General Theory of Topological Insulators

Lyons 2009 Shoucheng Zhang, Stanford University

Colloborators

Stanford group: Xiaoliang Qi, Taylor Hughes, Zhong Wang, Jiangping Hu, Andrei Bernevig

Universality Classes of Topological Insulators

Classification of universality classes in critical phenomena depends on the symmetry and dimensionality. $4-\epsilon$ expansion. Effective field theory.

Classification of topological universality classes depends on dimensionality and discrete anti-unitary symmetries, such as C and T. Topological field theory.

Time reversal breaking (TRB) topological insulators in D=2:

• TKNN 1982: Hall conductance is given by the first Chern number in momentum space.

• Haldane 1988: QH without Landau levels

• Zhang, Hansson & Kivelson; Read 1987: Topological field theory based on the Chern-Simons term.

$$
S = \int d^2k \, da(k) \int d^3x \, A(x) \wedge dA(x)
$$

Widely spread mis-conception: topological states require TRB and 2D.

Generalization of the QSH topology state to four dimensions in 2001

A Four-Dimensional Generalization of the Quantum Hall Effect

Shou-Cheng Zhang and Jiangping Hu

We construct a generalization of the quantum Hall effect, where particles move in four dimensional space under a $SU(2)$ gauge field. This system has a macroscopic number of degenerate single particle states. At appropriate integer or fractional filling fractions the system forms an incompressible quantum liquid. Gapped elementary excitation in the bulk interior and gapless elementary excitations at the boundary are investigated.

Time Reversal Invariant Topological Insulators

- Zhang & Hu 2001: TRI topological insulator in D=4. => Root state of all TRI topological insulators.
- Murakami, Nagaosa & Zhang 2004: Spin Hall insulator with spin-orbit coupled band structure.
- Kane and Mele, Bernevig and Zhang 2005: Quantum spin Hall insulator with and without Landau levels.
- Fu, Kane & Mele, Moore and Balents, Roy 2007: Topological band theory based on Z2
- Qi, Hughes and Zhang 2008: Topological field theory based on F F dual.

TRB Chern-Simons term in D=2: A_0 =even, A_i =odd

$$
S_{2D} = \int d^2k \, da(k) \int d^3x \, A(x) \wedge dA(x)
$$

TRI Chern-Simons term in D=4: A_0 =even, A_i =odd

$$
S_{4D} = \int d^4k \, da(k) \wedge da(k) \int d^5x \, A(x) \wedge dA(x) \wedge dA(x)
$$

Dimensional reduction

• From 4D QHE to the 3D topological insulator

Zhang & Hu, Qi, Hughes & Zhang

$$
S_{4DQH} = \int d^4x dt \, \varepsilon^{\mu\nu\rho\sigma\tau} A_{\mu} F_{\nu\rho} F_{\sigma\tau}
$$

\n
$$
\Rightarrow \int d^3x dt \big(\int dx_5 A_5(x, t) \big) \varepsilon^{\nu\rho\sigma\tau} F_{\nu\rho} F_{\sigma\tau}
$$

\n
$$
\Rightarrow S_{3D} = \int d^3x dt \theta(x, t) \varepsilon^{\nu\rho\sigma\tau} F_{\nu\rho} F_{\sigma\tau}
$$

• From 3D axion action to the 2D QSH

$$
S_{3D} = \int d^3x dt e^{v\rho\sigma\tau} A_v \partial_\rho \theta \partial_\sigma A_\tau
$$

\n
$$
\Rightarrow \int d^2x dt e^{\rho\sigma\tau} (\int dz A_z(x, t)) \partial_\rho \theta \partial_\sigma A_\tau
$$

\n
$$
\Rightarrow S_{2D} = \int d^2x dt e^{\rho\sigma\tau} \partial_\sigma \phi \partial_\rho \theta A_\tau
$$

$$
J_{2D}^{\mu} = \frac{e}{2\pi^2} \varepsilon^{\mu\rho\sigma} \partial_{\sigma} \phi \partial_{\rho} \theta
$$

$$
\Leftrightarrow J_{1D}^{\mu} = \frac{e}{2\pi} \varepsilon^{\mu\sigma} \partial_{\sigma} \phi
$$

