Magnetoelectric polarizability and axion electrodynamics in crystalline insulators

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References:
Andrew Essin (UCB), JEM, David Vanderbilt (Rutgers), arxiv:0810.2998
JEM, Ying Ran(UCB), Xiao-Gang Wen (MIT), arxiv:0804.4527, PRL to appear

1. abbreviated introduction
2. "prehistory" of 3D topological insulators
3. axion electrodynamics in a general crystalline insulators

Motivation for spin Hall effect and topological insulators:

Physics allows at least two ways to drive charge currents without dissipation:

Superconductivity:

$$J = \frac{n(e^*)^2 \mathbf{A}}{m} \quad \to \frac{e}{h} \quad \text{(Josephson constant)}$$

Quantum Hall effect:

$$J_x = \frac{\nu e^2}{h} E_y \quad \to \frac{e^2}{h}$$

Note: QHE (and SQHE) is dissipationless; it is the process of going from 3D to 1D that introduces the contact resistance

$$R = \left(\frac{2e^2}{h}\right)^{-1} = 13\ k\Omega$$

Are there similar phases that are related to spin?

IQHE Background:

1. A system of noninteracting lattice fermions with broken time-reversal symmetry (***T***) can show the integer quantum Hall effect (Haldane model, PRL 1988).

2. The IQHE is characterized by a topological invariant ("Chern number") and is stable to interactions and disorder.

Basic idea:

2D and 3D systems of noninteracting Bloch fermions with unbroken ***T*** have "topological insulator" phases. In 2D, these can show a spin Hall effect carried by edge states.

The topological insulator phase is stable to *nonmagnetic* disorder, and to sufficently weak interactions.

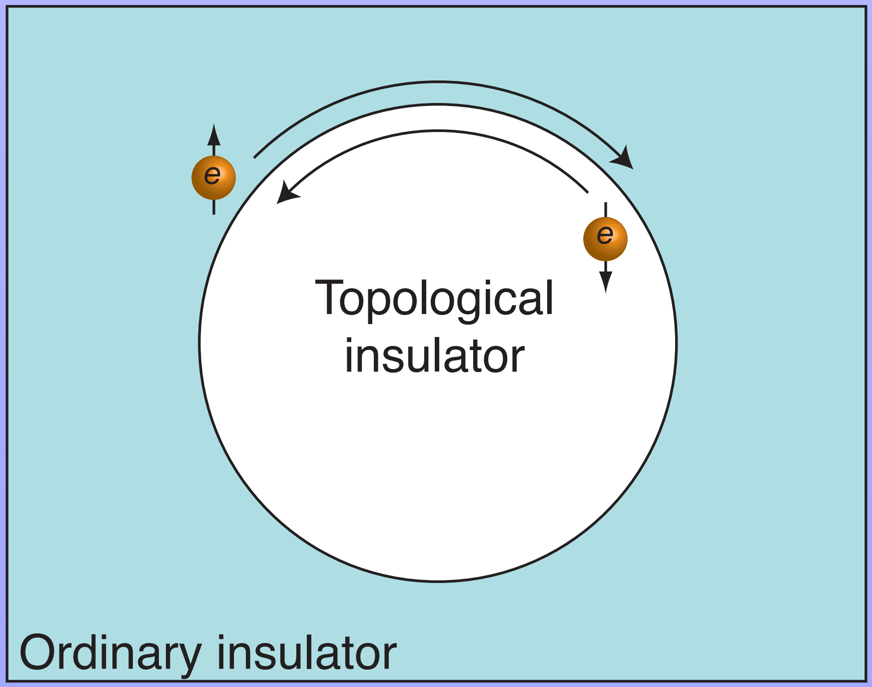
The quantum spin Hall effect

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



from JEM, Nature Physics N&V, 2008

Motivation beyond the SQHE

It turns out that in realistic models with an odd number of Kramers pairs of edge states, there is a stable phase. There are

exactly two phases of T-invariant band insulators (Kane and Mele, 2005; Bernevig, Haldane, Murakami, Nagaosa, Zhang, ...)

the "ordinary" insulator, which has an *even* number of Kramers pairs of edge modes (possibly zero)

and the "topological" insulator, which has an *odd* number of Kramers pairs of edge modes (requires SO coupling and broken inversion symmetry)

In 3D there are 16 classes of insulators, but only 2 are stable to disorder: ordinary and "strong topological"

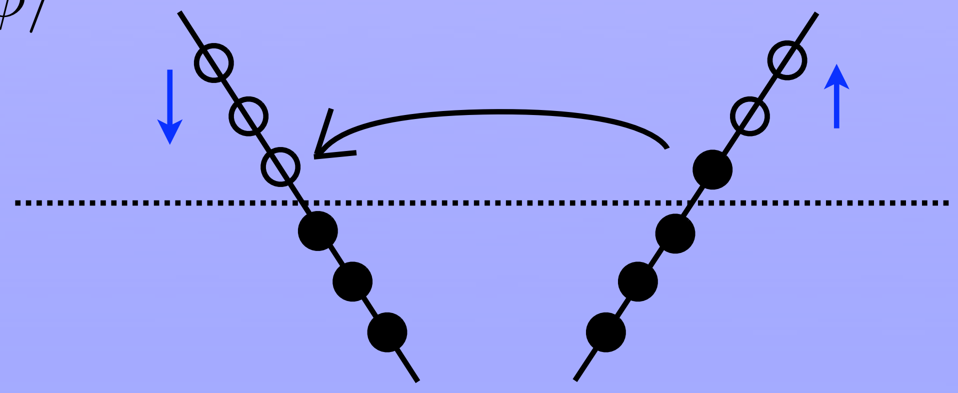
Some intuition for stability of edge state

The edge of the zero-Rashba model has a spin up mode moving clockwise and a spin-down mode moving counterclockwise.

There is an enhanced stability to backscattering when there is a *single pair* of time-reversed edge modes, i.e., one right-mover and one left-mover: a spin-half particle cannot scatter within a time-reversed pair (a "Kramers pair")

if the Hamiltonian is *time-reversal invariant.*

$$\langle\psi|H'|\phi\rangle = \langle T\phi|H'|T\psi\rangle = \langle\psi|H'|T^2\phi\rangle = -\langle\psi|H'|\phi\rangle$$



(Xu and JEM, PRB 2006;
Wu, Bernevig, and Zhang, PRL 2006)
Note that this absence of mixing is required to preserve Kramers degeneracies.

How can we tell, just from the band structure of a 2D or 3D material, whether that material will have this edge state?

Topological states of lattice fermions

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 and vanishes with *T* invariance. The integrand is the "Berry flux" *F*, where

$$A = -i \langle u | \nabla_k | u \rangle \qquad F = (\nabla_k \times \mathbf{A})_z$$

What about T-invariant systems?

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

Instead, a fairly technical analysis shows

1. each pair of spin-orbit-coupled bands in 2D has a Z2 invariant (is either "even" or "odd"), essentially as an integral over half the Brillouin zone;

2. the state is given by the overall Z2 sum of occupied bands:
if the sum is odd, then the system is in the "topological insulator" phase

The fundamental object in T-invariant systems is a Kramers-degenerate pair of bands, and "half" the Brillouin zone is sufficient to characterize the system....

