Topological Insulators and Superconductors
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I. Topological Insulators and Band Theory

Unifying theme: bulk – boundary correspondence

- Integer Quantum Hall Effect
- 2D Quantum Spin Hall Insulator
- 3D Topological Insulator
- Topological Superconductivity, Majorana fermions

II. Summary and Outlook

- What we have accomplished
- Challenges for the Future

Thanks to Gene Mele, Liang Fu, Jeffrey Teo
The Insulating State

The Integer Quantum Hall State

IQHE with zero net magnetic field

Graphene with a periodic magnetic field $B(r)$ (Haldane PRL 1988)
Topological Band Theory

The distinction between a conventional insulator and the quantum Hall state is a topological property of the band structure

\( H(\mathbf{k}) : \text{Brillouin zone } (= \text{torus } T^2) \rightarrow \text{Bloch Hamiltonians with energy gap} \)

The set of \( N \) occupied Bloch wavefunctions \( \{|u_i(\mathbf{k})\rangle\}_{i=1}^{N} \) defines a \( U(N) \) vector bundle over the Brillouin zone torus.

Classified by the first Chern number (or TKNN invariant) \( \langle \text{Thouless et al, 1984} \rangle \)

Closely related to theory of electric polarization

- Berry connection \( A(\mathbf{k}) = -i \sum_{i=1}^{N} \langle u_i(\mathbf{k}) | \nabla_{\mathbf{k}} | u_i(\mathbf{k}) \rangle \)
- Berry curvature \( F(\mathbf{k}) = \nabla_{\mathbf{k}} \times A(\mathbf{k}) \)
- 1st Chern number \( n = \frac{1}{2\pi} \oint_{C} A \cdot d\mathbf{k} = \frac{1}{2\pi} \int_{T^2} F \cdot d^2\mathbf{k} \in \mathbb{Z} \)

Insulator : \( n = 0 \)
IQHE state : \( \sigma_{xy} = n e^2/h \)

The TKNN invariant can only change at a phase transition where the energy gap goes to zero.
Edge States

Gapless states must exist at the interface between different topological phases.

IQHE state $n=1$

Vacuum $n=0$

Edge states ~ skipping orbits

Dirac Equation:

$$H = -i \mathbf{v} \left( \sigma_x \partial_x + \sigma_y \partial_y \right) + M(x) \sigma_z$$

Haldane Model

Bulk – Boundary Correspondence:

$$\Delta n = \# \text{ Chiral Edge Modes}$$

Jackiw, Rebbi (1976)
Su, Schrieffer, Heeger (1980)
### Time Reversal Invariant $Z_2$ Topological Insulator

Time Reversal Symmetry:

$$\Theta H(\mathbf{k})\Theta^{-1} = H(-\mathbf{k})$$

$$\Theta \psi = i\sigma^y \psi^*$$

Kramers’ Theorem:

$$\Theta^2 = -1 \implies \text{All states doubly degenerate}$$

**$Z_2$ topological invariant ($\nu = 0,1$)** for 2D T-invariant band structures

Understand via Bulk-Boundary correspondence: **Edge States for $0 \leq k < \pi/a$**

#### $\nu = 0$: Conventional Insulator
- Even number of bands crossing Fermi energy

#### $\nu = 1$: Topological Insulator
- Odd number of bands crossing Fermi energy

Kramers degenerate at **time reversal invariant momenta**

$$\mathbf{k}^* = -\mathbf{k}^* + G$$
2D Quantum Spin Hall Insulator

I. Graphene  
Kane, Mele PRL ’05
- Intrinsic spin orbit interaction  
  ⇒ small (~10mK-1K) band gap
- $S_z$ conserved: “| Haldane model $|$ 2
- Edge states: $G = 2 e^2/h$

II. HgCdTe quantum wells
Theory: Bernevig, Hughes and Zhang, Science ’06  
Experiment: Konig et al. Science ‘07

$d < 6.3 \text{ nm}: \text{Normal band order}$

$d > 6.3 \text{ nm}: \text{Inverted band order}$

Conventional Insulator

$\prod \xi_{2n}(\Lambda_a) = +1$

QSH Insulator

$\prod \xi_{2n}(\Lambda_a) = -1$

G ~ $2e^2/h$ in QSHI
3D Topological Insulators

There are 4 surface **Dirac Points** due to Kramers degeneracy

Surface Brillouin Zone

\[ \Lambda_4 \quad \Lambda_3 \quad \Lambda_1 \quad \Lambda_2 \]

\[ k_x \quad k_y \]

2D Dirac Point

\[ E_k = \pm \sqrt{\Lambda_a} \]

\[ E_k = \pm \sqrt{\Lambda_b} \]

\[ k = \Lambda_a \quad k = \Lambda_b \]

**How do the Dirac points connect?** Determined by 4 bulk \( Z_2 \) topological invariants \( \nu_0 \); \( (\nu_1 \nu_2 \nu_3) \)

\( \nu_0 = 1 \) : Strong Topological Insulator

Fermi circle encloses **odd** number of Dirac points
Topological Metal :
1/4 graphene
Robust to disorder: impossible to localize