Goldstone & Wilzcek

Topological field theory and the family tree

• Topological field theory of the QHE: (Thouless et al, Zhang, Hansson and Kivelson)

$$
S = \int d^2k \, da(k) \int d^3x \, A(x) \wedge dA(x)
$$

• Topological field theory of the TI: (Qi, Hughes and Zhang, 2008)

$$
S = \int d^3k (a(k) \wedge da(k) + ..) \int d^4x dA(x) \wedge dA(x)
$$

General definition of a topological insulator

- Z2 topological band invariant in momentum space based on single particle states. (Fu, Kane and Mele, Moore and Balents, Roy)
- Topological field theory term in the effective action. Generally valid for interacting and disordered systems. Directly measurable physically. Relates to axion physics! (Qi, Hughes and Zhang)

$$
S_0 = \frac{1}{8\pi} \int d^3x dt \left(\varepsilon \mathbf{E}^2 - \frac{1}{\mu} \mathbf{B}^2 \right)
$$

- For a periodic system, the system is time reversal symmetric only when $\theta = 0$ = > trivial insulator
- $\theta = \pi$ => non-trivial insulator

$$
S_{\theta} = \left(\frac{\theta}{2\pi}\right) \left(\frac{\alpha}{2\pi}\right) \int d^3x dt \mathbf{E} \cdot \mathbf{B}
$$

$$
\alpha = \tfrac{e^2}{\hbar c}
$$

θ **term with open boundaries**

• θ=π implies QHE on the boundary with $\sigma_w = \frac{1}{2} \frac{e^2}{h}$

• $\theta = \pi$ implies QHE on the boundary with

$$
S_{\theta} = \frac{\theta}{2\pi} \frac{\alpha}{16\pi} \int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi} \frac{\alpha}{4\pi} \int d^3x dt \partial^{\mu} (\epsilon_{\mu\nu\rho\sigma} A^{\nu} \partial^{\rho} A^{\tau})
$$

• For a sample with boundary, it is only insulating when a small T-breaking field is applied to the boundary. The surface theory is a CS term, describing the half QH. • Each Dirac cone contributes $\sigma_{xy} = 1/2e^2/h$ to the QH.

Therefore, $\theta = \pi$ implies an odd number of Dirac cones on the surface!

• No-go theorem: it is not possible to construct a 2D model with an odd number of Dirac cones, in a system with T²=-1 TR symmetry. Surface states of a TI with $\theta = \pi$ is a holographic liquid! Wu, Bernevig & Zhang, Holographical principle

• TI surface states can not rust away by surface chemistry.

• For a sample with boundary, physics is not periodic in θ . However, T-invariant perturbations, like disorder, can induce plateau transitions with $\Delta\sigma_{xy}$ =1 e²/h, or $Δθ=2π$. For TI with $θ=π$, the surface QH can never disappear, no matter how strong the disorder! $\sigma_{xy} = 1/2$ e²/h => $\sigma_{xy} = -1/2$ e²/h.

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The Topological Magneto-Electric (TME) effect

• Equations of axion electrodynamics predict the robust TME effect.

• $P_3=θ/2π$ is the electro-magnetic polarization, microscopically given by the CS term over the momentum space. Change of $P_3=2^{nd}$ Chern number! (Qi, Hughes & Zhang)

$$
P_3(\theta_0) = \int d^3k \mathcal{K}^{\theta}
$$

=
$$
\frac{1}{16\pi^2} \int d^3k \epsilon^{\theta ijk} \operatorname{Tr} \left[\left(f_{ij} - \frac{1}{3} [a_i, a_j] \right) \cdot a_k \right]
$$

θ **terms in condensed matter and particle physics**

• Quantum spin chains:

$$
S[\theta] = \theta \int dt dx \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_t \mathbf{n}), \quad \theta = \frac{S}{2}
$$

• Quantum Hall transitions:

$$
S[\theta] = \theta \int d^2x \epsilon^{\mu\nu} \text{tr} \left(\mathbf{Q} \mathcal{D}_{\mu} \mathbf{Q} \mathcal{D}_{\nu} \mathbf{Q} \right), \quad \theta = -\frac{\sigma_{xy}}{8}
$$

Equivalence between the integral and the discrete topological invariants (Wang, Qi and Zhang, 0910.5954)

$$
\deg(f) = \frac{1}{2\pi} \int_{\phi=0}^{\phi=2\pi} d\theta(\phi) = \frac{1}{2\pi} \int_{\phi=0}^{\phi=2\pi} \frac{d\theta}{d\phi} d\phi = n \in \mathbb{Z}
$$

 $\deg(f) = N[f^{-1}(p), J_{f^{-1}(p)} > 0] - N[f^{-1}(p), J_{f^{-1}(p)} < 0]$

Equivalence between the integral and the discrete topological invariants (Wang, Qi and Zhang, 0910.5954)

$$
P_3 = \frac{1}{16\pi^2} \int d^3 \mathbf{k} \epsilon^{ijk} \text{Tr}\{ [f_{ij}(\mathbf{k}) - \frac{2}{3} i a_i(\mathbf{k}) \cdot a_j(\mathbf{k})] \cdot a_k(\mathbf{k}) \}
$$

