The phase diagram of the quantum spin Hall effect in 2D and 3D

SpinAps, Asilomar, 6/5/07

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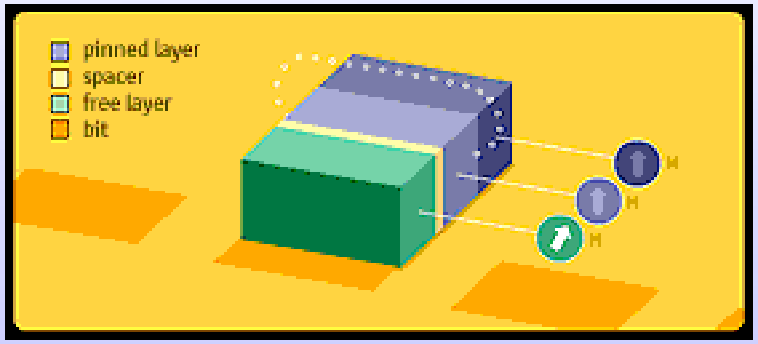
Current computers use, in general,

electron charge to manipulate information
electron spin or charge to store information
and electron charge or photons to move information



IBM magnetic read head

Can we use spin-based devices to reduce the dissipation of logic circuits?

Outline:

1. The dissipationless spin Hall effect in perfect materials

2. What happens in real materials with disorder and interactions?

3. Multiferroic manipulation of spin currents with applied voltage

Background:

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

Superconductivity:

$$J = \frac{n(e^*)^2\mathbf{A}}{m}$$

Quantum Hall effect:

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

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 useful analogues for spin currents?

Background:

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

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

3. Unlike broken symmetry phases, the IQHE state of a finite system can be defined via this invariant.

Background:

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Outline:

2D and 3D systems of noninteracting lattice fermions with unbroken ***T*** have "topological insulator" phases that show a spin quantum Hall effect carried by edge states.

The topological insulator phase is (1) intrinsically fermionic, unlike the IQHE; (2) stable to disorder; (3) at least perturbatively stable to interactions.

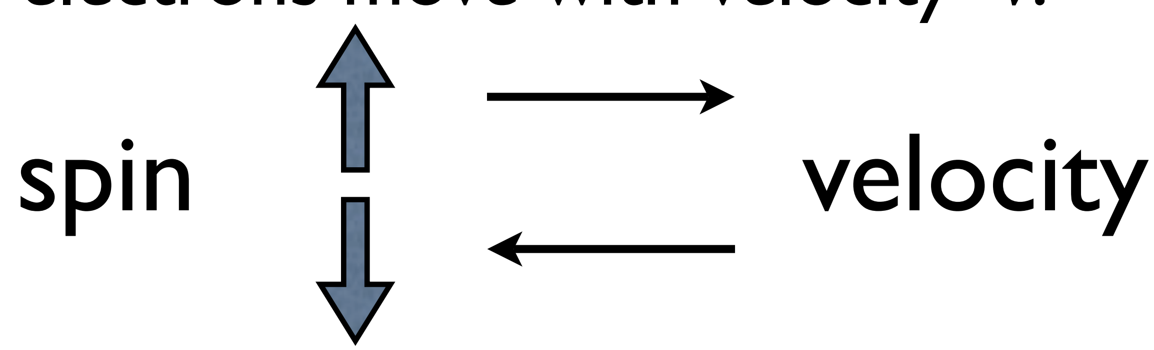
2. Signatures and possible materials.
3. Numerical studies and phase diagram.

What is a spin *current*?

Intuitive examples:

a *spin-polarized* current of electrons is one in which all electrons are in the same spin state: this current carries both charge and spin.

Example of a pure spin current:
suppose *n* spin-up electrons move with velocity *v*,
and *n* spin-down electrons move with velocity -*v*.



Then there is zero net charge current, but there is a current of spin:

More formally, spin current carries two vector indices

$\mathcal{J}_j^i$ = current of spin direction *i* in spatial direction *j*

Spin Hall effect

A fundamental difference between spin and charge currents is related to *symmetry*.

The ordinary Hall effect of electrons in a metal, and its quantized cousin (the *quantum Hall effect* or *QHE*), are both of the form

$$J_i = \alpha \epsilon_{ijk} E_j B_k$$

Symmetry permits a dissipationless *spin Hall effect*:

$$\mathcal{J}_j^i = \sigma_H^s \epsilon_{ijk} E_k$$

because spin currents are *even* under time-reversal

Background: types of SHE

$$\mathcal{J}_j^i = \sigma_H^s \epsilon_{ijk} E_k$$

One mechanism for a spin Hall current is via impurity scattering (the extrinsic SHE: theory 1970s, expt. 2004)

Recent excitement has centered on possible sources of of an "intrinsic" SHE that arises from the band structure of a clean material.

The first proposals (Murakami, Nagaosa, Zhang 2003; Sinova et al., 2004) involved doped semiconductors with no gap in the band structure.

Here we concentrate on the intrinsic SHE in materials that have zero diagonal conductivity.
(Kane and Mele PRL 2005, Haldane, Bernevig, Zhang, and others)

A proposed example is graphene with spin-orbit coupling.

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.

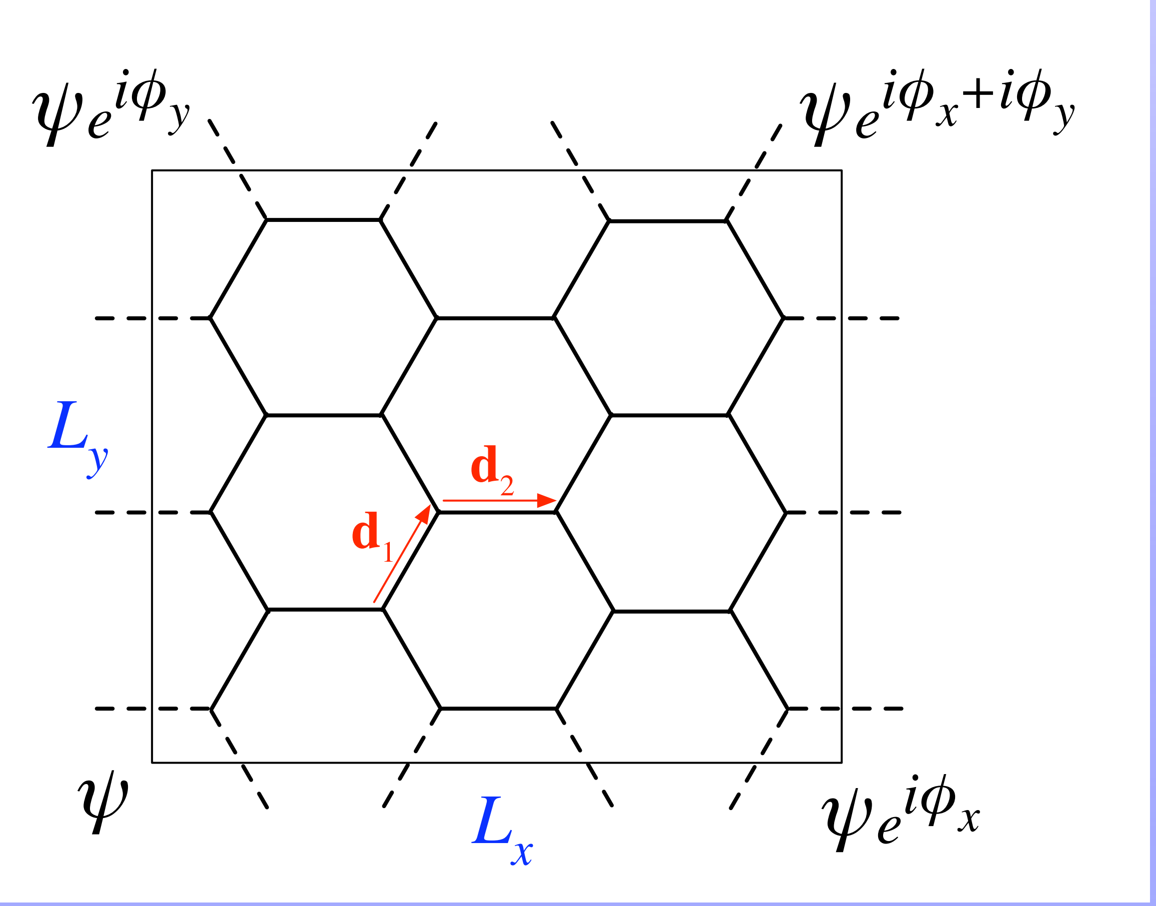
Imagine constructing a system for which spin-up electrons feel a pseudofield along z, and spin-down electrons feel a pseudofield along -z.

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

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



$$H_0 = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_v \sum_i \xi_i c_{i\sigma}^\dagger c_{i\sigma}$$

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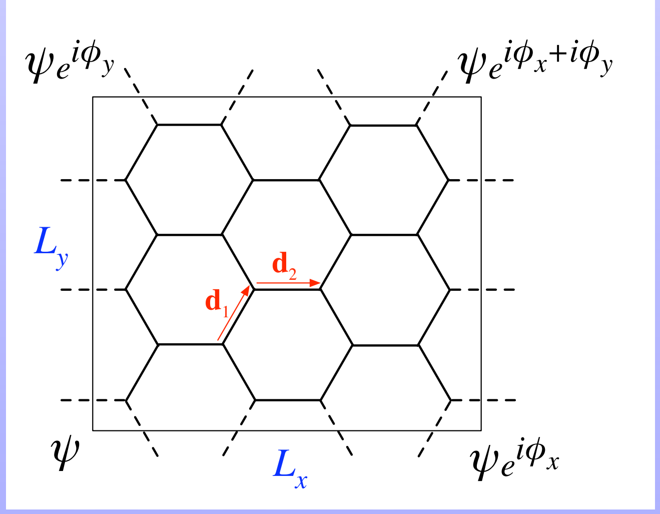

$$H_0 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + i\lambda_v \sum_i \xi_i c^\dagger_{i\sigma} c_{i\sigma}$$

The first term gives a semimetal with Dirac nodes (as in graphene).

