1. Magnetoelectric polarizability in 3D insulators and experiments!
2. Topological insulators with interactions
(3. Critical Majorana fermion chain at the QSH edge)

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References:
1, 2:
Andrew Essin (UCB), JEM, David Vanderbilt (Rutgers), arxiv:0810.2998
JEM, Ying Ran(UCB), Xiao-Gang Wen (MIT), PRL 2008.

3: Vasudha Shivamoggi and JEM, in preparation

"Axion electrodynamics" and magnetoelectric polarizability: outline

1. Z2 invariants in 2D and 3D materials with time-reversal invariance (intro)

2. Phenomenology of theta ("axion electrodynamics") in insulators (Wilczek, 1987)

3. Integer second Chern class invariants in 4D band structures (Avron et al., 1988)

4. Unified theory of theta term, including microscopics and connection to topological insulators (Qi, Hughes, Zhang, 2008)

5. Magnetoelectric polarizability and calculations for general 3D crystals/slabs; possible connection to existing experimental results (Essin, JEM, Vanderbilt)

Classification of T-invariant insulators

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 (4 Z2 invariants), but only 2 are stable to disorder: ordinary and "strong topological"

What about three 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*

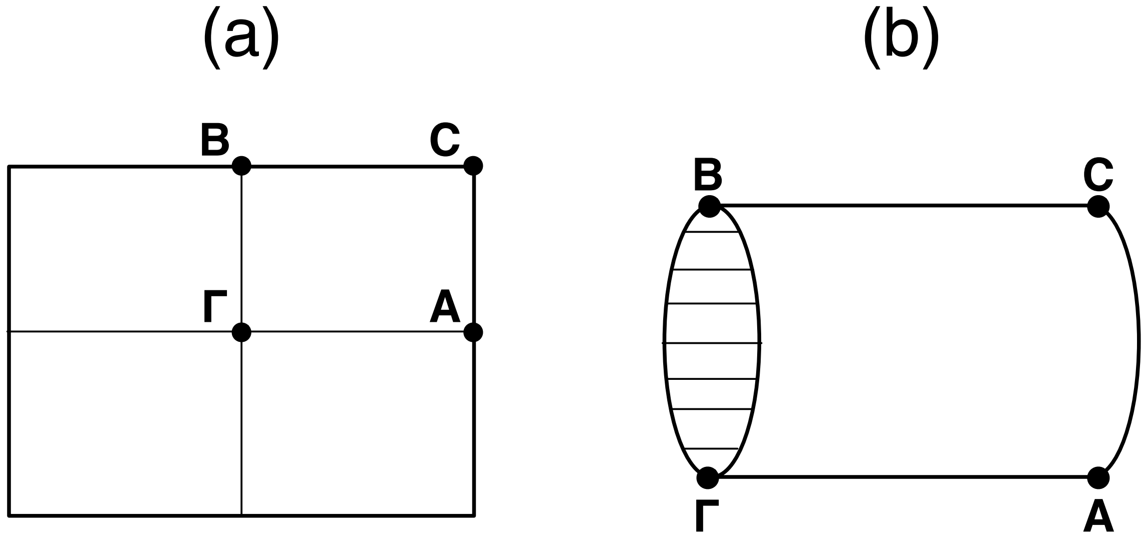
However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

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:

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

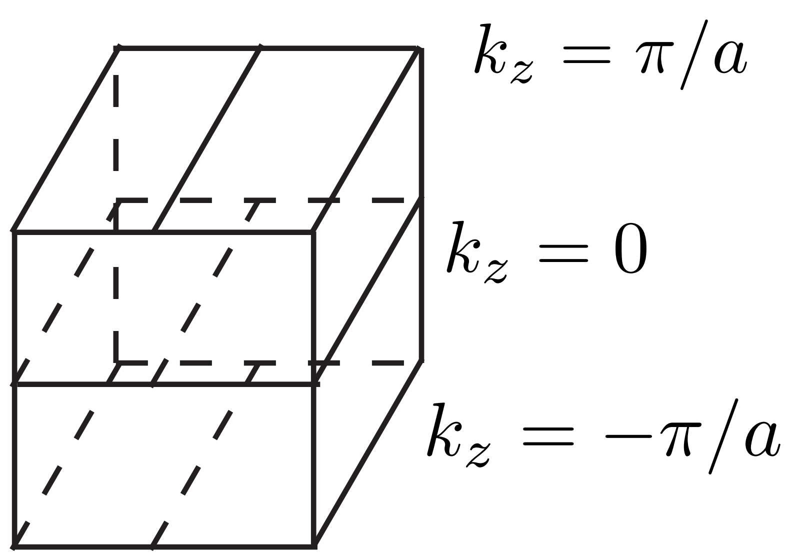


"effective BZ"

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



$$x_0 x_{\pm 1} = y_0 y_{\pm 1} = z_0 z_{\pm 1}$$

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.