Z2 topological invariants (results)

Each Kramers band pair of a time-reversal-invariant insulator has a Z2 invariant ("odd" or "even") analogous to the integer Chern number, even when no additional quantities are conserved.

Consider a 2D Brillouin torus.

In terms of the Berry field A and flux F, the topological invariant is (Fu and Kane, '07)

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

Where does this come from? *A* and *F* generalize the single-band formulas

$$A = -i\langle\psi(k)|\nabla_k\psi(k)\rangle \qquad F = (\nabla_k \times \mathbf{A})_z$$

A is a "Berry connection in momentum space".
Ordinary Chern number is integral of *F* over entire Brillouin zone.

What about higher dimensions?

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:

Cxy (for *xy* planes in the 3D Brillouin torus), *Cyz*, *Cxz*

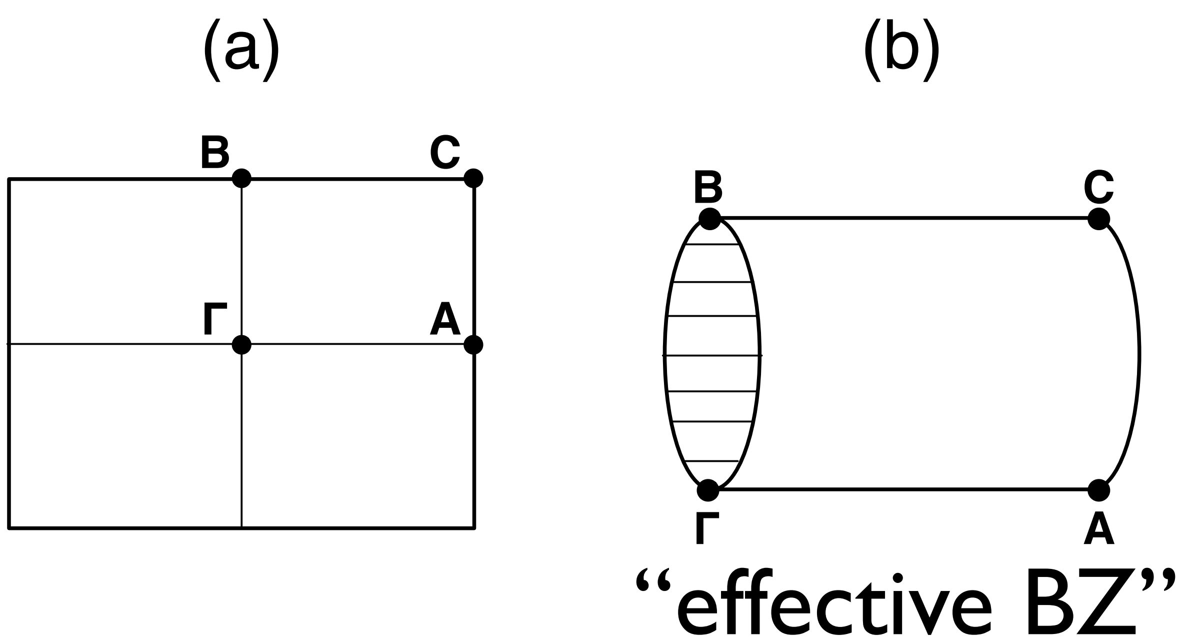
However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

General description of invariant from JEM and L. Balents, PRB RC 2007.
The connection to physical consequences in inversion-symmetric case: Fu, Kane, Mele, PRL 2007. See also R. Roy, arXiv.

Build 3D from 2D

Note that only at special momenta like k=0 is the "Bloch Hamiltonian" time-reversal invariant: rather, k and -k have T-conjugate Hamiltonians. Imagine a square BZ:

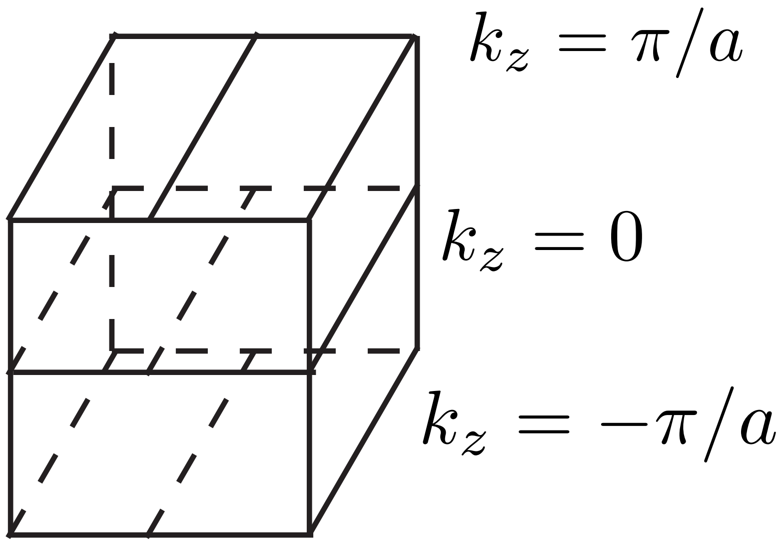
$$H(-k) = TH(k)T^{-1}$$



In 3D, we can take the BZ to be a cube (with periodic boundary conditions):

think about xy planes

2 inequivalent planes look like 2D problem



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

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

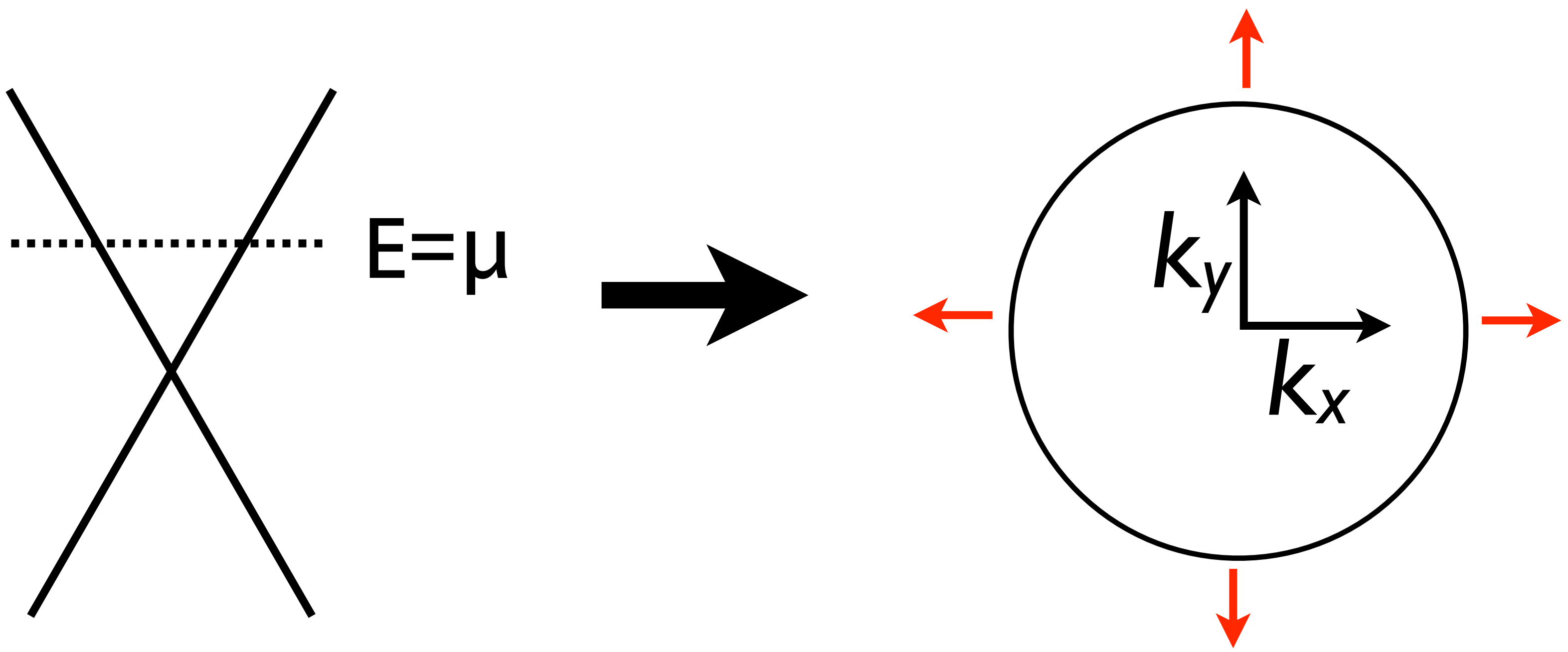
Physical consequences: "boundary chiral fermions"

