

# Electrodynamics in insulators

We know that the constants  $\epsilon$  and  $\mu$  in Maxwell's equations can be modified inside an ordinary insulator.

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

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

This term is a total derivative, unlike other magnetoelectric couplings.

The angle  $\theta$  is periodic and odd under T.

A T-invariant insulator can have two possible values: 0 or  $\pi$ .

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

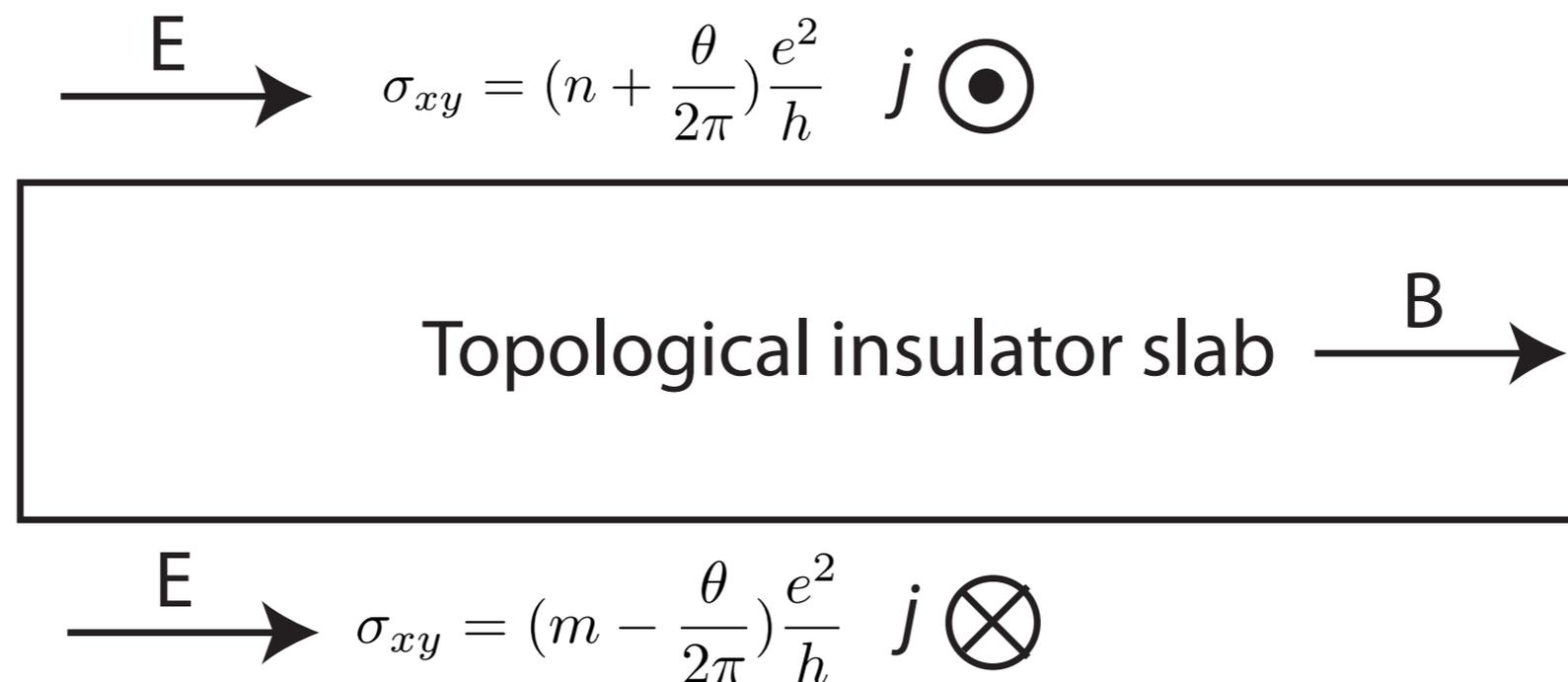
# Axion E&M, then and now

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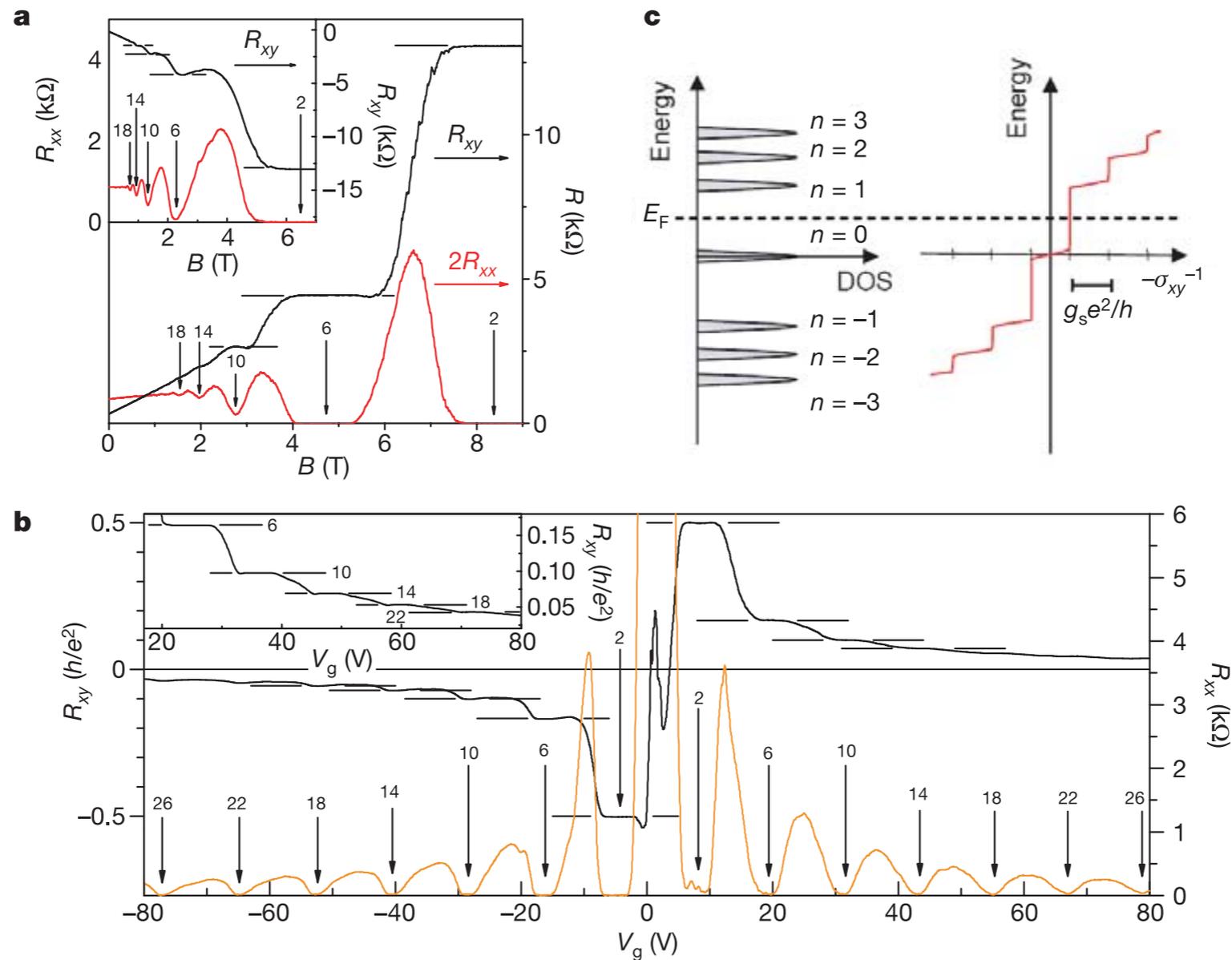
Magnetoelectric effect: (Qi, Hughes, Zhang 2008)

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



# Dirac fermion QHE: graphene

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



# Topological response

Idea of “axion electrodynamics in insulators”

there is a “topological” part of the magnetoelectric term

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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

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

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

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

# 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 (Xiao et al.), it is not at all clear why this should be the only magnetoelectric term from orbital motion of electrons.

