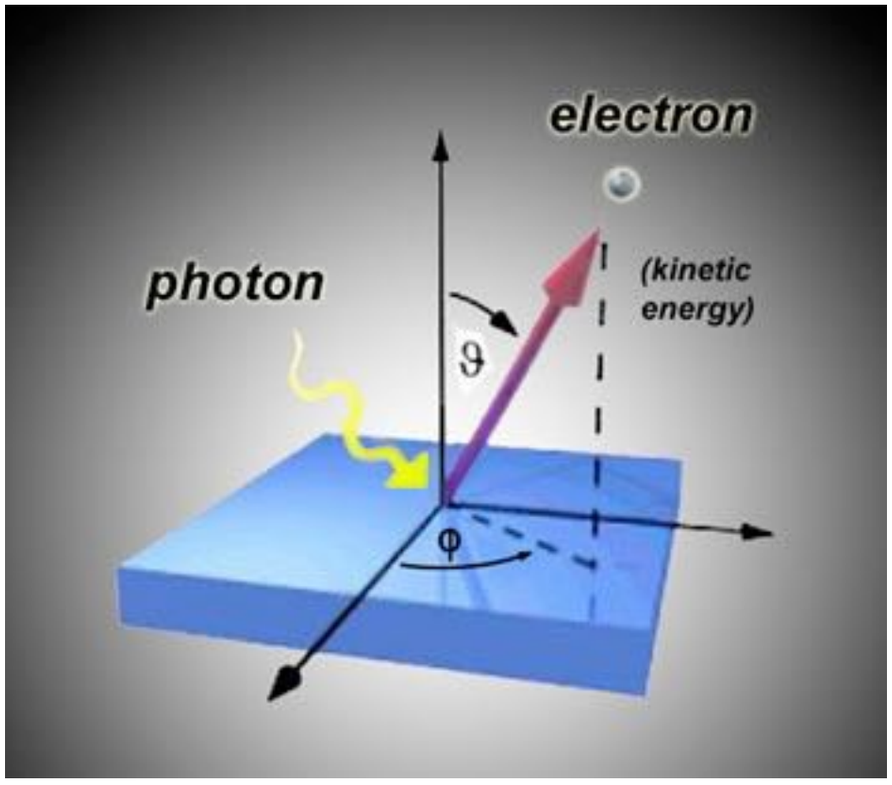
2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

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.



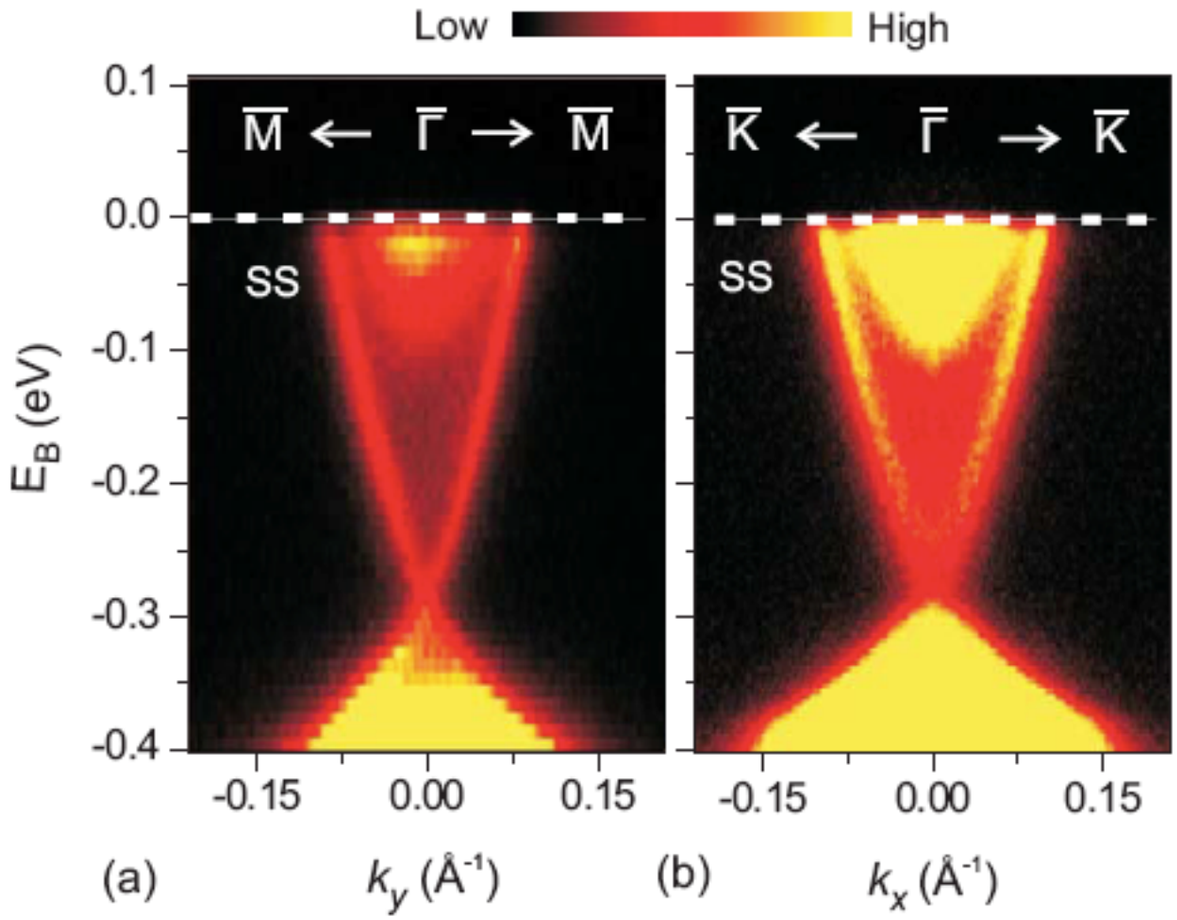
Measure as many properties as possible of the outgoing electron
to deduce the momentum, energy, and spin it had while still in the solid.

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.

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.

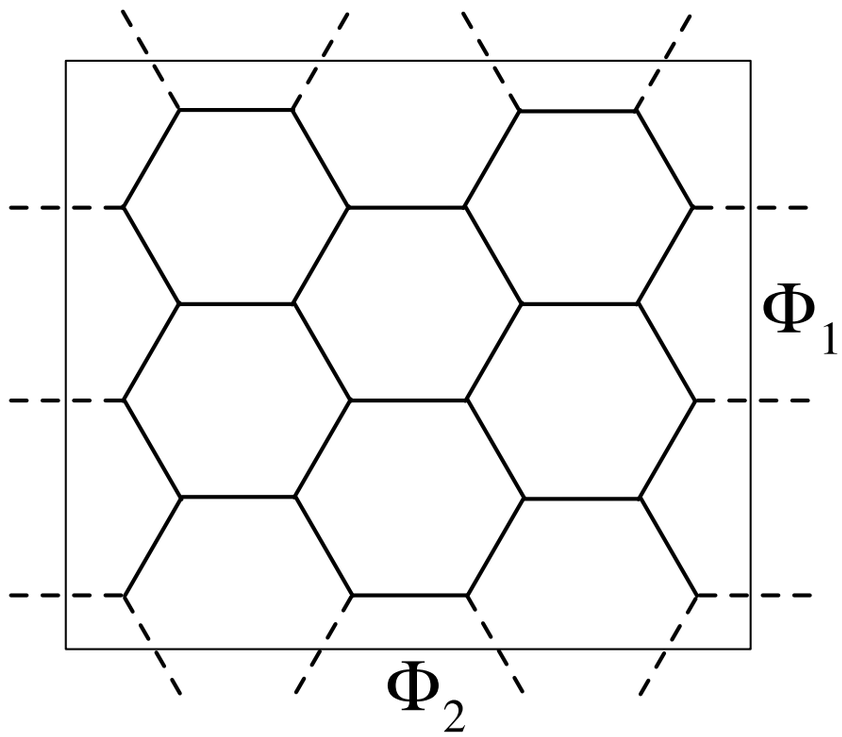
For T-invariant systems, all ordinary Chern numbers are zero.

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.

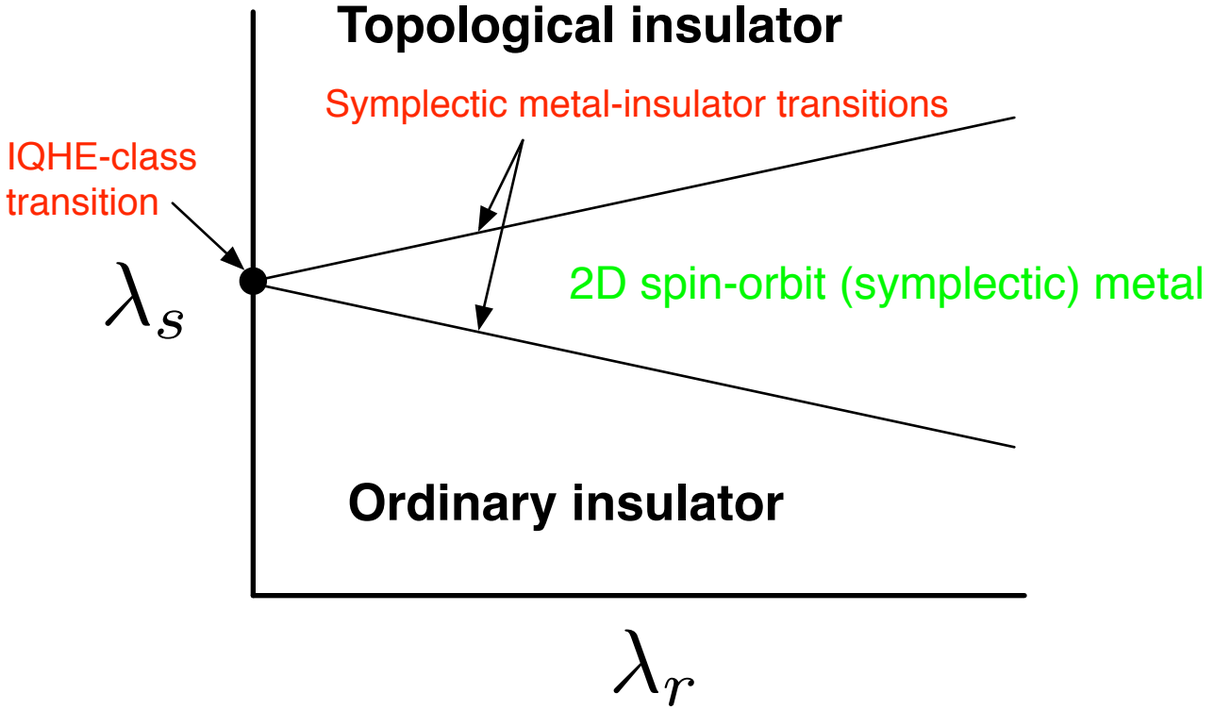
Effect of boundary phase is to shift *k*: alternate picture of topological invariant is in terms of half the (Φ_1,Φ_2) torus.

