Organizing Principles for Understanding Matter

Symmetry

- Conceptual simplification
- Conservation laws
- Distinguish phases of matter by pattern of broken symmetries

Topology

- Properties insensitive to smooth deformation
- Quantized topological numbers
- Distinguish topological phases of matter

Interplay between symmetry and topology has led to a new understanding of electronic phases of matter.
Topology and Quantum Phases

Topological Equivalence: Principle of Adiabatic Continuity

Quantum phases with an energy gap are topologically equivalent if they can be smoothly deformed into one another without closing the gap.

Topologically distinct phases are separated by quantum phase transition.

Topological Band Theory

Describe states that are adiabatically connected to non-interacting fermions.

Classify single particle Bloch band structures

\[ H(k) : \text{Brillouin zone (torus)} \rightarrow \text{Bloch Hamiltonians with energy gap} \]

Band Theory of Solids e.g. Silicon

\[ E_g \sim 1 \text{ eV} \]
Topological Electronic Phases

Many examples of topological band phenomena

States adiabatically connected to independent electrons:

- Quantum Hall (Chern) insulators
- Topological insulators
- Weak topological insulators
- Topological crystalline insulators
- Topological (Fermi, Weyl and Dirac) semimetals …..

Many real materials and experiments

Topological Superconductivity

Proximity induced topological superconductivity

Majorana bound states, quantum information

Tantalizing recent experimental progress

Beyond Band Theory: Strongly correlated states

State with intrinsic topological order

- fractional quantum numbers
- topological ground state degeneracy
- quantum information
- Symmetry protected topological states
- Surface topological order …..

Much recent conceptual progress, but theory is still far from the real electrons
Topological Band Theory

I. Introduction
   - Insulating State, Topology and Band Theory

II. Band Topology in One Dimension
   - Berry phase and electric polarization
   - Su Schrieffer Heeger model:
     - domain wall states and Jackiw Rebbi problem
   - Thouless Charge Pump

III. Band Topology in Two Dimensions
   - Integer quantum Hall effect
   - TKNN invariant
   - Edge States, chiral Dirac fermions

IV. Generalizations
   - 3D Quantum Hall Effect
   - Topological Defects
   - Weyl Semimetal
**Insulator vs Quantum Hall state**

**The Insulating State**
- Atomic insulator

**2D Cyclotron Motion, \( \sigma_{xy} = \frac{e^2}{h} \)**

**What's the difference?**

**The Integer Quantum Hall State**
- Distinguished by Topological Invariant

**Landau levels**

**Topological Invariant**

\[ g_c \]

\[ \omega_c = \frac{h}{e} \]

**atomic energy levels**

\[ E_g = \hbar \omega_c \]
Topology

The study of geometrical properties that are insensitive to smooth deformations

Example: 2D surfaces in 3D

A closed surface is characterized by its genus, \( g = \# \text{ holes} \)

\( g = 0 \)

\( g = 1 \)

\( g \) is an integer topological invariant that can be expressed in terms of the gaussian curvature \( \kappa \) that characterizes the local radii of curvature

\[
\kappa = \frac{1}{r_1 r_2} > 0 \\
\kappa = 0 \\
\kappa < 0
\]

Gauss Bonnet Theorem:

\[
\int \kappa dA = 4\pi (1 - g)
\]

Band Theory of Solids

Bloch Theorem:

Lattice translation symmetry

\[ T(R)\psi = e^{i\mathbf{k} \cdot \mathbf{R}} \psi \quad \text{and} \quad \psi = e^{i\mathbf{k} \cdot \mathbf{r}} u(\mathbf{k}) \]

Bloch Hamiltonian

\[ H(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{r}} H e^{i\mathbf{k} \cdot \mathbf{r}} \quad \text{and} \quad H(\mathbf{k}) \left| u_n(\mathbf{k}) \right\rangle = E_n(\mathbf{k}) \left| u_n(\mathbf{k}) \right\rangle \]

\( \mathbf{k} \in \text{Brillouin Zone} \)

\( = \text{Torus, } T^d \)

Band Structure:

A mapping \( \mathbf{k} \mapsto H(\mathbf{k}) \)

(or equivalently to \( E_n(\mathbf{k}) \) and \( \left| u_n(\mathbf{k}) \right\rangle \))
Berry Phase

Phase ambiguity of quantum mechanical wave function

\[ |u(k)\rangle \rightarrow e^{i\phi(k)} |u(k)\rangle \]

Berry connection: like a vector potential

\[ A = -i \langle u(k)| \nabla_k |u(k)\rangle \]

\[ A \rightarrow A + \nabla_k \phi(k) \]

Berry phase: change in phase on a closed loop \( C \)

\[ \gamma_C = \oint_C A \cdot dk \]

Berry curvature:

\[ F = \nabla_k \times A \]

\[ \gamma_C = \int_S F d^2k \]

Famous example: eigenstates of 2 level Hamiltonian

\[ H(k) = d(k) \cdot \sigma = \begin{pmatrix} d_z & d_x - id_y \\ d_x + id_y & -d_z \end{pmatrix} \]

\[ H(k)|u(k)\rangle = +|d(k)||u(k)\rangle \]

\[ \gamma_C = \frac{1}{2} \left( \text{Solid Angle swept out by } \hat{d}(k) \right) \]
Topology in one dimension: Berry phase and electric polarization

Classical electric polarization:

\[ P = \frac{\text{dipole moment}}{\text{length}} \]

Bound charge density

\[ \rho_{\text{bound}} = \nabla \cdot P \]

End charge

\[ Q_{\text{end}} = P \cdot \hat{n} \]

Proposition: The quantum polarization is a Berry phase

\[ P = \frac{e}{2\pi} \oint_{BZ} A(k) \, dk \]

\[ A = -i \langle u(k) | \nabla_k | u(k) \rangle \]

BZ = 1D Brillouin Zone = S^1
Quantum Polarization

Bloch states $\psi_k(r) = e^{ikr} u_k(r)$ are defined for periodic boundary conditions.