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

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

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

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

# Orbital magnetoelectric polarizability

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

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

$$\alpha_j^i = (\alpha_I)_j^i + \alpha_{CS} \delta_j^i$$

$$(\alpha_I)_j^i = \sum_{\substack{n \text{ occ} \\ m \text{ unocc}}} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \text{Re} \left\{ \frac{\langle u_{n\mathbf{k}} | e \mathbf{r}_{\mathbf{k}}^i | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | e (\mathbf{v}_{\mathbf{k}} \times \mathbf{r}_{\mathbf{k}})_j - e (\mathbf{r}_{\mathbf{k}} \times \mathbf{v}_{\mathbf{k}})_j - 2i \partial H_{\mathbf{k}}' / \partial B^j | u_{n\mathbf{k}} \rangle}{E_{n\mathbf{k}} - E_{m\mathbf{k}}} \right\}$$

$$\alpha_{CS} = -\frac{e^2}{2\hbar} \epsilon_{abc} \int_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \text{tr} \left[ \mathcal{A}^a \partial^b \mathcal{A}^c - \frac{2i}{3} \mathcal{A}^a \mathcal{A}^b \mathcal{A}^c \right].$$

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.

# Multiferroicity/magnetolectricity

So we have a general theory for the orbital magnetolectric response tensor in a crystal (which essentially includes the orbital “toroidal moment”).

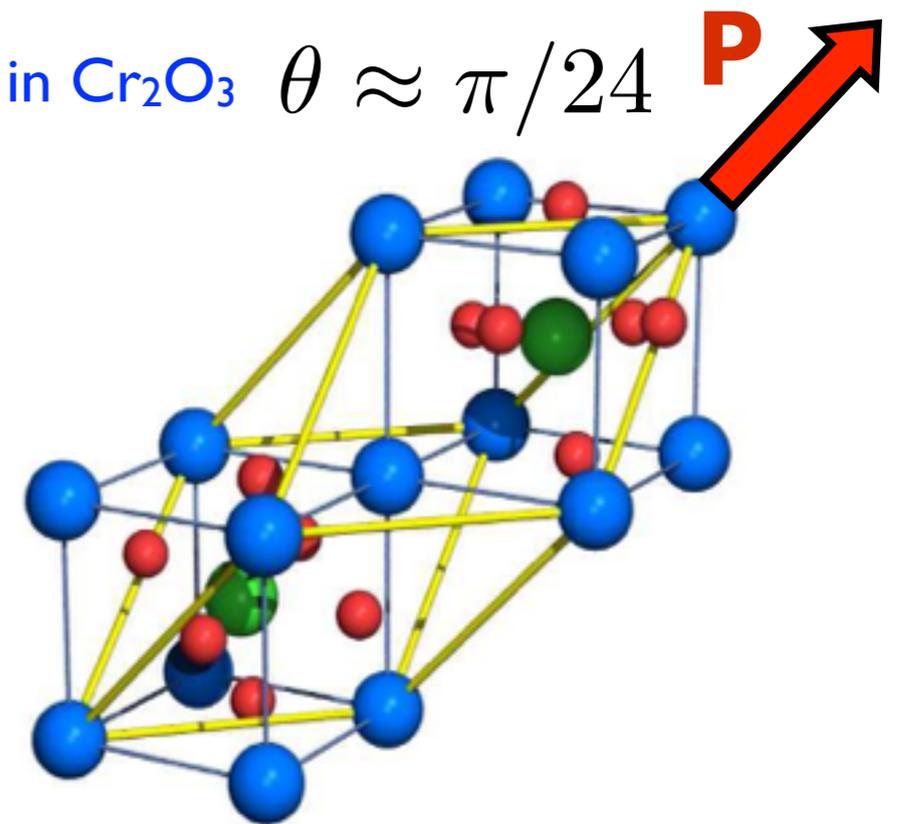
It is not a pure Berry phase in general, but *it is in topological insulators*.

Such magnetolectric responses have been measured, e.g., in  $\text{Cr}_2\text{O}_3$   $\theta \approx \pi/24$  (Obukhov, Hehl, et al.).

Example of the ionic “competition”:  $\text{BiFeO}_3$

Can make a 2x2 table of “magnetolectric 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 magnetolectric effects requiring ionic motion.

# Summary of recent experiments

1. There are now at least 3 strong topological insulators that have been seen experimentally ( $\text{Bi}_x\text{Sb}_{1-x}$ ,  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$ ).
2. Their metallic surfaces exist in zero field and have the predicted form.
3. These are fairly common bulk 3D materials (and also  $^3\text{He B}$ ).
4. The temperature over which topological behavior is observed can extend up to room temperature or so.

## What's left

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

(What are they good for?)

Are there more profound consequences of geometry and topology?

*Lecture 2: Many basic phenomena in matter*

*Lecture 3: New types of particles, with new types of statistics*

*Lecture 4: The future*

But first we need a few basic notions from topology.

# Outline of lecture 2

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

Insulators: Polarization, IQHE, “topological insulators”, ...

Metals: New semiclassical term for electron motion.

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

3. What do we learn about magnetoelectric effects more generally? (“multiferroic” materials)

4. Introduction to topological field theories. Candidate “BF theory” for topological insulators.

# Berry phase review

Why do we write the phase in this form?

Does it depend on the choice of reference wavefunctions?

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

If the ground state is non-degenerate, then the only freedom in the choice of reference functions is a local phase:

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

Under this change, the “Berry connection”  $\mathcal{A}$  changes by a gradient,

$$\mathcal{A} \rightarrow \mathcal{A} + \nabla_{\mathbf{k}} \chi$$

*just like the vector potential in electrodynamics.*

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

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

# How can we picture $A$ ?

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

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

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

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

# What about non-magnetic insulators?

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

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

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

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

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

There is an ambiguity of  $e$  per transverse unit cell, the “polarization quantum.”

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

Fact from cohomology:

Odd dimensions have Chern-Simons forms that have a “quantum” ambiguity;

Even dimensions have Chern forms that are quantized.

# But what does $F$ do?

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

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

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

a “magnetic field” in momentum space.