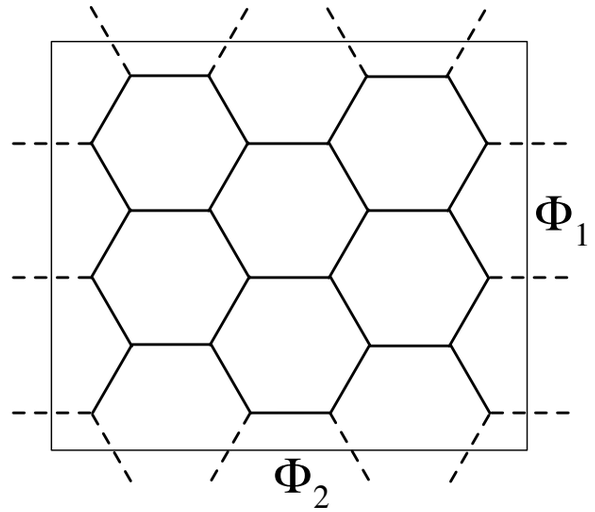


Can define Chern parities by pumping, analogous to Chern numbers, and study phase diagram w/disorder

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.

Berry phase in solids

Every simple gauge-invariant object made from A and F seems to mean something physically. We can identify several types of Berry-phase phenomena of nearly free electrons:

Insulators:

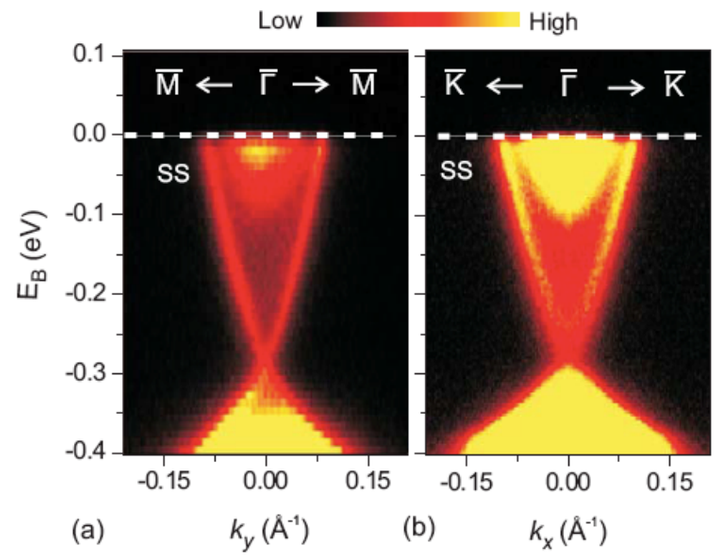
Topological phases independent of symmetry:
Examples: 2D and 4D QHE (1982,1988)

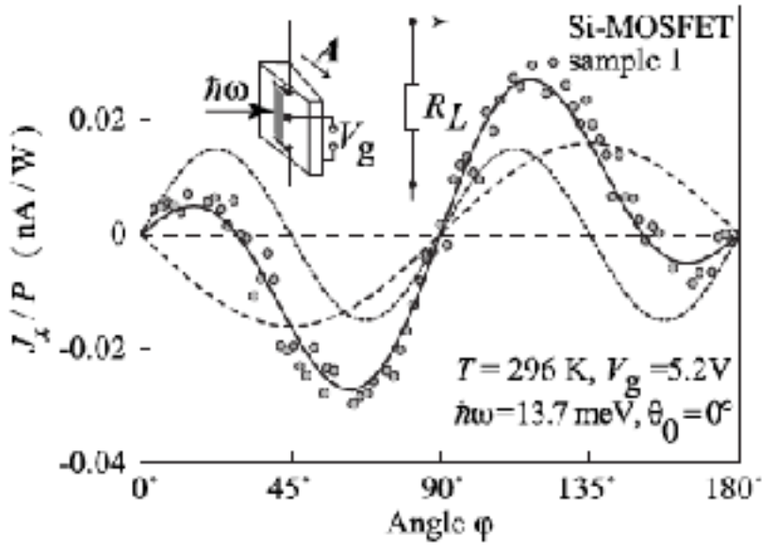
Topological phases dependent on symmetry
Examples: 2D and 3D Z2 topological insulators (2005,2007)

The Berry-phase approach to understanding these leads to expressions that are physically meaningful without symmetries:

Examples: electrical polarization (1987-1990); magnetoelectric effect (2009-2010)

Metals: Several long-observed phenomena in metals are now believed to be Berry-phase effects. I will give a quick descriptio of 3 (1999,2010,2012).





Warmup for magnetoelectricity and metals: polarization in insulators

Electrical polarization: "simple" Berry phase effect in solids (took about 50 years to understand how to calculate polarization of a solid from its unit cell)

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

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

More seriously: relate changes in *P* to currents moving through the unit cell.

Polarization isn't quantized in general; it is just a simple physical observable determined by the Berry phase. Note that there is an ambiguity *ne*.

Broader reason, in hindsight: E(k), the band structure, is k-symmetric with time-reversal, even with broken inversion. Anything related to inversion-breaking has to come from the wavefunction, and at low energy, usually from the Berry phase.

Warmup for magnetoelectricity and metals: polarization in insulators

Note an interesting property of this integral: its value changes by *ne* (a multiple of the "polarization quantum" in d=1) under "large gauge transformations")

This is connected to how Thouless derived the 1D polarization formula: a change in polarization corresponds to a pumping of charge through the unit cell, and changing polarization by a quantum corresponds to moving a charge from the left boundary to the right boundary.

The same concept applies in higher dimensions (King-Smith and Vanderbilt) and the generalization of this formula is widely used to compute polarization of crystals.

The key is the relation dA = F.

Can we imitate something like this in higher dimensions? We know that the "second Chern form" F ^ F underlies the 4D IQHE…

What is quantized in a 3D TI? 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.

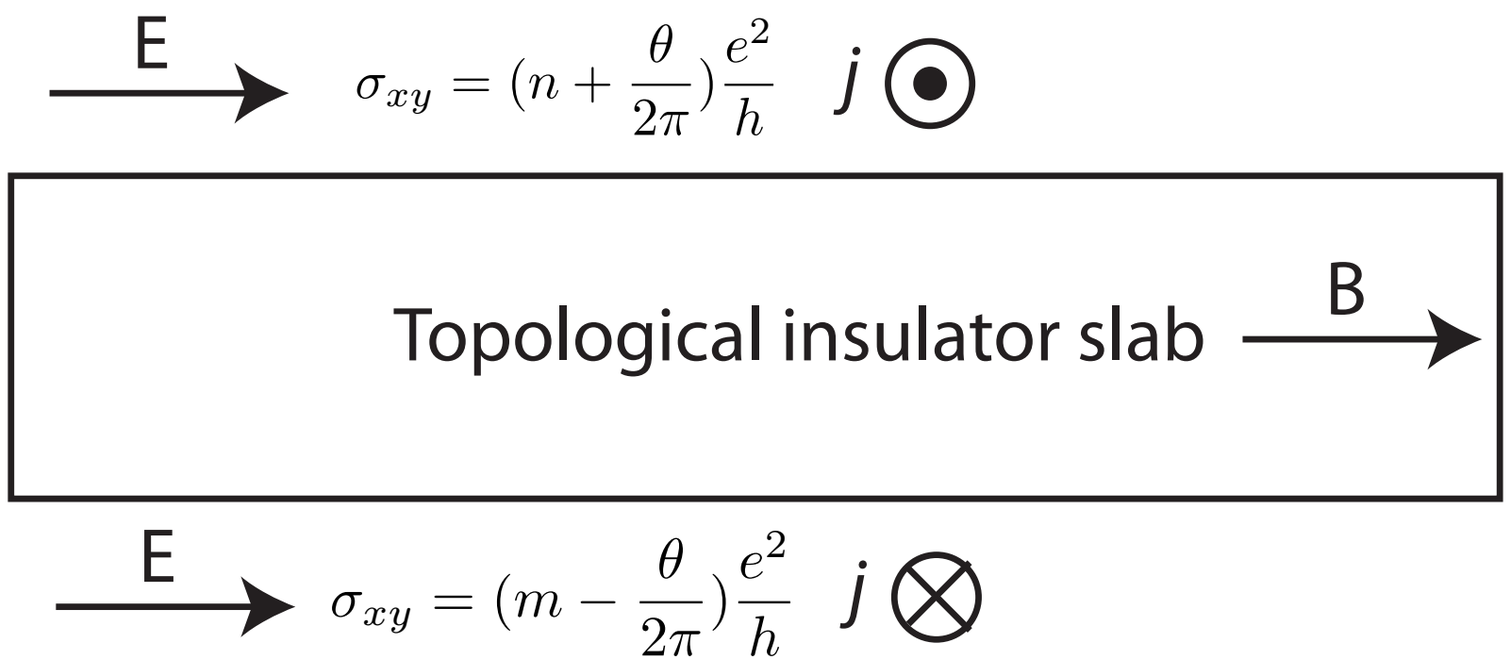
A T-invariant insulator can have *two* possible values: 0 or π.