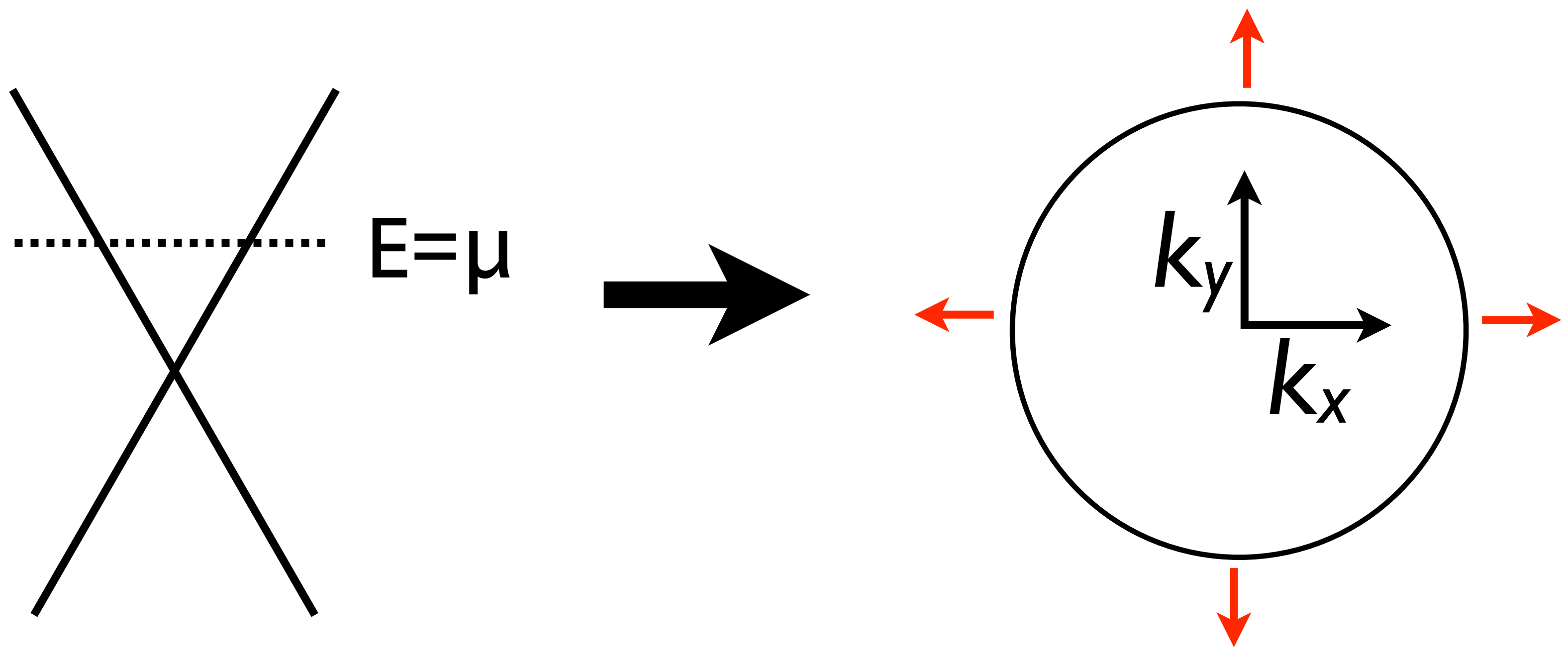
Physical consequences: "boundary chiral fermions"

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 definition).