The topological invariant predicts a gapless surface state. In the 1D edge, this was "half" of an ordinary quantum wire. In the 2D surface of the topological insulator, it seems:

1. The one-surface (2D) Fermi surface encloses an *odd* number of Dirac points (say 1);

2. The Fermi surface has only one spin state at each k;

3. The Berry's phase in going around the Fermi surface is π (Haldane).

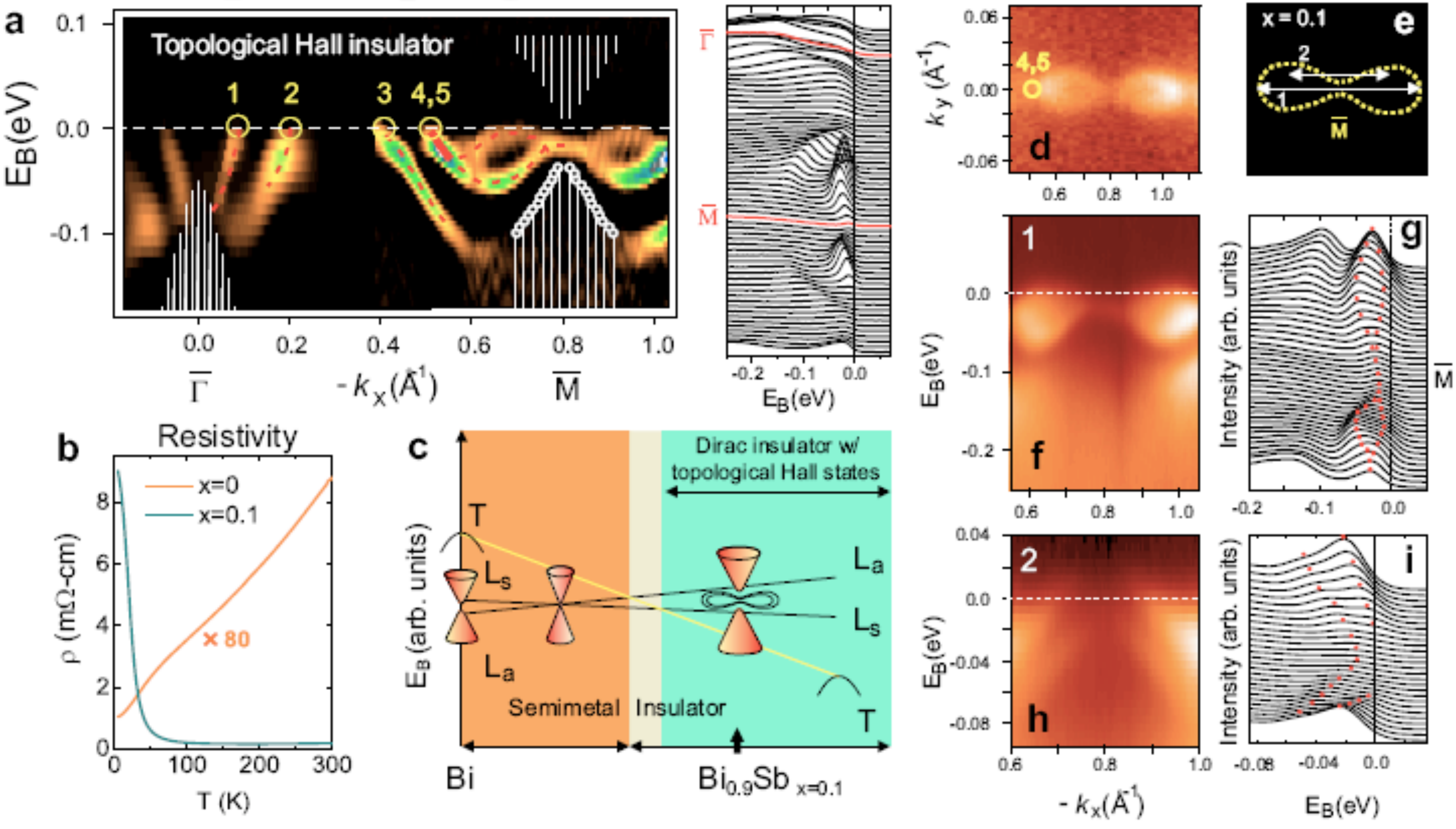


Note that T is still unbroken, but there is a single spin state (the # of degrees of freedom is like a spinless Fermi surface).

Topological Insulator with surface Hall modes

D. Hsieh, M.Z. Hasan et.al., Princeton University (*Nature*, 2008)

STI: $Z_2 = -1$ topological surface modes



Prehistory of topological insulators in 3D: Part I

For any 3D insulator, consider the possibility of an induced coupling between electric and magnetic fields:

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

("axion electrodynamics": Wilczek, PRL 1987)

The angle θ turns out to be periodic with period 2π. The values θ=0 *and* θ=π are consistent with time-reversal invariance. The boundary between the two supports massless Dirac fermions.
(Volkov and Pankratov, 1985;
Fradkin, Dagotto, and Boyanovsky, 1986)

Axion electrodynamics involves the second Chern invariant (the 4D Chern form) of the *electromagnetic fields*, a U(1) bundle in 3+1 dimensions. How to compute this in solids?

Prehistory of topological insulators in 3D:

Physical consequences (Wilczek,1987) of the total derivative term

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

1. In a T-invariant system, 2D boundaries between regions of different θ (0 and π) are gapless.

2. A small T-breaking perturbation at the edge, or a material with T-breaking in bulk, leads to a quantum Hall layer at a boundary with conductance

$$\sigma_{xy} = \frac{\Delta\theta}{2\pi}e^2/h$$

(The metallic behavior = an ambiguity in how to go from 0 to π.)

3. These surface currents mean that an electric field induces a magnetic dipole, or a magnetic field induces an electric dipole.

4. "Witten effect": magnetic monopoles pick up electrical charge & vv.