Axion E&M

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

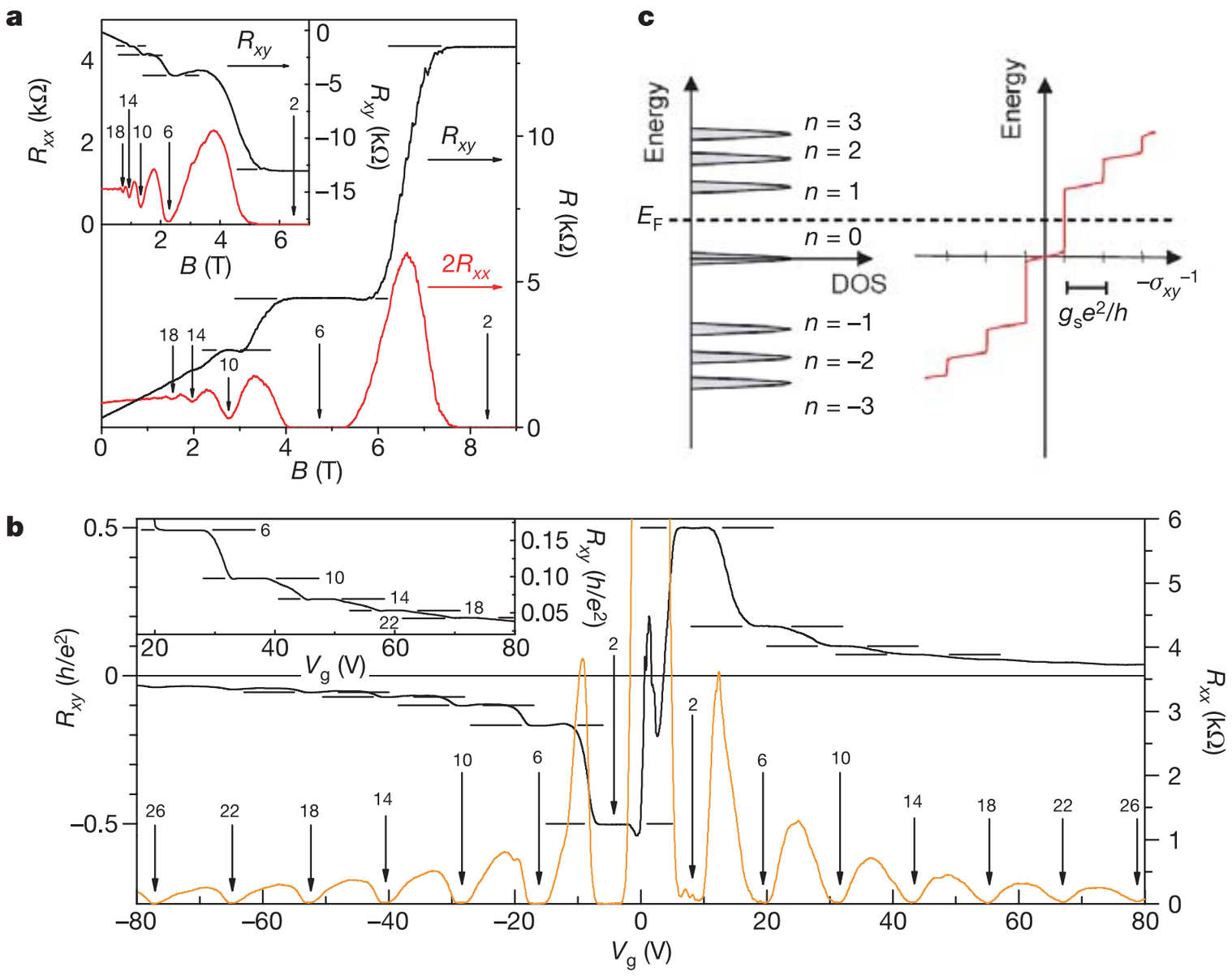
This explains a number of properties of the 3D topological insulator when its surfaces become gapped by breaking T-invariance:

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.
Data shown below from Y. Zhang et al. (Kim group, Columbia)



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.
Has just the right gauge ambiguity under "large gauge transformations".

Non-Abelian Berry gauge fields phase in insulators

Note: If more than 1 degenerate state, the connection is *non-Abelian*:

$$\mathcal{A}^{\alpha\beta} = \langle \psi_k^\alpha | - i\nabla_k | \psi_k^\beta \rangle$$

Two-fold degeneracies are automatic if nothing depends on spin.

1. Even with spin-orbit, certain momenta with *k* equal to -*k* still have degeneracies in non-magnetic materials, due to Kramers degeneracies;
2. Frequently, even if the occupied bands of a material are non-degenerate, calculation shows that physical properties depend on the non-Abelian connection as if they were degenerate.

So far, the orbital magnetoelectric polarizability is the only d <= 3 quantity I know of that depends on the non-Abelian Berry phase. It has an analogue in metallic dynamics (Varjas et al., arXiv, June '16).

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

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.

$$
\begin{aligned}
\alpha_j^i &= (\alpha_I)_j^i + \alpha_{CS}\delta_j^i \\
(\alpha_I)_j^i &= \sum_{n\,\mathrm{occ}}^{m\,\mathrm{unocc}} \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \mathrm{Re}\left\{ \frac{\langle u_{n\mathbf{k}}|e\,\not{r}^i_{\mathbf{k}}|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|e(\mathbf{v}_{\mathbf{k}}\times \not{r}_{\mathbf{k}})_j - e(\not{r}_{\mathbf{k}}\times \mathbf{v}_{\mathbf{k}})_j - 2i\partial H'_{\mathbf{k}}/\partial B^j|u_{n\mathbf{k}}\rangle}{E_{n\mathbf{k}} - E_{m\mathbf{k}}} \right\} \\
\alpha_{CS} &= -\frac{e^2}{2\hbar}\epsilon_{abc}\int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\,\mathrm{tr}\left[\mathcal{A}^a\partial^b\mathcal{A}^c - \frac{2i}{3}\mathcal{A}^a\mathcal{A}^b\mathcal{A}^c\right].
\end{aligned}
$$

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.

Warmup for metals: polarization in insulators

Electrical polarization: "simple" Berry phase effect in solids (took about 50 years to understand how to calculate polarization of a solid from its unit cell)

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

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What about metals?

Claim: the biggest omission in Ashcroft and Mermin (standard solids text) is a term in the semiclassical equations of motion, the (Karplus-Luttinger) ***anomalous velocity***.

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

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 (Fe, e.g.)

Example II: helicity-dependent photocurrents in optically active materials

Example III: optical rotation in gyrotropic/chiral materials with T symmetry

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Example III: optical rotation in gyrotropic/chiral materials with T symmetry

Can we get anything quantized/interesting in a metal?

Anomalous Hall effect (100+ years)

From Nagaosa et al., RMP 2011

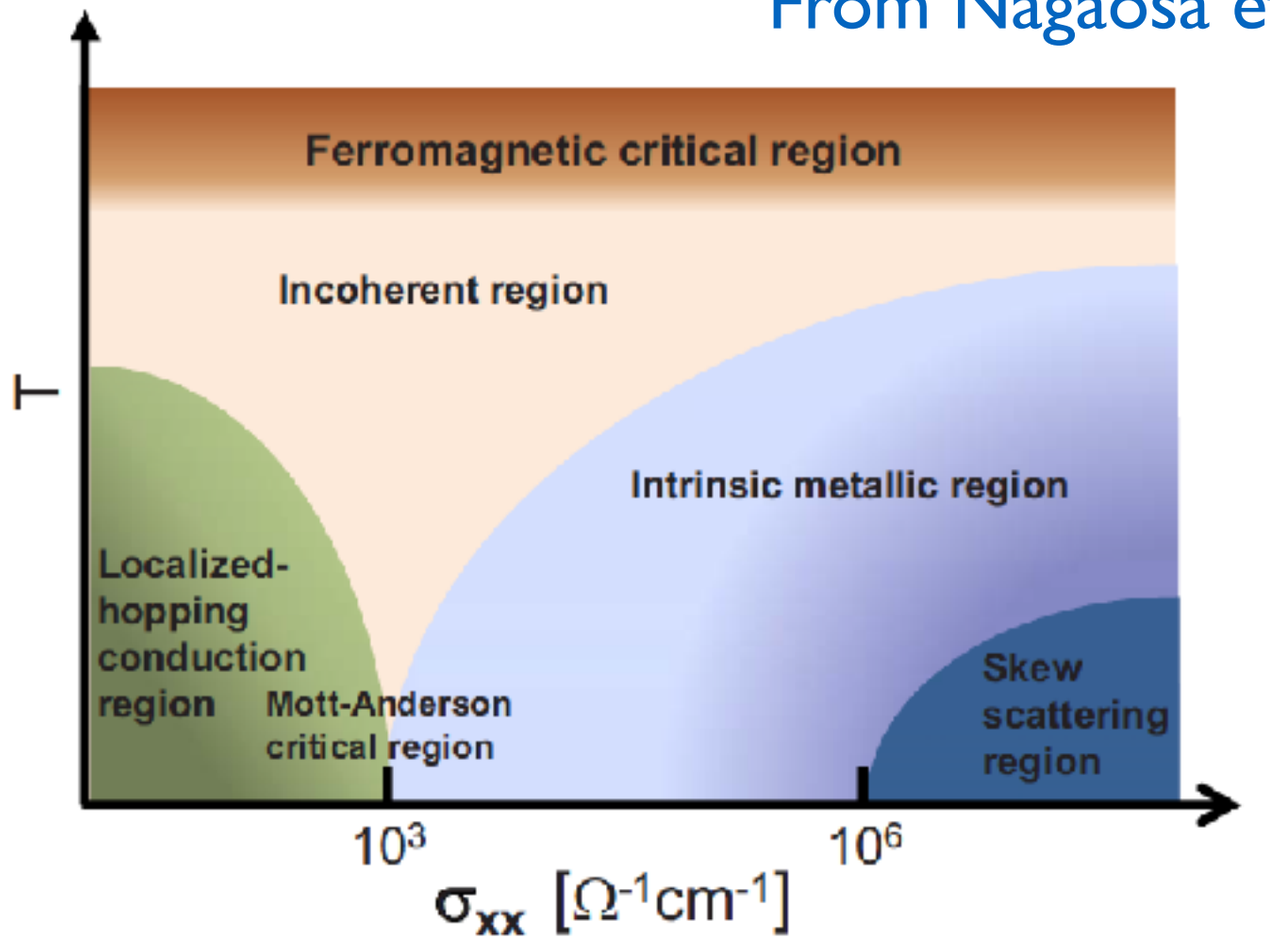


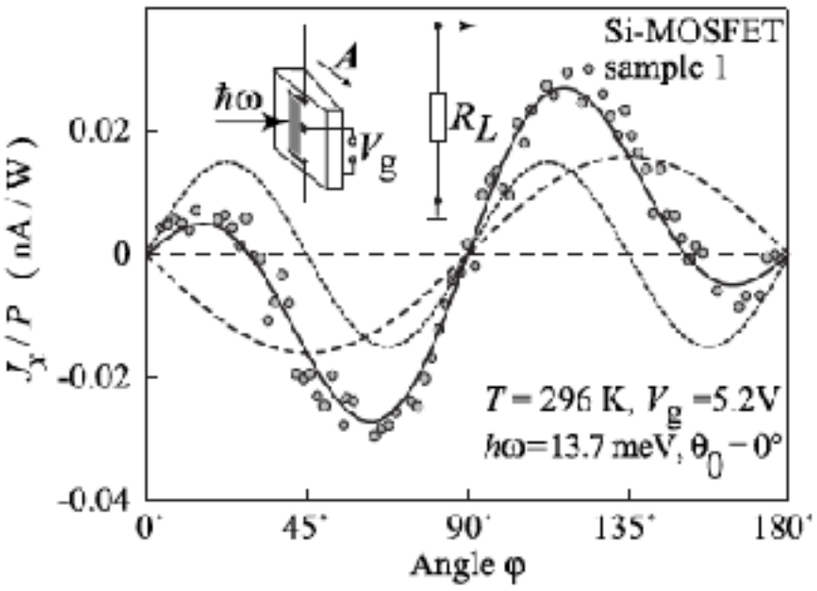
FIG. 47. (Color online) A speculative and schematic phase diagram for the anomalous Hall effect in the plane of the diagonal conductivity σ_{xx} and the temperature T.