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

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

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

# But what does $F$ do?

Example I: the anomalous Hall effect in itinerant magnets

An electrical field  $\mathbf{E}$  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

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

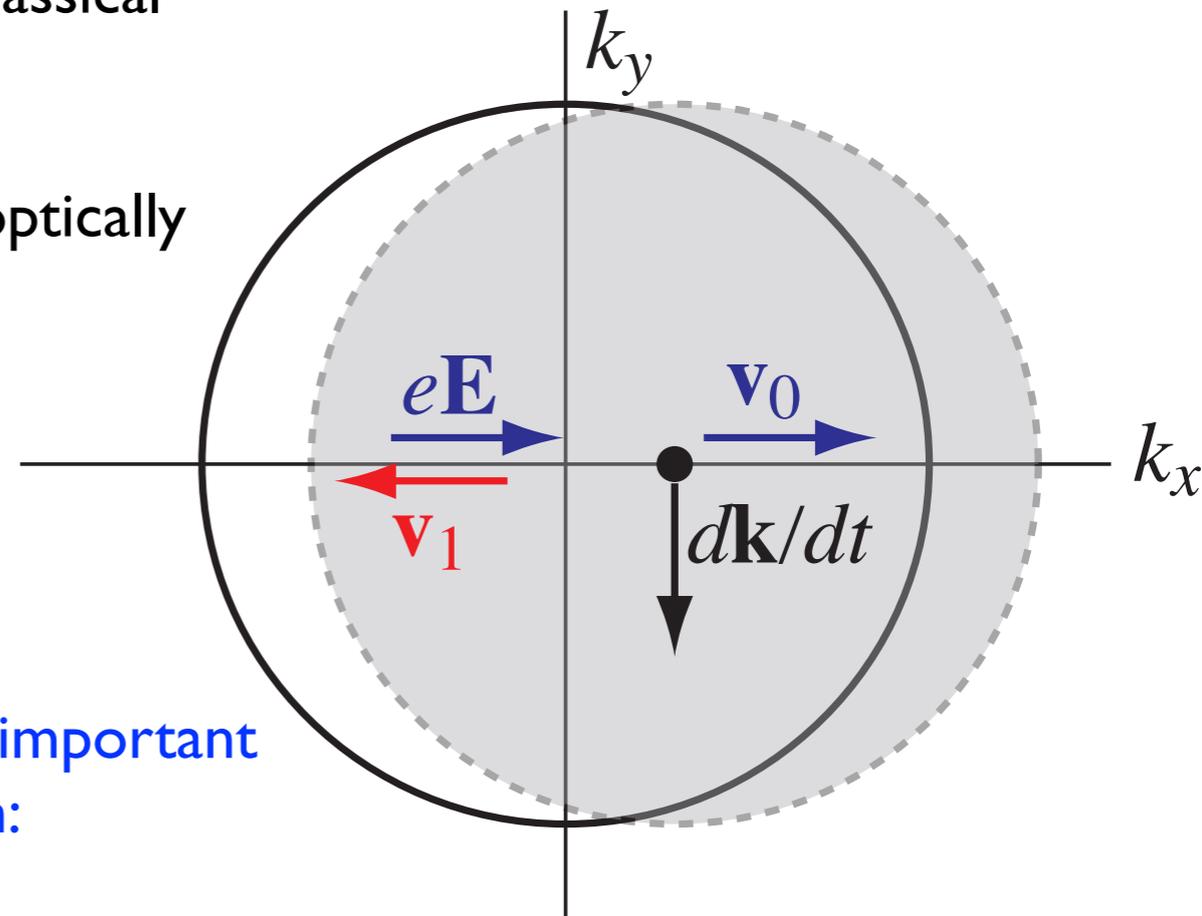
Smit's objection: in steady state the electron distribution is stationary; why should the anomalous velocity contribute at all?

(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  $\mathbf{E}$ ) and two are “Luttinger-type”.

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

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

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

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

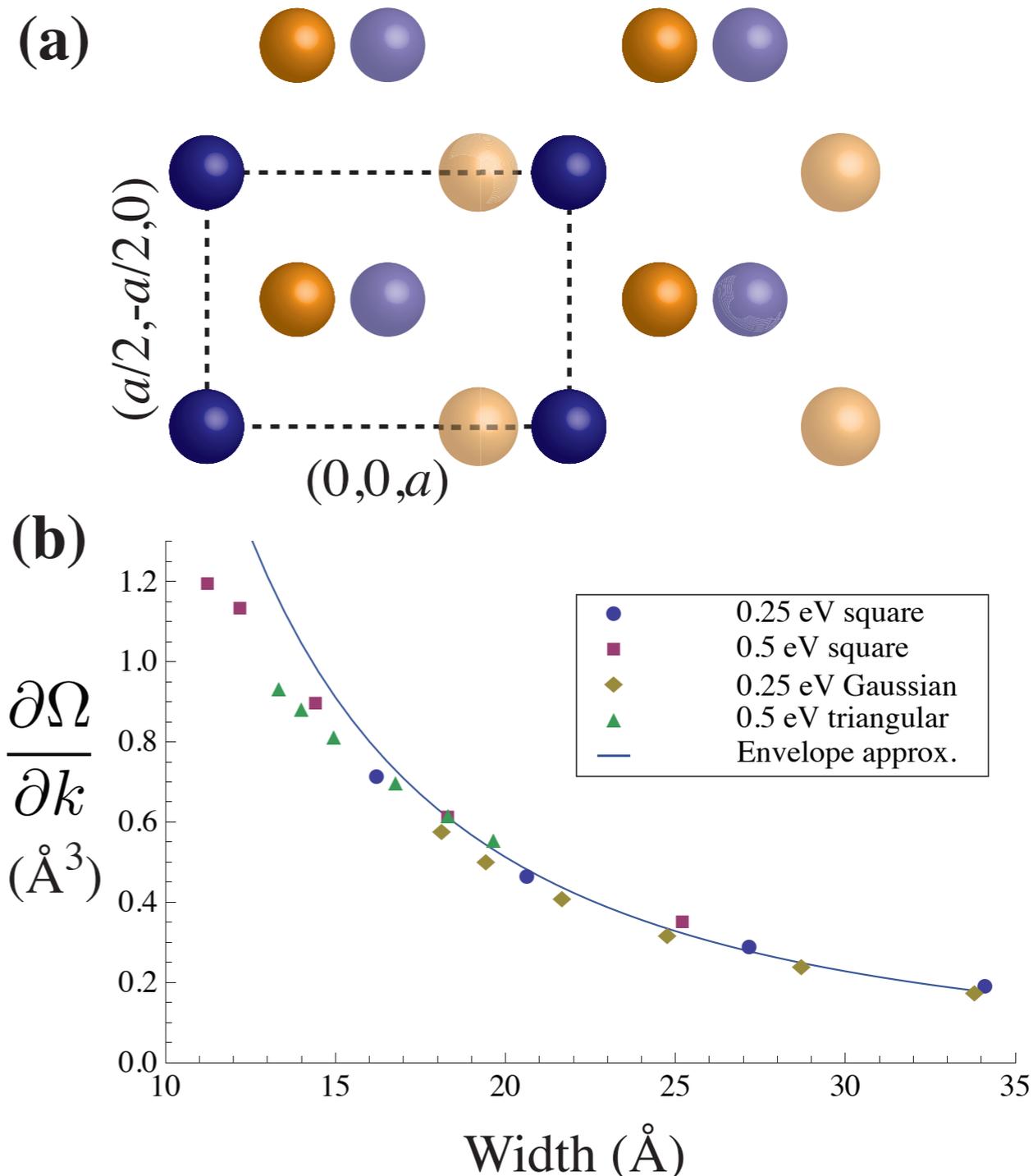
# Confinement-induced Berry phases

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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  $\mathcal{F}$  at the Brillouin zone origin: symmetries force