The second term, which appears if the sublattices are inequivalent, 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

$$H_0 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + i\lambda_v \sum_i \xi_i c^\dagger_{i\sigma} c_{i\sigma}$$

The spin-dependent part contains two SO couplings

$$H' = i\lambda_{SO} \sum_{\langle\langle ij \rangle\rangle} v_{ij} c^\dagger_i s^z c_j + i\lambda_R \sum_{\langle ij \rangle} c^\dagger_i (\mathbf{s} \times \hat{\mathbf{d}}_{ij})_z c_j$$

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.

KEY: the system with an SO-induced gap is fundamentally different from the system with a sublattice gap: **it is in a different phase.**

Example: Kane-Mele-Haldane model for graphene

$$H_0 = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda_v \sum_i \xi_i c_{i\sigma}^\dagger c_{i\sigma}$$

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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?

The quantum spin Hall effect

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.*

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

(Wu, Bernevig, and Zhang, PRL 2006; Xu and Moore, PRB 2006)
Stability to **both** disorder and interactions can be argued by looking at the edge (later)
Add B field->edge conductance set by *inelastic* processes (phase-breaking rate).

How can we tell, just from the band structure of a 2D or 3D material, whether that material will show an SQHE?

Importance beyond the SQHE

Aside from possible spin transport measurements, the deeper significance of this idea is that in 2D there are

exactly two phases of T-invariant band insulators

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.

Importance beyond the SQHE

Terminology:

The "topological" insulator phases
(a. k. a. topological band insulator, topologically nontrivial insulator, ...)

are *phases* of time-reversal invariant band insulators for which a dissipationless SQHE is *generic*.

How can we tell the phases possible in a given band structure?

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.

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

What about the SQHE?

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 the QSHE?

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

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

Z2 topological invariants

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.
(Moore and Balents, PRB RC '07)
For the "odd" class, there must be spin-orbit coupling and broken inversion.
Consider a 2D Brillouin torus.

In terms of the Berry field A and flux F, the topological invariant is

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

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

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

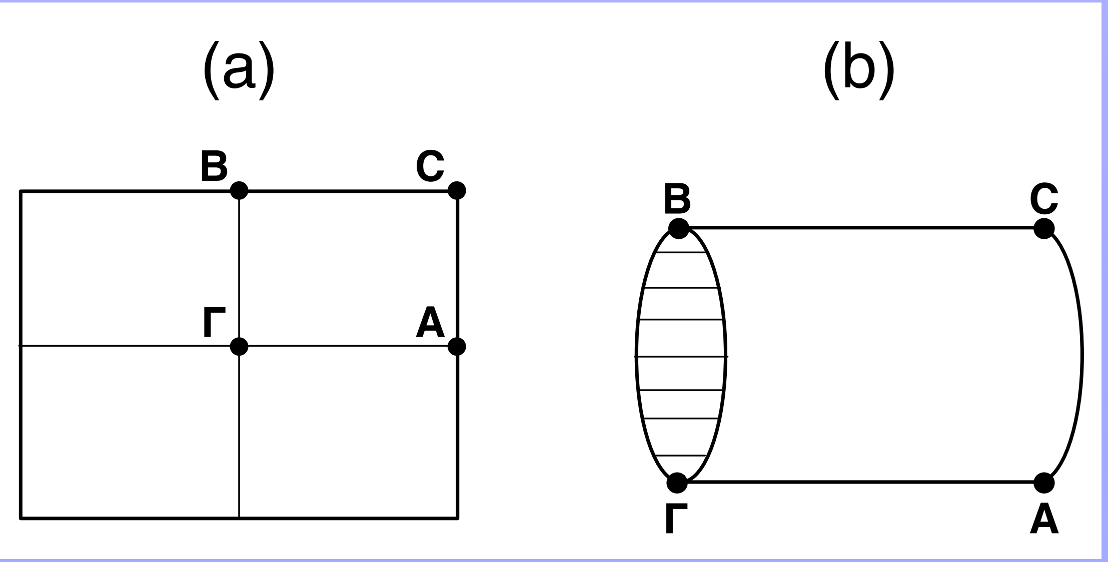
Sketch of where Z2 invariants come from

Avron, Seiler, Simon: (IQHE, 1983)
classify maps from the Brillouin zone (a 2-torus) to the space of *n* by *n* Bloch Hamiltonians with no accidental degeneracies:

$$\pi_2(\mathcal{C}) = \mathbb{Z}^{n-1}, \quad \pi_1(\mathcal{C}) = 0.$$

$$\pi_n(M) = \text{equivalence classes of maps from } S^n \text{ to } M$$

We classify maps from "half the Brillouin zone" in T-invariant systems: there is a Z2 for each band *pair* conjugate under T.



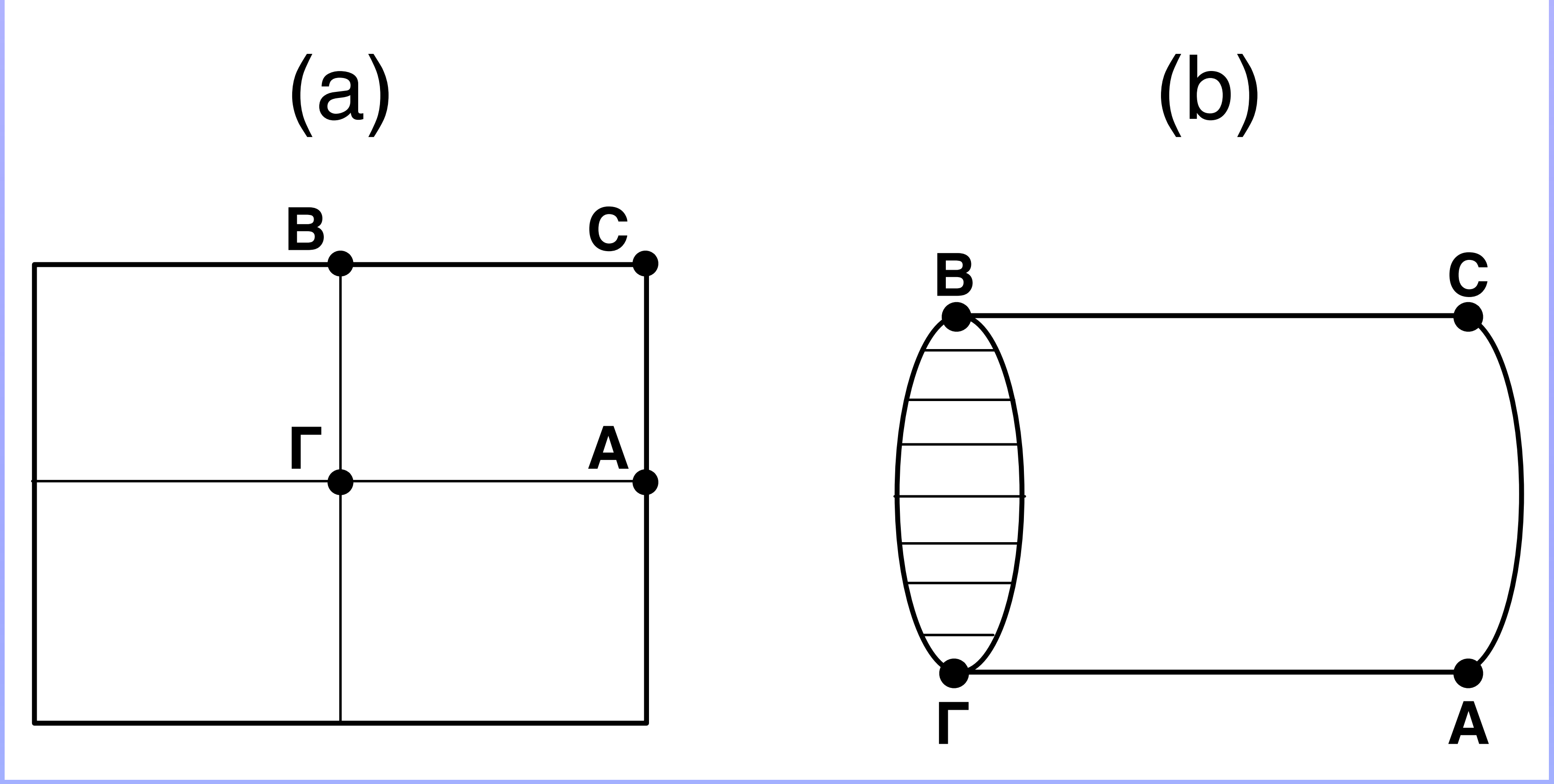
Ordinary Chern numbers are *ambiguous* except for parity (oddness or evenness).

Z2 topological invariants

The Bloch Hamiltonians at points in the Brillouin zone related by time-reversal are *conjugate* to each other, not necessarily identical.

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

The set of *independent* points (the effective Brillouin zone or EBZ) is then shown in (b) below: it has the topology of a cylinder with special boundary conditions.