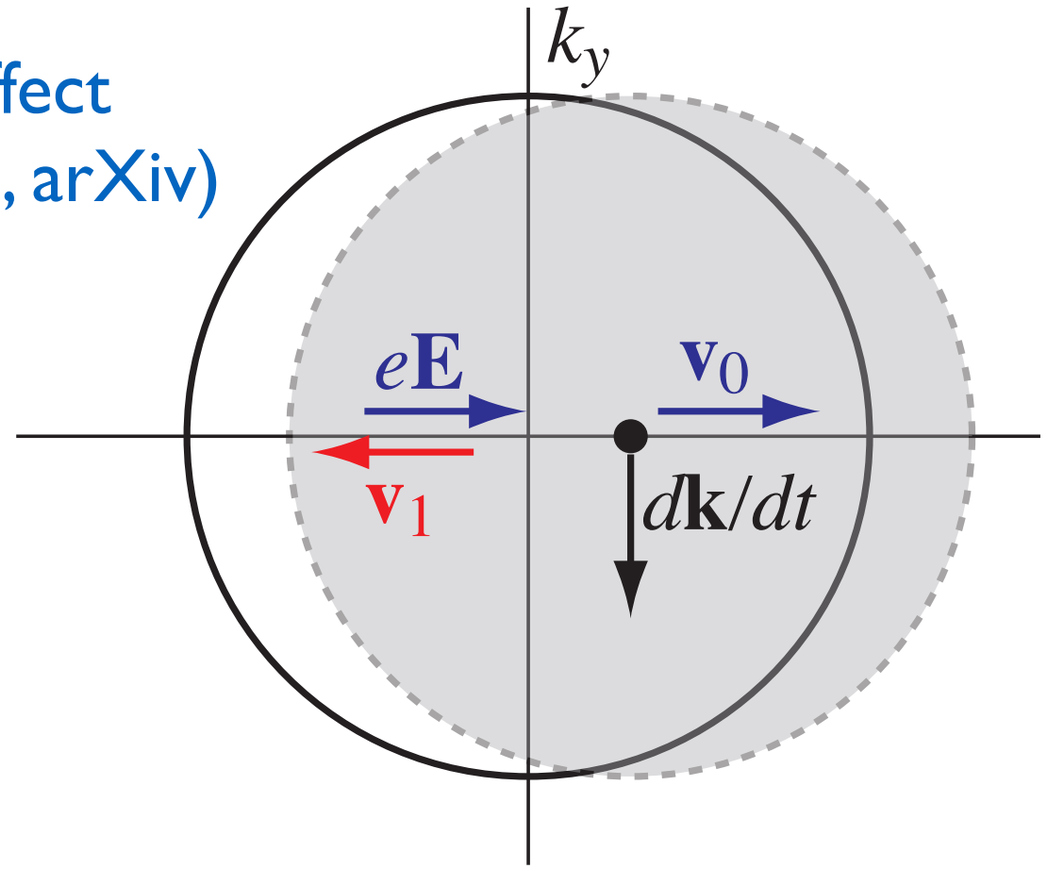
Sundaram and Niu, 1999
A topological approach:
J. Dahlhaus et al., PRB to appear

$$\sigma_{xy} = \frac{e^2}{h} \int_{\mathrm{FS}} d^2k \, \frac{F}{2\pi} + \text{extrinsic}$$

Two other "mystery" effects:

I. Nonlinear optics: circular photogalvanic effect
(JEM and J. Orenstein, PRL 2010; Deyo et al., arXiv)





Currents are switched by the sense of circular polarization, as previously observed in a series of experiments by S.D. Ganichev et al. We believe this is entirely or almost entirely a Berry-phase effect.

Next problem:

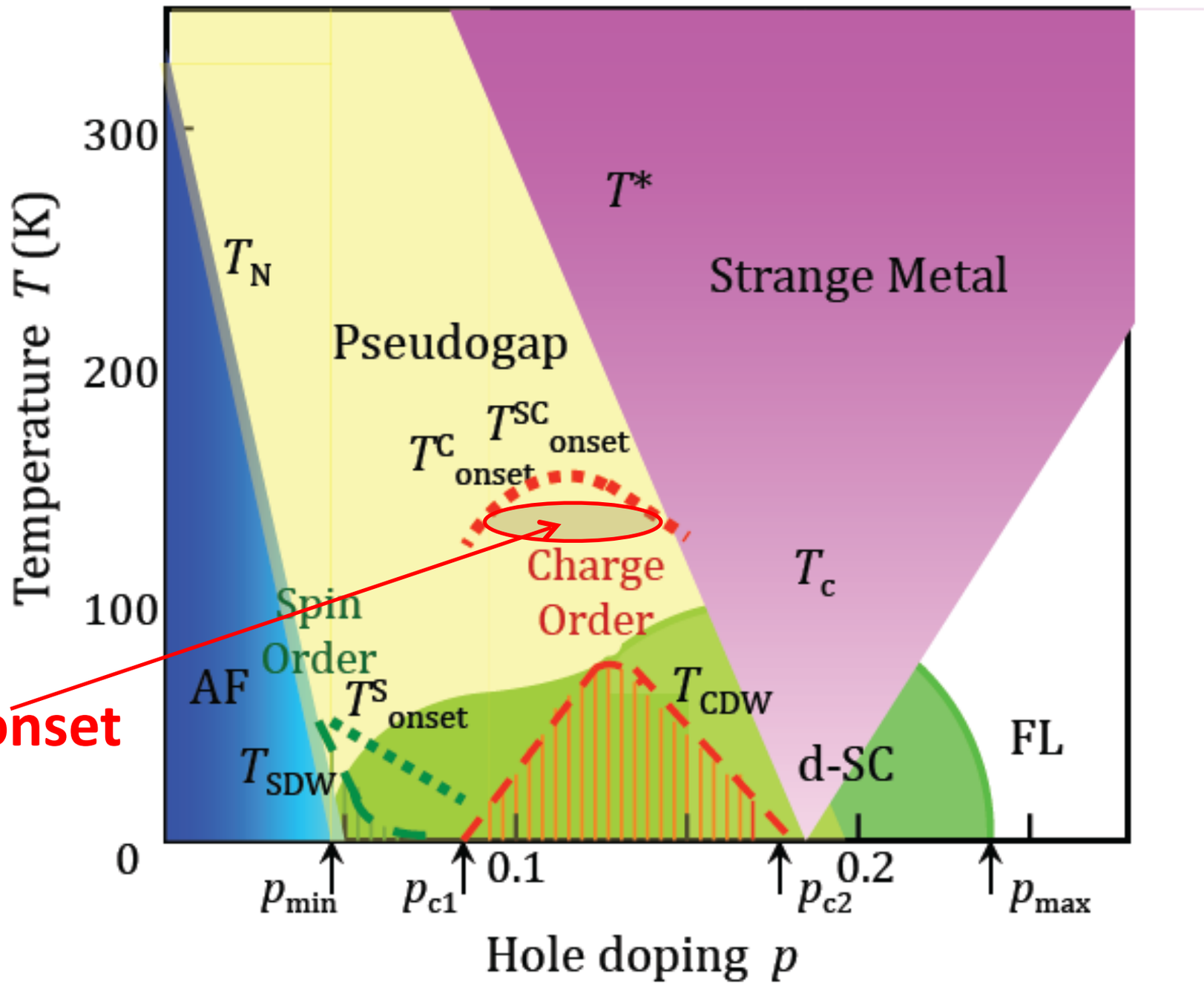
Linear optics: Chiral materials (and sugar water!) can show optical rotation in transmission, the Faraday effect, even without time-reversal breaking. (J. Orenstein and JEM, PRB 2012, motivated by cuprates)

1. Why they do not show Kerr effect (rotation in *reflection*, rather than transmission). (Zhong, Orenstein, Moore, PRL 2015)

2. Surprise: this problem is intimately connected to the "chiral magnetic effect" proposed in Weyl semimetals, although as sometimes described that effect is actually *zero* for topological reasons. (Zhong, Moore, Souza, PRL 2016)

Cuprate phase diagram: updated

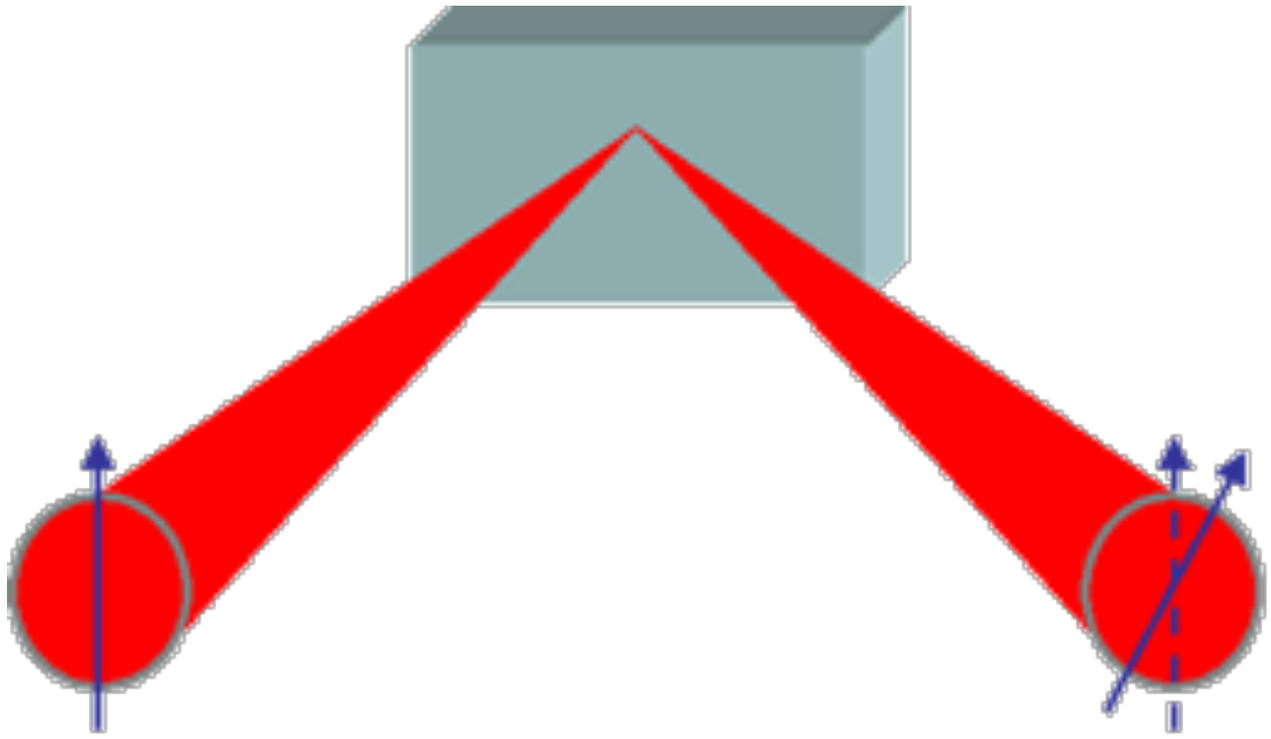
B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, J. Zaanen



What is new is signature of **charge order** by X-ray diffraction

Evidence **for local breaking of C4 symmetry** with short coherence length

What is the Kerr effect?