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



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

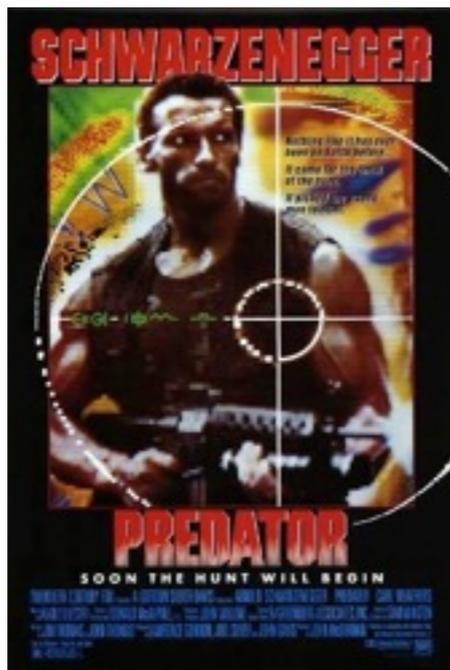
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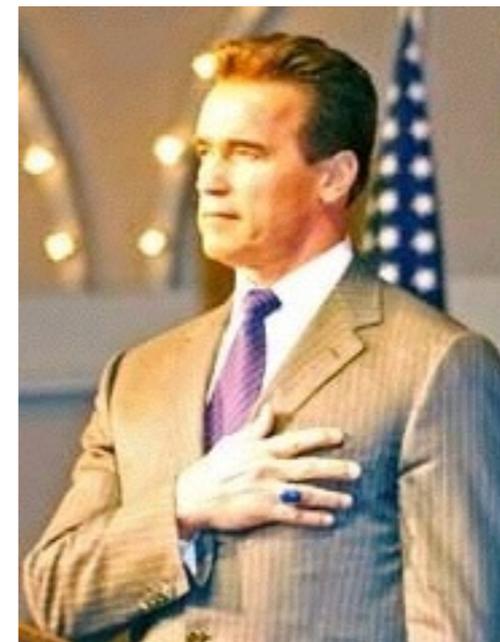
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1987



2007

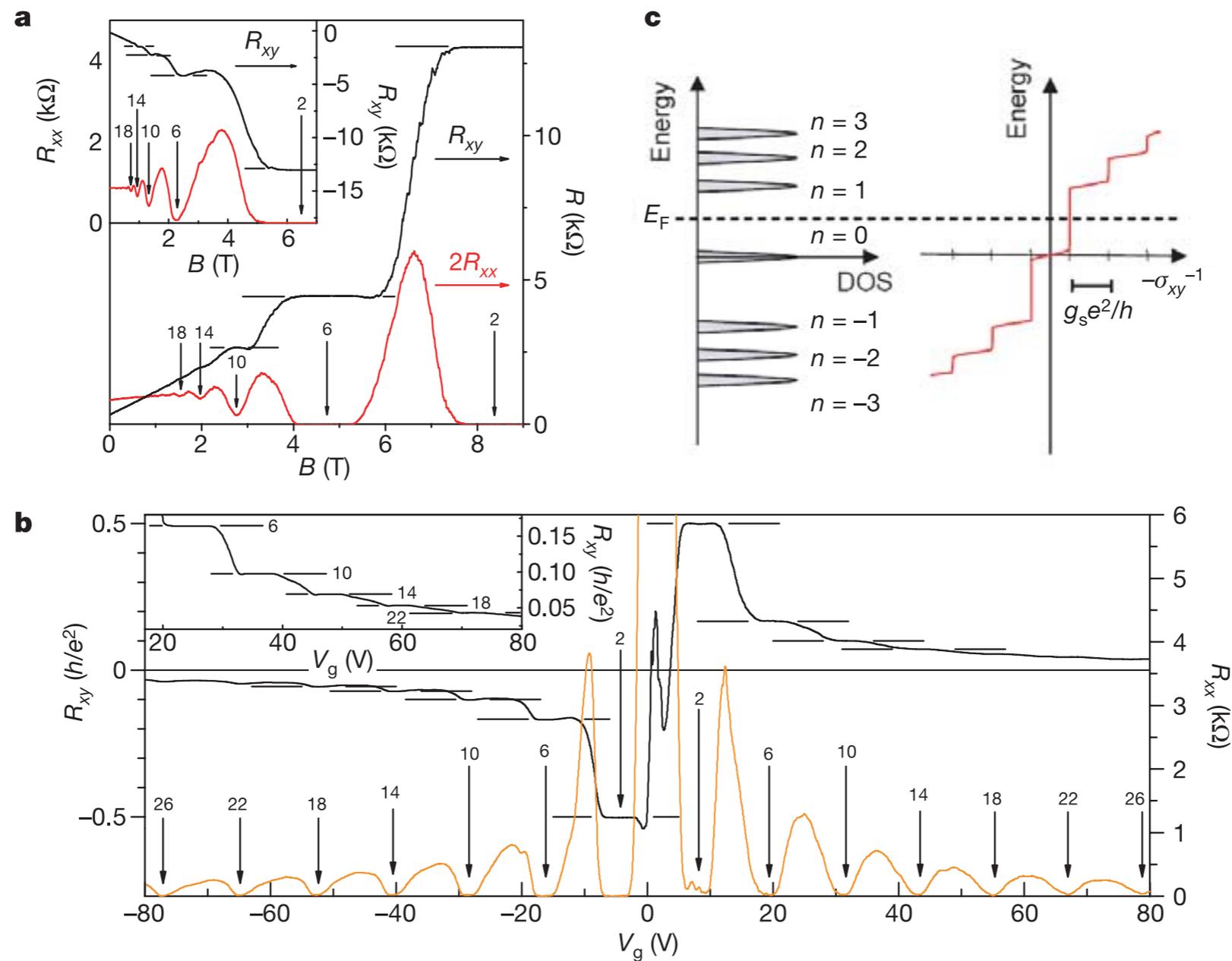


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These two values correspond to ordinary and topological 3D insulators.  
(Qi, Hughes, and Zhang, 2008)