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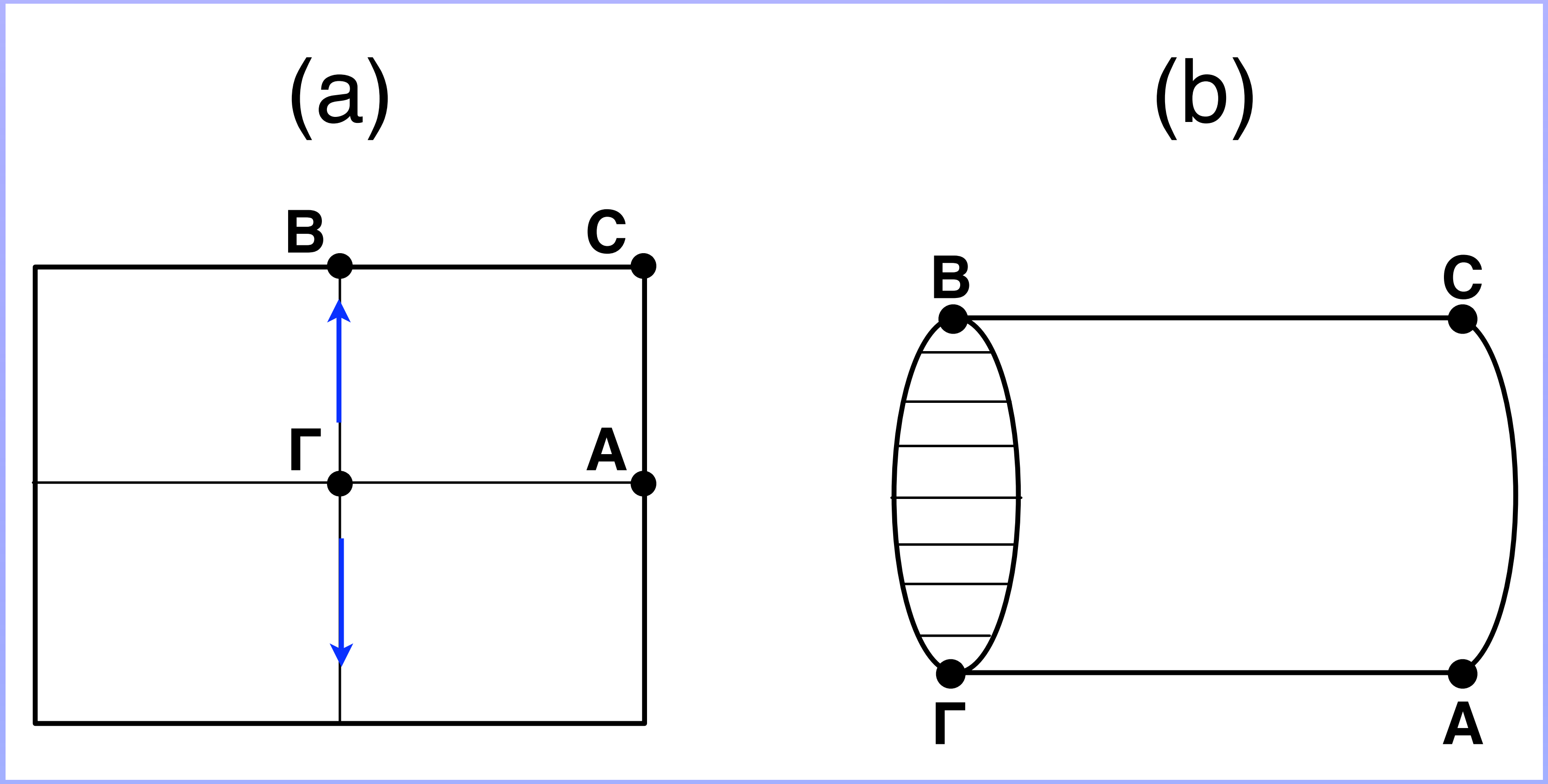


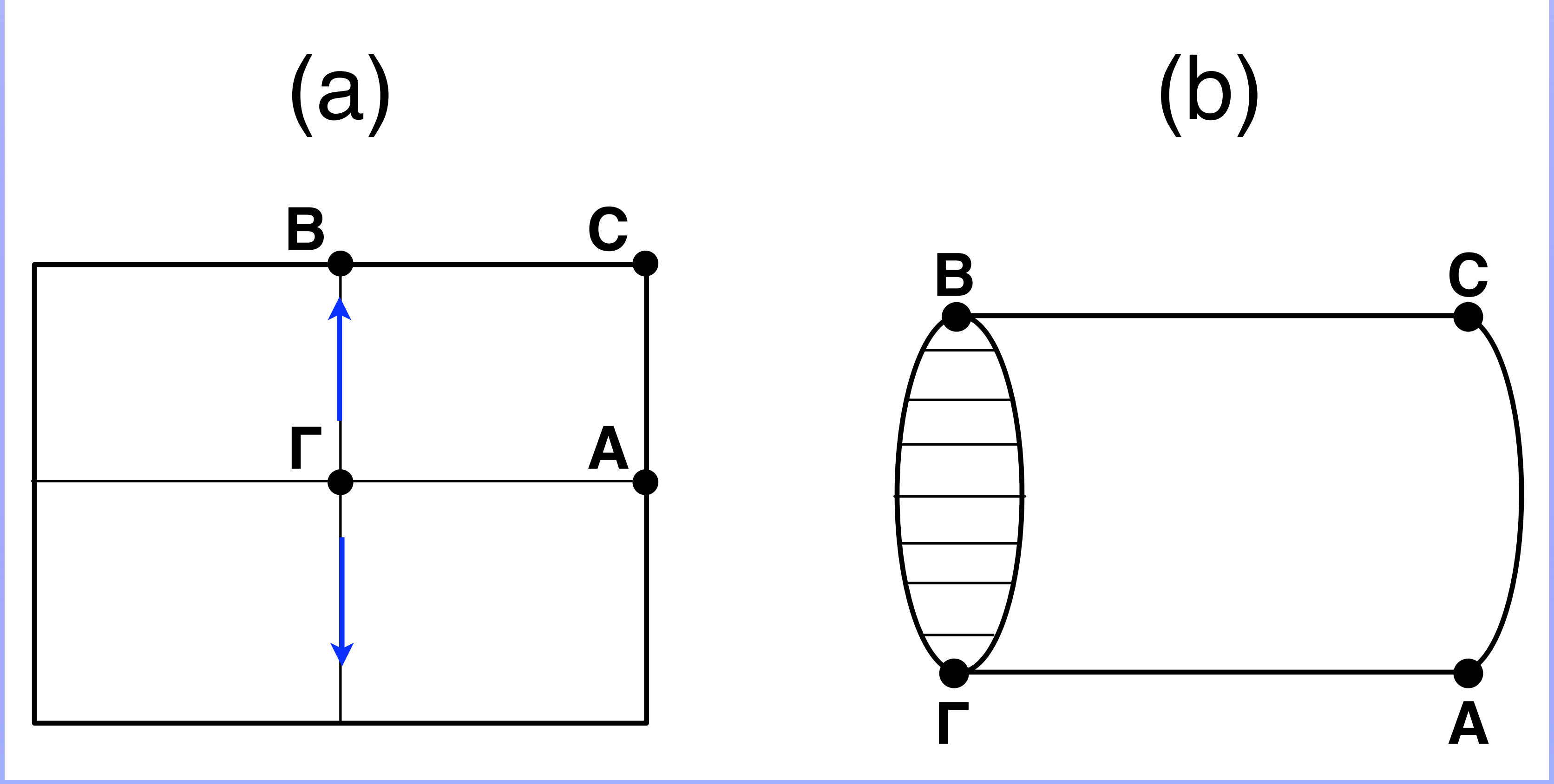
Z2 topological invariants

An abstract definition of the ordinary Chern number (Avron, Seiler, Simon):

if *C* is the space of Bloch Hamiltonians, then mappings from the Brillouin torus to *C* are classified by *one integer for each band*, with a zero sum rule.
Why?