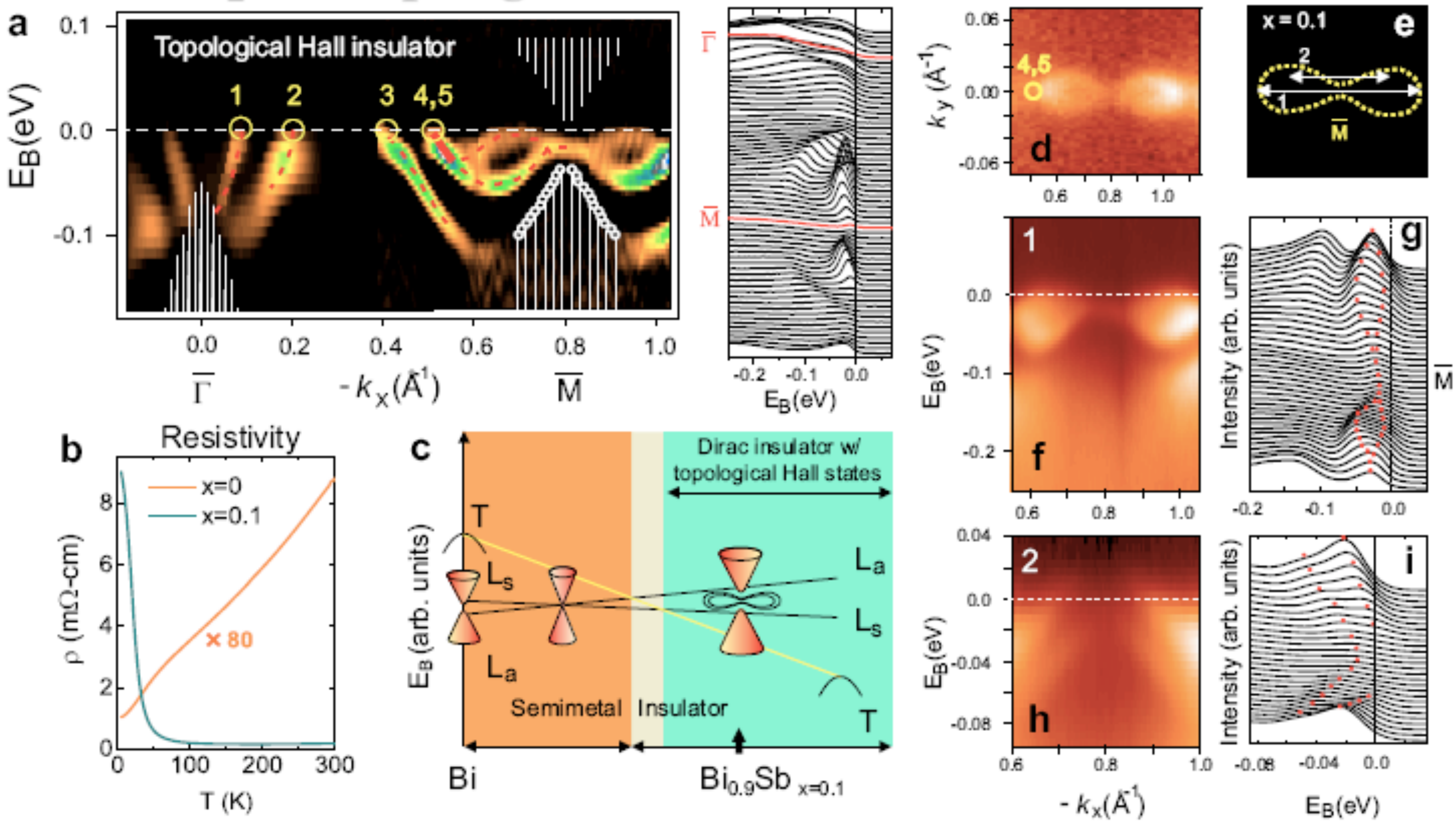


Note that T is still unbroken, but there is a single spin state (the # of degrees of freedom is like a spinless Fermi surface).

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; but "too many" fermions, i.e., an even number)