# 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)



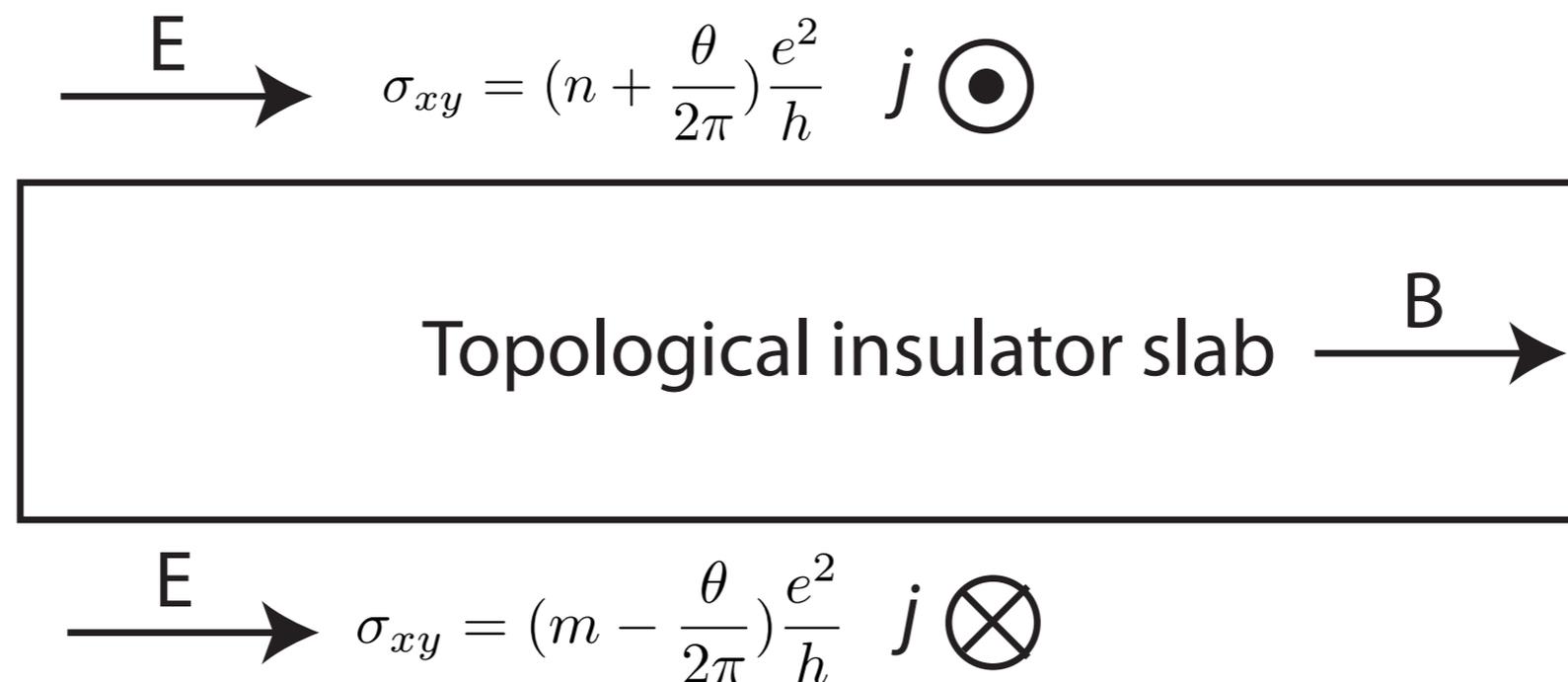
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(Qi, Hughes, Zhang, 2008; Essin, JEM, Vanderbilt 2009)

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

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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

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(The antisymmetric part is related to the “toroidal moment” in multiferroics;  
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The “ordinary part” indeed looks like a Kubo formula of electric and magnetic dipoles.

Not inconsistent with previous results:

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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.

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# Magnetoelectric theory: a spinoff of TIs

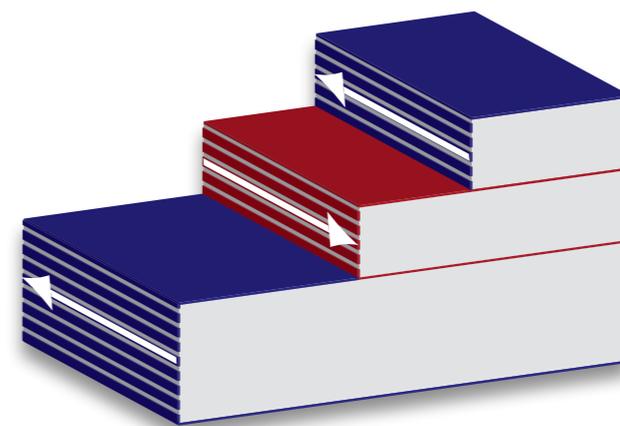
This leads to a general theory for the orbital magnetoelectric response tensor in a crystal, including contributions of all symmetries.

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

Such magnetoelectric responses have been measured, e.g., in  $\text{Cr}_2\text{O}_3$   $\theta \approx \pi/24$  (Obukhov, Hehl, et al.). But this required gapped surfaces.

The magnetoelectric theory helps understand some related phases that are protected by inversion or by the combination of time-reversal and translation:

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



# Magnetolectric theory: a spinoff of TIs

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

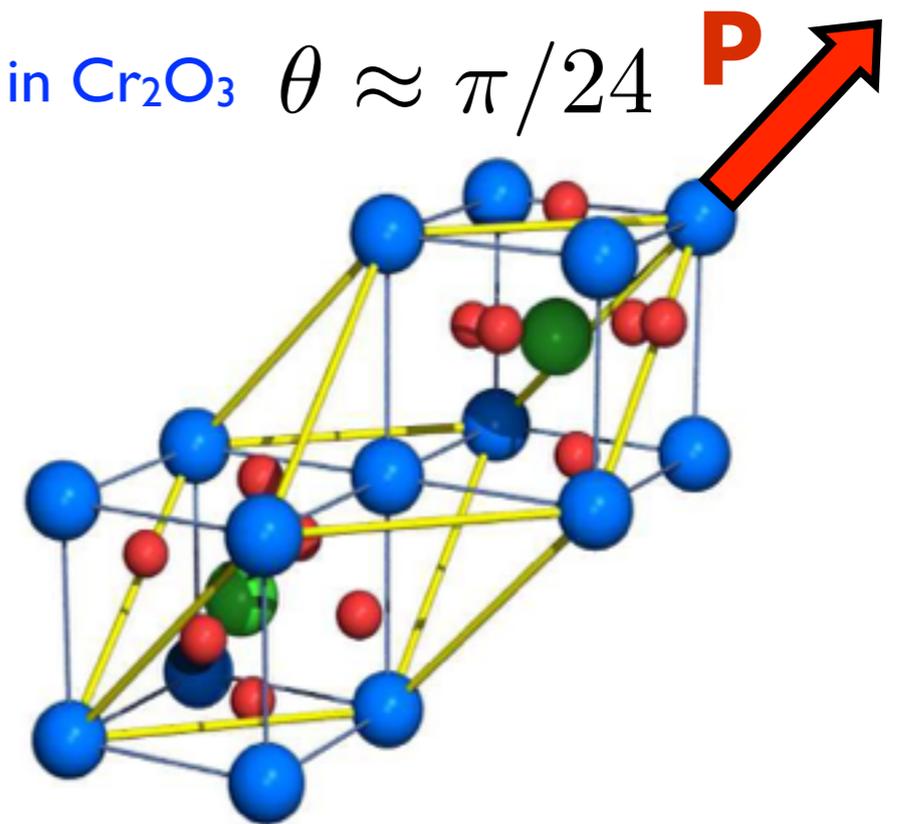
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(ignore nuclear magnetism)

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

# Topological field theory of QHE

How can we describe the topological order in the quantum Hall effect?