$$\pi_2(\mathcal{C}) = \mathbb{Z}^{n-1}, \quad \pi_1(\mathcal{C}) = 0.$$

$$\pi_n(M) = \text{equivalence classes of maps from } S^n \text{ to } M$$

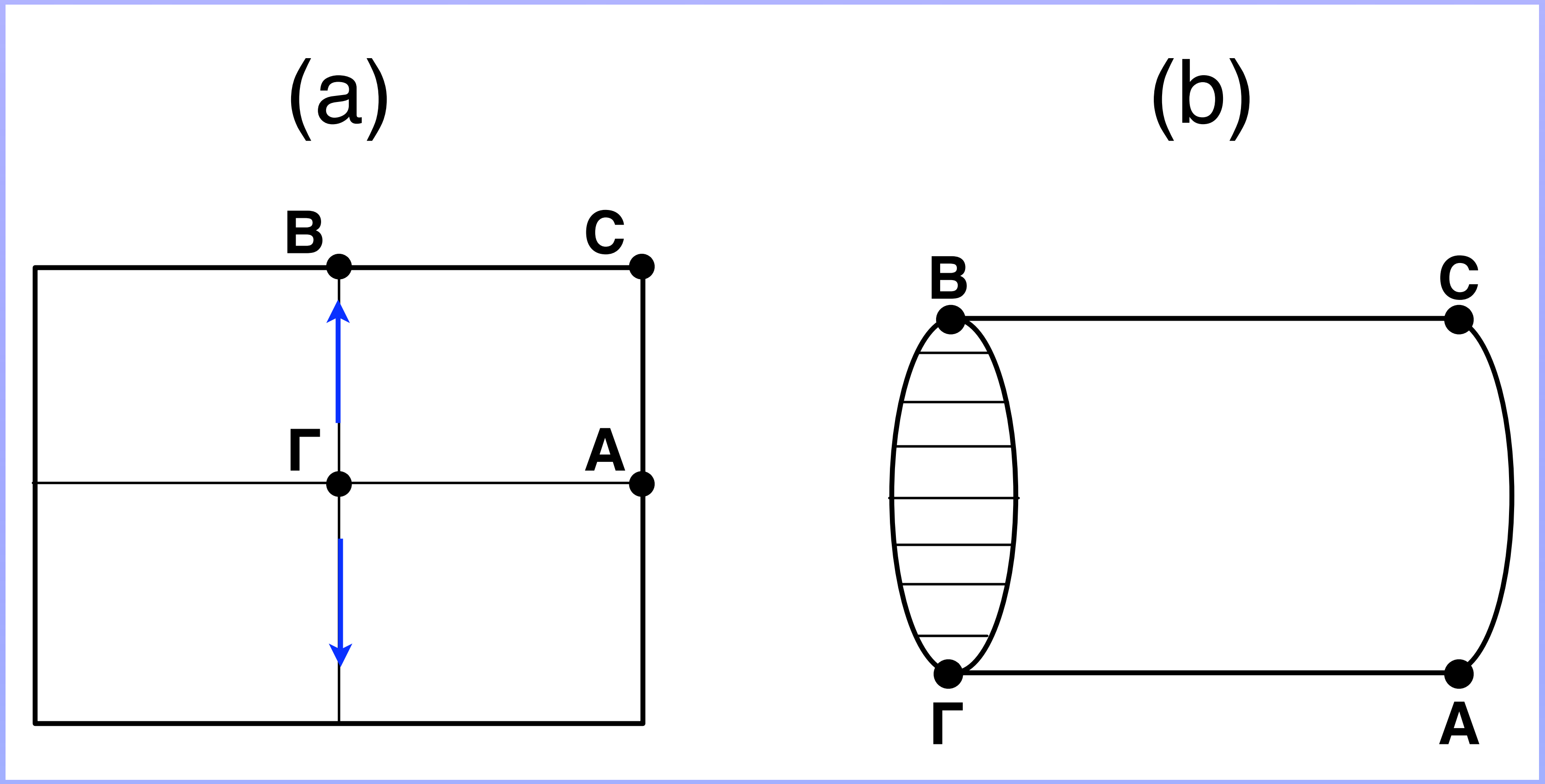


Z2 topological invariants

Key idea for the *T*-invariant case:
Consider all possible ways of "contracting" a mapping from the EBZ to one from a sphere, to define a Chern integer.

There are an *infinite* number of possible ways, differing by all *even* Chern numbers.

We will show that the difference between two "contractions" is even:



Z2 topological invariants

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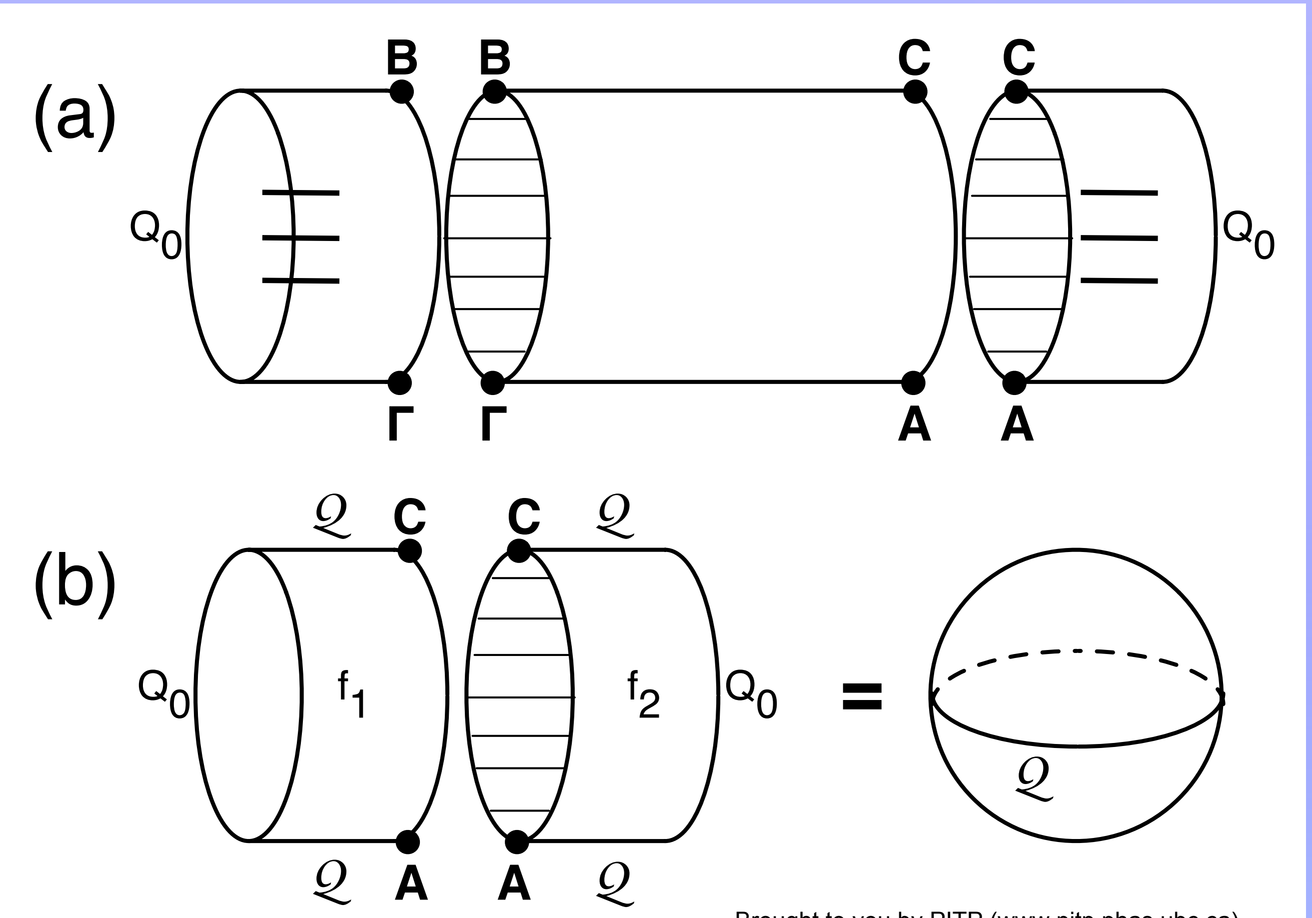
Consider all possible ways of "contracting" a mapping from the EBZ to one from a sphere, to define a Chern integer.

There are an *infinite* number of possible ways, differing by all *even* Chern numbers.
The symmetries at the two circular boundaries of the cylinder mean that contractions have more symmetry in their interior than the EBZ:
two contractions can be combined to give a sphere with even Chern numbers.

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

The flux part counts the contribution from the EBZ itself, which is unambiguous.
The field part counts the contribution from the contraction, which is ambiguous by even integers.
The sum is always an integer.



Z2 topological invariants

Conclusions on topological classes:

there is 1 Z2 invariant (even Chern numbers or odd Chern numbers) per T-related pair of bands, with a zero sum rule;

the state of a system is the sum of Z2 invariants of occupied bands, just like the sum of ordinary Chern number determines the IQHE phase:

if the sum is odd, then the system is a *topological insulator*, with a robust spin Hall effect; if the sum is even, then the system is deformable to an ordinary insulator.

Z2 topological invariants

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In three dimensions, we find 4 Z2 invariants per band (only a little more complicated to show). Surprising because there are only 3 Chern integers: 3 of the 4 Z2 invariants correspond to layered versions of 2D.

The fourth is more interesting and also thought to be more stable.
Examples with nontrivial fourth invariant were found by Fu, Kane, and Mele (PRL '07 and Bernevig, Chen, and Zhang.

Z2 topological invariants in 3D

In three dimensions, we find 4 Z2 invariants per band pair.

But there are only 3 Chern numbers! (*xy*, *xz*, *yz* planes)

The Z2 invariants can be enumerated as follows: there are six inequivalent planes in the 3D Brillouin zone that reduce to the 2D case and have a Z2 invariant.

Call these $x_0, x_1, y_0, y_1, z_0, z_1$. Each is ±1 (even or odd).
These are not independent, however:

$$x_0 x_1 = y_0 y_1 = z_0 z_1$$

Hence there are only *four* invariants. Three are layered versions of the IQHE, but the nontrivial fourth invariant can not be realized in any model in which up and down spin decouple.

Physical consequences

What do we learn about the SQHE?

1. The *existence of propagating edge modes* is universal in the topological insulator, but the amount of S_z that propagates is not quantized.

2. Corrections at finite temperature T or voltage V are power-law rather than exponential, because the transport is protected by a *symmetry* rather than a *gap*.

3. The SQHE is perturbatively stable to electron-electron interactions and disorder (from bosonization looking at the edge), but maybe not as stable as the IQHE.

We have a set of integrals on the Brillouin zone that, given any 2D or 3D band insulator with SO coupling, will predict whether the system is a topological insulator (has edge states) or not.

Are there topological insulator phases
at accessible temperatures in real materials?
How could we tell?

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 infer the phase.

Materials recently proposed: Bi, InSb, strained Sn (3d), HgTe (2d) (Bernevig, Hughes, and Zhang, *Science* (2006); *experiments...)*

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.