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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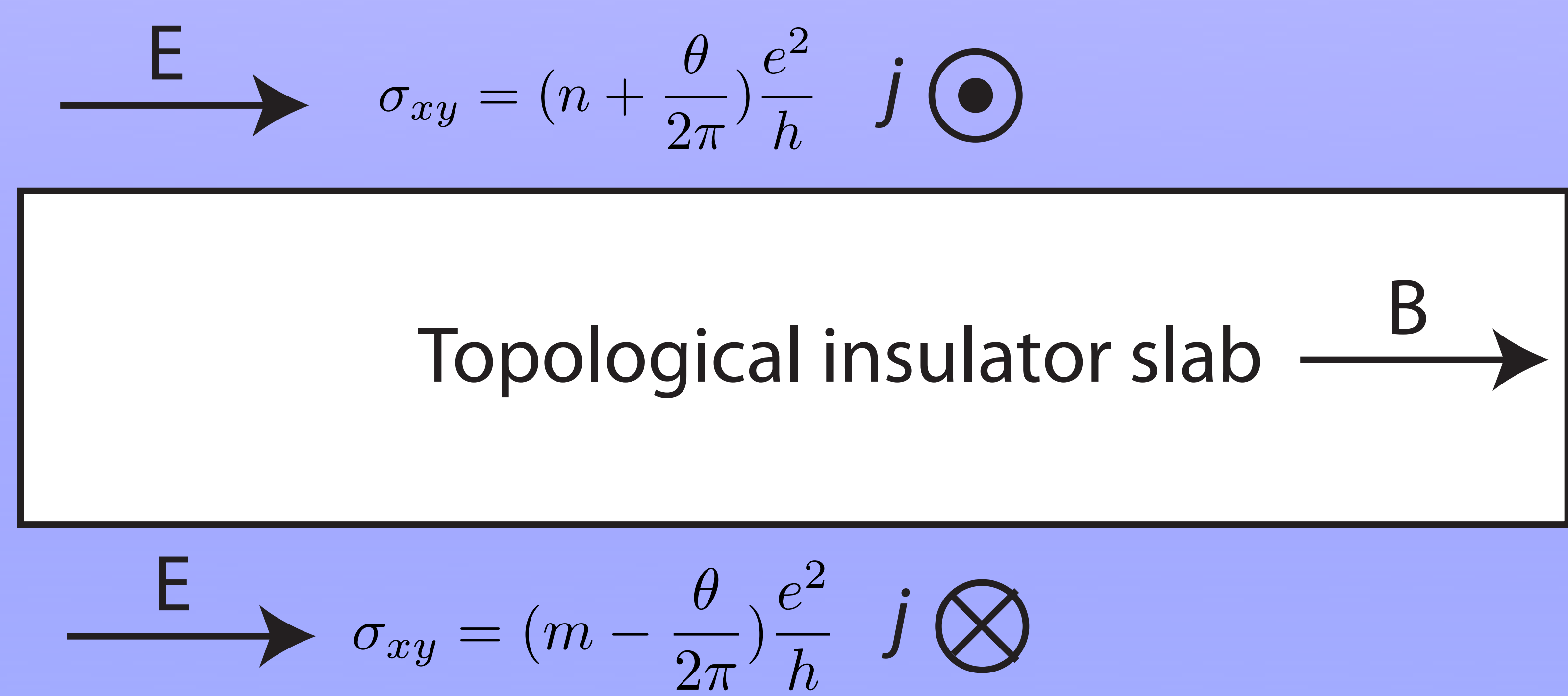


Connection between θ=π and 3D topological insulator:

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

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:

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

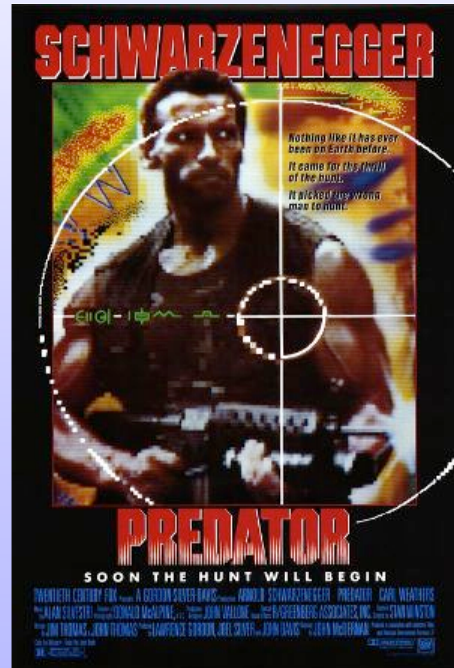
Here *n* is the quaternionic dimension (twice the complex dimension), and *n-1* appears because of a zero sum rule.

This is a 4D version of the 2D IQHE ("TKNN integer"),

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

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.)

1987



2008

We 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 was the connection made 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 noninteracting fermions; 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)
See also B. A. Bernevig and H.-D. Chen, arxiv.

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:

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

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.

This OMP is the same as the "magneto-electric polarization" defined by Qi et al.