Standard answer: Chern-Simons Landau-Ginzburg theory  
(Girvin & MacDonald; Zhang, Hansson, and Kivelson; Read; ...)

$$L_{CS} = -\frac{k}{4\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda + j^\mu a_\mu, \quad j^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} \partial_\nu A_\lambda$$

There is an “internal gauge field”  $a$  that couples to electromagnetic  $A$ .

Integrating out the internal gauge field  $a$  gives a Chern-Simons term for  $A$ , which just describes a quantum Hall effect:

$$L_{QHE} = -\frac{1}{4k\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda$$

There is a difference in principle between the topological field theory and the topological term generated for electromagnetism; they are both Chern-Simons terms.

# Topological field theory of QHE

What good is the Chern-Simons theory? (Wen)

$$L_{CS} = -\frac{k}{4\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda + j^\mu a_\mu, \quad j^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} \partial_\nu A_\lambda$$

The bulk Chern-Simons term is not gauge-invariant on a manifold with boundary.

It predicts that a quantum Hall droplet must have a chiral boson theory at the edge:

$$S = \frac{k}{4\pi} \int \partial_x \phi (\partial_t \phi - v \partial_x \phi) dx dt$$

For fractional quantum Hall states, the chiral boson is a “Luttinger liquid” with strongly non-Ohmic tunneling behavior.

Experimentally this is seen qualitatively--perhaps not quantitatively.

# Topological field theory of TI

For the topological insulator, we know many properties.

Two standard defining properties in the 3D case:

1. When T is unbroken, there are gapless surfaces with an odd number of Dirac fermions.
2. When T is broken weakly, there is a half-integer quantum Hall effect at the surface, which is equivalent to a bulk EM term

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

Can we find an internal topological field theory that can capture the gapless surface and, when gapped, capture the “axion electrodynamics” term for electromagnetism?

In the 2D case, a useful defining property is that a pi flux insertion in the bulk captures an odd number of Kramers singlets (Fu-Kane, Essin-Moore, Ran-Vishwanath-Lee, Qi-Zhang)

# Topological field theory of TI

For the two-dimensional topological insulator, we know that an example of the state is provided by a pair of integer quantum Hall states for “spin-up” and “spin-down”.

We can write the resulting combination of two Chern-Simons theories in a basis of two fields  $a$  and  $b$  with different time-reversal properties:

$$L_{BF} = \frac{1}{\pi} \varepsilon^{\mu\nu\lambda} (b_\mu \partial_\nu a_\lambda + A_\mu \partial_\nu b_\lambda)$$

This is known as 2D “BF theory”, since the topological part couples the field  $b$  and the field strength  $F$  of  $a$ . It is time-reversal even, unlike CS theory.

Its edge has two oppositely propagating boson modes. In the above we have written the coupling to electromagnetism, and indeed we obtain the localized states around a pi flux.

The sources of  $a$  and  $b$  are charge density and spin density.

This theory was previously studied in CM in the context of superconductivity (Oganesyan, Hansson, Sondhi 2004).

# What about 3D?

Unlike Chern-Simons theory, BF theory exists in 3D and still describes time-reversal-invariant systems.

$$L_{BF} = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_{\lambda\rho} + \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} A_\mu \partial_\nu b_{\lambda\rho} + C \varepsilon^{\mu\nu\lambda\rho} \partial_\mu a_\nu \partial_\lambda A_\rho$$

Now  $b$  is a two-form and there are two possible couplings to the EM field.

One is T-invariant and the other is not; we expect it to be generated by a T-breaking perturbation at a surface, and indeed it is a boundary term.

The electromagnetic current contains both contributions from  $a$  and  $b$ .

$$J_{EM}^\mu = J_b^\mu + J_a^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu b_{\lambda\rho} + \frac{1}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu (\theta \partial_\lambda a_\rho)$$

The two-form  $b$  contains information about electric and magnetic polarizations, which can be viewed as a density of intrinsically line-like objects (think about field lines).

# Facts about 3D BF

1. With the T-breaking perturbation, we obtain “axion electrodynamics”.

2. Without it, we obtain a bosonized representation of a 2D Fermi surface.

Sketch:

As in the FQHE, the bulk topological field theory is not gauge invariant on a manifold with boundary.

It forces boundary degrees of freedom and a topological zero-energy kinetic term.

For BF theory in 3D, the boundary degrees of freedom are a scalar and vector boson, coupled in a first-order Lagrangian. (Hansson-Oganesyan-Sondhi)

These are exactly the degrees of freedom required to represent canonically a single Dirac fermion with time-reversal symmetry (Cho-Moore).

The velocity and filling of the Dirac fermion are set by nonuniversal surface physics, as in the FQHE case.

# Facts about 3D BF

1. With the T-breaking perturbation, we obtain “axion electrodynamics”.
2. Without it, we obtain a bosonized representation of a 2D Fermi surface.
3. We can reproduce the flow of charge through flux tubes (“wormhole effect”, Rosenberg, Guo, Franz, PRB 2010).

We can modify the bulk coefficient of BF theory and obtain fractional braiding statistics of point-like and line-like objects. This seems to be different from the existing “parton” constructions of 3D fractional topological insulators.

A challenge in connecting to experimental reality: at the 1D edge of the FQHE, needed not just the chiral boson but “vertex operators”

$$e^{i\alpha\phi}$$

A microscopic derivation of our bulk BF Lagrangian, and a generalization to other symmetry classes, has recently been given by Chan, Ryu, Hughes, and Fradkin.

# Topological field theory of TIs

When the edge is gapped, the magnetoelectric effect results. We can view the surface T-breaking coupling as arising from a bulk polarization tensor (in addition to normal current piece)

$$L_{\text{surf}} = \frac{1}{8\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu a_\nu \partial_\lambda A_\rho = \frac{1}{2} P^{\mu\nu} \partial_\mu A_\nu = \frac{1}{2} (\vec{P} \cdot \vec{E} + \vec{M} \cdot \vec{B})$$

What does it mean to “bosonize the surface state”? We can canonically represent a Dirac fermion using the emergent surface fields (first-order scalar and vector bosons):

$$\begin{aligned} \tilde{\psi}(y, \hat{n}) &= C \exp(i\sqrt{\pi} [\tilde{A}(y, \hat{n}) + \tilde{B}(y, \hat{n})]) \\ O_{\hat{n}} &= \exp\left(\frac{i\sqrt{\pi}}{2} \int_0^\theta d\theta' [\alpha(\hat{n}(\theta')) + \beta(\hat{n}(\theta'))]\right) \\ \alpha(\hat{n}) &= \int_{-\infty}^{\infty} \partial_0 \tilde{A}(y, \hat{n}) \\ \beta(\hat{n}) &= \int_{-\infty}^{\infty} \partial_0 \tilde{B}(y, \hat{n}). \end{aligned}$$

A difference from the FQHE case: there the surface details set the velocity, but the chemical potential is essentially irrelevant; here the surface still determines the velocity and chemical potential, and *both* matter for the low-energy theory.