Construct Localized Wannier Orbitals:

$$|\varphi(R)\rangle = \int_{BZ} \frac{dk}{2\pi} e^{-ik(R-r)} |u(k)\rangle$$

Wannier states are gauge dependent, but for a sufficiently smooth gauge, they are localized states associated with a Bravais Lattice point $R$.

$$P = e\langle \varphi(R)|r - R|\varphi(R)\rangle = \frac{ie}{2\pi} \int_{BZ} \langle u(k)|\nabla_k|u(k)\rangle$$
Gauge invariance and intrinsic ambiguity of $P$

- The end charge is not completely determined by the bulk polarization $P$ because integer charges can be added or removed from the ends:

$$Q_{\text{end}} = P \mod e$$

- The Berry phase is gauge invariant under continuous gauge transformations, but is not gauge invariant under “large” gauge transformations.

$$P \rightarrow P + en \quad \text{when} \quad |u(k)\rangle \rightarrow e^{i\phi(k)}|u(k)\rangle \quad \text{with} \quad \phi(\pi/a) - \phi(-\pi/a) = 2\pi n$$

Changes in $P$, due to adiabatic variation are well defined and gauge invariant

$$|u(k)\rangle \rightarrow |u(k, \lambda(t))\rangle$$

$$\Delta P = P_{\lambda=1} - P_{\lambda=0} = \frac{e}{2\pi} \oint_{C} A \, dk = \frac{e}{2\pi} \int_{S} F \, dk \, d\lambda$$

gauge invariant Berry curvature
Su Schrieffer Heeger Model

\[ H = \sum_i (t + \delta t) c_{Ai}^\dagger c_{Bi} + (t - \delta t) c_{Ai+1}^\dagger c_{Bi} + h.c. \]

\[ \delta t > 0 \]

\[ \delta t < 0 \]

\[ H(k) = d(k) \cdot \sigma \]

\[ d_x(k) = (t + \delta t) + (t - \delta t) \cos ka \]

\[ d_y(k) = (t - \delta t) \sin ka \]

\[ d_z(k) = 0 \]

Provided symmetry requires \( d_z(k) = 0 \), the states with \( \delta t > 0 \) and \( \delta t < 0 \) are distinguished by an integer winding number. Without extra symmetry, all 1D band structures are topologically equivalent.
Symmetries of the SSH model

“Chiral” Symmetry: \[ [H(k), \sigma_z] = 0 \] (or \( \sigma_z H(k) \sigma_z = -H(k) \))

- Artificial symmetry of polyacetylene. Consequence of bipartite lattice with only A-B hopping:
  - Requires \( d_z(k) = 0 \): integer winding number
  - Leads to particle-hole symmetric spectrum:
    \[ H\sigma_z |\psi_E\rangle = -E\sigma_z |\psi_E\rangle \implies \sigma_z |\psi_E\rangle = |\psi_E\rangle \]

Reflection Symmetry: \( H(-k) = \sigma_x H(k) \sigma_x \)

- Real symmetry of polyacetylene.
- Allows \( d_z(k) \neq 0 \), but constrains \( d_x(-k) = d_x(k), d_{y,z}(-k) = -d_{y,z}(k) \)
- No p-h symmetry, but polarization is quantized: \( Z_2 \) invariant
  \[ P = 0 \text{ or } e/2 \mod e \]
Domain Wall States

Single Particle Spectrum: zero mode

\[ t - \delta t = 0 : \text{decoupled } E=0 \text{ state} \]
\[ t - \delta t >0 : \text{protected by particle hole symmetry} \]

Many body ground state: charge fractionalization

Occupied:
charge \(+e/2\)

Empty:
charge \(-e/2\)

Splitting the electron:

\[ \text{split} \]
Jackiw Rebbi Problem

Low energy continuum theory for $\delta t \ll t$:

Focus on low energy states with $k \sim \pi/a$

$$H = -i\nu_F \sigma_x \partial_x + m(x)\sigma_y$$

$$\nu_F = ta; \quad m = 2\delta t$$

Massive 1+1 D Dirac Hamiltonian

Zero mode at boundary where $m(x)$ changes sign:

Solve $$(i/\nu_F)\sigma_x H \psi_0 = 0 \rightarrow \partial_x \psi_0 = -m(x)\sigma_z \psi_0 / \nu_F$$

Domain wall bound state $\psi_0$

$$E_{\text{gap}} = 2|m|$$

$$\psi_0(x) = e^{-\int_0^x m(x')dx'/\nu_F} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
Thouless Charge Pump

The integer charge pumped across a 1D insulator in one period of an adiabatic cycle is a topological invariant that characterizes the cycle.

\[ H(k, t + T) = H(k, t) \]

\[ \Delta P = \frac{e}{2\pi} \left( \oint A(k, T) dk - \oint A(k, 0) dk \right) = ne \]

\[ n = \frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} \mathbf{F} dk dt \]

The integral of the Berry curvature defines the first Chern number, \( n \), an integer topological invariant characterizing the occupied Bloch states, \(|u(k, t)\rangle\).