Prehistory of topological insulators in 3D:

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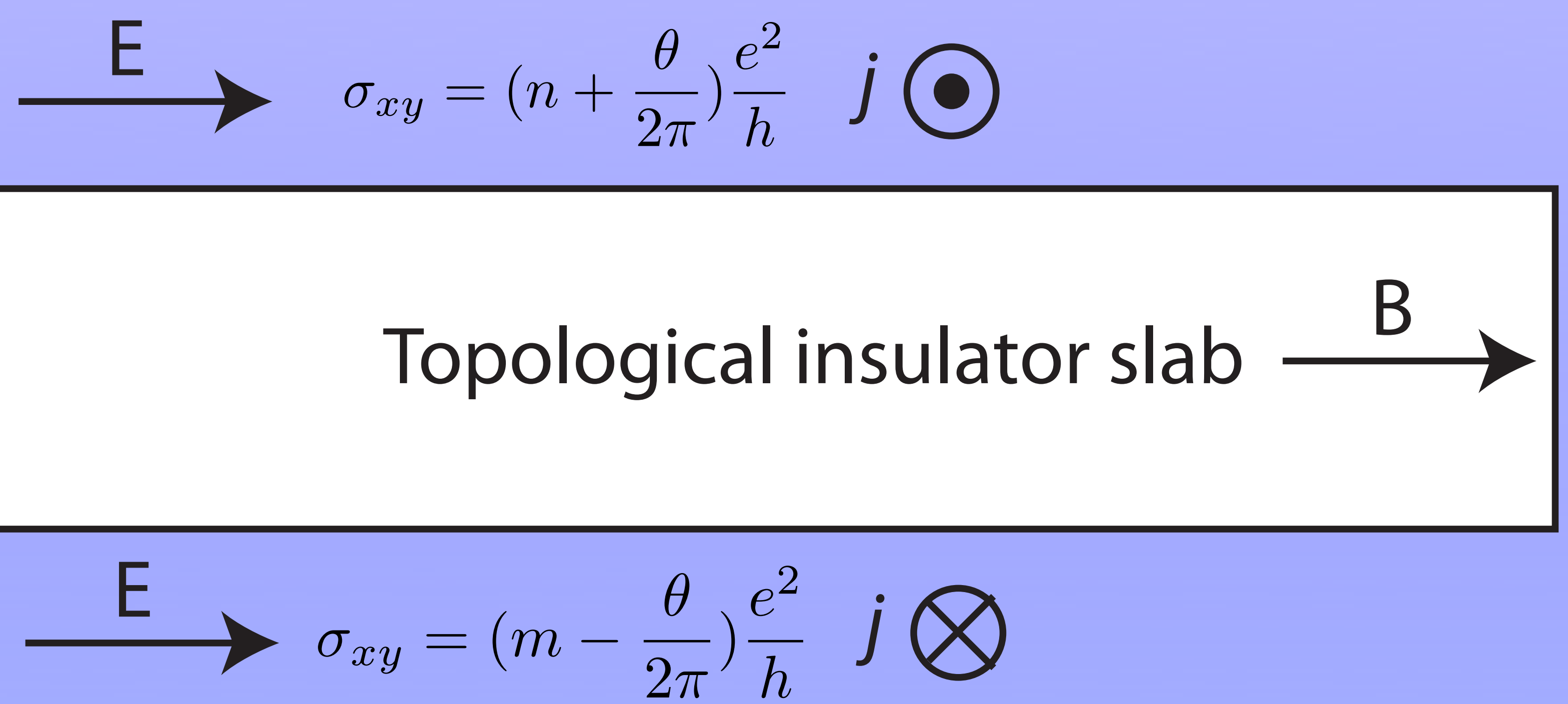


Connection between θ=π and 3D topological insulator:

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

A boundary at which θ changes shows a surface quantum Hall effect of magnitude $\sigma_{xy} = (\Delta\theta) e^2 / 2\pi h$

How is this consistent with what we said before?

We said before that the topological insulator has a metallic surface state with an odd number of Dirac fermions.

Under an infinitesimal T-breaking perturbation (e.g., a weak magnetic field), this becomes a half-integer quantum Hall effect.

Hence a boundary between θ=π and θ=0 is consistent with the "axion electrodynamics" picture, as long as some infinitesimal perturbation is present to eliminate the metallic surface.

Prehistory of topological insulators in 3D: Part II

Avron, Sadun, Seiler, Simon, 1988:
The set of "quaternionic Hermitian" matrices (i.e., Hamiltonians that can describe T-invariant Fermi systems) without accidental degeneracies has a nontrivial *fourth* homotopy group:

$$\pi_4(M_n(\mathcal{H})) = \mathbb{Z}^{n-1}$$

Here *n* is the quaternionic dimension (twice the complex dimension), and *n-1* appears because of a zero sum rule.

This is a 4D version of the 2D IQHE homotopy,

$$\pi_2(C_n(\mathcal{H})) = \mathbb{Z}^{n-1}$$

The 4D invariant is the integral of the 4D Chern form of the nonabelian bundle. This corresponds in band structure to 4D systems with *PT* symmetry, but not *P* or *T* separately.
(*PT* symmetry forces every Bloch Hamiltonian H(k) to be T-invariant.)

General idea: this term describes the *orbital magnetic polarizability*, which is a bulk property in 3D in the same way as *polarization*. For crystals, this leads to a simple derivation.

In other words, given any 3D band insulator, we compute the coupling in

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

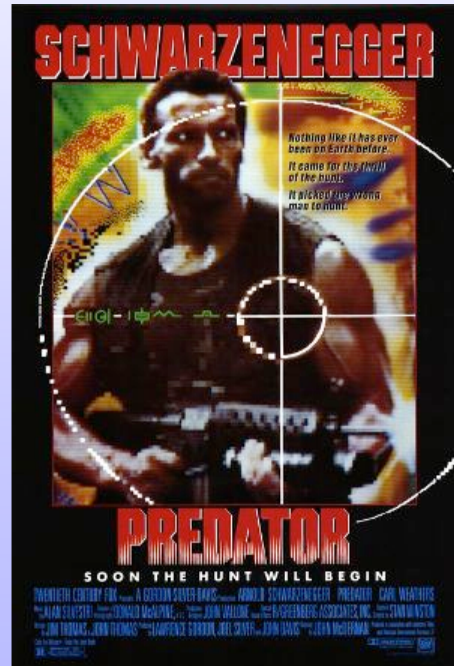
by the orbital magnetoelectric polarizability

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

from integrating the "Chern-Simons form" of Bloch states:

$$\theta = \frac{1}{2\pi}\int_{\mathrm{BZ}} d^3k\,\epsilon_{ijk}\,\mathrm{Tr}[A_i\partial_j A_k - i\frac{2}{3}A_iA_jA_k]$$

1987



2008

We already understand (since 2006) the odd-even effect of T-invariant fermions, and how to determine whether a given *T*-invariant band structure realizes the ordinary or topological insulator.

How can we make the connection directly between axion electrodynamics (the second Chern form of the EM field) and the Berry phases of a band structure?