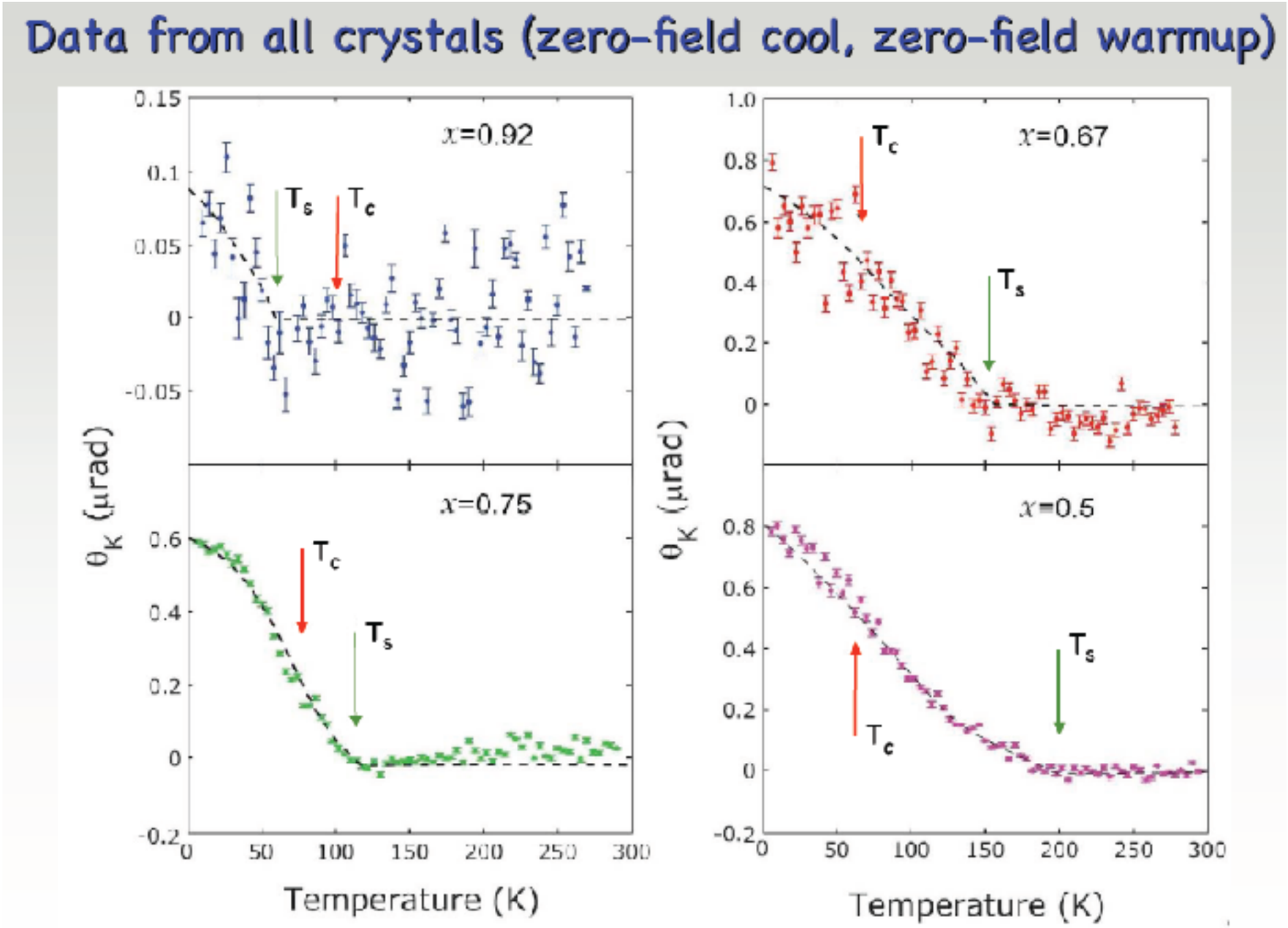
Rotation of the plane of polarization upon reflection

Stanford Sagnac measures the *polar Kerr effect* (normal incidence)
Faraday effect = rotation of the plane of polarization upon *transmission*

Both typically present in ferromagnets…

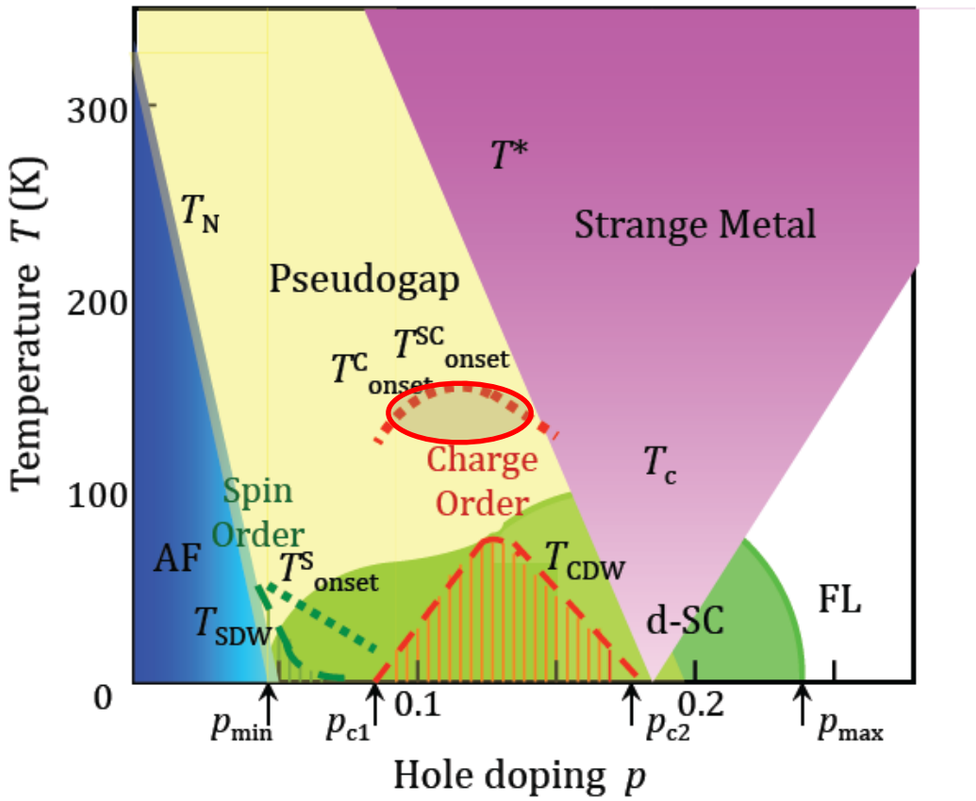
Observations of Kerr effect by Kapitulnik group

Kerr data in YBCO crystals



Onset of Kerr signal “always” coincides with charge order

YBCO



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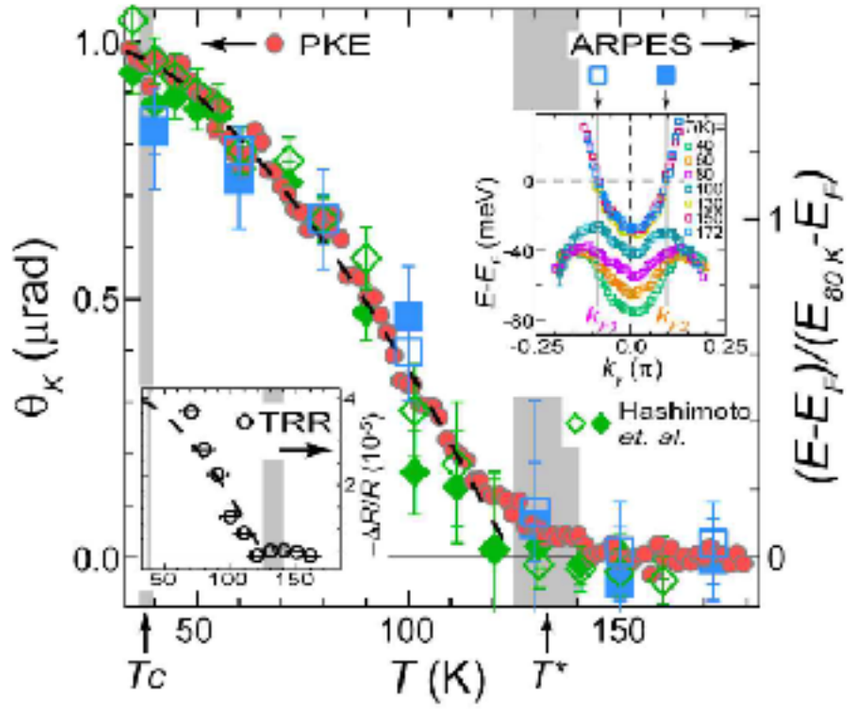
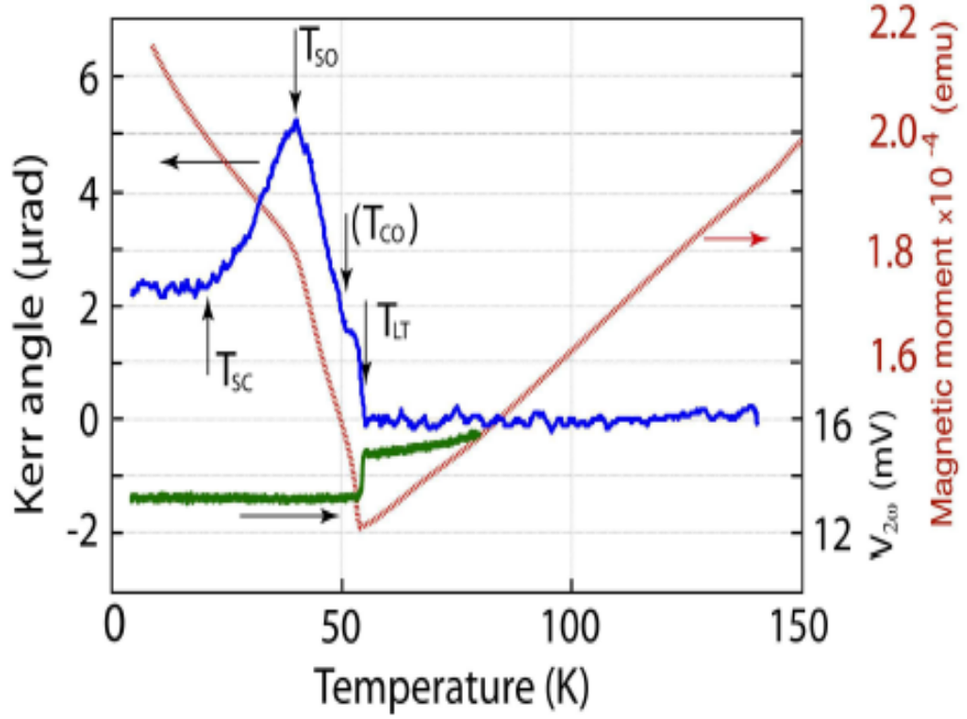


LBCO



Kerr conundrum in cuprates I

The most natural point group symmetry to be broken by charge order is C4→C2

This would lead to optical birefringence $n_x \neq n_y$

But, that is precisely what the Sagnac interferometer in the Stanford Kerr experiments is designed to reject!