The magnetoelectric polarizability, part of the polarizability tensor, has actually been measured experimentally and is always "topological" from the EM point of view:

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

Cr2O3: theta=pi/25, but mechanism is probably not orbital and doesn't involve surface QHE layers. arxiv:0708.2069

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 $m(\cos\beta + i \sin\beta \gamma^5)$

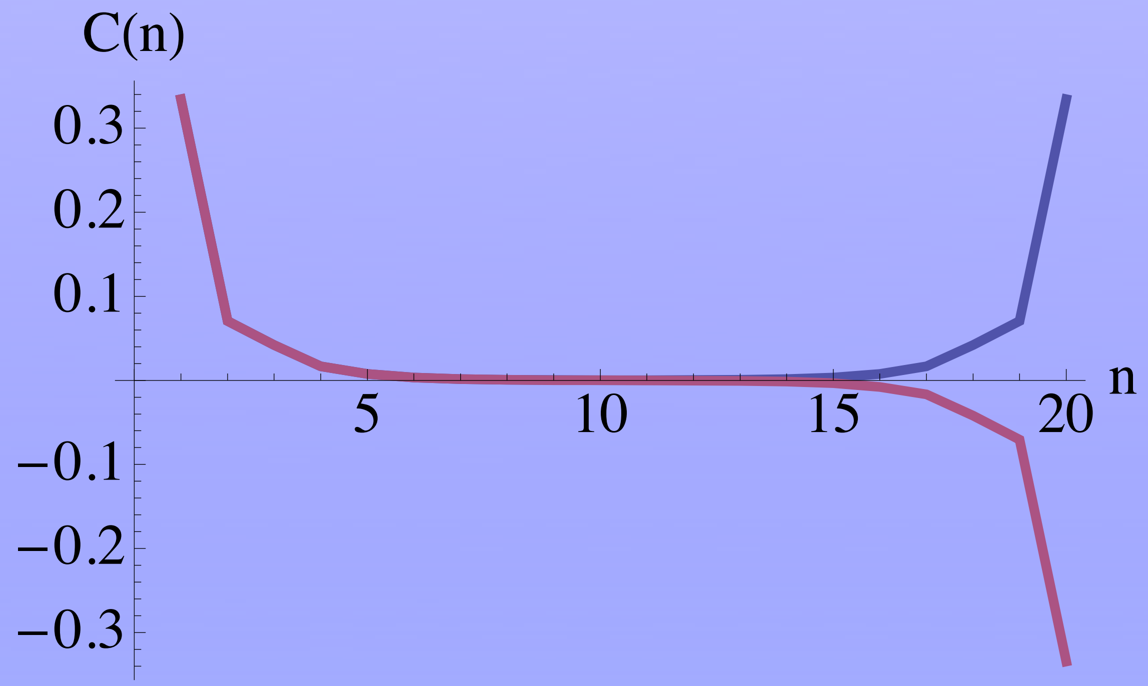
We first study this model in a slab geometry in order to see one of the "axion electrodynamics" signatures: applying *T*-breaking edge perturbations leads to half-IQHE surface layers.

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

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

the formula of Qi, Hughes, and Zhang.
(Can equally well derive by considering orbital *magnetization* response to an applied *electric* field.)