Recent appearances of second Chern form of a band structure:

Xiao, Shi, Clougherty and Q. Niu, arxiv:0711.1855

Second Chern form arises in computing the polarization induced by a slowly varying crystal inhomogeneity

Qi, Hughes, and Zhang, arxiv:0802.3537

Second Chern form of EM field arises in 4D from integrating out fermions; derived expression for theta in 3D in terms of non-Abelian Chern-Simons form.

$$\theta = \frac{1}{2\pi} \int_{\mathrm{BZ}} d^3k \; \epsilon_{ijk} \, \mathrm{Tr}[A_i \partial_j A_k - i \frac{2}{3} A_i A_j A_k]$$

JEM, Ran, and Wen, arxiv:0804.4527 (more later)

Here we focus on crystalline insulators: sufficiently far from a boundary, there is a well-defined unit cell.

We introduce an explicit model to compute physical consequences of axion electrodynamics:

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \frac{4\lambda_{SO}}{a^2} \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \sigma \cdot (d_{ij}^1 \times d_{ij}^2) c_j + h \cdot \left(\sum_{i \in A} c_i^\dagger \sigma c_i - \sum_{i \in B} c_i^\dagger \sigma c_i \right).$$

The first terms are the Fu-Kane-Mele diamond lattice model of a 3D topological insulator. The last term is a staggered Zeeman field,

$$|h| = m \sin\beta, \quad \beta = 0 \text{ ordinary}, \beta = \pi \text{ topological}$$

The linearized Dirac mass is $m(\cos\beta + i \sin\beta\gamma^5)$

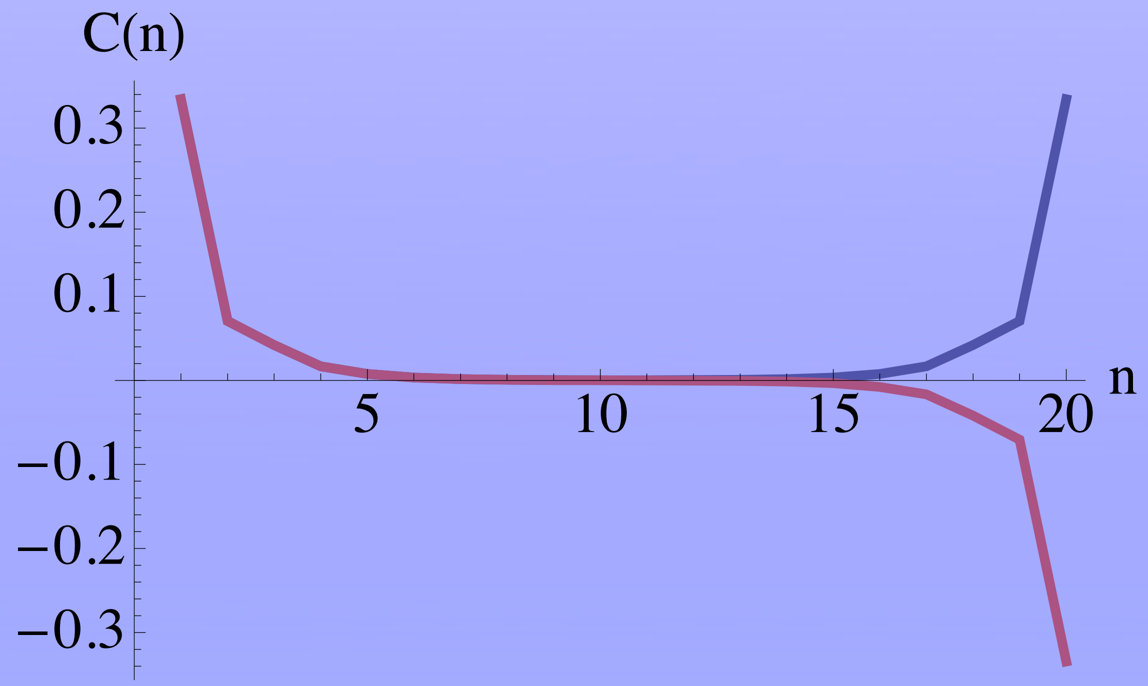
We first study this model in a slab geometry in order to see one of the "axion electrodynamics" signatures: applying *T*-breaking edge perturbations leads to half-IQHE surface layers.

To compute this we look at the Chern number,

$$C = \frac{1}{2\pi}\int d^2k \sum_{\nu} \mathcal{F}^{\nu\nu}_{xy} = \frac{i}{2\pi}\int d^2k \sum_{\nu} \epsilon_{ij}\partial_i u_\nu \partial_j u_\nu = \frac{i}{2\pi}\int d^2k \, \mathrm{Tr}\left[\mathcal{P}\epsilon_{ij}\partial_i\mathcal{P}\partial_j\mathcal{P}\right].$$

Can define layer-resolved Chern number using a real-space projection operator:

$$C(n) = \frac{i}{2\pi}\int d^2k \, \mathrm{Tr}\left[\mathcal{P}\epsilon_{ij}(\partial_i\mathcal{P})\tilde{\mathcal{P}}_n(\partial_j\mathcal{P})\right].$$



Computation for 20-layer slab in topological insulator phase
Changing boundary condition switches by an *integer* times e^2/h.

How can we understand why this surface Hall conductance is always a bulk property, for general theta?

Claim: Theta is nothing more or less than the bulk magnetoelectric polarizability, which can be computed in many ways:

This gives a quick derivation using the Xiao et al. formula for polarization in a smoothly inhomogeneous crystal:

Sketch: A weak magnetic field can be considered as inhomogeneity.

Choose a gauge with A along x and slowly increasing on y. The first semiclassical term in the polarization (Xiao et al.) corresponds to

$$\theta = \frac{1}{2\pi} \int_{\mathrm{BZ}} d^3k \, \epsilon_{ijk} \, \mathrm{Tr}[A_i \partial_j A_k - i\frac{2}{3} A_i A_j A_k]$$

(Can equally well derive by considering orbital *magnetization* response to an applied *electric* field.)