In the 2 band model, the Chern number is related to the solid angle swept out by \( \hat{\mathbf{d}}(k, t) \), which must wrap around the sphere an integer \( n \) times.

\[ n = \frac{1}{4\pi} \int_{-\pi/2}^{\pi/2} dk dt \hat{\mathbf{d}} \cdot (\partial_k \hat{\mathbf{d}} \times \partial_t \hat{\mathbf{d}}) \]
**TKNN Invariant**

For 2D band structure, define

\[ A(k) = -i \langle u(k) | \nabla_k | u(k) \rangle \]

\[
BZ = \begin{array}{c|c}
\pi/a & k_y \\
\hline
\pi/a & k_y \\
\end{array}
\begin{array}{c|c}
-\pi/a & C_1 \\
\hline
-\pi/a & C_2 \\
\end{array}
\]

BZ

Physical meaning: Quantized Hall conductivity

\[ \sigma_{xy} = n \frac{e^2}{h} \]

Laughlin argument: Thread flux \( \Delta \Phi = \frac{h}{e} \)

Thouless pump: Cylinder with circumference 1 lattice constant (a)

\[ \Phi \text{ plays role of } k_y \quad \Delta \Phi = \frac{h}{e} \quad \Rightarrow \quad \Delta k_y = 2\pi / a \quad \Delta P = ne \]

Alternative calculation: compute \( \sigma_{xy} \) via Kubo formula
Realizing a non trivial Chern number

Integer quantum Hall effect:

Landau levels

Chern insulator:

e.g. Haldane model

Band Inversion Paradigm
Lattice model for Chern insulator

\[ H(k) = \tau_z \left( 2t_0 \left[ \cos k_x a + \cos k_y a \right] + \Delta E_{sp} \right) \]
\[ + 2t_{sp} \left( \tau_x \sin k_x a + \tau_y \sin k_y a \right) = \mathbf{d}(k) \cdot \tau \]

Square lattice model with inversion of bands with \( s \) and \( p_x + ip_y \) symmetry near \( \Gamma \)

\[ |\Delta E_{sp}| > 4t : \text{Uninverted Trivial Insulator} \]
\[ |\Delta E_{sp}| < 4t : \text{Inverted Chern Insulator} \]

Regularized continuum model for Chern insulator

\[ H(k) = \tau_z \left( m + ak^2 \right) + \nu \left( k_x \tau_x + k_y \tau_y \right) = \mathbf{d}(k) \cdot \tau \]

Inverted near \( k = 0 \) for \( m < 0 \). Uninverted for \( m > \infty \)

\[ m = 4t_0 - \Delta E_{sp} \]
\[ a = t_0 a \]
\[ \nu = 2t_{sp} a \]
Edge States

Gapless states at the interface between topologically distinct phases

IQHE state
\[ n=1 \]

Vacuum
\[ n=0 \]

Edge states ~ skipping orbits
Lead to quantized transport

Band inversion transition : Dirac Equation

\[ H = v_F \left( -i\sigma_x \partial_x + \sigma_y k_y \right) + m(x)\sigma_z \]

\[ \psi_0(x) \sim e^{ik_yy}e^{-\int_0^x m(x')dx'/v_F} \]

\[ E_0(k_y) = v_F k_y \]

Chiral Dirac fermions are unique 1D states :

“One way” ballistic transport, responsible for quantized conductance. Insensitive to disorder, impossible to localize

Fermion Doubling Theorem :
Chiral Dirac Fermions can not exist in a purely 1D system.
Bulk - Boundary Correspondence

$\Delta N = N_R - N_L$ is a topological invariant characterizing the boundary.

$N_R \ (N_L) = \# \text{ Right (Left) moving chiral fermion branches intersecting } E_F$

$\Delta N = 1 - 0 = 1$

$\Delta N = 2 - 1 = 1$

**Bulk – Boundary Correspondence:**

The boundary topological invariant $\Delta N$ characterizing the gapless modes = Difference in the topological invariants $\Delta n$ characterizing the bulk on either side
Single particle edge spectrum: "one way edge states"

Vacuum: $n=0$

QHE state: $n=1$

Many body edge spectrum: "chiral Fermi liquid"

- Free Dirac fermion conformal field theory: $H = -i\nu \psi^\dagger \partial_x \psi$

- Quantized electrical conductance: $G = \frac{dI}{dV} = \nu \frac{e^2}{h}$

- Quantized thermal conductance: $\kappa = \frac{dI}{dT} = c \frac{\pi^2 \hbar^2 k_B^2 T}{3h}$

Chiral Anomaly:

In the presence of an electric field, the charge at the edge is not conserved

$$\frac{dQ_+}{dt} = \frac{e}{2\pi} \frac{dk}{dt} = \frac{e}{2\pi} \frac{eE}{\hbar} = \sigma_{xy} E$$
Generalizations

$d=4$: 4 dimensional generalization of IQHE

$$A_{ij} = \langle u_i(k) | \nabla_k | u_j(k) \rangle \cdot dk$$  Non-Abelian Berry connection 1-form

$$F = dA + A \wedge A$$  Non-Abelian Berry curvature 2-form

$$n = \frac{1}{8\pi^2} \int_{\mathbb{R}^4} \text{Tr}[F \wedge F] \in \mathbb{Z}$$  2nd Chern number = integral of 4-form over 4D BZ

Boundary states: 3+1D Chiral Dirac fermions

Higher Dimensions: “Bott periodicity”  $d \rightarrow d+2$

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More generally, the 3 independent Chern numbers \((n_x, n_y, n_z)\) define a reciprocal lattice vector \(\mathbf{G}\) that characterizes a family of lattice planes.