Subtleties of time-reversal symmetry

A magnetic material can have both Kerr (reflection) and Faraday (transmission) effects.

A "chiral" T-symmetric material with low spatial symmetry **can have Faraday but not Kerr**. (This was derived macroscopically from Onsager reciprocity by Halperin, then seemingly forgotten; see also recent work of Armitage, Freed, etc.) **So purely spatial "chiral" ordering without T breaking cannot explain the Stanford experiment, at least in linear response.**

Faraday rotation in chiral materials is a Berry-phase effect (2012).

Challenge: it was unclear how the absence of Kerr rotation arises microscopically. It turns out that this does follow from the Berry-Boltzmann equations, through a subtle "topological tracelessness". (2015)

The same topological identity gives a compact derivation of the vanishing static chiral magnetic effect in uniform Weyl semimetals.

Outline of CME and GME

Many papers have been written on the possibility of a “chiral magnetic effect” in Weyl semimetals and other materials, also of the form

$$J_i = -\alpha_{ij}^{\mathrm{gme}} B_j$$

This would be related to the chiral anomaly in particle physics, and to the Berry curvature around Weyl points.

Consensus now that it is zero at equilibrium (as “Bloch’s other theorem” says).

It can be nonzero in transport (non-commutation of q->0 and omega->0 limits) or at nonzero frequency (gyrotropy!), but in its simplest form does not involve the Berry phase but something else: (Zhong, JEM, Souza, PRL 2016; see also Ma-Pesin PRB 2016)

$$\alpha_{ij}^{\mathrm{gme}} = -\frac{1}{(2\pi)^2}\frac{e}{h}\sum_{na}\int_{S_{na}} dS\, \hat{v}_{\mathrm{F},i} m_{n,j}(\mathbf{k}_f)\,.$$

3D Dirac and Weyl metals

Can we find 3D materials that are massless semimetals like graphene?

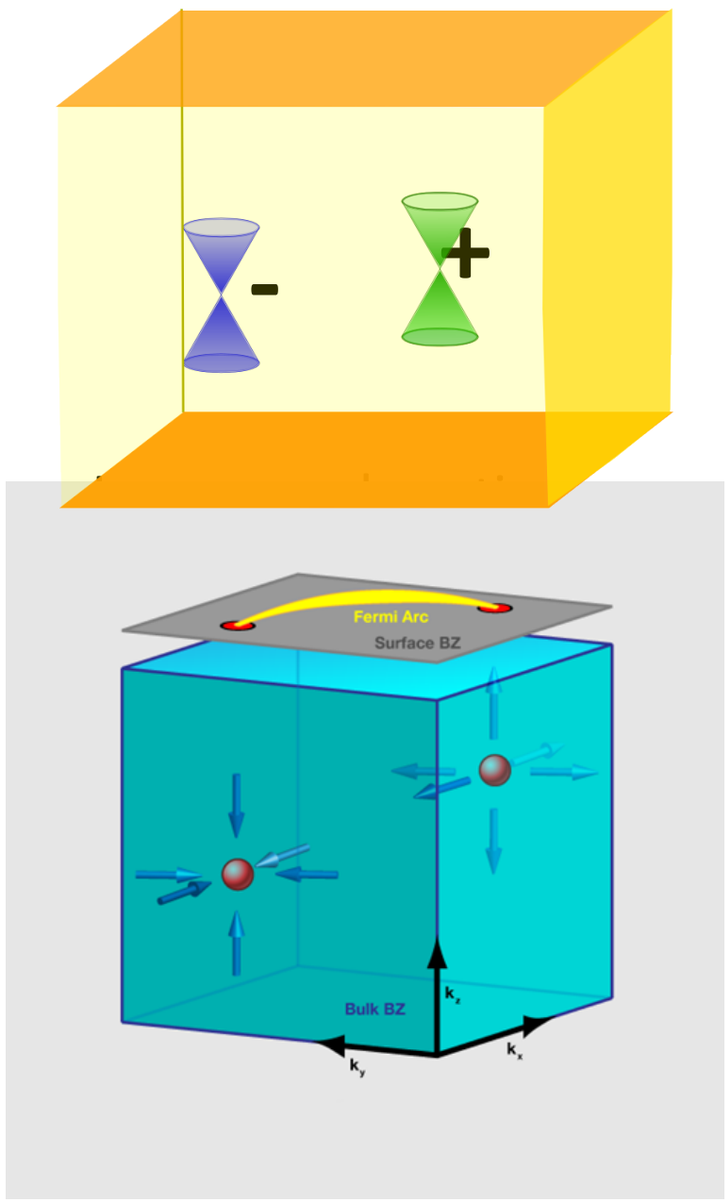
Yes! There are two ways to generalize graphene's massless "Dirac electrons" to 3D.

In the early days of quantum mechanics, two alternatives were put forward that are "half" of Dirac's celebrated equation for the electron.

Dirac: 4 by 4 matrix equation describes the electron and the positron
4-band semimetals found in Na3Bi, Cd2As3, 2013

Weyl: 2 by 2 matrix equation describes a particle with only one "handedness"
Does not seem to exist in the standard model; neutrinos were a possibility
2-band semimetals found in "inversion-breaking" TaAs, 2014-2015

Weyl semimetal
old theory idea (Herring, …);
trick is finding at Fermi surface



A Weyl point has topological charge: the Chern number from Berry flux through a small sphere around it is an integer. (Murakami, 2008)

There are surface Fermi arcs connecting Weyl points (Wan et al., 2010).

What are consequences of this topological property?

What is “chiral anomaly” in CM?
How is it related to chiral magnetic effect?

Chiral anomaly: current conservation is anomalous for a single Weyl fermion coupled to a U(1) gauge field:

$$\partial^\mu J^W_\mu = \frac{g^2 C}{16\pi^2}\mathbf{E}\cdot\mathbf{B}$$

CME idea: The total charge of Weyl points in a crystal is 0.

But they can occur at different energies. So maybe the (static) energy difference can replace the electric field, giving a scalar contribution to

$$J_i = -\alpha^{\mathrm{gme}}_{ij} B_j$$

A simpler, “topological” example: the uniform chiral magnetic effect

Apply a constant magnetic field **B** = B **z** to a solid. Solve the Berry-Boltzmann equation.

The currents in the **x** and **y** directions vanish trivially.

The current along **z** has “ordinary” and “anomalous” parts

$$j_z^{(o)} = -(e^2 B/\hbar) \int \frac{f^0 d^3k}{(2\pi)^3} \Omega_z v_z$$

$$j_z^{(a)} = -\frac{e^2 B}{\hbar} \int \frac{f^0 d^3k}{(2\pi)^3} (\Omega_x v_x + \Omega_y v_y).$$

Note for experts: the ordinary part comes from the phase-space volume correction (Xiao et al.). These cancel since

$$\langle \Omega_x(\mathbf{k}) v_x(\mathbf{k}) + \Omega_y(\mathbf{k}) v_y(\mathbf{k}) + \Omega_z(\mathbf{k}) v_z(\mathbf{k}) \rangle = 0$$

In a Weyl semimetal, the trace around one Weyl point is quantized to (Chern number) times (chemical potential), which gives a robust derivation of the “chiral magnetic effect”.

Vanishing of static CME via "tracelessness"

Berry mechanism leads to constraint on gyrotropic tensor

Proof is based on the fact that Ω is a curl of "Berry connection." (Hence div Ω = 0).

$$\int_{occ} d^3k \boldsymbol{\Omega}(\mathbf{k}) \cdot \mathbf{v}(\mathbf{k})$$
$$= \int_{occ} d^3k \boldsymbol{\Omega}(\mathbf{k}) \cdot \nabla \varepsilon(\mathbf{k})$$
$$= \int_{occ} d^3k \nabla \cdot [\varepsilon(\mathbf{k}) \boldsymbol{\Omega}(\mathbf{k})]$$
$$= \varepsilon_F \int_{FS} d^2k \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}(\mathbf{k})$$
$$= 0$$

But it was thought that different Weyl points at different energies could make this nonzero. Actually not: for a set of "monopoles" at different energies, the integral is a constant since

$$\frac{d}{dE}\left[\sum_i (E - E_i) m_i\right] = 0$$

by Nielsen-Ninomiya,

and the constant is actually zero by boundary conditions at the bottom of the band.

Supplemental Material for "Gyrotropic magnetic effect and the orbital moment on the Fermi surface"

DERIVATION OF THE EXPRESSION FOR CME AND GME USING KUBO FORMULA

The Kubo formula of the linear current response to a vector potential $\mathbf{A}e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$ is[S36]

$$J_i(\omega) = -e^2 \int [d^3k] \sum_{n,m} \frac{f(\epsilon_{n,\mathbf{k}-\mathbf{q}/2}) - f(\epsilon_{m,\mathbf{k}+\mathbf{q}/2})}{\epsilon_{n,\mathbf{k}-\mathbf{q}/2} - \epsilon_{m,\mathbf{k}+\mathbf{q}/2} + \omega} \langle n_{\mathbf{k}-\mathbf{q}/2}|\partial_i H|m_{\mathbf{k}+\mathbf{q}/2}\rangle\langle m_{\mathbf{k}+\mathbf{q}/2}|\partial_j H|n_{\mathbf{k}-\mathbf{q}/2}\rangle A_j(\omega,\mathbf{q}) \tag{24}$$

where we have set $\hbar = 1$ and in the following we would use the expression of the group velocity $\mathbf{v}_n = \nabla_{\mathbf{k}}\epsilon_n$. We are going to expand Eq. (24) and get the term which is zeroth order in ω and first order in q. As been discussed[S12] the result is different whether we set $\omega \to 0$ first or not. The two different results are related to CME and GME respectively.