\n
$$
2P_3(\text{mod } 2) = -\frac{1}{24\pi^2} \int d^3 \mathbf{k} \epsilon^{ijk} \text{Tr}[(B \partial_i B^{\dagger})(B \partial_j B^{\dagger})(B \partial_k B^{\dagger})] (\text{mod } 2)
$$

\n
$$
B_{\alpha\beta}(-\mathbf{k}) = \langle \mathbf{k}, \alpha | \Theta, -\mathbf{k}, \beta \rangle
$$

\n
$$
= -\langle -\mathbf{k}, \beta | \Theta, \mathbf{k}, \alpha \rangle
$$

\n
$$
A_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad A_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}
$$

\n
$$
= -B_{\beta\alpha}(\mathbf{k})
$$

$$
(-1)^{2P_3} = (-1)^{\sum_{m=1}^{N} \deg_2(g_m)} = \prod_m (-1)^{n_m}
$$

RHS=QHZ definition of TI, RHS=FKM definition of TI

I. Fractional charge effect in QSH insulators

- Motivation: when spin is not conserved, how to distinguish the QSH insulator from a trivial insulator *qualitatively*?
- QSH edge states consist of one left mover and one right mover (4=2+2)

I. Fractional charge effect in QSH insulators

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two possible mass terms

bond and site CDW $2\Delta \equiv m \cos \theta = m_1$ $V \equiv m \sin \theta = m_2$

Any mass term must breaks T

e.g., magnetic field

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Why "half" is special?

• Edge effective theory

$$
H_{\text{eff}} \ = \ \int\! \frac{dk}{2\pi} \left(\psi_{k\uparrow}^{\dagger} \psi_{k\downarrow}^{\dagger} \right) \left(\begin{array}{cc} v k & m_1 - im_2 \\ m_1 + im_2 & -vk \end{array} \right) \left(\begin{array}{c} \psi_{k\uparrow} \\ \psi_{k\downarrow} \end{array} \right)
$$

- Mass term $m_1 + im_2 = m(B)$ is time-reversal $m(B) = -m(-B)$ **odd.**
- This relation makes sure an *anti-phase* domain wall between **B** and **–B** carries half charge, no matter which direction is **B**.
- The magnetic domain wall is an "external field" detecting a T-invariant system. only QSH insulator can have half charge as the response

Half charge from the bulk effective theory

$$
J_{2D}^{\mu} = \frac{e}{2\pi^2} \varepsilon^{\mu\rho\sigma} \partial_{\sigma} \varphi \partial_{\rho} \theta
$$

$$
j^{\mu} = \frac{1}{8\pi} \epsilon^{\mu\nu\tau} \hat{\mathbf{n}} \cdot \partial_{\nu} \hat{\mathbf{n}} \times \partial_{\tau} \hat{\mathbf{n}}
$$

Experimental Proposal to measure the half charge

• Measurement of local charge density: single electron transistor (SET). (Kastner, RMP 64 849)

sourse \vdash QD \vdash drain **Gate** G M M F_g Charge in a confined region: $Q = -Ne + Q_b$ **Background** charge Q_b tunned by gate Tunneling occurs at $Q_b = e(N+1/2)$, N2**Z**

Creating an SET by magnetic double barrier

• Make an SET on QSHE edge by a "magnetic trap"

If magnetic field is rotated continuously….

The phase θ of mass term rotates continuously, leading to a shift of peaks. During each period of rotation, conductance peak also shifts by a period.

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- Experimental conditions: m(**B**) ' 3 meV for B=1T perpendicular to the HgTe quantum well.
- for B=1T, L>1 μ m, I_m ~100nm

$$
\begin{array}{c}\n\begin{array}{c}\n\uparrow \\
\hline\n\end{array}\n\end{array}
$$

• Summary: fractional charge in a magnetic domain wall provides a "quantized response property" of QSH insulator to an external field---magnetic domain wall.