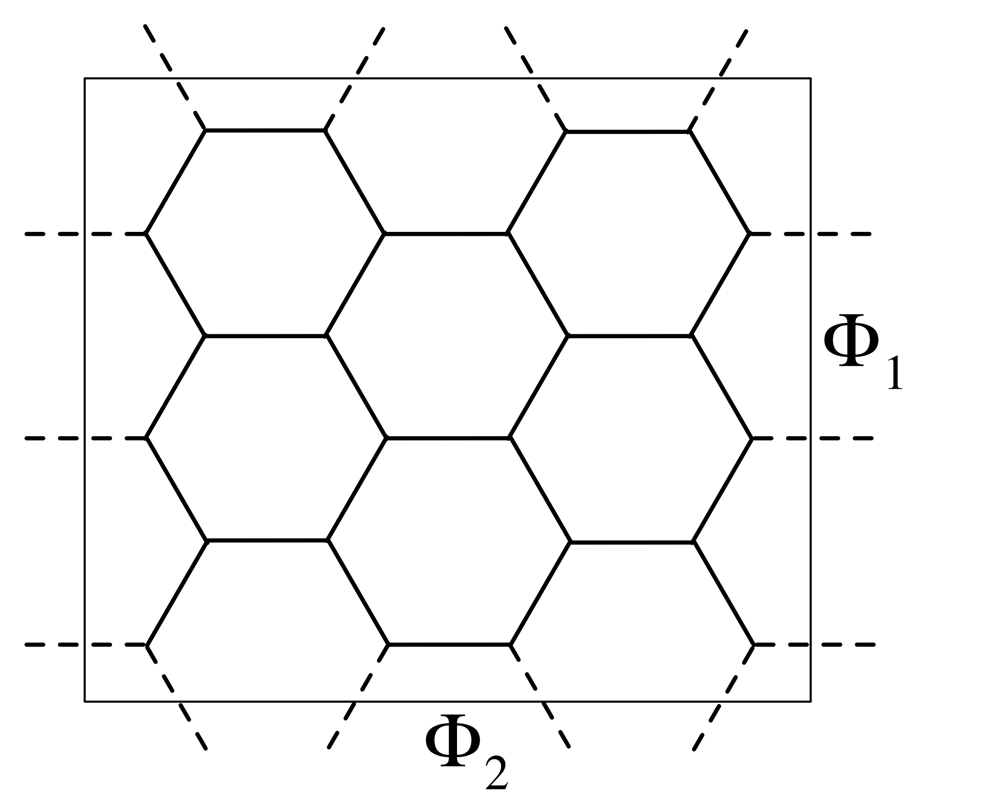
What about the SQHE? Is it a new phase of condensed matter?

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.

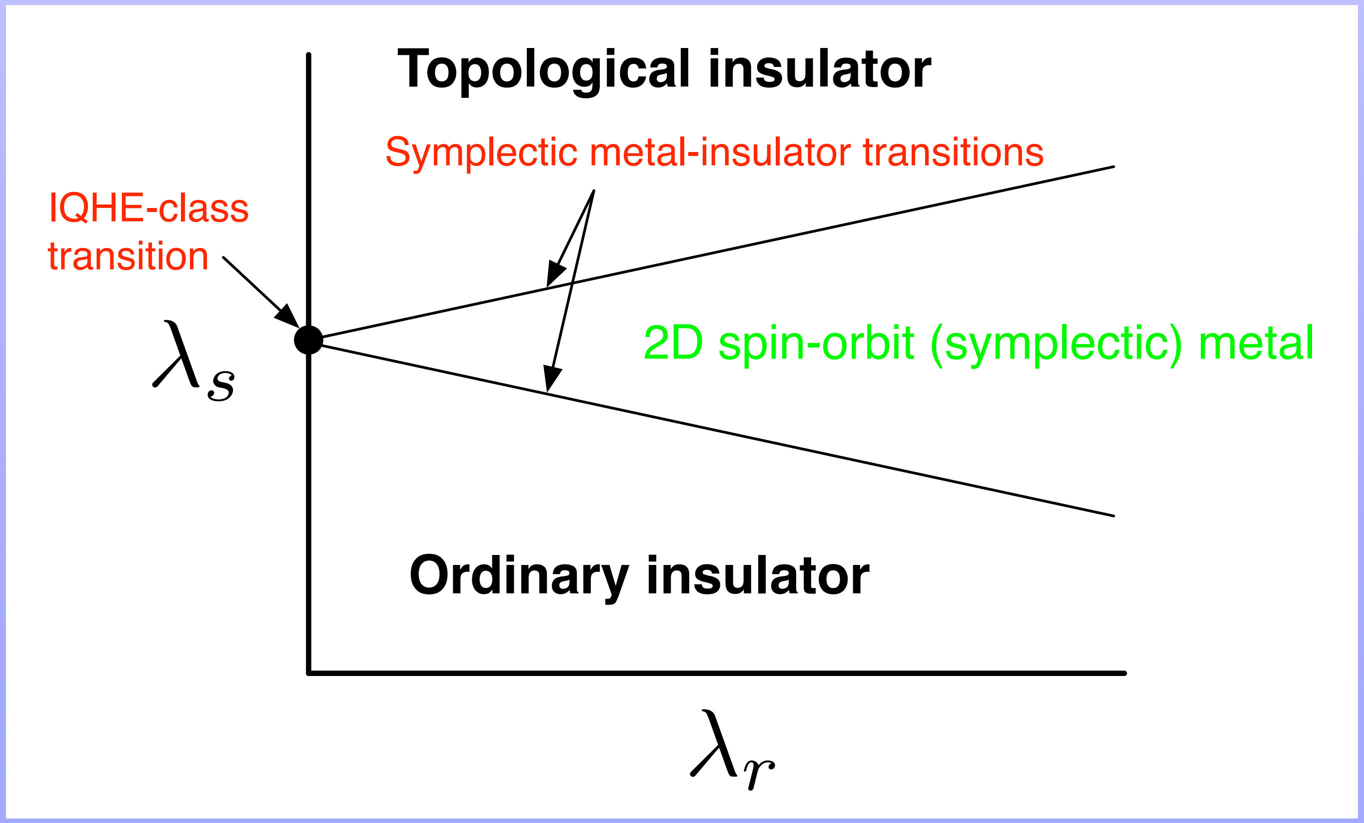
Effect of boundary phase is to shift *k*: alternate picture of topological invariant is in terms of half the (Φ_1,Φ_2) torus.

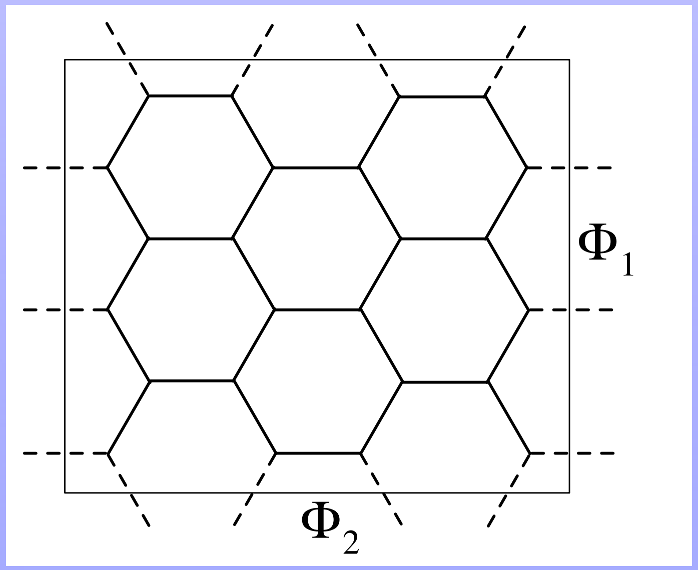


Can define Chern parities analogous to Chern numbers, and study phase diagram w/disorder