\( \nu_0 = 0 \) : Weak Topological Insulator

Fermi circle encloses **even** number of Dirac points
Related to layered 2D QSHI

Moore & Balents PRB 07
Roy, cond-mat 06
Fu, Kane & Mele PRL 07
Bi$_{1-x}$Sb$_x$ Theory: Predict Bi$_{1-x}$Sb$_x$ is a topological insulator by exploiting inversion symmetry of pure Bi, Sb (Fu, Kane PRL’07)

Experiment: ARPES (Hsieh et al. Nature ’08)

- Bi$_{1-x}$Sb$_x$ is a Strong Topological Insulator $\nu_0; (\nu_1, \nu_2, \nu_3) = 1; (111)$

- 5 surface state bands cross $E_F$ between $\Gamma$ and $M$

Bi$_2$Se$_3$


- $\nu_0; (\nu_1, \nu_2, \nu_3) = 1; (000)$: Band inversion at $\Gamma$

- Energy gap: $\Delta \sim 0.3$ eV: A room temperature topological insulator

- Simple surface state structure: Similar to graphene, except only a single Dirac point

Control $E_F$ on surface by exposing to NO$_2$
Surface Quantum Hall Effect

Orbital QHE: \( E=0 \) Landau Level for Dirac fermions. “Fractional” IQHE

\[
\sigma_{xy} = \frac{e^2}{2h} \left( n + \frac{1}{2} \right)
\]

\( \nu=1 \) chiral edge state

Anomalous QHE: Induce a surface gap by depositing magnetic material

\[
H_0 = \psi^\dagger (-i\nu \sigma \hat{\nabla} - \mu + \Delta_M \sigma_z)\psi
\]

Mass due to Exchange field

\[
\sigma_{xy} = \text{sgn}(\Delta_M) \frac{e^2}{2h}
\]

\( \uparrow E_{\text{gap}} = 2|\Delta_M| \)

Chiral Edge State at Domain Wall: \( \Delta_M \leftrightarrow -\Delta_M \)
Topological Magnetoelectric Effect

Qi, Hughes, Zhang ’08; Essin, Moore, Vanderbilt ’09

Consider a solid cylinder of TI with a magnetically gapped surface

\[ J = \sigma_{xy} E = \frac{e^2}{h} \left( n + \frac{1}{2} \right) E = M \]

Magnetoelectric Polarizability

\[ M = \alpha E \quad \alpha = \frac{e^2}{h} \left( n + \frac{1}{2} \right) \]

topological “\( \theta \) term”

\[ \Delta L = \alpha \mathbf{E} \cdot \mathbf{B} \]

\[ \alpha = \theta \frac{e^2}{2\pi h} \]

TR sym.: \( \theta = 0 \) or \( \pi \) mod 2\( \pi \)

The fractional part of the magnetoelectric polarizability is determined by the bulk, and independent of the surface (provided there is a gap)

Analogous to the electric polarization, \( P \), in 1D.

\[ \Delta L \text{ formula} \quad \text{“uncertainty quantum”} \]

<table>
<thead>
<tr>
<th>( d=1 ): Polarization ( P )</th>
<th>( P \cdot \mathbf{E} )</th>
<th>( \frac{e}{2\pi} \int_{BZ} \text{Tr} [\mathbf{A}] )</th>
<th>( e ) (extra end electron)</th>
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<tbody>
<tr>
<td>( d=3 ): Magnetoelectric polarizability ( \alpha )</td>
<td>( \alpha \mathbf{E} \cdot \mathbf{B} )</td>
<td>( \frac{e^2}{4\pi^2 h} \int_{BZ} \text{Tr} [\mathbf{A} \wedge d\mathbf{A} + \frac{2}{3} \mathbf{A} \wedge \mathbf{A} \wedge \mathbf{A}] )</td>
<td>( e^2 / h ) (extra surface quantum Hall layer)</td>
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Topological Superconductivity

BCS mean field theory: $\Psi^\dagger \Psi \Psi^\dagger \Psi \Rightarrow \braket{\Psi^\dagger \Psi^\dagger} \Psi \Psi = \Delta^* \Psi \Psi$

$$H = \frac{1}{2} \sum_k \left( \Psi^\dagger \Psi \right) H_{BdG} \left( \begin{array} {c} \Psi \\ \Psi^\dagger \end{array} \right)$$

Bogoliubov de Gennes Hamiltonian

$$H_{BdG} = \begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0 \end{pmatrix}$$

Intrinsic anti-unitary particle – hole symmetry

$$\Xi H_{BdG} \Xi^{-1} = -H_{BdG}$$

$$\Xi^2 = +1$$

Particle – hole redundancy

$$\varphi_{-E} = \Xi \varphi_E \Rightarrow \gamma_{E}^\dagger = \gamma_{-E}$$

Bloch - BdG Hamiltonians satisfy

$$\Xi H_{BdG}(k) \Xi^{-1} = -H_{BdG}(-k)$$

Topological classification problem similar to time reversal symmetry
1D $\mathbb{Z}_2$ Topological Superconductor: $\nu = 0, 1$ (Kitaev, 2000)