Noise Experiments on the helical edge, (Maciejko et al)

II. Spin-charge separation in QSH insulators

• A π -flux tube threaded into a QSH insulator induces spin-charge separation. (Qi & Zhang, see similar proposal, Ran, Vishwanath, Lee) φ*(t*

 $\uparrow \sigma_{H} = +e^{2}/h$

 $\frac{1}{\sqrt{6}}$ $\frac{1}{\sigma}$ $\frac{1}{\sigma}$ $\frac{1}{\sigma}$ $\frac{1}{\sigma}$

• Start from decoupled case

• Flux threading in quantum Hall system. (Laughlin PRB

$$
\mathbf{j} \stackrel{\mathbf{1981}}{=} \sigma_H \mathbf{E} \times \hat{\mathbf{z}} \qquad \frac{\partial Q}{\partial t} = -\oint \mathbf{j} \cdot d\mathbf{n} = -\sigma_H \oint \mathbf{E} \cdot d\mathbf{l} = \frac{\sigma_H \partial \phi}{c \partial t}
$$

 $Q = \sigma_H \Delta \phi / c = -e \Delta \phi / 2\pi$

)

 E

Charge flux creates a Spinon

 $Q = 0, S = \hbar/2$

$$
Q=e, S=0
$$

Why is this phenomena unique for QSH? Topological Stability protected by T

- Spin charge separation of π flux remains true for generic QSH insulators.
- Time reversal symmetry provides a definition of spinon even when spin is not conserved
- Spinon states: *T2=-1*, electron number *N* even chargeon/holon state: *T2=1, N* odd.
- Conventional electron system $T^2 = (-1)^{N_F}$
- Spin-charge separated system (locally)

$$
T^2 = -(-1)^{N_F}\,
$$

- Once spin-charge separated object is realized, it is topologically stable.
- Spinon+electron=chargeon/holon

General definition of flux threading

- Spin flux pumps charge \rightarrow Easier to generalize
- Generalization of the spin flux $(\phi_{\uparrow} = -\phi_{\downarrow})$:
- Redefine hopping leads to parameterized Hamiltonian *H*Γ*(*θ*)*
- Operator Γ plays the role of spin S ,

- Conclusion 1: When θ goes from 0 to π in $H_{\Gamma}(\theta)$ (i.e., when threading a "Γ flux"), integer charge Q=Ne is pumped to the flux tube.
- Conclusion 2: For any two different choices Γ_1 and Γ_2 , the charge pumped during $\theta=0 \rightarrow \pi$ satisfies $N_1-N_2=0$ mod 2 l_1l_2 does not

• Thus the parity of charge pumped by the spin flux $(-1)^N$ is independent of the choice of Γ

A new way to define QSH insulator more generically

When odd number of charge is pumped by a spin flux, the system is a QSH insulator.

Numerical evidence on HgTe $model\rightarrow$

Experimental proposal

 Ω

20

 λ (nm)

40

60

Physical flux has finite size (penetration depth)

Break T, splitting of two mid-gap states

Spinon or holon/ chargeon tuned by chemical potential

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Seeing the magnetic monopole thru the mirror of a TME insulator, (Qi et al, Science 323, 1184, 2009)

An electron-monopole dyon becomes an anyon!

Dynamic axions in topological magnetic insulators

$$
\theta = \frac{1}{4\pi} \int d^3k \epsilon^{ijk} Tr \left[A_i \partial_j A_k + \frac{2}{3} A_i A_j A_k \right]
$$

• Hubbard interactions leads to anti-ferromagnetic order

$$
H = H_0 + U \sum_i \left(n_{iA\uparrow} n_{iA\downarrow} + n_{iB\uparrow} n_{iB\downarrow} \right) + V \sum_i n_{iA} n_{iB}
$$

• Effective action for dynamical axion

$$
\mathcal{S}_{\text{tot}} = \mathcal{S}_{\text{Maxwell}} + \mathcal{S}_{\text{topo}} + \mathcal{S}_{\text{axion}}
$$

= $\frac{1}{8\pi} \int d^3x dt (\epsilon \mathbf{E}^2 - \frac{1}{\mu} \mathbf{B}^2)$
+ $\frac{\alpha}{4\pi^2} \int d^3x dt (\theta_0 + \delta\theta) \mathbf{E} \cdot \mathbf{B}$
+ $g^2 J \int d^3x dt [(\partial_t \delta\theta)^2 - (v_i \partial_i \delta\theta)^2 - m^2 \delta\theta^2]$

Axionic polariton

• Attenuated total reflection => optical modulator?