\[
\sigma_{ij} = \frac{e^2}{2\pi h} \varepsilon_{ijk} G_k
\]
Topological Defects

Consider insulating Bloch Hamiltonians that vary slowly in real space

$$H = H(k, s)$$

1 parameter family of 3D Bloch Hamiltonians

2nd Chern number: $$n = \frac{1}{8\pi^2} \int_{T^3 \times S^1} \text{Tr}[F \wedge F]$$

Generalized bulk-boundary correspondence:

$$n$$ specifies the number of chiral Dirac fermion modes bound to defect line

Example: dislocation in 3D layered IQHE

$$n = \frac{1}{2\pi} G_c \cdot B$$

3D Chern number
(vector \( \perp \) layers)

Are there other ways to engineer 1D chiral dirac fermions?
Weyl Semimetal

Gapless “Weyl points” in momentum space are topologically protected in 3D

A sphere in momentum space can have a Chern number:

\[ n_S = \int_S d^2 k F(k) \in \mathbb{Z} \]

\( n_s = +1 \): S must enclose a degenerate Weyl point:

Magnetic monopole for Berry flux

\[ H(k_0 + q) = v(q_x \sigma_x + q_y \sigma_y + q_z \sigma_z) \]

( or \( v_{ia} q_i \sigma_a \) with \( \det[v_{ia}] > 0 \) )

Total magnetic charge in Brillouin zone must be zero: Weyl points must come in +/- pairs.
Surface Fermi Arc

\[ n_1 = n_2 = 0 \]

\[ n_0 = 1 \]

Surface BZ
Chiral Anomaly

In the presence of $E$ and $B$, the charge at one (or the other) Weyl point is not conserved:

$$\frac{dn_+}{dt} = - \frac{dn_-}{dt} = \frac{e^2}{h^2} \mathbf{E} \cdot \mathbf{B}$$
Topological Band Theory II: Time reversal symmetry

I. Graphene
   - Haldane model
   - Time reversal symmetry and Kramers’ theorem

II. 2D quantum spin Hall insulator
   - $\mathbb{Z}_2$ topological invariant
   - Edge states
   - HgCdTe quantum wells, expts

III. Topological Insulators in 3D
   - Weak vs strong
   - Topological invariants from band structure

IV. The surface of a topological insulator
   - Dirac Fermions
   - Absence of backscattering and localization
   - Quantum Hall effect
   - $\theta$ term and topological magnetoelectric effect
Two band model: \[ H = - t \sum_{<ij>} c_A^\dagger c_B \]

\[ H(k) = d(k) \cdot \sigma \]

\[ E(k) = \pm |d(k)| \]

\[ d(k) = \sum_{j=1}^{3} - t (\hat{x} \cos k \cdot r_j + \hat{y} \sin k \cdot r_j) \]

Inversion and Time reversal symmetry require \( d_z(k) = 0 \)

2D Dirac points at \( k = \pm K \) point vortices in \((d_x, d_y)\)

\[ H(\pm K + q) = \nabla \sigma \cdot q \] Massless Dirac Hamiltonian

Berry's phase \( \pi \) around Dirac point
Topological gapped phases in Graphene

Break P or T symmetry:

\[ H(\pm K + q) = vq \sigma + m\pm \sigma_z \]

\[ E(q) = \pm \sqrt{v^2|q|^2 + m^2} \]

\[ n = \# \text{times } \hat{d}(k) \text{ wraps around sphere} \]

1. **Broken P**: eg Boron Nitride

   \[ m_+ = m_- \]

   Chern number \( n=0 \) : Trivial Insulator

2. **Broken T**: Haldane Model ’88

   \[ m_+ = - m_- \]

   Chern number \( n=1 \) : Quantum Hall state
Energy gaps in graphene:

\[ H = \frac{v_F}{2} \sigma \cdot p + V \]

\[ E(p) = \pm \sqrt{v_F^2 p^2 + \Delta^2} \]

1. Staggered Sublattice Potential (e.g. BN)

\[ V = \Delta_{CDW} \sigma^z \]

Broken Inversion Symmetry

2. Periodic Magnetic Field with no net flux (Haldane PRL ’88)

\[ V = \Delta_{Haldane} \sigma^z \tau^z \]

Broken Time Reversal Symmetry
Quantized Hall Effect \( \sigma_{xy} = \text{sgn} \Delta \frac{e^2}{h} \)

3. Intrinsic Spin Orbit Potential

\[ V = \Delta_{SO} \sigma^z \tau^z S^z \]

Respects ALL symmetries
Quantum Spin-Hall Effect
Quantum Spin Hall Effect in Graphene

The intrinsic spin orbit interaction leads to a small (~10mK-1K) energy gap

Simplest model:

\[ H = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} = \begin{pmatrix} H_{\text{Haldane}} & 0 \\ 0 & H_{\text{Haldane}}^* \end{pmatrix} \]

Bulk energy gap, but gapless edge states

“Spin Filtered” or “helical” edge states

Edge band structure

Edge states form a unique 1D electronic conductor

- HALF an ordinary 1D electron gas
- Protected by Time Reversal Symmetry
Quantum Spin Hall Effect in HgTe quantum wells

Theory: Bernevig, Hughes and Zhang, Science '06

d < 6.3 nm : Normal band order

d > 6.3 nm : Inverted band order

Conventional Insulator

Quantum spin Hall Insulator with topological edge states

\[ \prod \xi_{2n}(\Lambda_\alpha) = +1 \]

\[ \prod \xi_{2n}(\Lambda_\alpha) = -1 \]

BHZ Model : 4 band T-invariant band inversion model

\[ H(k) = \tau_z (m + ak^2) + \nu (k_x \tau_x \sigma_x + k_y \tau_x \sigma_y) \]
Experiments on HgCdTe quantum wells