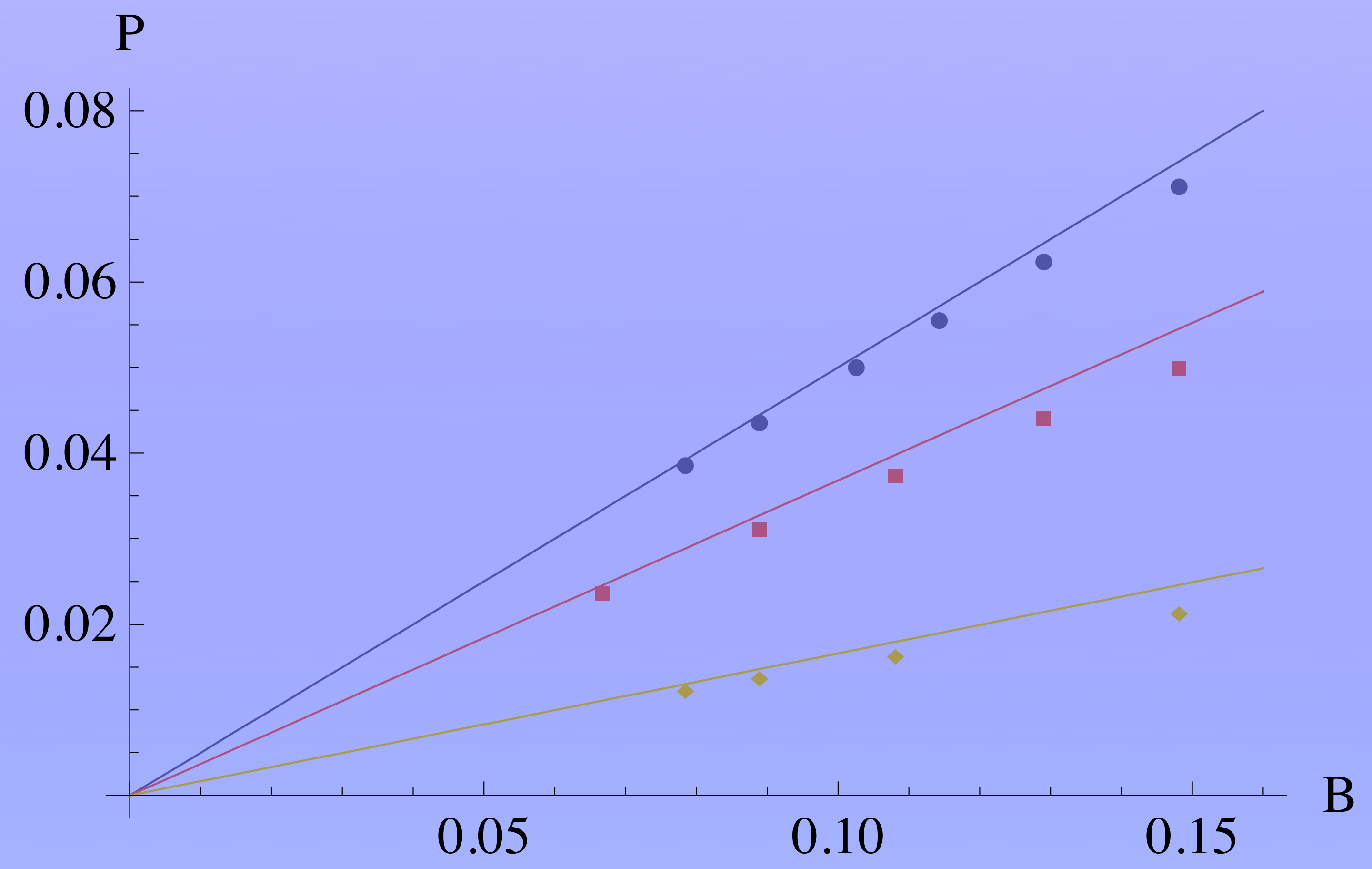
How can we confirm that this surface Hall conductance is always a bulk property, for general theta?

Claim: Theta is nothing more or less than the bulk magnetoelectric polarizability, which can be computed in many ways:

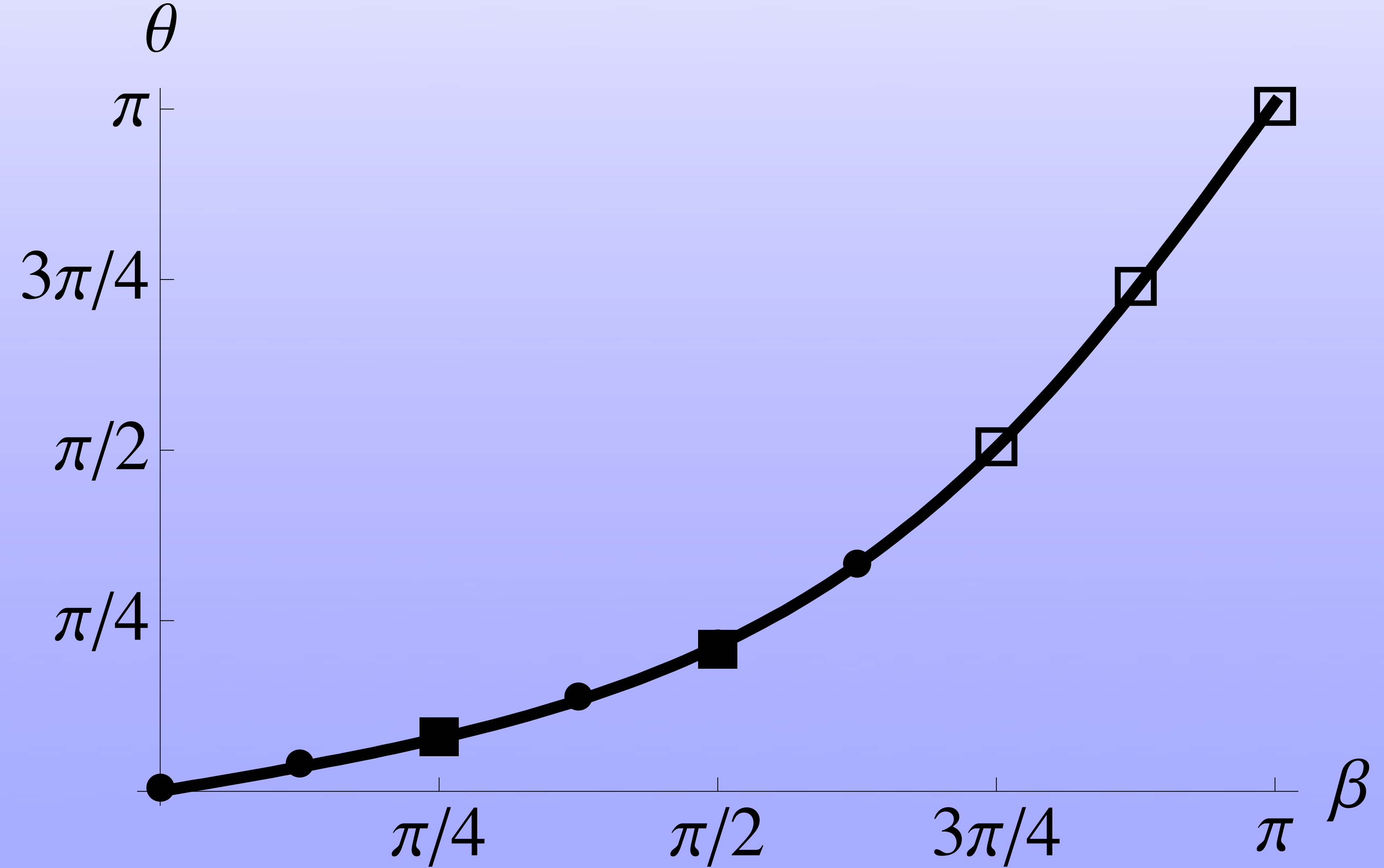
1. apply a flux through a supercell, and extrapolate to limit of small flux

2. compute Chern-Simons integral directly from a "smooth gauge"

Comparison:



Equivalence of four measures of theta:



The magnetoelectric polarizability θ (in units of $e^2/2\pi h$). The curve is obtained from the second Chern integral. The filled squares are computed by the Chern-Simons form. The open squares are the slopes of P *vs.* B. The remaining points are obtained from layer-resolved σ_{xy}.