Topological insulators and superconductors

Full pairing gap in the bulk, gapless Majorana edge and surface states

Qi, Hughes, Raghu and Zhang, PRL, 2009

Topological superconductors and superfluids

The BCS-BdG model for 2D equal spin pairing \Leftrightarrow model of 2D TI by BHZ

$$
H=\frac{1}{2}\int d^{2}x\tilde{\Psi}^{\dagger}\left(\begin{array}{ccc} \epsilon_{\mathbf{p}} & \Delta p_{+} & \\ \Delta p_{-} & -\epsilon_{\mathbf{p}} & \\ & & \epsilon_{\mathbf{p}} & -\Delta p_{-} \\ -\Delta p_{+} & -\epsilon_{\mathbf{p}} \end{array}\right)\tilde{\Psi}
$$

$$
\tilde{\Psi}(x) \ \equiv \ \Big(c_{\uparrow}(x), c_{\uparrow}^{\dagger}(x), c_{\downarrow}(x), c_{\downarrow}^{\dagger}(x) \Big)^T
$$

where $p_+ = p_x + ip_y$. The edge Hamiltonian is given by:

$$
H_{\text{edge}} = \sum_{k_y \geq 0} v_F k_y \left(\psi_{-k_y \uparrow} \psi_{k_y \uparrow} - \psi_{-k_y \downarrow} \psi_{k_y \downarrow} \right).
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forming a pair of Majorana fermions. Mass term breaks T symmetry=> topological protection!

Qi, Hughes, Raghu and Zhang, PRL, 2009 Schnyder et al, PRB, 2008 Kitaev Roy

Tanaka, Nagaosa et al, PRB, 2009 Sato, PRB, 2009

Probing He3B as a topological superfluid (Chung and Zhang, 2009)

The BCS-BdG model for He3B \Leftrightarrow Model of the 3D TI by Zhang et al

$$
\hat{\mathcal{H}}_{BdG} = \left[\begin{array}{ccc} \epsilon_{\mathbf{p}} - E_F & 0 & -\frac{\Delta}{p_F} \hat{p}_{-} & \frac{\Delta}{p_F} \hat{p}_{x} \\ 0 & \epsilon_{\mathbf{p}} - E_F & \frac{\Delta}{p_F} \hat{p}_{x} & \frac{\Delta}{p_F} \hat{p}_{+} \\ -\frac{\Delta}{p_F} \hat{p}_{+} & \frac{\Delta}{p_F} \hat{p}_{x} & -\epsilon_{\mathbf{p}} + E_F & 0 \\ \frac{\Delta}{p_F} \hat{p}_{x} & \frac{\Delta}{p_F} \hat{p}_{-} & 0 & -\epsilon_{\mathbf{p}} + E_F \end{array} \right]
$$

Surface Majorana state:

$$
\mathcal{H}_{surf} = v_F \boldsymbol{\sigma} \cdot (\mathbf{\hat{z}} \times \mathbf{p})
$$

Summary: discovery of new states of matter

Crystal Magnet S-wave superconductor

Quantum Spin Hall Topological insulators

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Strong to weak pairing transitionband inversion

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- This term defines and described the TI
- Frank Wilzcek: Topological insulator is a window into the universe! (Nature **458**, 129, 2009)

PHYSICS

A New State of Quantum Matter

Experiments show that electron spins can flow without dissipation in a novel electrical insulator.

Naoto Nagaosa

Quantum spin Hall effect shows
up in a quantum well insulator,
just as predicted

The effect, which occurs without a magnetic field, is a new and topological-Iv distinct electronic state.

Completing the table of Hall effects

Momentum space topology of the tight-binding model

$$
h(k) = d_a(k)\tau^a \qquad \qquad \sigma_{xy} = -\frac{1}{8\pi^2} \int \int dk_x dk_y \hat{\mathbf{d}} \cdot \partial_{\mathbf{x}} \hat{\mathbf{d}} \times \partial_{\mathbf{y}} \hat{\mathbf{d}}
$$

Topological quantum phase transition

Inversion symmetry breaking in zincblend lattices

Inversion breaking term comes in the form:

 $C(< k_z > +...$) $\{J_z, J_x^2 - J_y^2\}$, J_x, J_y, J_z -spin 3/2 matrices

which couples $E1+$, H1- and $E1-$, H1+ states and is a constant in quasi-2d systems

$$
H^{eff}_{\Delta} = \left(\begin{array}{cccc} 0 & 0 & 0 & -\Delta \\ 0 & 0 & \Delta & 0 \\ 0 & \Delta & 0 & 0 \\ -\Delta & 0 & 0 & 0 \end{array}\right)
$$

Gap closes at nodes away from $k=0$, gap reopens at non-zero value of M/2B. In the inverted regime, the helical edge state crossing is still robust.

Tight-binding model by X Dai, Z Fang, …

Quantum control of the electron spin

• The electron spin can be rotated by a pure AB flux, without any interaction with the electromagnetic field.