# Last topic:

From topological insulators to  
3D “semi-topological semi-metals” (Dirac and Weyl)

Motivation:

Allowing the possibility of crystalline symmetries greatly increases the variety of possible topological band structures (both metals and insulators).

Some of these have been found recently:  
topological crystalline insulators (proposed by L. Fu)

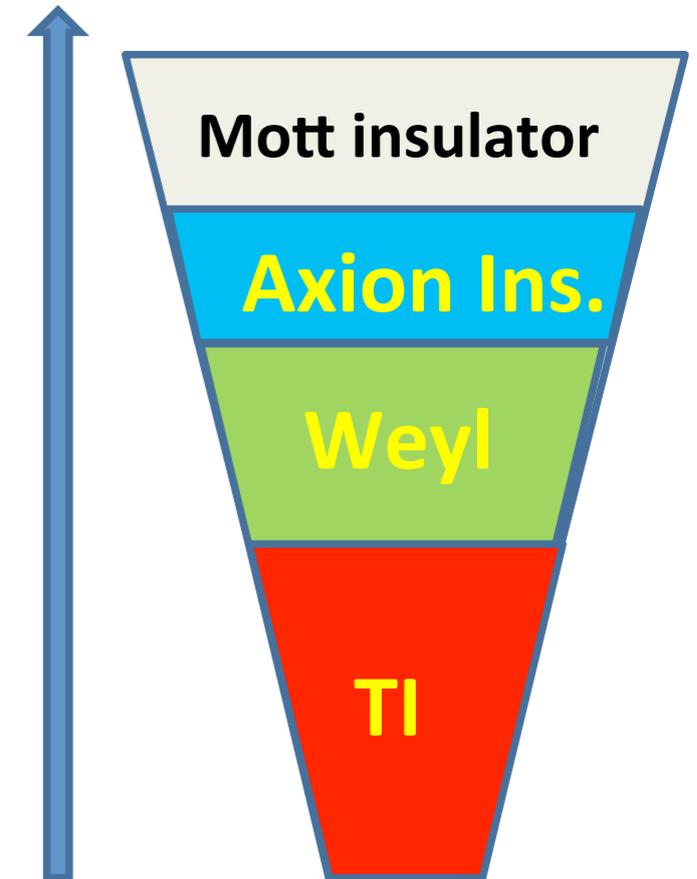
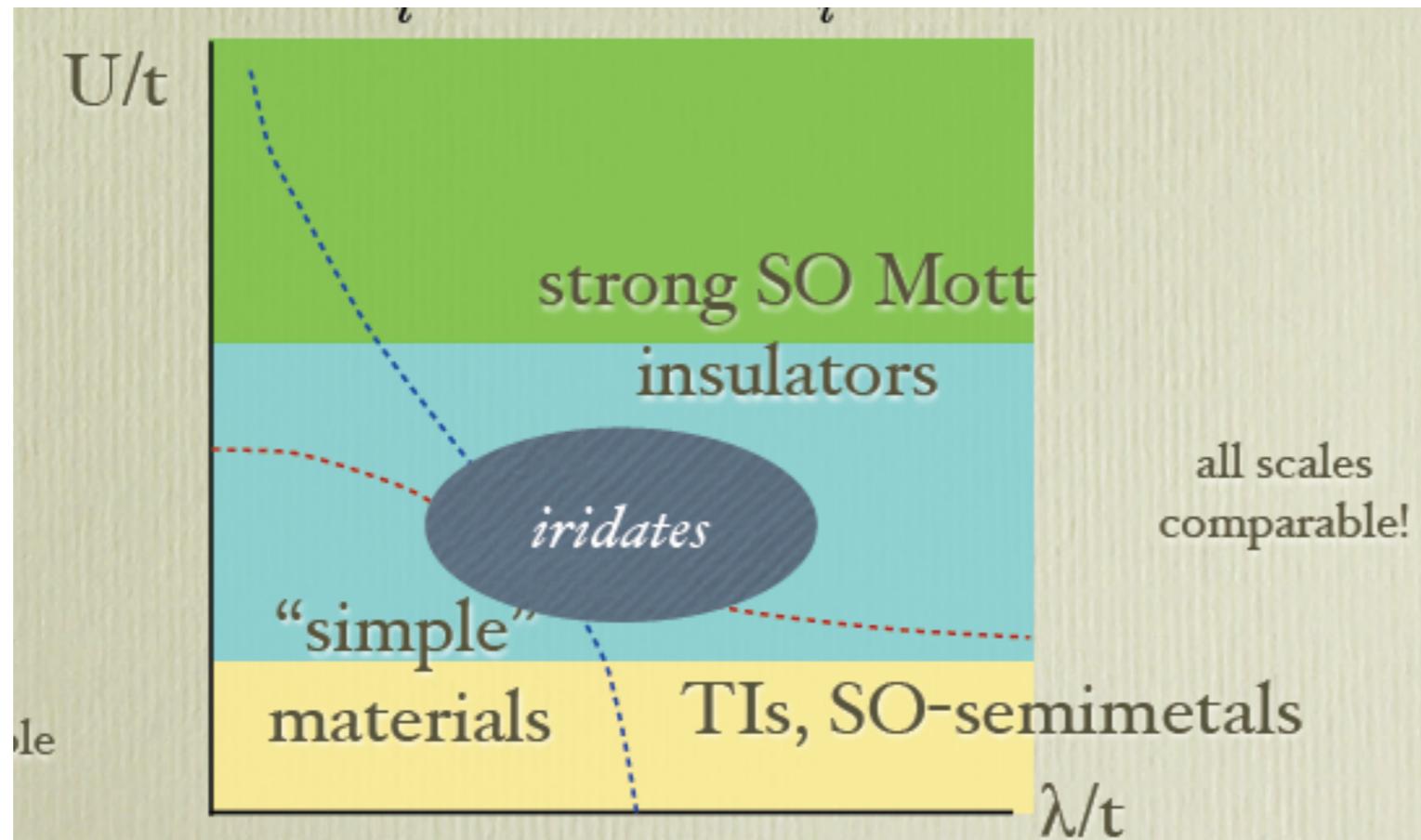
3D Dirac semimetals

(3 experimental papers; see CM Journal Club commentary, JEM)

# Novel states predicted with tuning of correlations

Iridates are weak Mott insulators  
(intermediate coupling)