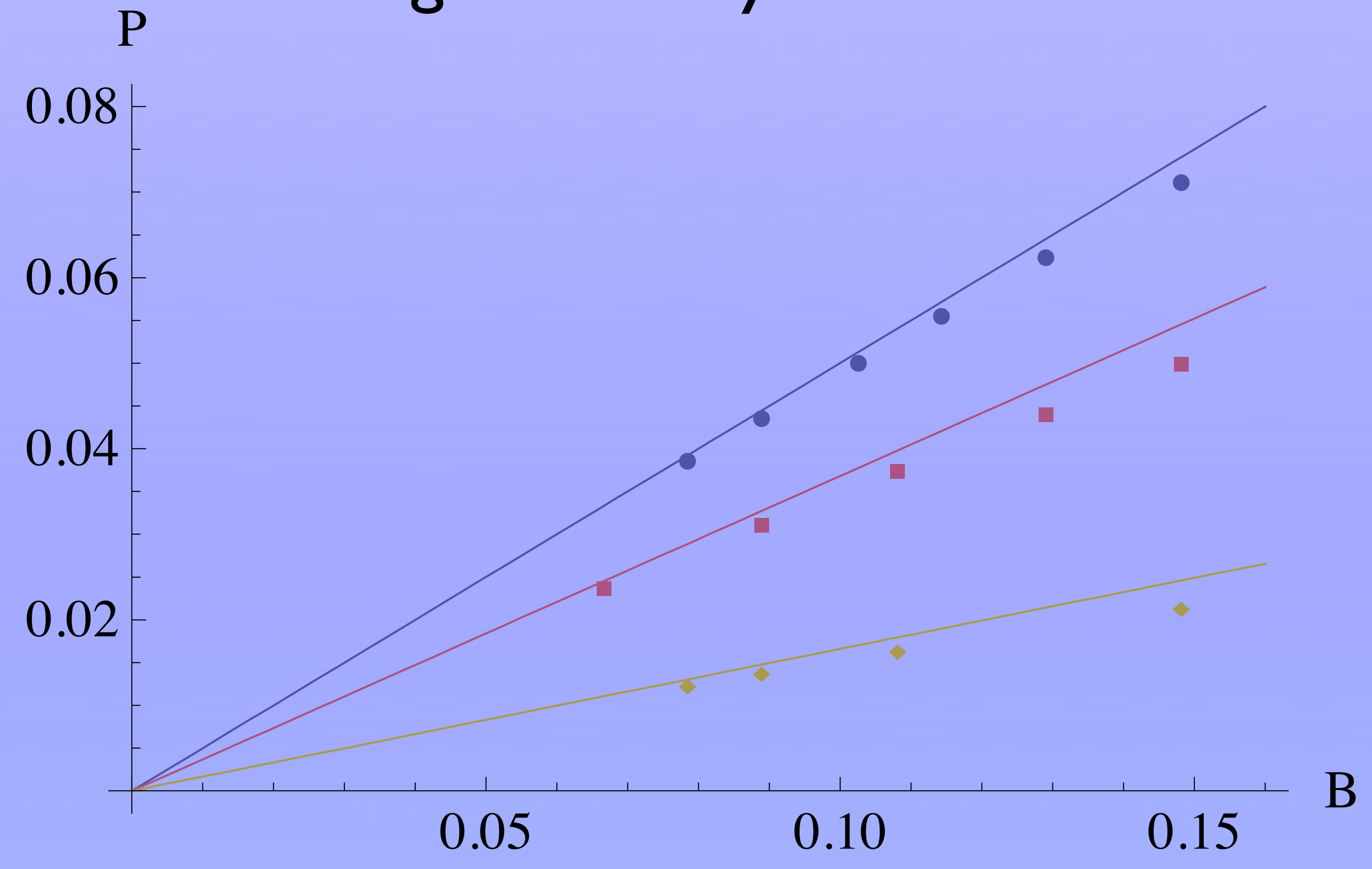
How can we confirm that this surface Hall conductance is always a bulk property, for general theta?

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

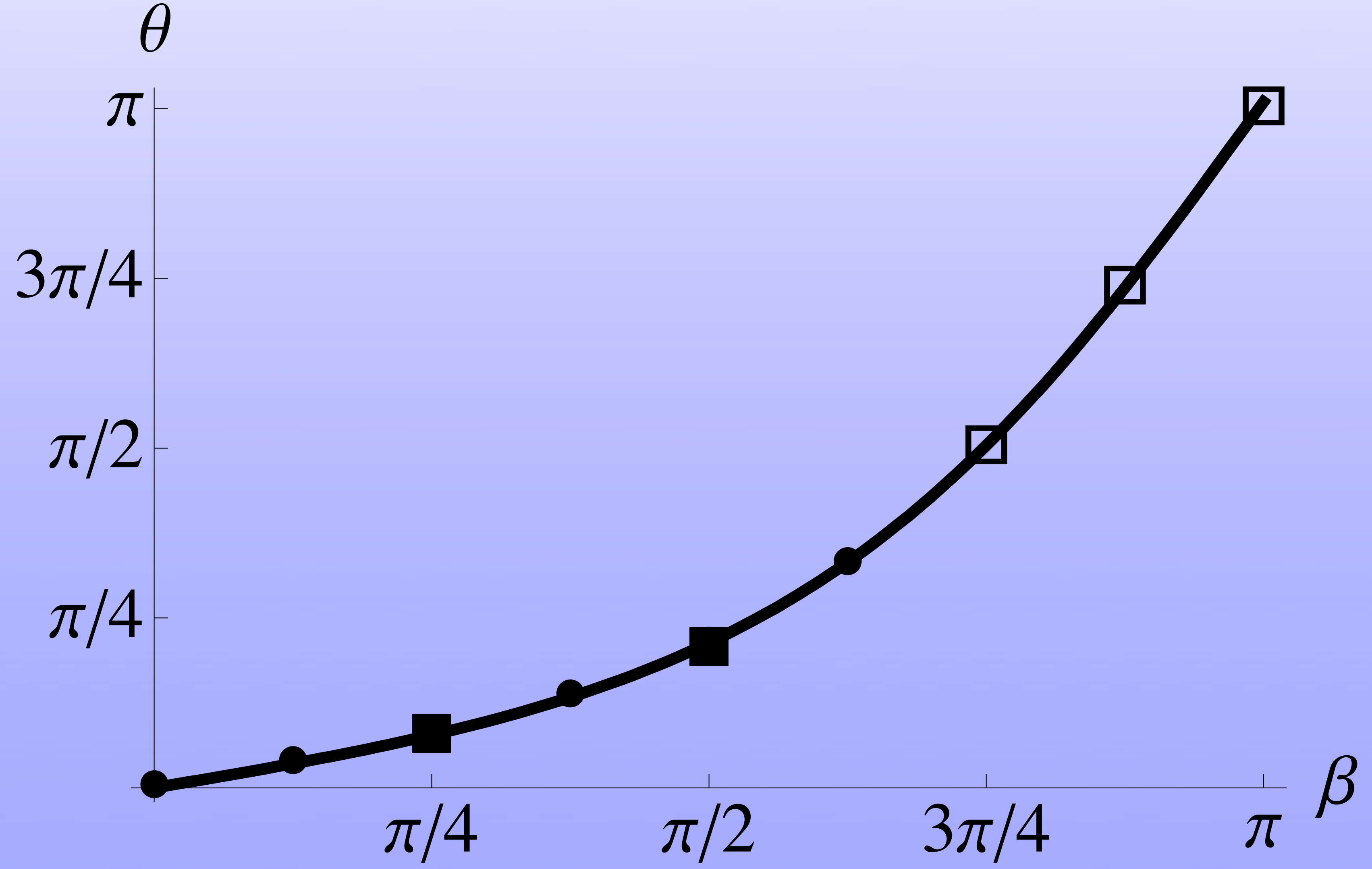
1. apply a flux through a supercell, and extrapolate to limit of small flux; compute polarization by conventional methods.