Measured conductance $2e^2/h$ independent of W for short samples ($L<L_{\text{in}}$)
Time Reversal Symmetry: \([H, \Theta] = 0\)

Anti Unitary time reversal operator: \(\Theta \psi = e^{i\pi S^y/\hbar} \psi^*\)

Spin \(\frac{1}{2}: \Theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix} \quad \Theta^2 = -1\)

Kramers’ Theorem: for spin \(\frac{1}{2}\) all eigenstates are at least 2 fold degenerate

Proof: for a non degenerate eigenstate

- \(\Theta |\chi\rangle = c |\chi\rangle\)
- \(\Theta^2 |\chi\rangle = \pm c^2 |\chi\rangle\)
- \(\Theta^2 \neq -1\)

Consequences for edge states:

States at “time reversal invariant momenta” \(k^*=0\) and \(k^*=-\pi/a\) are degenerate.

The crossing of the edge states is protected, even if spin conservation is violated.

Absence of backscattering, even for strong disorder. No Anderson localization
Time Reversal Invariant $\mathcal{Z}_2$ Topological Insulator

2D Bloch Hamiltonians subject to the T constraint $\Theta H(k) \Theta^{-1} = H(-k)$ with $\Theta^2 = -1$ are classified by a $\mathcal{Z}_2$ topological invariant ($\nu = 0, 1$).

Understand via Bulk-Boundary correspondence: \textbf{Edge States for } 0 < k < \pi/a\textbf{.}
Physical Meaning of $\mathbb{Z}_2$ Invariant

Sensitivity to boundary conditions in a multiply connected geometry

$\nu = N$ IQHE on cylinder: Laughlin Argument

$\Delta \Phi = \phi_0 = h/e$

$\Delta Q = Ne$

Flux $\phi_0 \Rightarrow$ Quantized change in Electron Number at the end.

Quantum Spin Hall Effect on cylinder

$\Delta \Phi = \phi_0 / 2$

Flux $\phi_0 / 2 \Rightarrow$ Change in Electron Number Parity at the end, signaling change in Kramers degeneracy.
Formula for the $\mathcal{K}_2$ invariant

- Bloch wavefunctions: $|u_n(k)\rangle$ (N occupied bands)

- $T$ - Reversal Matrix: $w_{mn}(k) = \langle u_m(k)|\Theta|u_n(-k)\rangle \in U(N)$

- Antisymmetry property: $\Theta^2 = -1 \Rightarrow w(k) = -w^T(-k)$

- $T$ - invariant momenta: $k = \Lambda_a = -\Lambda_a \Rightarrow w(\Lambda_a) = -w^T(\Lambda_a)$

- Pfaffian: $\det[w(\Lambda_a)] = (\text{Pf}[w(\Lambda_a)])^2$ e.g. $\det\begin{pmatrix} 0 & z \\ -z & 0 \end{pmatrix} = z^2$

- Fixed point parity: $\delta(\Lambda_a) = \frac{\text{Pf}[w(\Lambda_a)]}{\sqrt{\det[w(\Lambda_a)]}} = \pm 1$

- Gauge dependent product: $\delta(\Lambda_a)\delta(\Lambda_b)$

  “time reversal polarization” analogous to $\frac{e}{2\pi}\int A(k)dk$

- $\mathbb{Z}_2$ invariant: $(-1)^\nu = \prod_{a=1}^{4} \delta(\Lambda_a) = \pm 1$

  Gauge invariant, but requires continuous gauge
1. $S_z$ conserved: independent spin Chern integers:

$$n_{↑} = - n_{↓} \quad (\text{due to time reversal})$$

Quantum spin Hall Effect:

$$\nu = n_{↑,↓} \mod 2$$

2. Inversion (P) Symmetry: determined by Parity of occupied 2D Bloch states

$$P|\psi_n(\Lambda_a)\rangle = \xi_n(\Lambda_a)|\psi_n(\Lambda_a)\rangle$$

$$\xi_n(\Lambda_a) = \pm 1$$

In a special gauge:

$$\delta(\Lambda_a) = \prod_n \xi_n(\Lambda_a)$$

$$(-1)^\nu = \prod_{a=1}^{4} \prod_n \xi_{2n}(\Lambda_a)$$

Allows a straightforward determination of $\nu$ from band structure calculations.
3D Topological Insulators

There are 4 surface Dirac Points due to Kramers degeneracy

\[ \begin{align*}
\Lambda_4 & \quad \Lambda_3 \\
\Lambda_1 & \quad \Lambda_2
\end{align*} \]

Surface Brillouin Zone

2D Dirac Point

\[ \begin{align*}
E & = \mathcal{E}_k \\
k_x & = \mathcal{E}_k \\
k_y & = \mathcal{E}_k
\end{align*} \]

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

$\nu_0 = 0$: Weak Topological Insulator

Related to layered 2D QSHI; $(\nu_1 \nu_2 \nu_3) \sim$ Miller indices

Fermi surface encloses even number of Dirac points

$\nu_0 = 1$: Strong Topological Insulator

Fermi circle encloses odd number of Dirac points

Topological Metal:

1/4 graphene

Berry’s phase $\pi$

Robust to disorder: impossible to localize
Topological Invariants in 3D

1. 2D → 3D : Time reversal invariant planes

The 2D invariant

\[ (-1)^{\nu} = \prod_{a=1}^{4} \delta(\Lambda_a) \quad \delta(\Lambda_a) = \frac{\text{Pf}[w(\Lambda_a)]}{\sqrt{\det[w(\Lambda_a)]}} \]

Each of the time reversal invariant planes in the 3D Brillouin zone is characterized by a 2D invariant.