For CME we set $\omega \to 0$ first and the contribution from interband ($n \neq m$) is

$$\begin{aligned} -e^2 \sum_{n,m\neq n} \int [d^3k] \Big\{ &(\frac{\partial f}{\partial \epsilon_n} v_{nl} + \frac{\partial f}{\partial \epsilon_m} v_{ml}) \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle (\epsilon_n - \epsilon_m) - (f(\epsilon_n) - f(\epsilon_m))\,(v_{nl} + v_{ml}) \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle \\ &+ \frac{(f(\epsilon_n) - f(\epsilon_m))}{\epsilon_n - \epsilon_m} [-\langle \partial_l n|\partial_i H|m\rangle\langle m|\partial_j H|n\rangle + \langle n|\partial_i H|\partial_l m\rangle\langle m|\partial_j H|n\rangle \\ &+ \langle n|\partial_i H|m\rangle\langle \partial_l m|\partial_j H|n\rangle - \langle n|\partial_i H|m\rangle\langle m|\partial_j H|\partial_l n\rangle] \Big\} \frac{q_l}{2} . \end{aligned} \tag{25}$$

The contribution from intraband ($n = m$) is

$$-e^2 \sum_n \int [d^3k] \frac{\partial f}{\partial \epsilon_n} [-\langle \partial_l n|\partial_i H|n\rangle v_{nj} + \langle n|\partial_i H|\partial_l n\rangle v_{nj} + \langle \partial_l n|\partial_j H|n\rangle v_{ni} - \langle n|\partial_j H|\partial_l n\rangle v_{ni}] \frac{q_l}{2} . \tag{26}$$

Combining them together and with some simplification we get

$$-e^2 \sum_{n,m} i q_l \int [d^3k] \,\mathrm{Im} \left[\frac{\partial f}{\partial \epsilon_n} v_{nl} \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle - \frac{\partial f}{\partial \epsilon_n} v_{nj} \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle + \frac{\partial f}{\partial \epsilon_n} v_{ni} \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle \right] (\epsilon_n - \epsilon_m) \tag{27}$$

$$+ - e^2 \sum_{n,m} i q_l \int [d^3k]\, f(\epsilon_n) \,\{ \mathrm{Im}[-\langle \partial_l n|\partial_i H|m\rangle\langle m|\partial_j n\rangle + \langle n|\partial_i H|\partial_l m\rangle\langle m|\partial_j n\rangle] - (i \leftrightarrow j)\} \tag{28}$$

$$+ - e^2 \sum_{n,m} i q_l \int [d^3k]\, f(\epsilon_n)\, (v_{nl} + v_{ml})\, \mathrm{Im}\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle . \tag{29}$$

Integrate by parts for Eq. (27) we have

$$\begin{aligned} -e^2 \sum_{n,m} i q_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}\,\{ &[(\epsilon_n - \epsilon_m)(\langle \partial_i n|\partial_l m\rangle\langle m|\partial_j n\rangle + \langle \partial_l n|\partial_j m\rangle\langle m|\partial_i n\rangle + \langle \partial_l n|m\rangle\langle \partial_j m|\partial_i n\rangle) - (i \leftrightarrow j)] \\ &+ \langle \partial_i n|m\rangle\langle m|\partial_j n\rangle (v_{nl} - v_{ml}) + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle (v_{ni} - v_{mi}) - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle (v_{nj} - v_{mj})\} \end{aligned} \tag{30}$$

and adding Eq. (28) Eq. (29) together

$$\begin{aligned} -e^2 \sum_{n,m} i q_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}\,\{ &\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle (v_{nl} + v_{ml}) + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle (v_{ni} + v_{mi}) - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle (v_{nj} + v_{mj}) \\ &+ [(\epsilon_n - \epsilon_m)(\langle n|\partial_i m\rangle\langle \partial_l m|\partial_j n\rangle + \langle \partial_l n|\partial_i m\rangle\langle m|\partial_j n\rangle + \langle \partial_l n|m\rangle\langle \partial_i m|\partial jn\rangle) - (i \leftrightarrow j)]\} . \end{aligned} \tag{31}$$

Adding Eq. (30) and Eq. (31) together we get

$$-e^2 \sum_{n,m} 2 i q_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}[\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle v_{nl} + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle v_{ni} - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle v_{nj}] \tag{32}$$

There is a nonzero linear effect: “transport limit”

Recall that the q->0 and w->0 limits do not commute in an E field:

q->0 first (“uniform”) gives electrical *conductivity*

w->0 first (“static”) gives electrical *compressibility.*

Something similar happens for a magnetic field, and we can calculate in the transport limit.

But a magnetic field at nonzero omega necessarily involves an electrical field as well: the uniform or “transport limit” of the CME is really describing the low-frequency response to an electromagnetic wave.

We (e.g., Landau-Lifshitz) know a lot about the symmetry properties of such responses. What is their microscopic origin? Indeed it comes from the B field part of the wave, which couples to the *orbital moment of Bloch electrons.*

Orbital moment of Bloch electrons

Something that is not always taught (at least by me) in solid state courses is that a Bloch electron has an orbital moment

$$m_{n,j} = \frac{e}{2\hbar}\varepsilon_{jln}\mathrm{Im}\ \langle\partial_l n|H-\epsilon_n|\partial_n n\rangle\ .$$

This modifies the group velocity that appears in the semiclassical equations:

$$v_{\mathrm{group}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_k = \frac{1}{\hbar}\nabla_{\mathbf{k}}(\epsilon_{\mathbf{k}} + \mathbf{m}_{n\mathbf{k}}\cdot\mathbf{B}).$$

In other words, all the previous pieces found by us and other people come together in the full quantum Kubo formula in a very simple Fermi-surface expression that is pretty easy to calculate in actual materials.

The linear response CME is actually optical rotation! (“gyrotropic magnetic effect”)

Orbital moment should also modify other things, including collective modes.

Summary of CME and GME

Many papers have been written on the possibility of a “chiral magnetic effect” in Weyl semimetals and other materials, also of the form

$$J_i = -\alpha_{ij}^{\mathrm{gme}} B_j$$

The only linear response effect is not a scalar and is properly regarded as a “gyrotropic magnetic effect”, easily measured in optical rotation

$$\alpha_{ij}^{\mathrm{gme}} = -\frac{1}{(2\pi)^2}\frac{e}{h}\sum_{na}\int_{S_{na}} dS\, \hat{v}_{\mathrm{F},i} m_{n,j}(\mathbf{k}_f)\,.$$

Beyond linear response there are other effects, including those more like the chiral magnetic effect in particle physics (cf. Son-Spivak). So we would like to compute responses to higher order in EM fields and look for topological pieces.

Future work

We can give a systematic derivation of the nonlinear Berry-phase effect mentioned earlier using the Floquet approach (Morimoto, Zhang, JEM), and have computed semiclassically some other effects.

There is an interesting experiment by Phuan Ong's group on angle-dependent magnetoconductivity with a low-field regime that might be explained by our theory.

Some bigger challenges:

Are there any consequences of *non-Abelian* gauge fields in metals?

Which effects can be quantized/associated with nonzero topological invariants?

Additional effects in metals

In closing, I would like to say a few words about nonlinear effects in metals.

The point of the preceding section was that the linear response to A(q,omega) is not particularly quantized: for two Weyl nodes split in energy by *E*, the result is

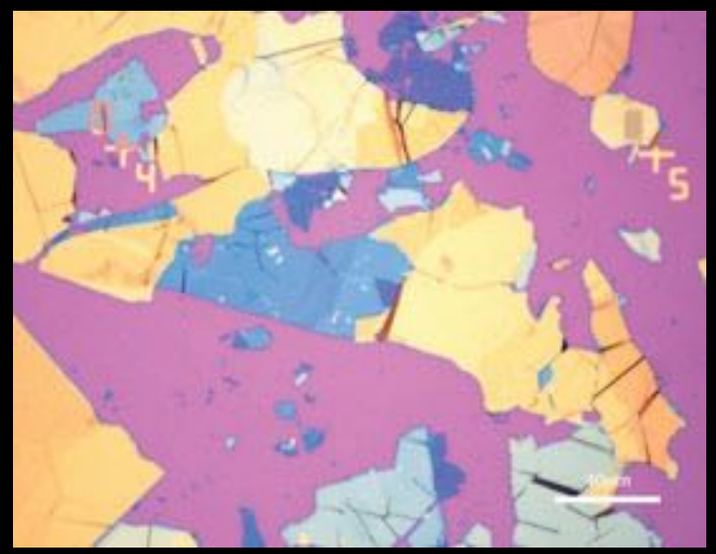
$$\mathbf{j} = \frac{e^2}{3h^2}(\epsilon_R - \epsilon_L)\mathbf{B}.$$

This is scalar, like the proposed CME, but with a different magnitude. More to the point, it depends on the energy difference between nodes, so isn't quantized.

Can we ever see quantized responses in metals? Yes, and even in optics…

Optical quantization in semimetals

Properties of the "semi-metallic" electrons in graphene:
effective mass is *zero*