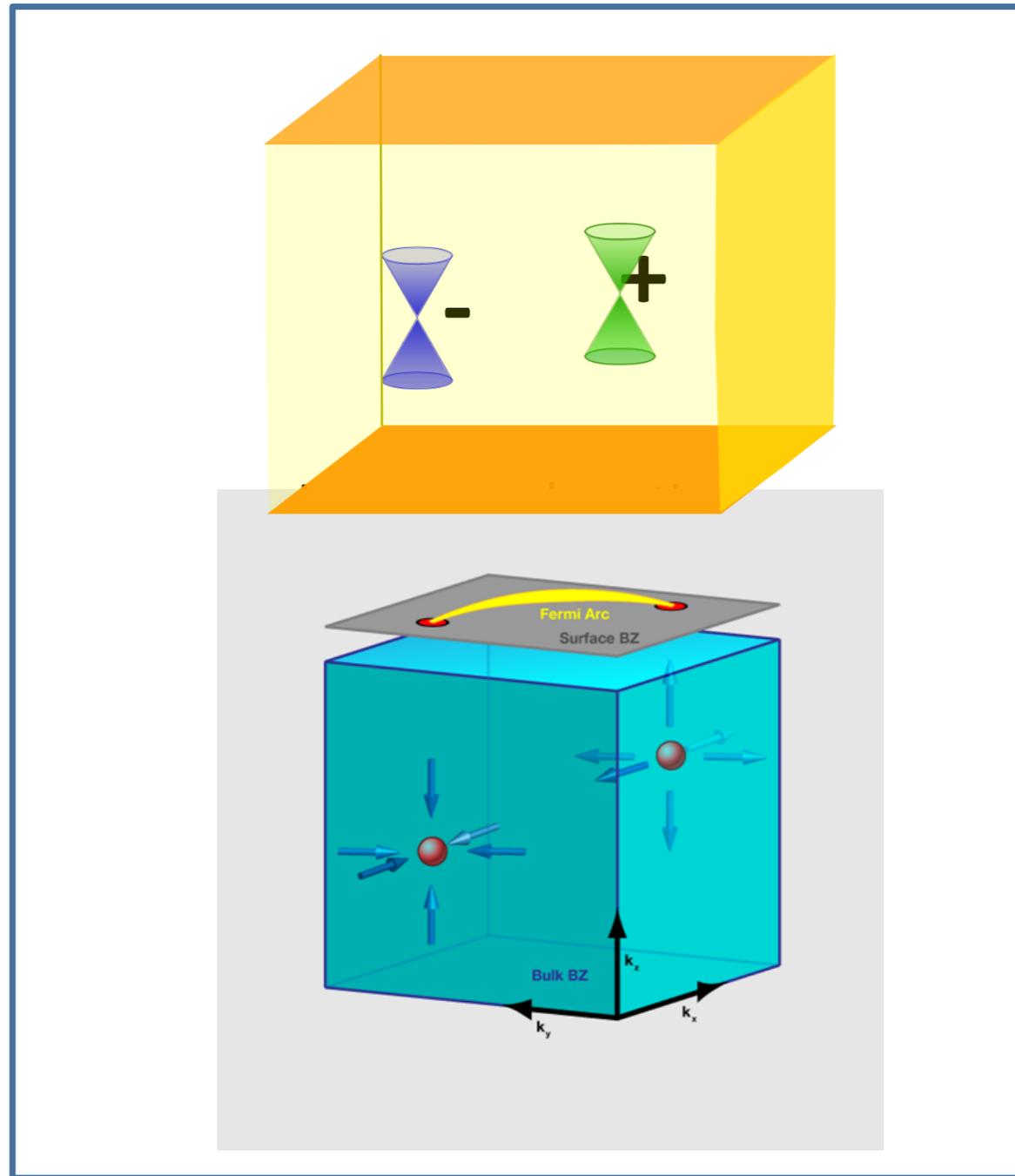
Increasing correlation



Correlations can be tuned by a variety of methods, such as chemical substitution and lattice strain due to substrate mismatch.

Slide from LBNL Quantum Materials Program

# Theoretical predictions: new phases of topological matter



## Scientific Achievement

- Prediction of Weyl semimetal, a 3D version of graphene, and possible realization in pyrochlore iridates.
- Arises in materials with strong-spin orbit coupling that break either time-reversal or inversion symmetry. The Dirac node is topologically protected.

## Significance

Leads to exotic 'Fermi arc' surface states. A Topological phase beyond topological insulators.

## Publications

X. Wan, A. M. Turner, Ashvin Vishwanath, and S. Y. Savrasov, Phys. Rev. B **83**, 205101 (2011).

X. Wan, , Ashvin Vishwanath and S. Y. Savrasov, Phys. Rev. Lett. 108 (2012).

P. Hosur, S. Parameswaran , Ashvin Vishwanath, Phys. Rev. Lett. 108 046602 (2012).

# Semi-topological semi-metals in 3D created by magnetic backgrounds

Graphene (2D) has a 2-band Dirac point (1947)

$$H = k_x \sigma_x + k_y \sigma_y$$

Stabilized by symmetries of honeycomb lattice.  
Unstable to adding 3rd Pauli matrix (opens gap).

Two versions in 3D: 2-band Weyl point (Herring, 1937)

$$H = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z.$$

Requires breaking of time-reversal or inversion symmetry

If not, combination of 2 Weyl points = 4-band Dirac point,  
which can be stabilized by crystalline symmetries.

Just seen via ARPES in  $\text{Cd}_3\text{As}_2$  (Princeton),  $\text{Na}_3\text{Bi}$  (Oxford).

# 3D Weyl and Dirac semimetals

1. The 3D Weyl semimetal is quite stable as long as crystal momentum is well-defined (there is a topological “Chern number” around the Weyl point).
2. It might appear in pyrochlore iridates (DFT+U says so).
3. It has an unusual “Fermi arc” surface state connecting the Weyl points.

Problem: We don't know whether the actual magnetic background in experiment is the right one for this phase, or even whether there is a single background or a spin-ice-like fluctuating one.

DFT+U is a useful technique, especially if some information about the magnetic structure is provided by experiment.

# Yet another spin liquid in iridates

A solvable *non-Abelian* spin liquid Hamiltonian written down by Kitaev on the honeycomb lattice, with strong spin-orbital coupling,

$$H = \sum_{\langle ij \rangle \parallel \mathbf{v}_1} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle \parallel \mathbf{v}_2} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle \parallel \mathbf{v}_3} \sigma_i^z \sigma_j^z.$$

may actually appear as the effective Hamiltonian of *honeycomb* iridates (Jackeli and Khaliullin, PRL 08).

Sodium iridate experiment: maybe not (S.K. Choi et al., 2012):

We report inelastic neutron scattering measurements on  $\text{Na}_2\text{IrO}_3$ , a candidate for the Kitaev spin model on the honeycomb lattice. We observe spin-wave excitations below 5 meV with a dispersion that can be accounted for by including substantial further-neighbor exchanges that stabilize zig-zag magnetic order. The onset of long-range magnetic order below  $T_N = 15.3$  K is confirmed via the observation of oscillations in zero-field muon-spin rotation experiments. Combining single-crystal diffraction and density functional calculations we propose a revised crystal structure model with significant departures from the ideal  $90^\circ$  Ir-O-Ir bonds required for dominant Kitaev exchange.

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