The topological insulator with disorder

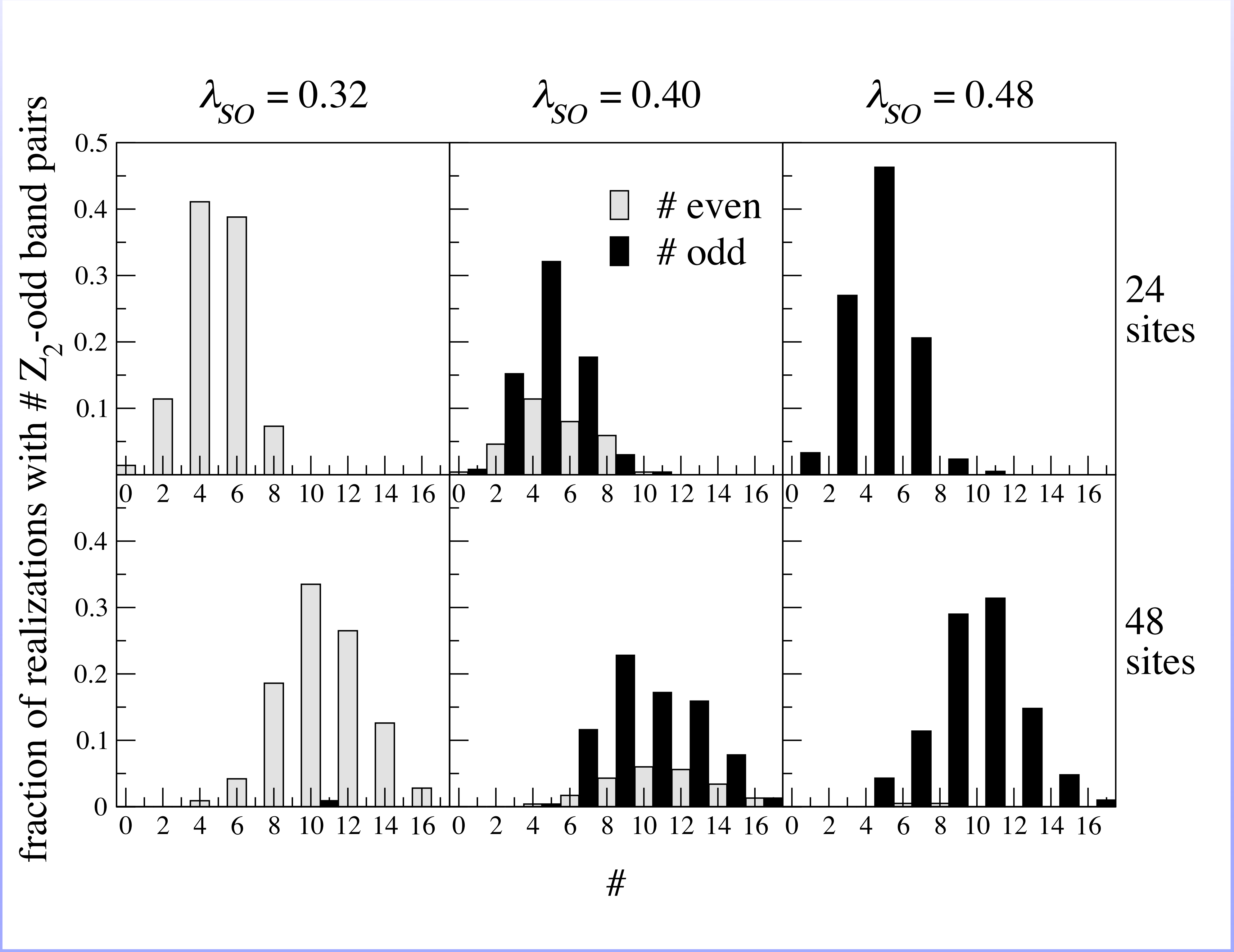
Spin-orbit *T=0* phase diagram (fix spin-independent part): instead of a point transition between ordinary and topological insulators, have a symplectic metal in between.





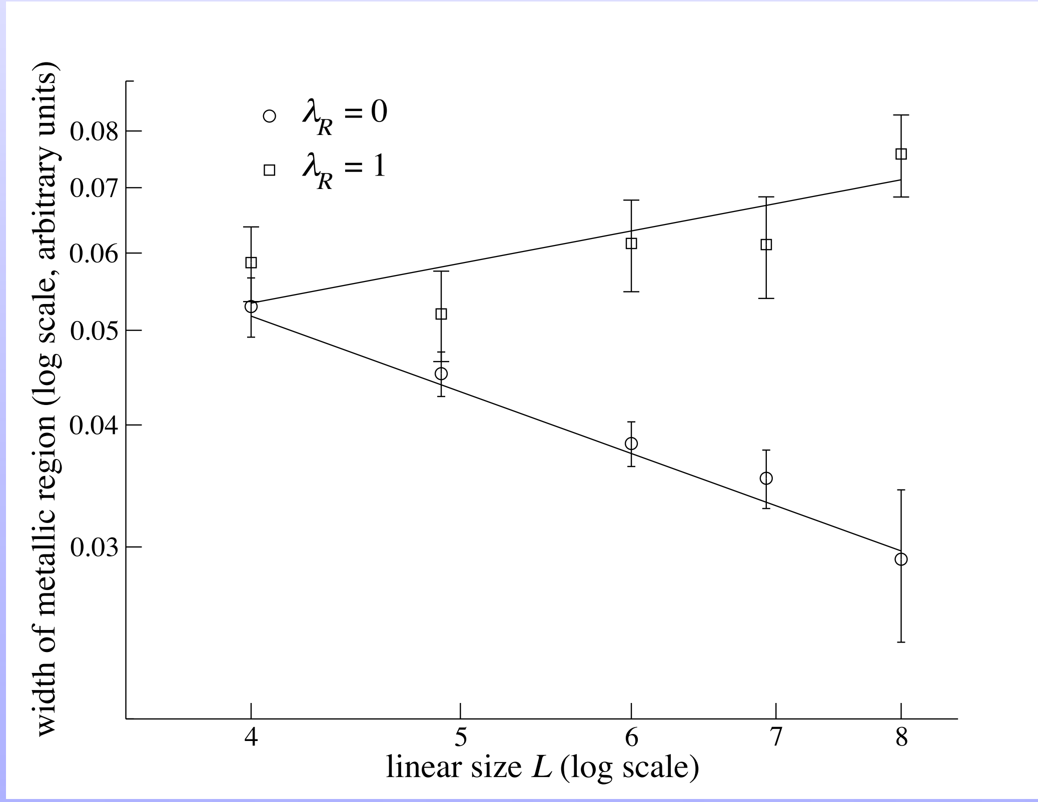
We can observe this numerically using Fukui-Hatsugai algorithm (cond-mat/ 0611423) to compute invariants (A. Essin and JEM, cond-mat).

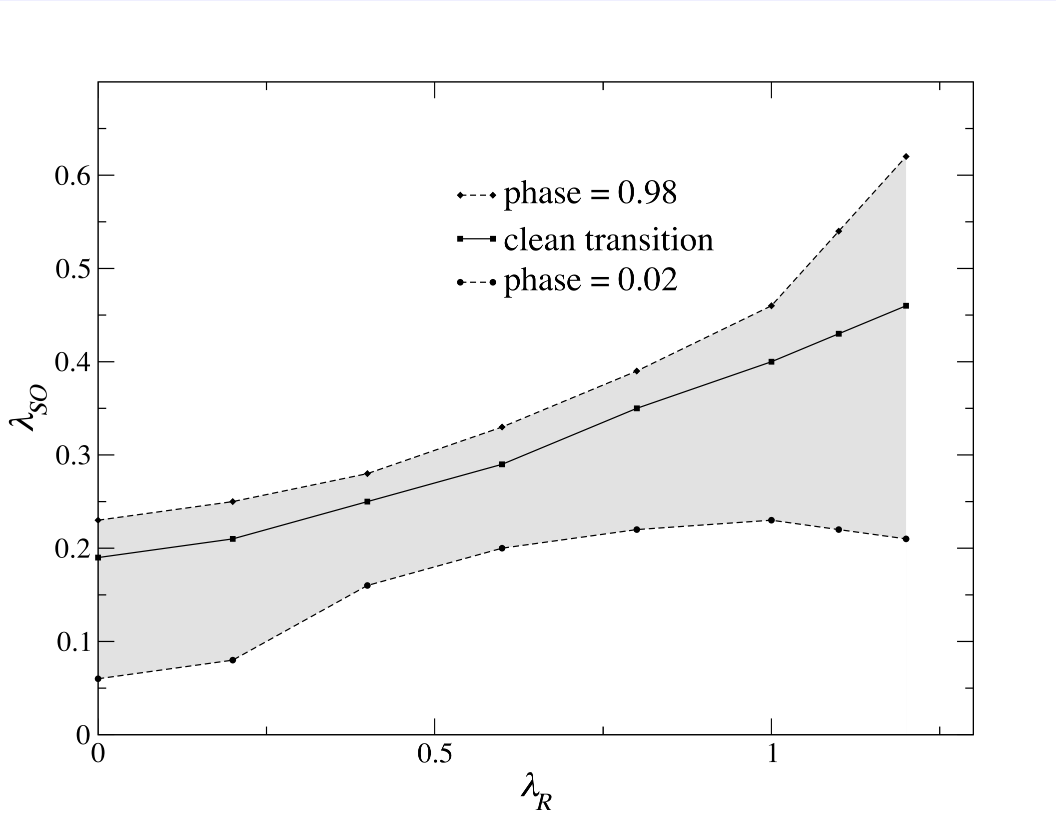
Numerical evidence



Identification of phases

Numerical evidence





Transition width

Phase diagram

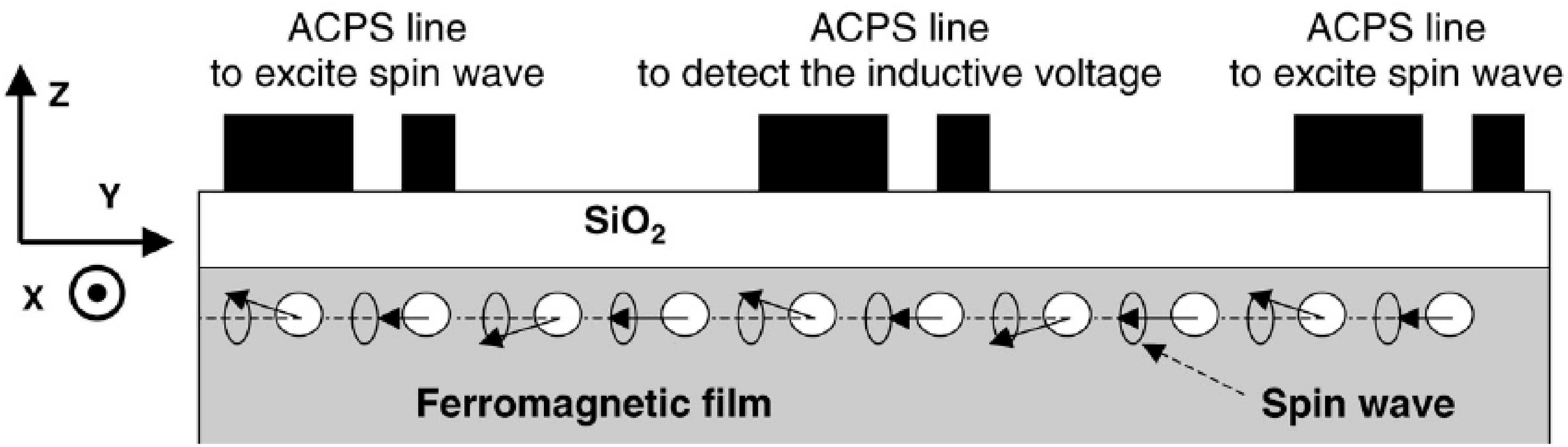
All numerics done on UC Berkeley Shared Nanoscience Computer Facility
(IBM SUR donation)