Weak Topological Invariants (vector):

\[ (-1)^{\nu_i} = \prod_{a=1}^{4} \delta(\Lambda_a) \bigg|_{k_i=0} \quad \mathbf{G}_v = \frac{2\pi}{a} (\nu_1, \nu_2, \nu_3) \]

“mod 2” reciprocal lattice vector indexes lattice planes for layered 2D QSHI

Strong Topological Invariant (scalar)

\[ (-1)^{\nu_o} = \prod_{a=1}^{8} \delta(\Lambda_a) \]
2. 4D → 3D : Dimensional Reduction

Add an extra parameter, \( k_4 \), that smoothly connects the topological insulator to a trivial insulator (while breaking time reversal symmetry)

\( H(k, k_4) \) is characterized by its second Chern number

\[
n = \frac{1}{8\pi^2} \int d^4 k \text{Tr}[F^\wedge F]
\]

\( n \) depends on how \( H(k) \) is connected to \( H_0 \), but due to time reversal, the difference must be even.

\[
\nu_0 = n \mod 2
\]

Express in terms of Chern Simons 3-form:

\[
\text{Tr}[F^\wedge F] = dQ_3
\]

\[
\nu_0 = \frac{1}{4\pi^2} \int d^3 k Q_3(k) \mod 2
\]

\[
Q_3(k) = \text{Tr}[A^\wedge dA + \frac{2}{3} A^\wedge A^\wedge A]
\]

Gauge invariant up to an even integer.
Topological Superconductivity

0. ... from last time: The surface of a topological insulator
1. Bogoliubov de Gennes Theory
2. Majorana bound states, Kitaev model
3. Topological superconductor
4. Periodic Table of topological insulators and superconductors
5. Topological quantum computation
6. Proximity effect devices
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: $\Delta \sim .3$ 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$_2$
Unique Properties of Topological Insulator Surface States

“Half” an ordinary 2DEG ; ¼ Graphene

Spin polarized Fermi surface

- Charge Current ~ Spin Density
- Spin Current ~ Charge Density

\(\pi\) Berry’s phase

- Robust to disorder
- Weak Antilocalization
- Impossible to localize, Klein paradox

Broken symmetry can lead to surface energy gap:

- Quantum Hall state, topological magnetoelectric effect (broken Time Reversal)
  Fu, Kane '07; Qi, Hughes, Zhang '08, Essin, Moore, Vanderbilt '09

- Superconducting state (broken gauge symmetry)
  Fu, Kane '08
Surface Quantum Hall Effect

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

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

Anomalous QHE: Induce a surface gap by depositing magnetic material

\[
H_0 = \psi^\dagger (-i v \sigma \cdot \nabla - \mu + \Delta_M \sigma_z) \psi
\]

Mass due to Exchange field

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

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

\[
E_{\text{gap}} = 2|\Delta_M|
\]
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

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

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.

**d=1 : Polarization P**

\[
P \cdot E = \frac{e}{2\pi} \int_{BZ} \text{Tr}[A]
\]

“uncertainty quantum” (extra end electron)

**d=3 : Magnetoelectric polarizability \(\alpha\)**

\[
\alpha E \cdot B = \frac{e^2}{4\pi^2 h} \int_{BZ} \text{Tr}[A^\wedge dA + \frac{2}{3} A^\wedge A^\wedge A]
\]

\[
e^2 / h \quad \text{(extra surface quantum Hall layer)}
\]
Strong Interactions

Topological Insulator coupled to compact U(1) gauge field, A

For a compact gauge field, magnetic monopoles are excitations in the theory. Useful diagnostic for strongly interacting theories.

Low energy theory for A:  \( \theta \) term  

\[
S = i\theta N \\
N = \frac{1}{32\pi^2} \int d^3x d\tau \epsilon_{\mu\nu\lambda\rho} F_{\mu\nu} F_{\lambda\rho} \in \mathbb{Z}
\]

- Time reversal symmetry:  \( \theta = 0 \) or \( \pi \mod 2\pi \).  \( \theta = \pi \mod 2\pi \) for electron TI

- Witten Effect: Magnetic monopoles are charged  
  \[
  Q = \frac{\theta}{2\pi} e
  \]

- Monopoles (or dyons) are bosons with half integer charge  
  \[
  Q = e \left( n + \frac{1}{2} \right)
  \]
Can the surface of a TI be gapped without breaking symmetry?

Pass monopole from inside to outside of TI:

\[ Q = \frac{e}{2} \text{ boson} \]

Break T at surface:

\[ \sigma_{xy} = \frac{e^2}{2h} : \text{ charge } \frac{e}{2} \text{ flows away on surface} \]

Superconductor at surface:

Charge conservation is violated at surface

Keep U(1) and T at surface:

Charge e/2 stays at surface: Requires a topologically ordered surface state with e/2 quasiparticle
Requirements for a Topological Surface Phase on TI

It should be impossible in 2D if symmetry is preserved, but if symmetry is broken there should be a 2D state with the same topological order

Broken T: Topo – M slab

A 2D Non-Abelian quantum Hall state with

- Hall conductance $\nu \frac{e^2}{h}; \quad \nu = 1/2$
- Thermal Hall cond. $c \pi^2 k_B^2/6h; \quad c = 1/2$

Theories of symmetry preserving gapped state:

Related to Moore-Read (Pfaffian) state of FQHE at $\nu=1/2$

- “T-Pfaffian state” Bonderson, Nayak, Qi ‘13 ; Chen, Fidkowski, Vishwanath ‘13
- “Moore-Read/antisemion state” Metlitski, Kane, Fisher ‘13 ; Wang, Potter, Senthil ‘13
BCS Theory of Superconductivity

mean field theory: \[ \Psi^\dagger \Psi \Psi^\dagger \Psi \Rightarrow \langle \Psi^\dagger \Psi^\dagger \rangle \Psi \Psi = \Delta^* \Psi \Psi \]

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

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

\[ \varphi_{-E} = \Xi \varphi_E \Rightarrow \varphi_{E}^\dagger = \varphi_{-E} \]

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

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

Real part of a Dirac fermion:
$$\begin{align*}
\gamma_1 &= \Psi + \Psi^\dagger \\
\gamma_2 &= -i(\Psi - \Psi^\dagger)
\end{align*}$$

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

$\gamma_i^2 = 1$  
$\gamma_i, \gamma_j = 2\delta_{ij}$

"Half a state"

Two Majorana fermions define a single two level system

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

Zero mode
$$\Gamma^{\dagger}_{E=0} = \Gamma_{E=0} \equiv \gamma$$

Majorana fermion bound state
Kitaev Model for 1D p wave superconductor

\[ H - \mu N = \sum_{i} t (c_{i}^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_{i}) - \mu c_{i}^{\dagger} c_{i} + \Delta (c_{i} c_{i+1} + c_{i+1}^{\dagger} c_{i}^{\dagger}) \]

\[ = \sum_{k} \left( c_{k}^{\dagger} c_{-k}^{\dagger} \right) H_{BdG}(k) \left( \begin{array}{c} c_{k} \\ c_{-k}^{\dagger} \end{array} \right) \]

\[ H_{BdG}(k) = \tau_{z} (2t \cos k - \mu) + \tau_{x} \Delta \sin k = \mathbf{d}(k) \cdot \tau \]

\[ |\mu| > 2t : \text{Strong pairing phase} \]
\[ \text{trivial superconductor} \]

\[ |\mu| < 2t : \text{Weak pairing phase} \]
\[ \text{topological superconductor} \]

Similar to SSH model, except different symmetry:
\[ (d_{x}, d_{y}, d_{z})_{k} = (-d_{x}, -d_{y}, d_{z})_{-k} \]
Majorana Chain

\[ c_i \rightarrow \gamma_{1i} + i\gamma_{2i} \]

\[ H = 2i \sum_{i} t_1 \gamma_{1i} \gamma_{2i} + t_2 \gamma_{2i} \gamma_{1i+1} \]

For \( \Delta = t \): nearest neighbor Majorana chain

\[ t_1 = \mu, \quad t_2 = 2t \]

\[ \mu c_i^\dagger c_i \rightarrow 2i\mu \gamma_{1i} \gamma_{2i} \]

\[ t (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) \rightarrow 2it(\gamma_{1i} \gamma_{2i+1} - \gamma_{2i} \gamma_{1i+1}) \]

\[ \Delta (c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger) \rightarrow 2i\Delta (\gamma_{1i} \gamma_{2i+1} + \gamma_{2i} \gamma_{1i+1}) \]

\( t_1 > t_2 \)

trivial SC

\( t_1 < t_2 \)

topological SC

Unpaired Majorana Fermion at end
2D topological superconductor (broken T symmetry)

Bulk-Boundary correspondence: \( n = \# \) Chiral Majorana Fermion edge states

\[ \gamma_k = \gamma_k^\dagger \]

Examples
- Spinless \( p_x + ip_y \) superconductor (n=1)
- Chiral triplet \( p \) wave superconductor (eg Sr$_2$RuO$_4$) (n=2)

Read Green model:
\[
H = \sum_k \left( \frac{k^2}{2m} - \mu \right) c_k^\dagger c_k + (\Delta(k)c_k c_{-k} + c.c.)
\]
\[
\Delta(k) = \Delta_0 \left( k_x + ik_y \right)
\]

Lattice BdG model:
\[
H_{BdG}(k) = \tau_z \left( 2t \left[ \cos k_x + \cos k_y \right] - \mu \right) + \Delta \left( \tau_x \sin k_x + \tau_y \sin k_y \right) = d(k) \cdot \tau
\]

\( |\mu| > 4t \) : Strong pairing phase
- trivial superconductor

\( |\mu| < 4t \) : Weak pairing phase
- topological superconductor

Chern number 0

Chern number 1
Majorana zero mode at a vortex

Hole in a topological superconductor threaded by flux

Boundary condition on fermion wavefunction

\[ \psi(L) = (-1)^{p+1}\psi(0) \]

\[ \psi(x) \propto e^{iq_mx} \quad ; \quad q_m = \frac{\pi}{L}(2m + 1 + p) \]

Without the hole: Caroli, de Gennes, Matricon theory (’64)

\[ \Delta \varepsilon \sim \frac{\Delta^2}{E_F} \]
### 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:**  
\[ \Pi H(k)\Pi^{-1} = - H(k) ; \quad \Pi \propto \Theta \Xi \]

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**K-theory Classes:**

- **Real K-theory**
  - Altland-Zirnbauer Random Matrix Classes
- **Complex K-theory**

**Bott Periodicity**  
\[ d \rightarrow d+8 \]

---

Kitaev, 2008  
Schnyder, Ryu, Furusaki, Ludwig 2008
Majorana Fermions and Topological Quantum Computing

(Kitaev ’03)

The degenerate states associated with Majorana zero modes define a topologically protected quantum memory