2. compute Chern-Simons integral directly

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

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

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 the origin. One argument: 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).

2. What do we learn about interactions?

Preliminary result: the 4D *second* Chern number, unlike the first, does not generalize directly to an interacting system (i.e., a many-body wavefunction). There is no remaining "symplectic structure" given only the many-body wavefunction, separated by a gap.

However, the magnetoelectric polarizability (a response in the *first* Chern number) does.

In other words, given an arbitrary *finite* "black box", we can compute the IQHE by applying boundary phases. We can compute if it is a 3D TI by a physical flux *through* the box: the polarization responds in a topological insulator, not in an ordinary insulator.

This works (at least for parallelpipeds) because of the relationship between geometry of flux quantization and polarization: both depend on transverse area.

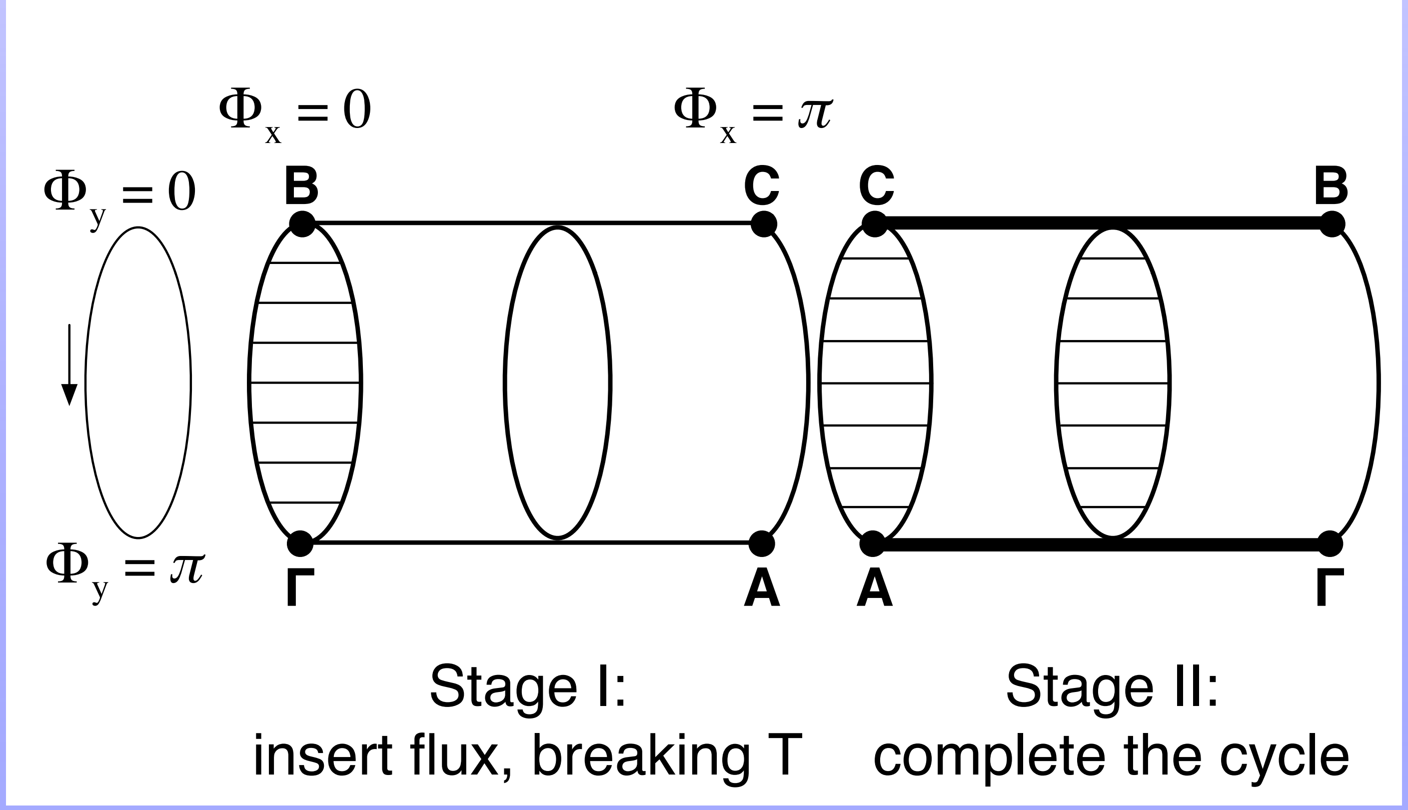
See also Sung-Sik Lee and Shinsei Ryu, PRL/talk in this session.