one layer of graphene attenuates 2.3% of light

(π times the fine structure constant) $\frac{\pi e^2}{hc}$

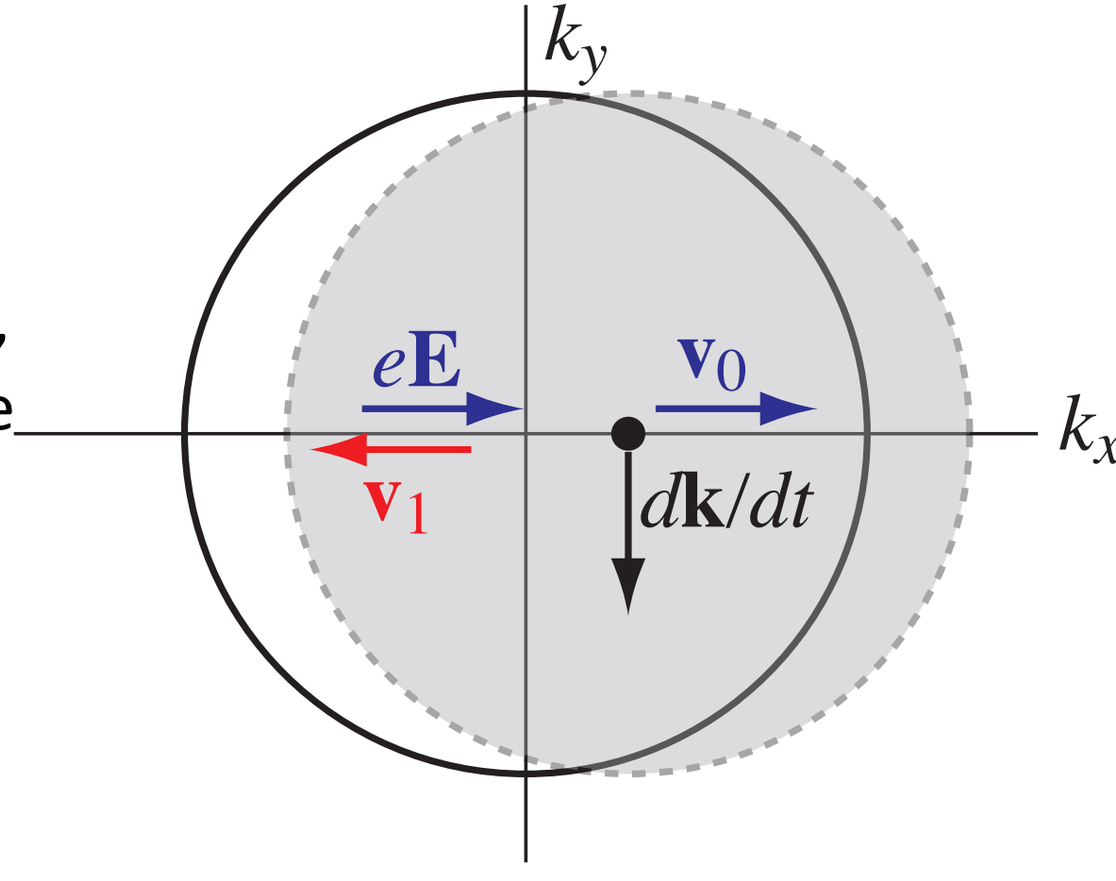
1. A quantized effect in Weyl semimetals

We believe that the “circular photogalvanic effect”, which made a quick appearance earlier, is effectively quantized in energy-split Weyl semimetals.

First, recall the semiclassical Berry phase CPGE in metals:

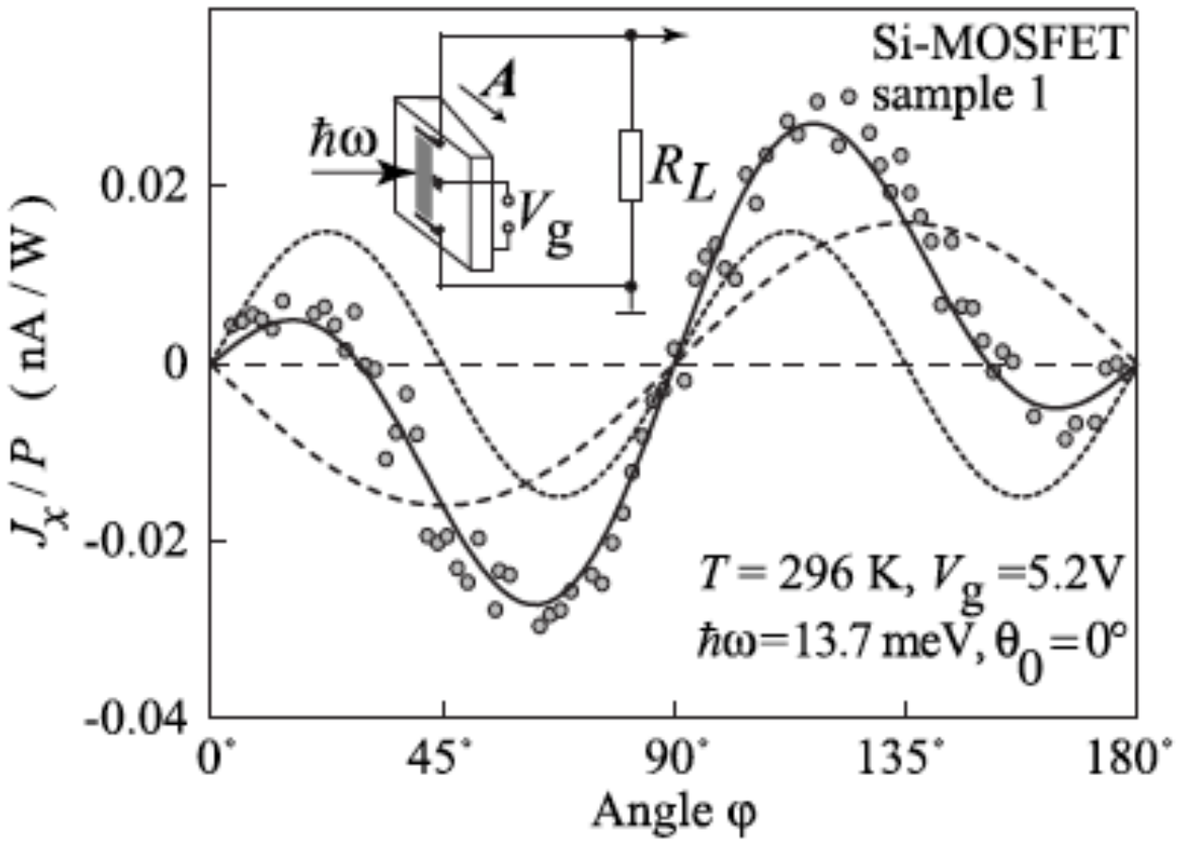
$$\frac{dx^a}{dt} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k})\frac{dk_b}{dt}.$$

Around a period of the circular incident wave, the ordinary velocity averages to zero, but the anomalous velocity does not, if F is linear in k (requires low symmetry).



Non-quantized CPGE

Measure the part of photocurrent that changes sign when the incident polarization changes from right circular to left circular:

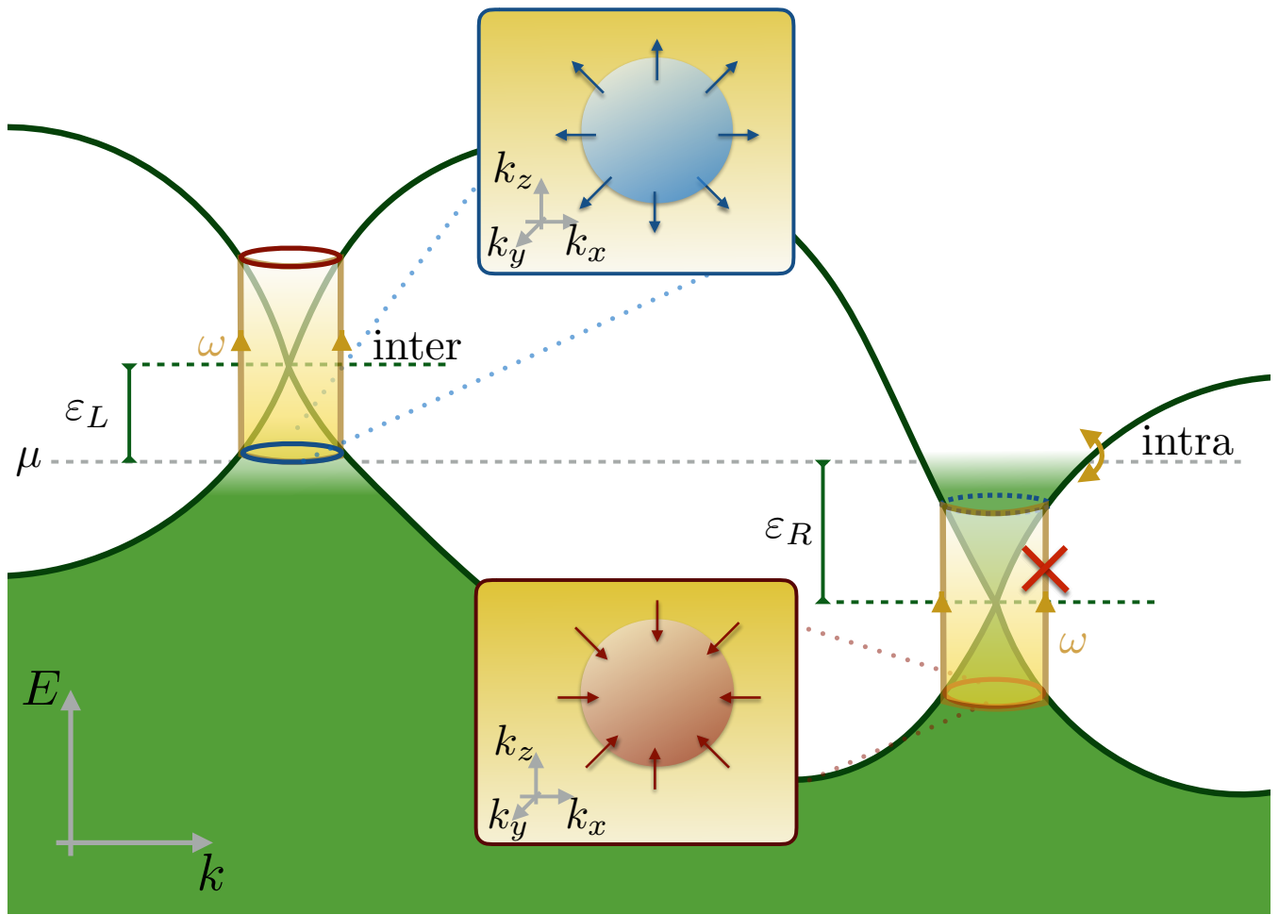


The Berry-phase theory (JEM and Orenstein, PRL 2010; Fu-Sodemann, PRB 2015) may explain many experiments from the group of Ganichev (Regensburg) on a variety of low-symmetry quantum wells.

Original explanation was in terms of spin-orbit, but signal strength in Si seems inconsistent with that. Strength is determined by degree of inversion breaking. Effect is pretty weak (pA photocurrents).

Quantized CPGE

The quantum calculation of CPGE from a Weyl node gives a surprising result: there is a large quantized value, over a broad range of frequencies, that will dominate metallic contributions from other parts of the Brillouin zone.



(F. de Juan, A. Grushin, T. Morimoto, JEM, Nat. Comm. 2017)

What is the “quantum”?

Because this is a nonlinear effect, the quantum is different from the standard e^2/h. Instead, it is e^3/(h^2 c):

$$\frac{1}{2}\left[\frac{dj_{\circlearrowright}}{dt}-\frac{dj_{\circlearrowleft}}{dt}\right]=\frac{2\pi e^3}{h^2 c\epsilon_0}IC_n,$$

Here I is the incident intensity and C is the Chern number of a Weyl node.

Some quick notes: what’s quantized is the “rate of current injection”. The DC photocurrent will then involve a non-universal relaxation time factor, that would have to be extracted by other means.