Bulk-Boundary correspondence: Discrete end state spectrum

Bulk:

- $\nu = 0$ “trivial”
- $\nu = 1$ “topological”

Boundary:

- $\Delta$
- $0$
- $-\Delta$

$\Gamma_E = \Gamma_{-E} = \Gamma_E^\dagger$

Majorana Fermion: Particle = Antiparticle $\gamma = \gamma^\dagger$

Real part of a Dirac fermion:

$$\gamma_1 = \Psi + \Psi^\dagger$$
$$\gamma_2 = -i(\Psi - \Psi^\dagger)$$

$\Psi = \gamma_1 + i\gamma_2$

$\gamma_1^2 = 1$

$\{\gamma_i, \gamma_j\} = 2\delta_{ij}$

“Half a state”

Two Majorana fermions define a single two level system

$$H = 2i\varepsilon_0 \gamma_1 \gamma_2 = \varepsilon_0 \Psi^\dagger \Psi$$

$\varepsilon_0$ empty

Majorana fermion bound state

Zero mode

$\Gamma_{E=0}^\dagger = \Gamma_{E=0} \equiv \gamma$
Periodic Table of Topological Insulators and Superconductors

Anti-Unitary Symmetries:
- Time Reversal: \[ \Theta H (k) \Theta^{-1} = + H (-k) ; \quad \Theta^2 = \pm 1 \]
- Particle-Hole: \[ \Xi H (k) \Xi^{-1} = - H (-k) ; \quad \Xi^2 = \pm 1 \]

Unitary (chiral) symmetry: \[ \Pi H (k) \Pi^{-1} = - H (k) ; \quad \Pi = \Theta \Xi \]

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<tr>
<th>( \Theta^2 )</th>
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<th>( \Pi^2 )</th>
<th>( d = 1 )</th>
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Schnyder, Ryu, Furusaki, Ludwig 2008
Kitaev, 2008

Altland-Zirnbauer Random Matrix Classes

Complex K-theory

Real K-theory

Bott Periodicity
Further Reading:

Hasan and Kane, Rev Mod Phys 82, 3045 (2010).


Major accomplishments:

Topological band theory of insulators and superconductors is well understood:

- Topological Invariants and bulk-boundary correspondence
- Robustness to disorder and weak interactions
- Electromagnetic and/or gravitational response

Rapid materials progress:

- Several materials have been identified and characterized experimentally.
- Even more materials have been predicted, based on band structure calculations.
- Detailed characterization of topological insulators via transport, optics and spectroscopy is developing.
Grand Challenges

• Perfect existing and new materials
• Design and implement heterostructure devices
• Find Majorana
• Classify and characterize many body topological phases
• Find applications for technology
Perfect New and Existing Materials

Real 3D topological insulator materials are not such great insulators. Electrical conductance is dominated by the bulk.

Challenge for materials theory in conjunction with experiments.

Success Story: Bi$_2$Te$_2$Se


Electrical resistivity in Bi$_2$Se$_3$

(Checkelsky et al ‘09)
Topological insulator devices

Requires control interfaces between materials. Challenge for materials theory and experiment

- **Topological Insulator – Trivial Insulator**
  - protect the surface states
  - control the surface state Fermi energy (modulation doping)

- **Topological Insulator – Magnetic Insulator**
  - achieve magnetically gapped surface states
  - anomalous quantum Hall effect
  - topological magnetoelectric effect

- **Topological Insulator – Superconductor**
  - achieve proximity induced superconductivity in the surface states.
Find Majorana

1937: Majorana publishes his modification of the Dirac equation that allows spin $\frac{1}{2}$ particles to be their own antiparticle.

1938: Majorana mysteriously disappears at sea

Observation of a Majorana fermion is among the great challenges of physics today

Potential Hosts:

Particle Physics: Neutrino (maybe)

- Allows neutrinoless double $\beta$-decay.

Condensed matter physics: Possible due to pair condensation $\left\langle \Psi^\dagger \Psi^\dagger \right\rangle \neq 0$

- $\nu=5/2$ Fractional quantum Hall effect
- Topological superconductivity

Topological Quantum Computation
What is the best way to achieve topological superconductivity?

• Exotic superconductors (superfluids)
  - Surface of $^4$He
  - p+ip superconductor (eg Sr$_2$RuO$_4$
  - Cu$_x$Bi$_2$Se$_3$ ?

• Ordinary superconductor heterostructures
  - superconductor – topological insulator
  - superconductor – semiconductor (eg InAs wire)

What are the most feasible experimental signatures of Majorana modes?
Classify and Characterize Interacting Topological States

Topological Insulators are like the Integer Quantum Hall effect. The single particle energy gap is correctly described by non-interacting band theory.

Interacting systems exhibit a much richer collection of fractional quantum Hall states. Understanding these was one of the greatest triumphs of many body physics.
What is a fractional topological insulator?

Classify possible states
Characterize quasiparticle excitations and surface states.

Need to develop new techniques:
- Parton construction?
- B-F theory?
- Entanglement spectrum?

What is the generalization of the bulk – boundary correspondence for interacting systems?