2. What do we learn about interactions?

The other process (applying an electric field to generate an orbital magnetic moment) is probably related to the previous definition of the Z2 invariant via *pumping* (of Z2, Fu and Kane PRB with open boundary; of charge, Essin and JEM PRB in closed system).

Picture for 2D case:

Z2 ambiguity comes from difference between different ways to close pumping cycle.



This is a Niu-Thouless-Wu version of Fu-Kane formula (see also JEM and LB),

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

2. What do we learn about interactions?

Are there similar response definitions for other 3D TI's?
(Schnyder, Ryu, Furusaki, Ludwig 08; Kitaev 08)

Is the dual response more appropriate for the T-invariant case (orbital magnetization in response to E field)?

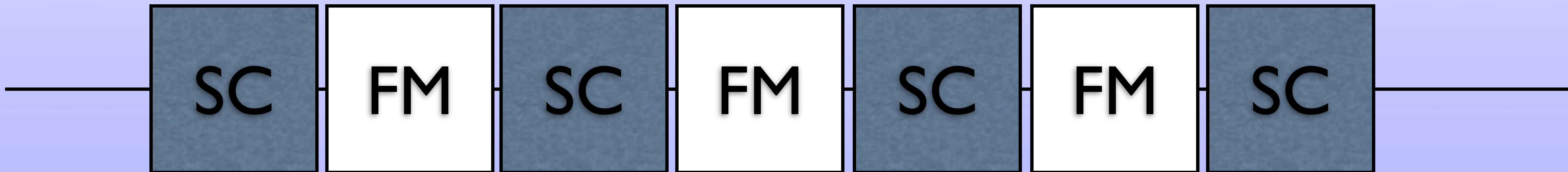
Is there anything topological about "ferrotoroidic response", which has been an active experimental area?
(E cross B rather than E dot B responses)
(cf. Batista, Ortiz, Aligia, PRL 2008)

Are switching/dynamical properties of theta useful?
Example: apply parallel E and B fields to induce a structural change between θ and -θ.

Majorana fermion chains at TI edges

(V. Shivamoggi and JEM, in progress)

Imagine superconducting and ferromagnetic regions randomly distributed along the quantum spin Hall edge.



At each SC/FM boundary there is a local Majorana fermion (Kitaev; Fu and Kane; Beenakker et al.).

The Hamiltonian if the SC and FM regions are large is H=0. When tunneling becomes possible, we realize the random Majorana hopping problem,

$$H = i \sum_j t_j \gamma_j \gamma_{j+1}$$ = random quantum Ising (Bonesteel and Yang, PRL 2006)

This is a critical *c=1/2* delocalization problem. (Roughly, SC and FM have a duality like h and J in quantum Ising: both are U(1) because one direction of the FM just shifts the chemical potential and can be neglected.)

It is very similar to the *c=1* particle-hole symmetric Dirac chain (Balents and Fisher, 1997, and references therein) which maps onto the XX spin chain.