112-processor IBM Linux on POWER cluster

6 groups
Louie, Moore (lead PI), Souza: nanoelectronics
Chrzan: structural properties of nanomaterials
Geissler: biological nanomaterials
Whaley: quantum computation

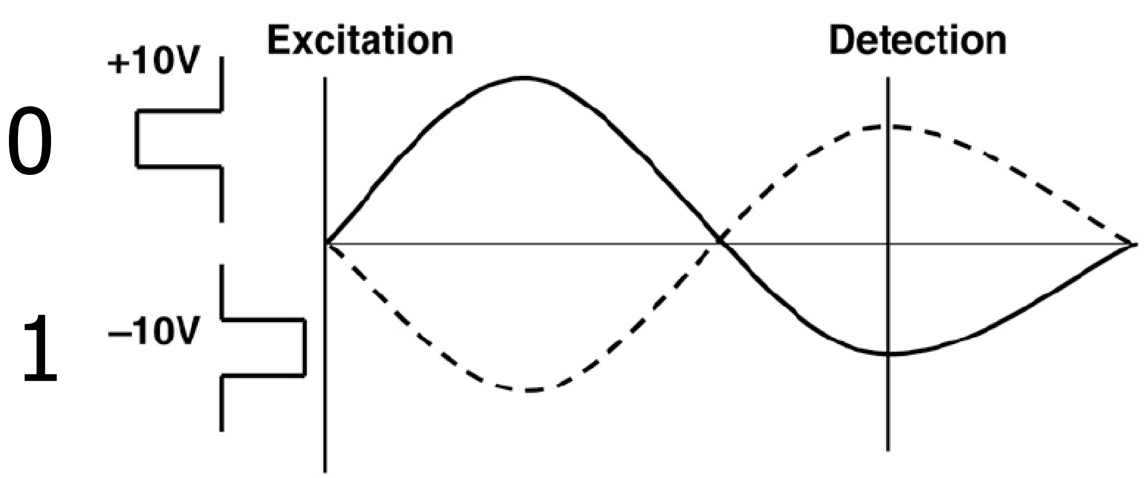
Multiferroics for spin-wave devices

Khitun and Wang Sup. & Mic. 2005; Kostylev et al APL 2005



$$M_{out} = e^{i(\phi_1 - \omega t)} + e^{i(\phi_2 - \omega t)}, \; t = \frac{(2n+1)\pi}{\omega}, \; V_{\text{ref}} > 0$$

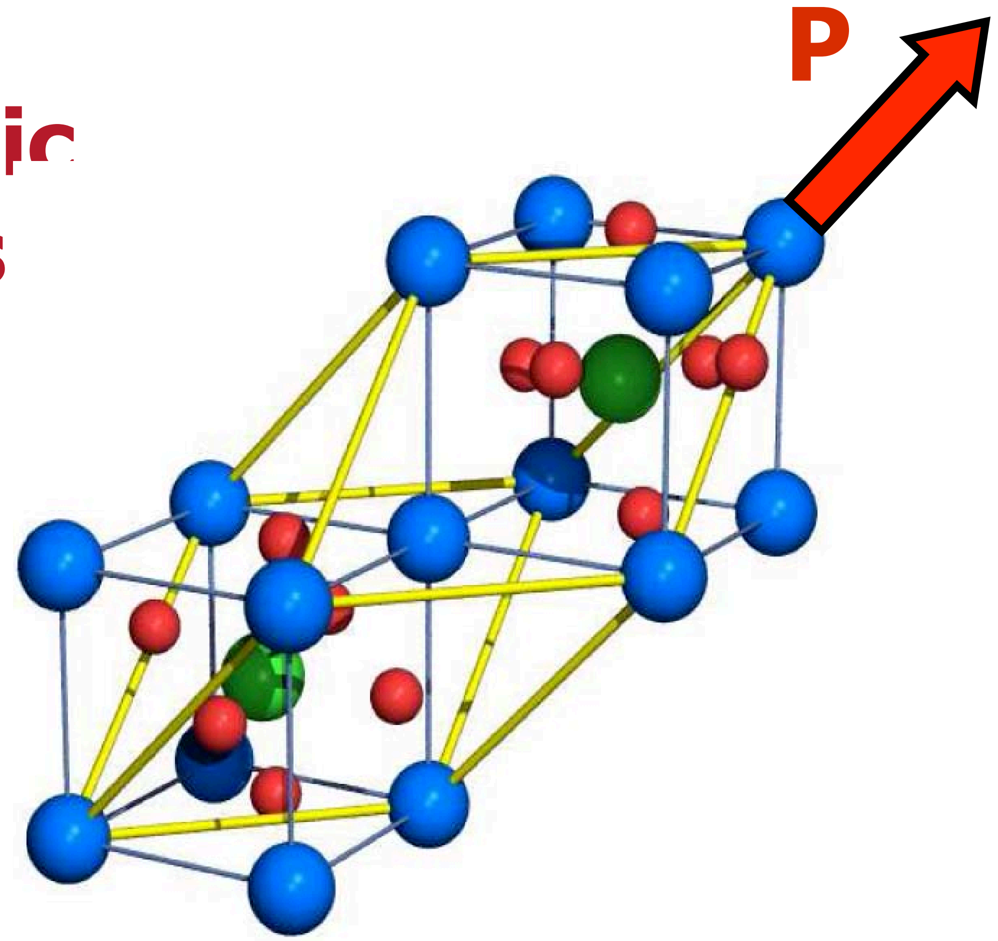
NOT gate:



AND gate:

ϕ_1	ϕ_2	M_{out}
0	0	$2e^{-i\omega t}$
0	π	0
π	0	0
π	π	$2e^{i(\pi - \omega t)}$

$BiFeO_3$, a high-T multiferroic Coupled polar (P), antiferromagnetic (L), and ferromagnetic (M) orders



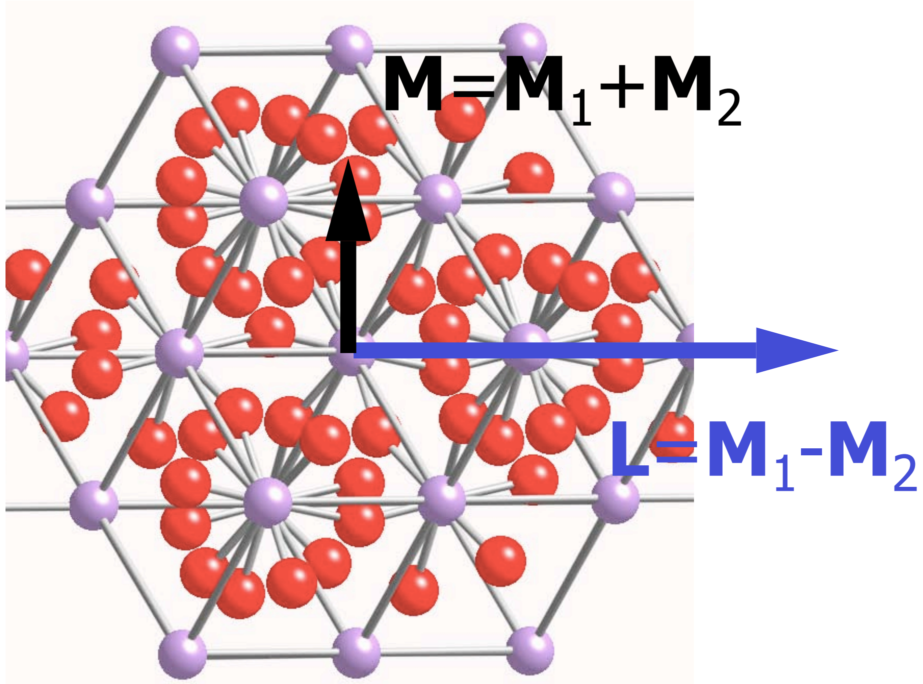
Figs. courtesy R. Ramesh

$BiFeO_3$ BULK

- Rhombohedral R3c: a=3.96Å, α=89.46º
- No inversion symmetry, but "close"
- T_N~ 650K; T_C ~ 1120K
- Cycloidal, possibly canted AFM order
- P ~ 6 $\mu C/cm^2$

$BiFeO_3$ FILM on (100) $SrTiO_3$

- Tetragonal distortion a=3.91Å, c=4.06Å
- Homogeneous, canted AFM order
- Giant ME effect: P ~ 90 $\mu C/cm^2$



Electrical coupling to **fast** (AF) spin waves

Landau model for $BiFeO_3$

$$F = F_P + F_{LM} + F_{ani} + F_{DM} + F_{Lif.}$$

Important interactions allowed in BFO due to "near" inversion symmetry:

$$\vec{L} \to -\vec{L}, \vec{P} \to -\vec{P}, \vec{\nabla} \to -\vec{\nabla}$$

Dzyaloshinskii-Moriya interaction: Explains canted AF

$$F_{DM} = -d\vec{P} \cdot \vec{M} \times \vec{L}$$

Allows generation and detection of magnetic spin waves through AC electric fields