We can make many analogies between the Berry phases that determine magnetoelectric polarizability, and the Berry-phase theory of polarization (King-Smith and Vanderbilt, '93)

	Polarization	Magnetoelectric polarizability
$d_{\min}$	1	3
Observable	$\mathbf{P} = \partial\langle H\rangle/\partial E$	$M_{ij} = \partial\langle H\rangle/\partial E_i \partial B_j$ $= \delta_{ij}\theta e^2/(2\pi h)$
Quantum	$\Delta\mathbf{P} = e\mathbf{R}/\Omega$	$\Delta M = e^2/h$
Surface	$q = (\mathbf{P}_1 - \mathbf{P}_2)\cdot\hat{\mathbf{n}}$	$\sigma_{xy} = (M_1 - M_2)$
EM coupling	$\mathbf{P}\cdot\mathbf{E}$	$M\mathbf{E}\cdot\mathbf{B}$
CS form	$\mathcal{A}_i$	$\epsilon_{ijk}(\mathcal{A}_i\mathcal{F}_{jk} + i\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k/3)$
Chern form	$\epsilon_{ij}\partial_i\mathcal{A}_j$	$\epsilon_{ijkl}\mathcal{F}_{ij}\mathcal{F}_{kl}$

A difference: magnetoelectric polarizability results from twisting of bands around each other (i.e., includes off-diagonal parts), unlike polarization

Mathematical properties of Chern-Simons band structure integral for theta

$$\theta = \frac{1}{2\pi} \int_{\mathrm{BZ}} d^3k \, \epsilon_{ijk} \, \mathrm{Tr}[A_i \partial_j A_k - i\frac{2}{3} A_i A_j A_k]$$

Not gauge-invariant: a "large" (non-null-homotopic) gauge transformation changes the magnetoelectric polarizability by

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

which corresponds to adding an integer quantum Hall layer, or the periodicity of theta (closely related to gauge-dependence of polarization in a crystal).

$\frac{e^2}{h}$ = contact resistance in 0D or 1D
= Hall conductance quantum in 2D
= magnetoelectric polarizability in 3D

"Band twisting" as origin of theta

Electric polarization is diagonal in band indices. The magnetoelectric polarizability is not, and off-diagonal terms can be significant.

Actually some "twisting" of occupied bands around each other is necessary. To see this, note that in a 2-band model with one occupied band, the Chern-Simons integral (now Abelian)

$$n = \frac{1}{4\pi^2} \int d^3k \, \epsilon_{ijk} F_{ij} A_k$$

computes a gauge-invariant integer; this is the Hopf invariant $\pi_3(S^2) = \mathbb{Z}$ (JEM, Ran, Wen),

because nondegenerate 2-band Hamiltonians are the sphere and maps from T3 with zero Chern are like maps from S3 (Pontryagin).

Hence any model that can be separated into occupied bands that do not mix in Hilbert space has zero theta.

Conclusions

1. There are experimentally observed 1D edge states that are predicted to have spin direction perfectly correlated with direction of motion. Can we test this and use this?

(2. The disorder physics of this system shows some interesting differences from the IQHE, including a metallic phase.)

3. Some 3D insulators show protected surface states. This phase is less like the IQHE, and the description of its surface states has more in common with graphene physics.

4. 3D insulators have an "orbital magnetoelectric polarizability" analogous to polarization in 1D. For T-invariant insulators there are only two possible values; general insulators are characterized by a magnetoelectric polarizability *angle*.

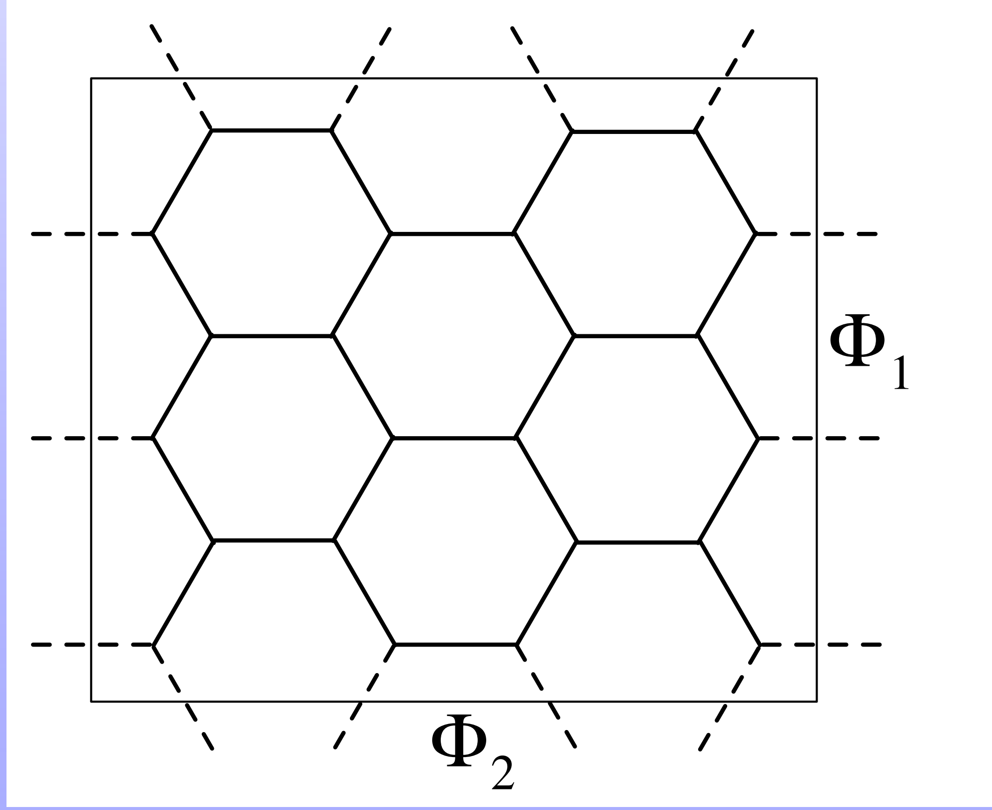
Surface optical conductivity can measure this in principle.

Defining the topological insulator 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.