- 2 Majorana separated bound states = 1 fermion
  - 2 degenerate states (full/empty) = 1 qubit
- 2N separated Majoranas = N qubits
- Quantum Information is stored non locally
  - Immune from local decoherence

Braiding performs unitary operations

Non-Abelian statistics

Interchange rule (Ivanov 03)

\[ \gamma_i \rightarrow \gamma_j \]

\[ \gamma_j \rightarrow -\gamma_i \]

These operations, however, are not sufficient to make a universal quantum computer

\[ \Psi = \gamma_1 + i \gamma_2 \]
Potential condensed matter hosts for topological superconductivity

- **Quasiparticles in fractional Quantum Hall effect at** $v=5/2$  Moore Read ‘91

- **Unconventional superconductors**
  - $\text{Sr}_2\text{RuO}_4$ Das Sarma, Nayak, Tewari ‘06
  - Fermionic atoms near feshbach resonance Gurarie ‘05
  - $\text{Cu}_x\text{Bi}_2\text{Se}_3$ ?

- **Proximity Effect Devices using ordinary superconductors**
  - Topological Insulator devices Fu, Kane ‘08
  - 2D Semiconductor/Magnet devices Sau, Lutchyn, Tewari, Das Sarma ‘09, Lee ‘09
  - 1D Semiconductor devices:
    - eg In As quantum wires Oreg, von Oppen, Alicea, Fisher ‘10
      Lutchyn, Sau, Das Sarma ‘10
      Expt: Maurik et al. (Kouwenhoven) ‘12
  - 1D Ferromagnetic atomic chains on superconductors
    Expt: Nadj-Perg et al. (Yazdani) ‘14
Topological Superconductors

Spinless p-wave superconductor:

\[ \langle c_{k}^{\dagger} c_{-k}^{\dagger} \rangle \propto \Delta e^{i\varphi} (k_x + ik_y) \]

Ordinary Superconductor:

\[ \langle c_{k_{\uparrow}}^{\dagger} c_{-k_{\downarrow}}^{\dagger} \rangle \propto \Delta e^{i\varphi} \]

(s-wave, singlet pairing)

Surface of topological insulator

\[ \langle c_{k}^{\dagger} c_{-k}^{\dagger} \rangle \propto \Delta_{\text{surface}} e^{i\varphi} \]

(s-wave, singlet pairing)

Half an ordinary superconductor
Nontrivial ground state supports Majorana fermions at vortices
Majorana Bound States on Topological Insulators

1. $\frac{\hbar}{2e}$ vortex in 2D superconducting state

2. Superconductor-magnet interface at edge of 2D QSHI

Quasiparticle Bound state at $E=0$

Majorana Fermion $\gamma_0$ “Half a State”

$$m = |\Delta_S| - |\Delta_M|$$

$m > 0$

$E_{\text{gap}} = 2|m|$

$m < 0$

Domain wall bound state $\gamma_0$
1D Majorana Fermions on Topological Insulators

1. 1D Chiral Majorana mode at superconductor-magnet interface

\[ \gamma_k = \gamma_{-k} : \text{“Half” a 1D chiral Dirac fermion} \]

2. S-TI-S Josephson Junction

Gapless non-chiral Majorana fermion for phase difference \( \phi = \pi \)

\[ H = - i \hbar v_F \left( \gamma_L \partial_x \gamma_L - \gamma_R \partial_x \gamma_R \right) + i \Delta \cos(\phi/2) \gamma_L \gamma_R \]
Another route to the 2D p+ip superconductor

Semiconductor - Magnet - Superconductor structure

• Single Fermi circle with Berry phase $\pi - \epsilon$
• Topological superconductor with Majorana edge states and Majorana bound states at vortices.
• Variants:
  - use applied magnetic field to lift Kramers degeneracy (Alicea ’10)
  - Use 1D quantum wire (e.g., InSb). A route to 1D p wave superconductor with Majorana end states. (Oreg, von Oppen, Alicea, Fisher ’10)
Experiments semiconductor nanowires

- Superconductor + Semiconductor nanowire
  Sau, Lutchyn, Tewari, Das Sarma ’09;
  Alicea ’10;
  Oreg, Refael, von Oppen ’10

First experiment: 1D Semiconductor quantum wire on superconductor

Mourik, …, Kouwenhoven, et al. ’12

Observe zero bias peak in tunneling conductance:

Attributed to Majorana end state.
Ferromagnetic Atomic Chains on Superconductors (Iron on lead)
Nadj-Perg, Science ’14

STM topography

Vortex in Iron based superconductor

Vortex at superconductor TI interface
HH Sun, et al. PRL 116, 257003 (2016)

STM Spectroscopy
E=0

4π periodic Josephson effect in HgTe SC – 2D TI – SC junctions

Ferromagnet
Superconductor

Majorana end mode

STM tip

STM Spectroscopy
E=0

“A TI with SC on inside”
Fractional Josephson Effect

- $4\pi$ periodicity of $E(\phi)$ protected by local conservation of fermion parity.

- AC Josephson effect with half the usual frequency: $f = eV/h$
A $Z_2$ Interferometer for Majorana Fermions

A signature for neutral Majorana fermions probed with charge transport

- Chiral electrons on magnetic domain wall split into a pair of chiral Majorana fermions
- "$Z_2$ Aharonov Bohm phase" converts an electron into a hole

\[
\begin{align*}
\Phi &= N \frac{h}{2e} \\
\gamma_1 &= \gamma_1 - i\gamma_2 \\
\gamma_2 &= \gamma_1 + i\gamma_2
\end{align*}
\]

Akhmerov, Nilsson, Beenakker, PRL '09
Fu and Kane, PRL '09