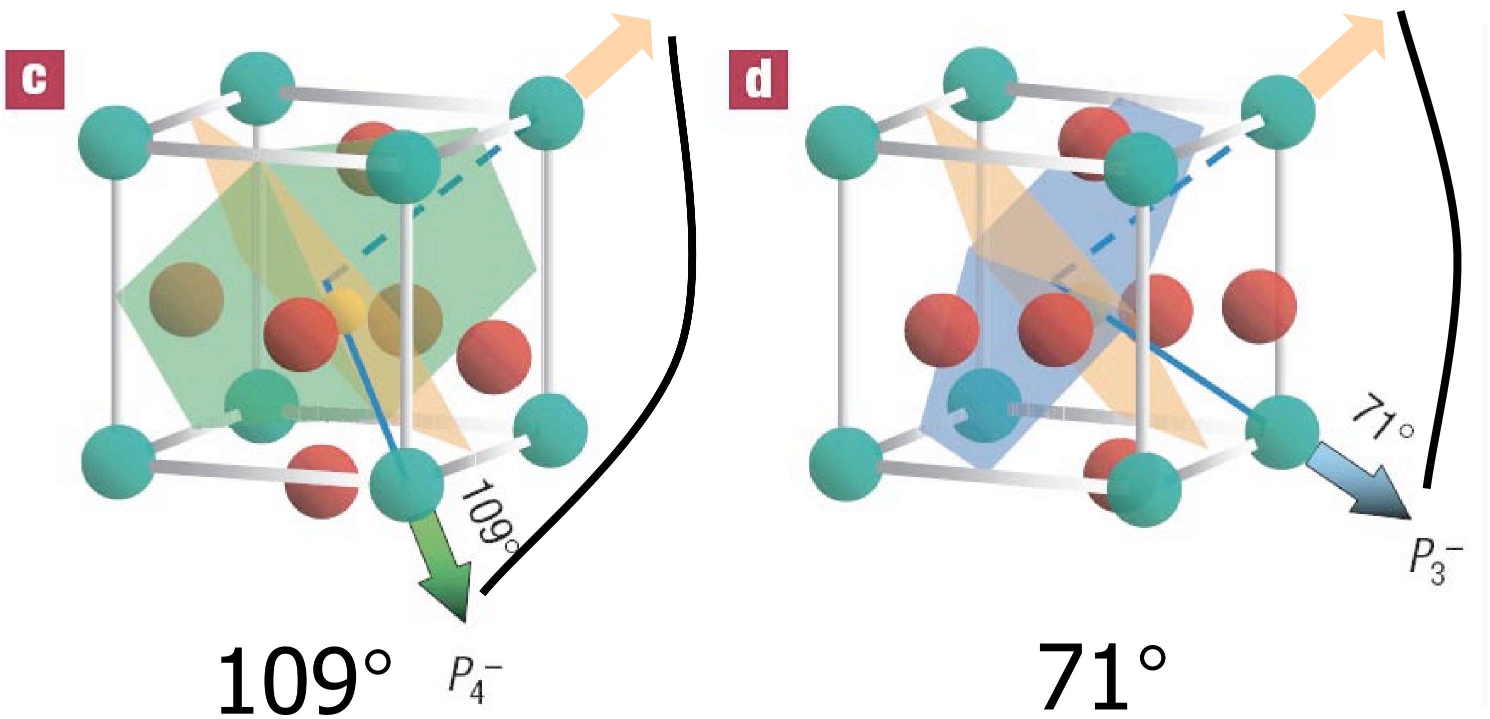
Lifshitz interaction: Explains spiral AF in bulk BFO

$$F_{Lif.} = \alpha \vec{P} \cdot \left[\vec{L}\vec{\nabla} \cdot \vec{L} + \vec{L} \times \left(\vec{\nabla} \times \vec{L} \right) \right]$$

Electric control via polarization vector orientation

AF order maintains orthogonality to P as shown by Ramesh et al.:

T. Zhao et al, Nature Mat. 2006



109° 71°

How does this operation affect the electromagnon spectrum?

Main conclusion of TDGL study (cf. poster of Rogerio de Sousa)

- Multiferroic $BiFeO_3$ combines multiferroicity with incommensurate magnetism: this allows strong coupling between k = 0 AC electric fields and **spin waves** at the cycloid wavevector
- Spin-wave propagation characteristics depend strongly on relative orientation of **k** and **P**, allowing electrical switching of spin wave propagation
- Next steps: experimental tests & dynamics of switching
- Demonstrate spin-wave device using correlated materials

Conclusions

1. Topological insulators: a new phase of 2D or 3D solids with universal spin and charge transport that is stable to disorder.

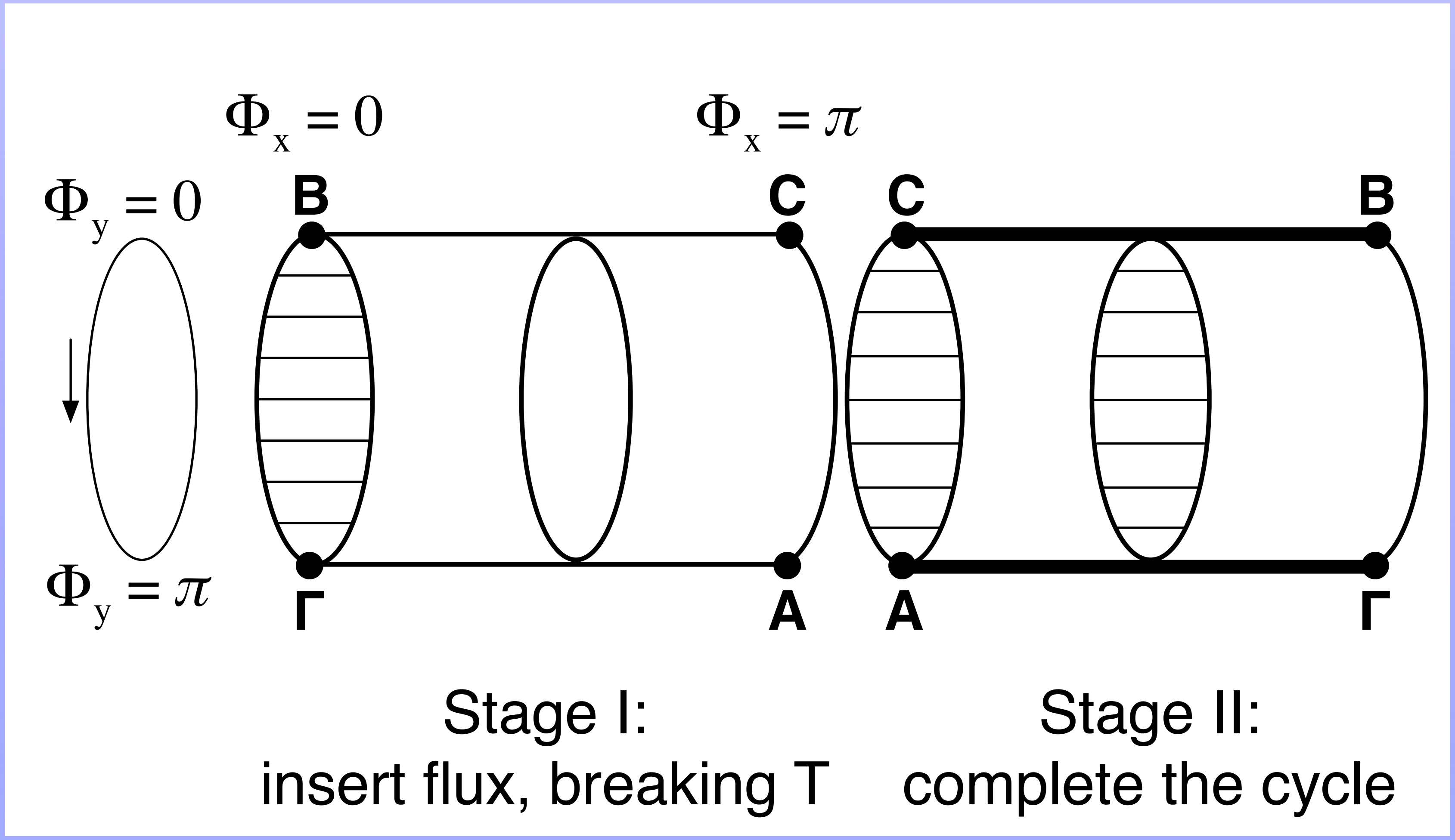
2. There is a simple prescription, given a gapped band structure, to compute whether the material is an ordinary or topological insulator.

3. The 2D phase transition to the ordinary insulator is split into two transitions separated by a metallic phase.

4. BFO and other incommensurate multiferroics show novel responses to nonzero-frequency electric fields.

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:



Interactions

The SQHE can be defined nonperturbatively for Slater determinants, as above.

However, we would like a definition using the full many-body wavefunction: This is difficult because time-reversal behaves differently with an even number of fermions (no Kramers degeneracies, etc.). In this sense the SQHE is "intrinsically fermionic."

Perturbatively, even though single-particle scattering is forbidden since

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

multiple-particle scattering is important, and the full SHE phase diagram can be obtained using a bosonization analysis.

1. There is a wide range of stability with interactions when the Z^2 index predicts stability without interactions.

2. interactions can actually stabilize the edge, even when the Z^2 index predicts an instability in the noninteracting case (**example: 2 pairs of edge modes**).