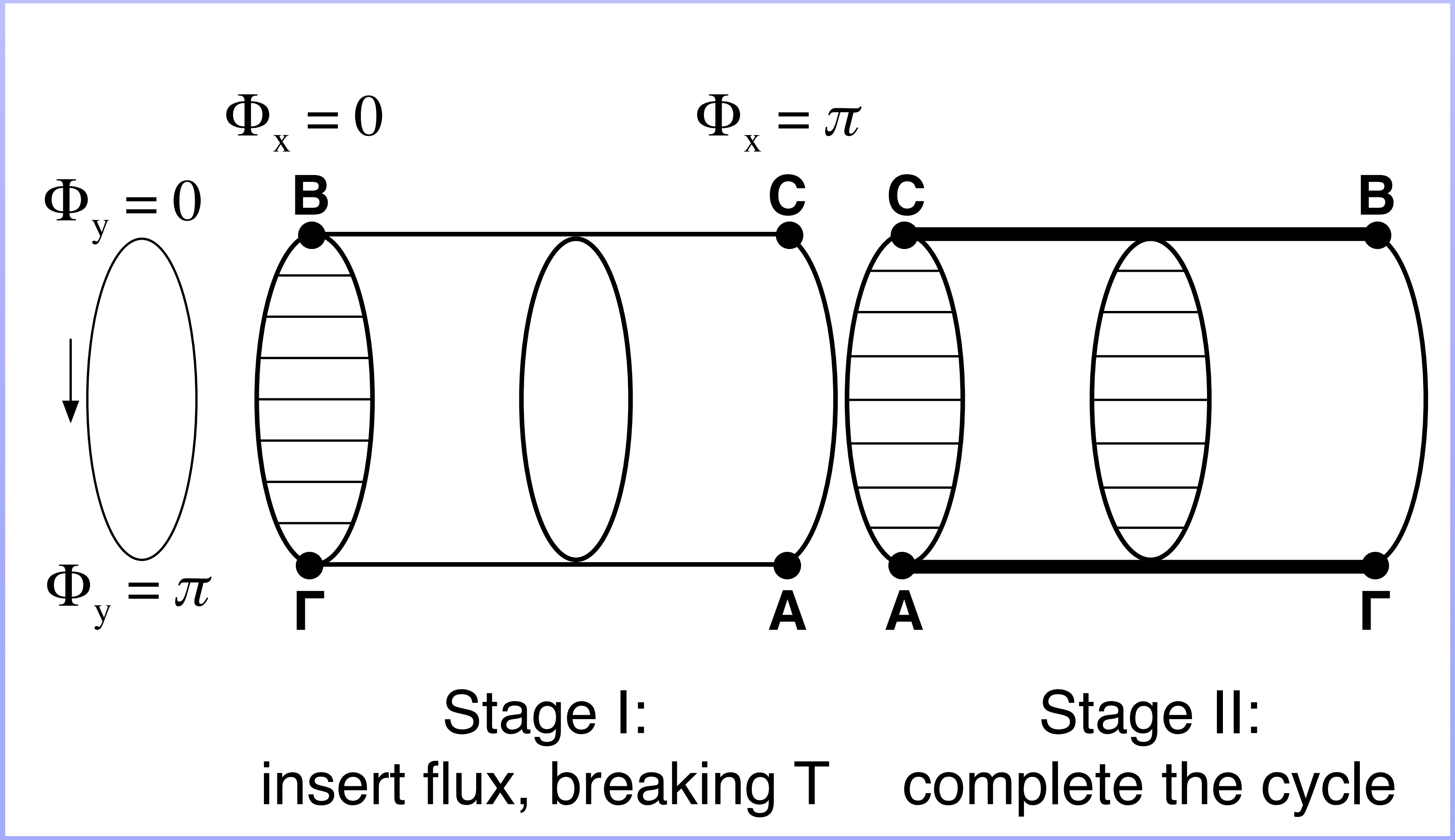
Effect of boundary phase is to shift *k*: alternate picture of topological invariant is in terms of half the (Φ_1, Φ_2) torus.



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

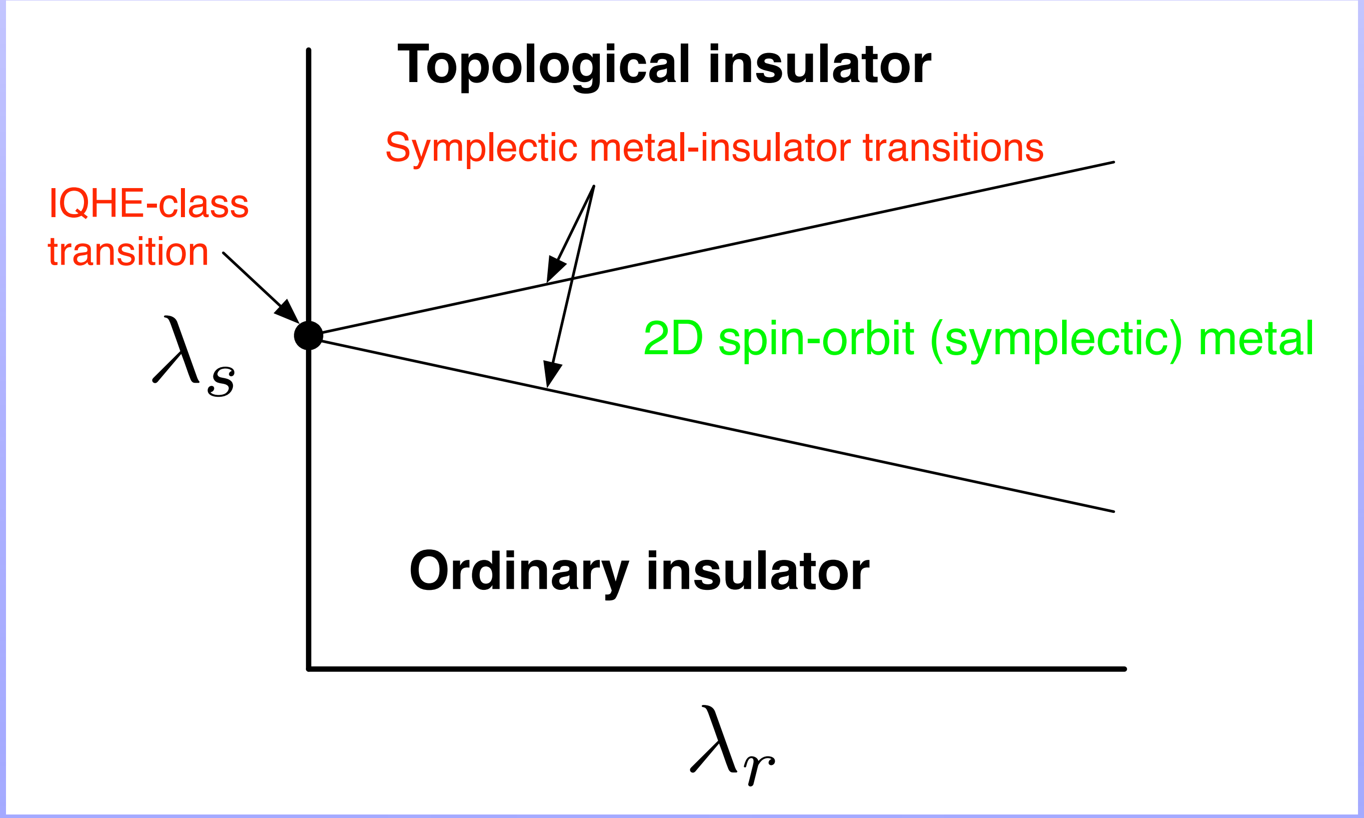
Pumping and interactions

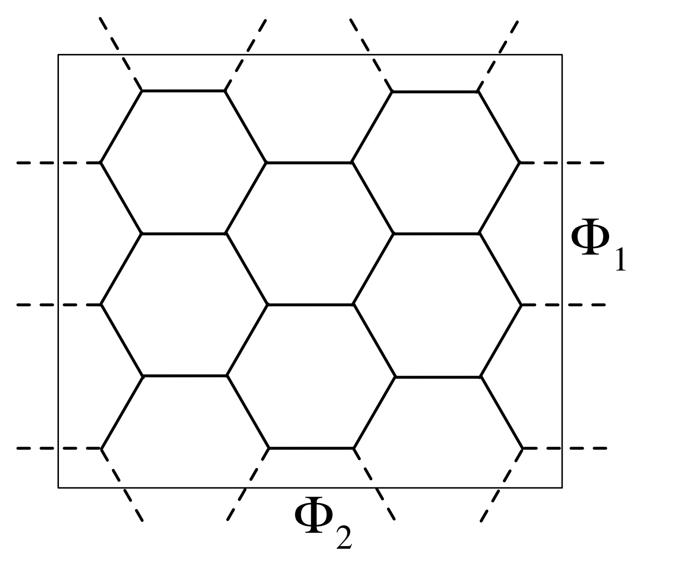
In addition to the supercell argument, we can give a physical definition of the topological insulator in a disordered system as follows: (mathematical content is the same)



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.